



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:20 PM BST

PDB ID : 2J0G
Title : L-ficolin complexed to N-acetyl-mannosamine
Authors : Garlatti, V.; Gaboriaud, C.
Deposited on : 2006-08-03
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

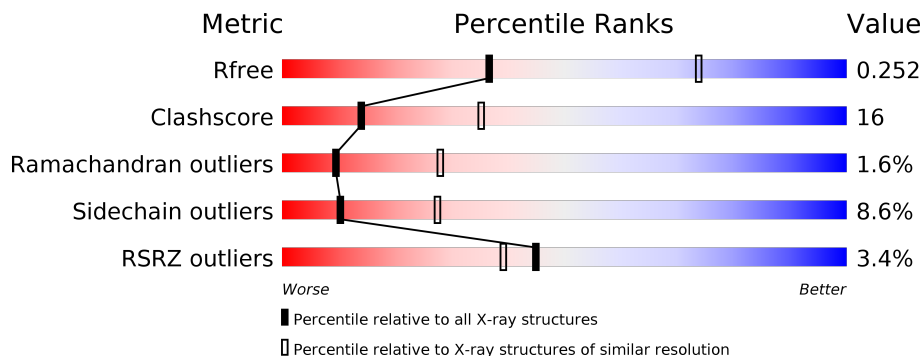
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	218	
1	B	218	
1	C	218	
1	D	218	
1	E	218	
1	F	218	

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Mol	Chain	Length	Quality of chain
2	G	5	 60% 40%
3	H	4	 50% 50%

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
2	MAN	G	3	X	-	-	-
3	NAG	H	2	-	-	-	X
3	MAN	H	3	X	-	-	-
3	FUC	H	4	-	-	-	X
5	BM3	B	400	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10580 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.

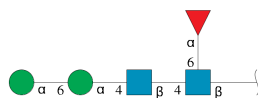
- Molecule 1 is a protein called FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	Total 1702	C 1071	N 300	O 323	S 8	0	0	0
1	B	217	Total 1744	C 1097	N 307	O 331	S 9	0	1	0
1	C	216	Total 1728	C 1087	N 304	O 328	S 9	0	0	0
1	D	214	Total 1715	C 1078	N 302	O 327	S 8	0	0	0
1	E	218	Total 1744	C 1096	N 307	O 332	S 9	0	0	0
1	F	212	Total 1715	C 1078	N 304	O 325	S 8	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

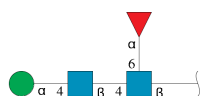
Chain	Residue	Modelled	Actual	Comment	Reference
A	168	THR	VAL	conflict	UNP Q15485
A	247	THR	VAL	conflict	UNP Q15485
B	168	THR	VAL	conflict	UNP Q15485
B	247	THR	VAL	conflict	UNP Q15485
C	168	THR	VAL	conflict	UNP Q15485
C	247	THR	VAL	conflict	UNP Q15485
D	168	THR	VAL	conflict	UNP Q15485
D	247	THR	VAL	conflict	UNP Q15485
E	168	THR	VAL	conflict	UNP Q15485
E	247	THR	VAL	conflict	UNP Q15485
F	168	THR	VAL	conflict	UNP Q15485
F	247	THR	VAL	conflict	UNP Q15485

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-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
			Total	C	N	O			
2	G	5	60	34	2	24	0	0	0

- Molecule 3 is an oligosaccharide called alpha-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.

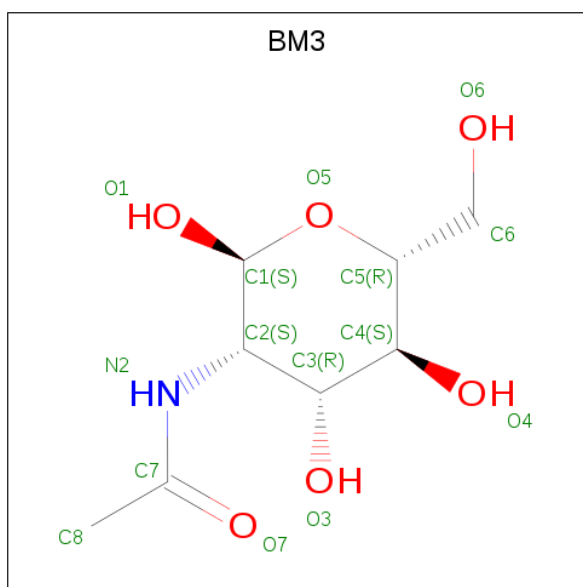


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	H	4	49	28	2	19	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

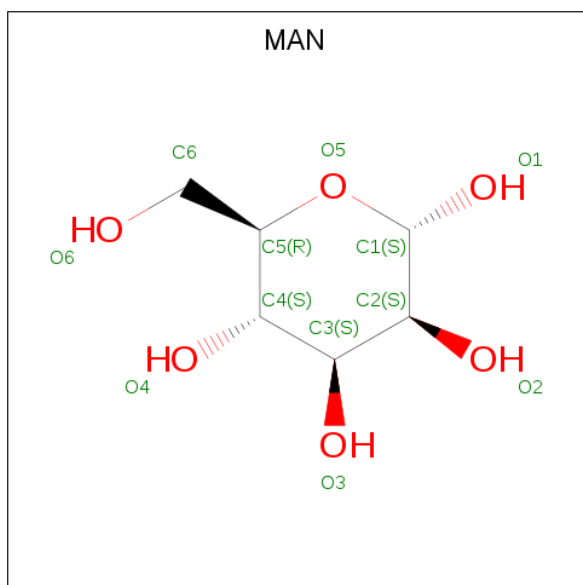
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-alpha-D-mannopyranose (three-letter code: BM3) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	15	8	1	6	2	0
5	C	1	15	8	1	6	0	0
5	E	1	15	8	1	6	2	0
5	F	1	15	8	1	6	11	0

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	C O	0	0
			11	6 5		

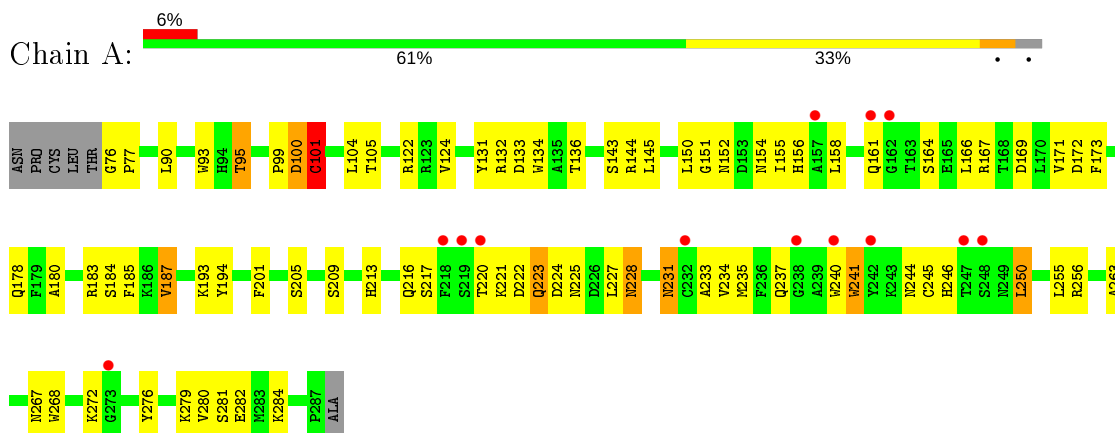
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	O	0	0
			5	5		
7	B	11	Total	O	0	0
			11	11		
7	C	7	Total	O	0	0
			7	7		
7	D	4	Total	O	0	0
			4	4		
7	E	9	Total	O	0	0
			9	9		
7	F	10	Total	O	0	0
			10	10		

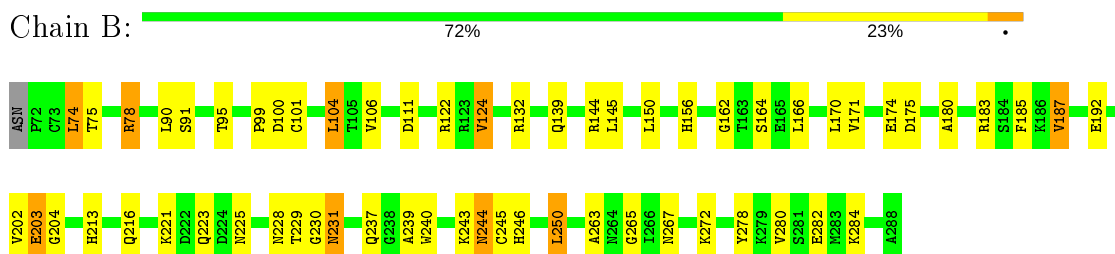
3 Residue-property plots [i](#)

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.

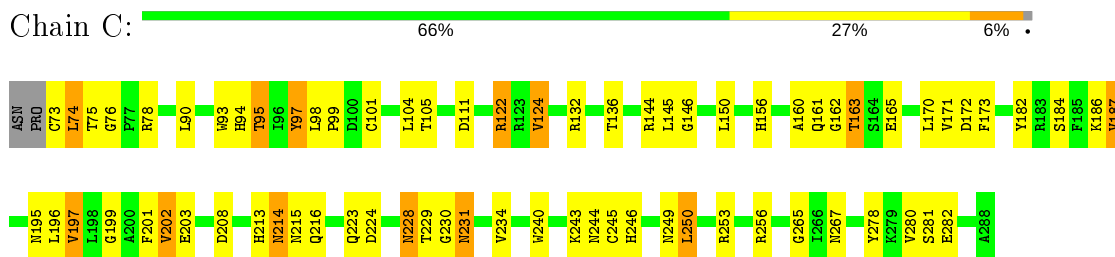
- Molecule 1: FICOLIN-2



- Molecule 1: FICOLIN-2

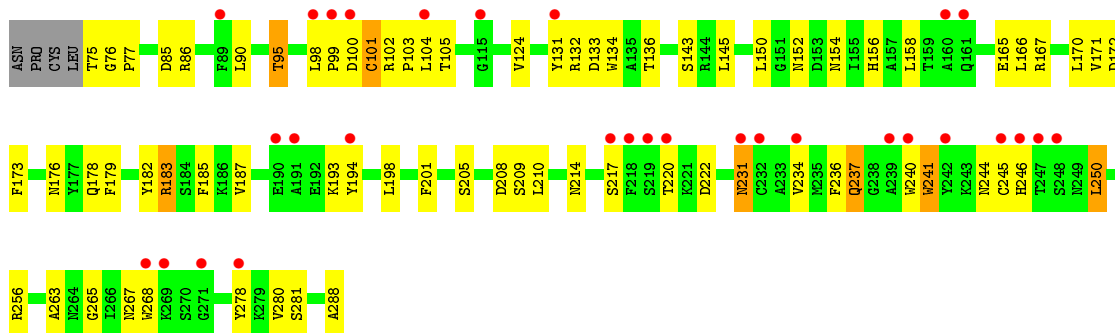


- Molecule 1: FICOLIN-2



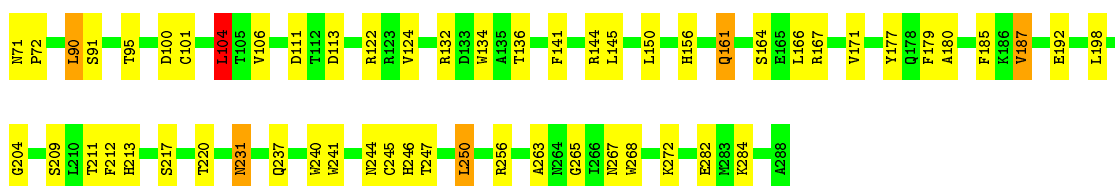
- Molecule 1: FICOLIN-2





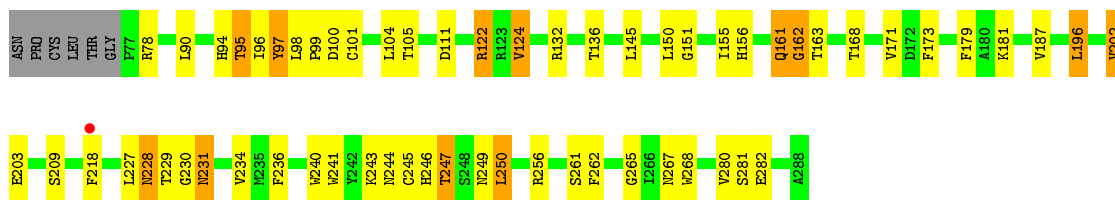
- Molecule 1: FICOLIN-2

Chain E: 74% 23%



- Molecule 1: FICOLIN-2

Chain F: 69% 22% 6%



- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-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 G: 60% 40%



- Molecule 3: alpha-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: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.94Å 96.94Å 139.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.85 48.47 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.85) 98.9 (48.47-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 2.86Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.248 0.202 , 0.252	Depositor DCC
R_{free} test set	1691 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtrriage
Anisotropy	0.073	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.037 for -h,-k,l 0.447 for h,-h-k,-l 0.038 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10580	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BM3, CA, MAN, NAG, FUC

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	0.55	1/1749 (0.1%)	0.66	0/2366
1	B	0.60	0/1792	0.71	0/2423
1	C	0.62	2/1775 (0.1%)	0.69	1/2400 (0.0%)
1	D	0.50	0/1762	0.64	0/2383
1	E	0.56	0/1792	0.71	1/2425 (0.0%)
1	F	0.56	0/1762	0.68	1/2381 (0.0%)
All	All	0.56	3/10632 (0.0%)	0.68	3/14378 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	GLN	C-N	-11.37	1.07	1.34
1	A	224	ASP	C-N	-8.45	1.14	1.34
1	C	224	ASP	C-N	-6.08	1.20	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	228	ASN	CB-CA-C	-8.89	92.62	110.40
1	C	228	ASN	CB-CA-C	-7.86	94.67	110.40
1	E	104	LEU	CA-CB-CG	5.61	128.20	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1702	0	1572	60	0
1	B	1744	0	1613	52	0
1	C	1728	0	1600	55	0
1	D	1715	0	1585	58	0
1	E	1744	0	1611	46	0
1	F	1715	0	1588	51	0
2	G	60	0	52	1	0
3	H	49	0	43	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	B	15	0	14	17	0
5	C	15	0	14	1	0
5	E	15	0	14	3	0
5	F	15	0	14	4	0
6	F	11	0	10	1	0
7	A	5	0	0	0	0
7	B	11	0	0	1	0
7	C	7	0	0	2	0
7	D	4	0	0	1	0
7	E	9	0	0	0	0
7	F	10	0	0	0	0
All	All	10580	0	9730	318	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 16.

All (318) 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:132:ARG:HD2	5:B:400:BM3:C8	1.32	1.53
5:B:400:BM3:C6	5:B:400:BM3:O6	1.75	1.33
5:C:400:BM3:C6	5:C:400:BM3:O6	1.77	1.31
1:B:132:ARG:HD2	5:B:400:BM3:H8C3	1.25	1.14
1:F:132:ARG:HD2	5:F:400:BM3:H8C1	1.22	1.10
1:B:132:ARG:CD	5:B:400:BM3:C8	2.29	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ARG:HG3	1:D:183:ARG:HH11	0.98	1.08
1:A:133:ASP:HB2	1:A:222:ASP:OD2	1.53	1.07
1:B:132:ARG:HD2	5:B:400:BM3:H8C2	1.16	1.07
1:C:186:LYS:HB3	1:C:197:VAL:HG23	1.37	1.05
1:D:95:THR:HG22	7:D:2001:HOH:O	1.62	0.99
1:F:132:ARG:CD	5:F:400:BM3:H8C1	1.94	0.98
1:D:231:ASN:HD21	1:D:234:VAL:H	1.13	0.95
1:D:244:ASN:N	1:D:245:CYS:HA	1.78	0.94
1:B:132:ARG:CD	5:B:400:BM3:H8C2	1.95	0.92
1:D:183:ARG:HG3	1:D:183:ARG:NH1	1.79	0.90
1:B:132:ARG:HH11	5:B:400:BM3:C8	1.83	0.90
1:A:133:ASP:CB	1:A:222:ASP:OD2	2.19	0.89
1:D:183:ARG:CG	1:D:183:ARG:HH11	1.83	0.89
1:F:132:ARG:HD2	5:F:400:BM3:C8	2.05	0.87
1:A:244:ASN:N	1:A:245:CYS:HA	1.90	0.85
1:B:132:ARG:HH11	5:B:400:BM3:H8C1	1.41	0.85
1:C:231:ASN:C	1:C:231:ASN:HD22	1.82	0.83
1:E:71:ASN:N	1:E:72:PRO:HD2	1.95	0.82
1:B:183:ARG:HD2	1:D:288:ALA:O	1.80	0.81
1:A:183:ARG:HH11	1:A:183:ARG:HB3	1.45	0.80
1:E:161:GLN:HA	1:E:161:GLN:NE2	1.94	0.80
1:D:231:ASN:ND2	1:D:234:VAL:H	1.79	0.80
2:G:3:MAN:H5	2:G:4:MAN:H2	1.63	0.80
1:B:132:ARG:CD	5:B:400:BM3:H8C3	2.05	0.80
1:C:228:ASN:O	1:C:230:GLY:N	2.15	0.79
1:F:228:ASN:O	1:F:230:GLY:N	2.15	0.79
1:C:216:GLN:HE21	1:C:243:LYS:NZ	1.80	0.79
1:F:231:ASN:HD22	1:F:231:ASN:C	1.87	0.78
1:B:100:ASP:O	1:B:101:CYS:HB2	1.83	0.78
1:A:100:ASP:O	1:A:101:CYS:HB2	1.81	0.77
1:D:198:LEU:H	1:D:214:ASN:ND2	1.83	0.77
1:D:231:ASN:HD22	1:D:231:ASN:C	1.88	0.77
1:B:244:ASN:HB3	7:B:2008:HOH:O	1.85	0.76
1:E:156:HIS:HD2	1:E:187:VAL:O	1.67	0.75
1:F:122:ARG:HD2	1:F:282:GLU:OE2	1.85	0.75
1:D:217:SER:O	1:D:241:TRP:HA	1.86	0.75
1:B:244:ASN:N	1:B:245:CYS:HA	2.01	0.74
1:C:186:LYS:HE2	1:C:197:VAL:HG21	1.70	0.74
1:D:209:SER:HB2	1:D:268:TRP:CE2	2.23	0.73
1:E:132:ARG:CD	5:E:400:BM3:H8C1	2.18	0.73
1:D:98:LEU:O	1:D:100:ASP:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ARG:HD2	5:E:400:BM3:H8C1	1.71	0.72
1:C:214:ASN:HD22	1:C:215:ASN:N	1.86	0.72
1:A:156:HIS:HD2	1:A:187:VAL:O	1.73	0.72
1:D:75:THR:HG23	1:D:76:GLY:H	1.54	0.71
1:A:228:ASN:HB2	1:A:244:ASN:OD1	1.90	0.70
1:B:156:HIS:HD2	1:B:187:VAL:O	1.74	0.70
1:A:173:PHE:CZ	1:A:256:ARG:HA	2.26	0.70
1:B:180:ALA:HA	1:B:204:GLY:HA3	1.72	0.70
1:E:71:ASN:N	1:E:72:PRO:CD	2.55	0.69
1:C:186:LYS:HB3	1:C:197:VAL:CG2	2.20	0.69
1:C:171:VAL:HB	1:C:280:VAL:HB	1.74	0.69
1:F:228:ASN:O	1:F:230:GLY:O	2.10	0.69
1:E:180:ALA:HA	1:E:204:GLY:HA3	1.74	0.68
1:A:132:ARG:NH2	1:B:111:ASP:OD2	2.26	0.68
1:D:156:HIS:HD2	1:D:187:VAL:O	1.75	0.68
1:B:228:ASN:O	1:B:230:GLY:N	2.26	0.68
1:E:213:HIS:CD2	1:E:247:THR:HG22	2.29	0.68
1:F:98:LEU:HB3	1:F:99:PRO:HD2	1.76	0.68
1:E:244:ASN:N	1:E:245:CYS:HA	2.09	0.68
1:B:231:ASN:HD22	1:B:231:ASN:C	1.95	0.68
1:B:132:ARG:HA	5:B:400:BM3:H8C2	1.76	0.67
1:E:231:ASN:HD22	1:E:231:ASN:C	1.98	0.67
1:E:212:PHE:HB3	1:E:247:THR:HG21	1.76	0.67
1:C:73:CYS:O	1:C:76:GLY:N	2.28	0.67
1:D:132:ARG:NH2	1:E:111:ASP:OD2	2.29	0.66
1:F:100:ASP:O	1:F:101:CYS:HB2	1.95	0.66
1:F:209:SER:HB3	1:F:247:THR:HG22	1.77	0.66
1:D:231:ASN:HD21	1:D:234:VAL:N	1.90	0.66
1:E:209:SER:HB2	1:E:268:TRP:CE2	2.30	0.66
1:E:122:ARG:HD2	1:E:282:GLU:OE2	1.96	0.65
1:B:132:ARG:HH11	5:B:400:BM3:H8C3	1.59	0.65
1:F:97:TYR:N	1:F:97:TYR:CD2	2.64	0.65
1:C:216:GLN:HE21	1:C:243:LYS:HZ3	1.44	0.65
1:A:134:TRP:HA	1:A:220:THR:HG21	1.77	0.64
1:A:246:HIS:CE1	1:A:263:ALA:HB1	2.31	0.64
1:D:77:PRO:HD3	1:D:86:ARG:HH12	1.63	0.64
1:B:132:ARG:HD2	5:B:400:BM3:H8C1	1.66	0.64
1:D:231:ASN:C	1:D:231:ASN:ND2	2.51	0.64
1:A:166:LEU:HD13	1:A:185:PHE:CG	2.32	0.64
1:F:97:TYR:HD2	1:F:97:TYR:N	1.96	0.64
1:B:265:GLY:H	1:B:267:ASN:HD21	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:HIS:HD2	1:C:187:VAL:O	1.81	0.63
1:C:97:TYR:CD2	1:C:97:TYR:N	2.66	0.63
1:F:161:GLN:O	1:F:162:GLY:O	2.16	0.63
1:C:122:ARG:NH1	1:C:124:VAL:HG21	2.14	0.62
1:D:152:ASN:HB3	1:D:194:TYR:CD1	2.33	0.62
1:B:132:ARG:NH1	5:B:400:BM3:H8C3	2.15	0.62
1:B:228:ASN:O	1:B:230:GLY:O	2.17	0.62
1:B:74:LEU:HD12	1:B:74:LEU:H	1.65	0.62
1:F:156:HIS:HD2	1:F:187:VAL:O	1.81	0.62
1:E:161:GLN:HA	1:E:161:GLN:HE21	1.64	0.61
1:D:240:TRP:CH2	1:D:250:LEU:HB2	2.37	0.60
1:E:240:TRP:CH2	1:E:250:LEU:HB2	2.36	0.60
1:A:183:ARG:NH1	1:A:183:ARG:HB3	2.16	0.60
1:B:166:LEU:HD22	1:B:185:PHE:CD1	2.37	0.60
1:D:246:HIS:CE1	1:D:263:ALA:HB1	2.36	0.60
1:A:240:TRP:CH2	1:A:250:LEU:HB2	2.37	0.60
1:C:122:ARG:HD2	1:C:282:GLU:OE2	2.02	0.60
1:E:132:ARG:NH2	1:F:111:ASP:OD2	2.33	0.59
1:E:132:ARG:NH1	1:E:136:THR:HG21	2.17	0.59
1:A:151:GLY:O	1:A:155:ILE:HG13	2.03	0.59
1:C:216:GLN:NE2	1:C:243:LYS:HZ2	2.01	0.59
1:B:132:ARG:NH1	5:B:400:BM3:C8	2.62	0.58
1:D:236:PHE:O	1:D:237:GLN:C	2.42	0.58
1:C:186:LYS:CB	1:C:197:VAL:HG23	2.24	0.58
1:A:231:ASN:C	1:A:231:ASN:HD22	2.06	0.58
1:C:97:TYR:N	1:C:97:TYR:HD2	2.01	0.58
1:C:231:ASN:C	1:C:231:ASN:ND2	2.55	0.57
1:C:216:GLN:NE2	1:C:243:LYS:NZ	2.53	0.57
1:E:100:ASP:C	1:E:100:ASP:OD1	2.41	0.57
1:F:209:SER:HB2	1:F:268:TRP:CE2	2.39	0.57
1:A:133:ASP:CA	1:A:222:ASP:OD2	2.52	0.57
1:A:143:SER:HA	1:B:91:SER:HB2	1.85	0.57
1:A:166:LEU:HB2	1:A:185:PHE:HB2	1.87	0.57
1:A:166:LEU:HD13	1:A:185:PHE:CD1	2.40	0.57
1:A:213:HIS:CE1	1:A:246:HIS:HA	2.40	0.57
1:D:173:PHE:CZ	1:D:256:ARG:HA	2.41	0.56
1:D:166:LEU:HD13	1:D:185:PHE:CG	2.41	0.56
1:C:214:ASN:HD22	1:C:215:ASN:H	1.53	0.56
1:A:223:GLN:OE1	1:A:225:ASN:ND2	2.38	0.55
1:D:133:ASP:HB2	1:D:222:ASP:OD2	2.06	0.55
1:E:132:ARG:HD3	5:E:400:BM3:H8C1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ARG:NH1	1:F:124:VAL:HG21	2.21	0.55
1:A:227:LEU:HD23	1:A:227:LEU:N	2.21	0.55
1:E:100:ASP:O	1:E:101:CYS:HB2	2.05	0.55
1:A:180:ALA:HB1	1:A:201:PHE:HE1	1.72	0.55
1:C:253:ARG:HD2	7:C:2006:HOH:O	2.07	0.55
1:F:246:HIS:CE1	1:F:249:ASN:HB2	2.41	0.55
1:C:216:GLN:HE21	1:C:243:LYS:HZ2	1.52	0.54
1:A:231:ASN:HD21	1:A:233:ALA:HB3	1.72	0.54
1:D:231:ASN:ND2	1:D:234:VAL:N	2.52	0.54
1:E:265:GLY:H	1:E:267:ASN:HD21	1.56	0.54
1:F:228:ASN:OD1	1:F:230:GLY:N	2.38	0.54
1:D:143:SER:HA	1:E:91:SER:HB2	1.89	0.54
1:D:198:LEU:H	1:D:214:ASN:HD21	1.53	0.54
1:F:228:ASN:C	1:F:230:GLY:N	2.59	0.54
1:F:231:ASN:C	1:F:231:ASN:ND2	2.60	0.53
1:B:202:VAL:O	1:B:203:GLU:HB3	2.07	0.53
1:B:216:GLN:HA	1:B:216:GLN:OE1	2.08	0.53
1:C:265:GLY:H	1:C:267:ASN:HD21	1.56	0.53
1:A:231:ASN:HD22	1:A:234:VAL:H	1.56	0.53
1:F:132:ARG:NH1	5:F:400:BM3:H8C3	2.23	0.53
1:A:246:HIS:HE1	1:A:263:ALA:O	1.90	0.53
1:F:265:GLY:H	1:F:267:ASN:HD21	1.55	0.53
1:C:228:ASN:ND2	1:C:244:ASN:OD1	2.35	0.53
1:C:132:ARG:NH1	1:C:136:THR:HG21	2.24	0.52
1:E:213:HIS:NE2	1:E:247:THR:HG22	2.24	0.52
1:C:228:ASN:C	1:C:230:GLY:H	2.11	0.52
1:B:228:ASN:C	1:B:230:GLY:N	2.62	0.52
1:F:228:ASN:C	1:F:230:GLY:H	2.12	0.52
1:B:183:ARG:CD	1:D:288:ALA:O	2.55	0.52
1:A:263:ALA:HA	1:A:267:ASN:ND2	2.25	0.52
1:C:228:ASN:C	1:C:230:GLY:N	2.59	0.51
1:F:181:LYS:O	1:F:202:VAL:HG13	2.10	0.51
1:F:95:THR:HA	1:F:105:THR:HA	1.91	0.51
1:A:99:PRO:HB2	1:A:161:GLN:HE22	1.75	0.51
1:F:96:ILE:C	1:F:97:TYR:CD2	2.84	0.51
1:A:99:PRO:HB2	1:A:161:GLN:NE2	2.25	0.51
1:A:171:VAL:HB	1:A:280:VAL:HB	1.93	0.51
1:D:75:THR:HG23	1:D:76:GLY:N	2.22	0.51
1:F:96:ILE:C	1:F:97:TYR:HD2	2.14	0.51
1:B:265:GLY:H	1:B:267:ASN:ND2	2.08	0.51
1:A:154:ASN:O	1:A:158:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:LEU:HD13	1:E:106:VAL:CG1	2.41	0.50
1:D:132:ARG:NH1	1:D:136:THR:HG21	2.27	0.50
1:F:171:VAL:HB	1:F:280:VAL:HB	1.94	0.50
1:F:228:ASN:ND2	1:F:244:ASN:OD1	2.39	0.50
1:B:132:ARG:NH2	1:C:111:ASP:OD2	2.38	0.50
1:D:265:GLY:H	1:D:267:ASN:ND2	2.10	0.50
1:B:223:GLN:HE21	1:B:225:ASN:HD21	1.60	0.50
1:D:201:PHE:HB2	1:D:208:ASP:OD2	2.11	0.50
1:A:255:LEU:O	1:A:256:ARG:HB2	2.13	0.49
1:B:213:HIS:CE1	1:B:246:HIS:HA	2.47	0.49
1:C:265:GLY:H	1:C:267:ASN:ND2	2.09	0.49
1:B:228:ASN:C	1:B:230:GLY:H	2.16	0.49
1:C:202:VAL:O	1:C:203:GLU:HB3	2.11	0.49
1:D:95:THR:HA	1:D:105:THR:HA	1.94	0.49
1:E:217:SER:O	1:E:241:TRP:HA	2.13	0.49
1:A:132:ARG:NH1	1:A:136:THR:HG21	2.27	0.49
1:B:132:ARG:CA	5:B:400:BM3:H8C2	2.42	0.49
1:D:244:ASN:H	1:D:245:CYS:HA	1.70	0.49
1:F:244:ASN:N	1:F:245:CYS:HA	2.27	0.49
1:A:246:HIS:CE1	1:A:263:ALA:O	2.66	0.49
1:F:265:GLY:H	1:F:267:ASN:ND2	2.09	0.49
1:D:167:ARG:NH1	1:D:179:PHE:CD1	2.81	0.49
1:D:265:GLY:H	1:D:267:ASN:HD21	1.60	0.48
1:A:133:ASP:HA	1:A:222:ASP:OD2	2.14	0.48
1:E:156:HIS:CD2	1:E:187:VAL:O	2.57	0.48
1:A:156:HIS:CD2	1:A:187:VAL:O	2.60	0.48
1:A:178:GLN:HG2	1:A:205:SER:OG	2.13	0.48
1:A:95:THR:HA	1:A:105:THR:HA	1.95	0.48
1:D:156:HIS:CD2	1:D:187:VAL:O	2.63	0.48
1:F:173:PHE:CE1	1:F:256[B]:ARG:HA	2.48	0.48
1:D:198:LEU:HD13	1:D:210:LEU:HD23	1.96	0.48
1:D:244:ASN:N	1:D:245:CYS:CA	2.62	0.48
1:F:173:PHE:CZ	1:F:256[B]:ARG:HA	2.49	0.48
1:D:77:PRO:HD3	1:D:86:ARG:NH1	2.27	0.47
1:D:131:TYR:CE1	1:D:237:GLN:HA	2.50	0.47
1:A:217:SER:O	1:A:241:TRP:HA	2.13	0.47
1:C:165:GLU:HB2	1:C:182:TYR:O	2.14	0.47
1:A:169:ASP:OD1	1:A:284:LYS:HE3	2.15	0.47
1:E:171:VAL:HG22	1:E:177:TYR:CD1	2.50	0.47
1:A:231:ASN:C	1:A:231:ASN:ND2	2.67	0.47
1:A:244:ASN:N	1:A:245:CYS:CA	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:HIS:HE1	1:E:263:ALA:O	1.97	0.47
1:F:173:PHE:CZ	1:F:256[A]:ARG:HA	2.50	0.47
1:A:209:SER:HB2	1:A:268:TRP:CE2	2.49	0.46
1:C:231:ASN:ND2	1:C:234:VAL:H	2.12	0.46
1:A:221:LYS:HG2	1:A:222:ASP:N	2.30	0.46
1:D:172:ASP:OD2	1:D:176:ASN:HB2	2.15	0.46
1:C:173:PHE:CZ	1:C:256:ARG:HA	2.50	0.46
1:F:202:VAL:O	1:F:203:GLU:HB3	2.15	0.46
1:B:156:HIS:CD2	1:B:187:VAL:O	2.63	0.46
1:C:98:LEU:HB3	1:C:99:PRO:HD2	1.97	0.46
1:F:262:PHE:HZ	6:F:402:MAN:HO4	1.57	0.46
1:B:104:LEU:HD13	1:B:106:VAL:CG1	2.45	0.46
1:B:239:ALA:O	1:B:240:TRP:HB2	2.14	0.46
1:A:231:ASN:ND2	1:A:234:VAL:H	2.13	0.46
1:B:231:ASN:ND2	1:B:231:ASN:C	2.67	0.46
1:C:95:THR:HA	1:C:105:THR:HA	1.96	0.46
1:D:183:ARG:NH1	1:D:183:ARG:CG	2.54	0.46
1:B:122:ARG:NH1	1:B:282:GLU:OE2	2.47	0.46
1:E:198:LEU:HD23	1:E:211:THR:HA	1.97	0.46
1:C:73:CYS:O	1:C:74:LEU:C	2.54	0.46
1:E:265:GLY:H	1:E:267:ASN:ND2	2.14	0.45
1:A:172:ASP:HB2	1:A:276:TYR:CE1	2.52	0.45
1:E:231:ASN:C	1:E:231:ASN:ND2	2.69	0.45
1:B:246:HIS:HE1	1:B:263:ALA:O	1.99	0.45
1:C:213:HIS:CE1	1:C:246:HIS:HA	2.51	0.45
1:A:131:TYR:CE1	1:A:237:GLN:HA	2.51	0.45
1:B:240:TRP:CH2	1:B:250:LEU:HB2	2.52	0.45
1:C:246:HIS:CE1	1:C:249:ASN:HB2	2.52	0.45
1:D:100:ASP:O	1:D:101:CYS:HB2	2.16	0.45
1:F:231:ASN:ND2	1:F:234:VAL:HG23	2.31	0.45
1:E:246:HIS:CE1	1:E:263:ALA:HB1	2.52	0.45
1:C:73:CYS:O	1:C:75:THR:N	2.50	0.45
1:C:173:PHE:CE1	1:C:256:ARG:HA	2.53	0.44
1:C:240:TRP:CH2	1:C:250:LEU:HB2	2.52	0.44
1:F:173:PHE:CE1	1:F:256[A]:ARG:HA	2.51	0.44
1:A:244:ASN:H	1:A:245:CYS:HA	1.79	0.44
1:D:131:TYR:CD1	1:D:237:GLN:HB3	2.53	0.44
1:D:171:VAL:HB	1:D:280:VAL:HB	1.99	0.44
1:F:240:TRP:CH2	1:F:250:LEU:HB2	2.53	0.44
1:F:227:LEU:HD12	1:F:243:LYS:HG3	2.00	0.44
1:B:244:ASN:N	1:B:245:CYS:CA	2.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HB3	1:A:217:SER:HB3	1.99	0.44
1:A:272:LYS:HA	1:A:272:LYS:HE2	2.00	0.44
1:B:144:ARG:NH2	1:C:94:HIS:NE2	2.66	0.44
1:B:284:LYS:HB3	1:B:284:LYS:HE2	1.82	0.44
1:A:122:ARG:HD3	1:A:282:GLU:OE2	2.17	0.44
1:B:124:VAL:O	1:B:124:VAL:CG1	2.64	0.44
1:B:170:LEU:HD13	1:B:278:TYR:CE1	2.53	0.44
1:F:218:PHE:HA	1:F:241:TRP:HA	1.99	0.44
1:C:124:VAL:O	1:C:124:VAL:CG1	2.63	0.44
5:B:400:BM3:O6	5:B:400:BM3:C5	2.61	0.43
1:B:216:GLN:HG3	1:B:243:LYS:HB2	2.00	0.43
1:F:124:VAL:CG1	1:F:124:VAL:O	2.65	0.43
5:B:400:BM3:C6	5:B:400:BM3:H6	2.18	0.43
1:C:124:VAL:O	1:C:124:VAL:HG12	2.18	0.43
1:C:78:ARG:HG2	1:C:97:TYR:O	2.18	0.43
1:E:179:PHE:CE2	1:E:204:GLY:HA2	2.54	0.43
1:A:164:SER:O	1:A:184:SER:HA	2.18	0.43
1:D:263:ALA:HA	1:D:267:ASN:ND2	2.34	0.43
1:C:184:SER:OG	1:C:199:GLY:HA3	2.19	0.43
1:E:90:LEU:HD12	1:E:90:LEU:HA	1.88	0.43
1:A:152:ASN:HB3	1:A:194:TYR:CD1	2.53	0.43
1:D:165:GLU:HB2	1:D:182:TYR:O	2.19	0.43
1:E:263:ALA:HA	1:E:267:ASN:ND2	2.34	0.42
1:E:284:LYS:HB3	1:E:284:LYS:HE2	1.85	0.42
1:C:146:GLY:HA3	7:C:2003:HOH:O	2.18	0.42
1:D:250:LEU:HD12	1:D:250:LEU:HA	1.88	0.42
1:E:136:THR:HG22	1:E:141:PHE:CD1	2.54	0.42
1:E:144:ARG:NH2	1:F:94:HIS:NE2	2.68	0.42
1:F:168:THR:O	1:F:179:PHE:HA	2.20	0.42
1:D:167:ARG:NH1	1:D:179:PHE:CE1	2.88	0.42
1:B:78:ARG:HH21	1:B:99:PRO:HA	1.85	0.42
1:E:212:PHE:HB3	1:E:247:THR:CG2	2.47	0.42
1:C:172:ASP:C	1:C:172:ASP:OD1	2.58	0.42
1:C:93:TRP:CZ2	1:C:144:ARG:HA	2.55	0.41
1:C:195:ASN:HD21	1:C:216:GLN:N	2.18	0.41
1:A:231:ASN:ND2	1:A:234:VAL:HG23	2.34	0.41
1:A:76:GLY:HA2	1:A:77:PRO:HD3	1.87	0.41
1:A:93:TRP:CE2	1:A:144:ARG:HG2	2.55	0.41
1:C:244:ASN:N	1:C:245:CYS:HA	2.34	0.41
1:E:113:ASP:OD2	1:E:167:ARG:NH1	2.54	0.41
1:E:240:TRP:CZ3	1:E:250:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:HG2	1:C:97:TYR:HB2	2.02	0.41
1:D:166:LEU:HB2	1:D:185:PHE:HB2	2.02	0.41
1:E:256:ARG:HG3	1:E:256:ARG:NH1	2.35	0.41
1:F:151:GLY:O	1:F:155:ILE:HG13	2.20	0.41
1:C:161:GLN:O	1:C:163:THR:N	2.54	0.41
1:D:178:GLN:HG2	1:D:205:SER:OG	2.21	0.41
1:B:171:VAL:HB	1:B:280:VAL:HB	2.02	0.41
1:D:154:ASN:O	1:D:158:LEU:HB2	2.21	0.41
1:D:170:LEU:HD13	1:D:278:TYR:CE1	2.55	0.41
1:A:166:LEU:HG	1:A:167:ARG:N	2.36	0.41
1:D:102:ARG:HA	1:D:103:PRO:HD3	1.89	0.41
1:E:166:LEU:HD22	1:E:185:PHE:CD1	2.55	0.41
1:F:132:ARG:NH1	1:F:136:THR:HG21	2.35	0.41
1:F:236:PHE:HE2	1:F:245:CYS:SG	2.44	0.41
1:D:134:TRP:HA	1:D:220:THR:HG21	2.02	0.40
1:F:209:SER:HB3	1:F:247:THR:CG2	2.47	0.40
1:E:244:ASN:N	1:E:245:CYS:CA	2.82	0.40
1:F:231:ASN:ND2	1:F:234:VAL:H	2.18	0.40
1:F:196:LEU:HB2	1:F:241:TRP:CD1	2.56	0.40
1:C:170:LEU:HB3	1:C:278:TYR:CD2	2.57	0.40
1:E:134:TRP:HA	1:E:220:THR:HG21	2.04	0.40
1:A:216:GLN:HE22	1:A:227:LEU:HD11	1.86	0.40
1:A:246:HIS:HE1	1:A:263:ALA:HB1	1.83	0.40
1:C:201:PHE:CD2	1:C:208:ASP:HB2	2.57	0.40
3:H:2:NAG:O3	3:H:3:MAN:H2	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	210/218 (96%)	189 (90%)	18 (9%)	3 (1%)	11 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	216/218 (99%)	193 (89%)	19 (9%)	4 (2%)	8	24
1	C	214/218 (98%)	190 (89%)	19 (9%)	5 (2%)	6	20
1	D	212/218 (97%)	189 (89%)	19 (9%)	4 (2%)	8	24
1	E	216/218 (99%)	196 (91%)	19 (9%)	1 (0%)	29	57
1	F	211/218 (97%)	185 (88%)	22 (10%)	4 (2%)	8	24
All	All	1279/1308 (98%)	1142 (89%)	116 (9%)	21 (2%)	9	28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	CYS
1	C	162	GLY
1	F	162	GLY
1	B	162	GLY
1	B	229	THR
1	C	74	LEU
1	C	229	THR
1	D	237	GLN
1	F	161	GLN
1	F	229	THR
1	D	99	PRO
1	B	203	GLU
1	C	160	ALA
1	D	241	TRP
1	A	241	TRP
1	F	124	VAL
1	A	124	VAL
1	B	124	VAL
1	C	124	VAL
1	D	124	VAL
1	E	124	VAL

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	178/183 (97%)	163 (92%)	15 (8%)	11	28
1	B	183/183 (100%)	163 (89%)	20 (11%)	6	17
1	C	181/183 (99%)	164 (91%)	17 (9%)	8	23
1	D	179/183 (98%)	167 (93%)	12 (7%)	16	39
1	E	183/183 (100%)	170 (93%)	13 (7%)	14	36
1	F	179/183 (98%)	163 (91%)	16 (9%)	9	26
All	All	1083/1098 (99%)	990 (91%)	93 (9%)	10	27

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	95	THR
1	A	100	ASP
1	A	101	CYS
1	A	104	LEU
1	A	145	LEU
1	A	150	LEU
1	A	187	VAL
1	A	223	GLN
1	A	228	ASN
1	A	231	ASN
1	A	235	MET
1	A	250	LEU
1	A	279	LYS
1	A	281	SER
1	B	74	LEU
1	B	75	THR
1	B	78	ARG
1	B	90	LEU
1	B	95	THR
1	B	104	LEU
1	B	139	GLN
1	B	145	LEU
1	B	150	LEU
1	B	164	SER
1	B	174	GLU
1	B	175	ASP
1	B	187	VAL
1	B	192	GLU
1	B	221	LYS

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Mol	Chain	Res	Type
1	B	231	ASN
1	B	237	GLN
1	B	244	ASN
1	B	250	LEU
1	B	272	LYS
1	C	90	LEU
1	C	95	THR
1	C	97	TYR
1	C	101	CYS
1	C	104	LEU
1	C	122	ARG
1	C	145	LEU
1	C	150	LEU
1	C	163	THR
1	C	187	VAL
1	C	196	LEU
1	C	197	VAL
1	C	202	VAL
1	C	214	ASN
1	C	231	ASN
1	C	250	LEU
1	C	281	SER
1	D	85	ASP
1	D	90	LEU
1	D	95	THR
1	D	101	CYS
1	D	104	LEU
1	D	145	LEU
1	D	150	LEU
1	D	183	ARG
1	D	193	LYS
1	D	231	ASN
1	D	250	LEU
1	D	281	SER
1	E	90	LEU
1	E	95	THR
1	E	104	LEU
1	E	145	LEU
1	E	150	LEU
1	E	161	GLN
1	E	164	SER
1	E	187	VAL

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Mol	Chain	Res	Type
1	E	192	GLU
1	E	231	ASN
1	E	237	GLN
1	E	250	LEU
1	E	272	LYS
1	F	78	ARG
1	F	90	LEU
1	F	95	THR
1	F	97	TYR
1	F	104	LEU
1	F	122	ARG
1	F	145	LEU
1	F	150	LEU
1	F	163	THR
1	F	196	LEU
1	F	202	VAL
1	F	231	ASN
1	F	247	THR
1	F	250	LEU
1	F	261	SER
1	F	281	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	156	HIS
1	A	161	GLN
1	A	178	GLN
1	A	195	ASN
1	A	216	GLN
1	A	231	ASN
1	A	246	HIS
1	A	267	ASN
1	B	139	GLN
1	B	156	HIS
1	B	223	GLN
1	B	231	ASN
1	B	244	ASN
1	B	246	HIS
1	B	267	ASN
1	C	139	GLN

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Mol	Chain	Res	Type
1	C	156	HIS
1	C	195	ASN
1	C	214	ASN
1	C	216	GLN
1	C	231	ASN
1	C	267	ASN
1	D	139	GLN
1	D	156	HIS
1	D	214	ASN
1	D	228	ASN
1	D	231	ASN
1	D	246	HIS
1	D	267	ASN
1	E	139	GLN
1	E	156	HIS
1	E	161	GLN
1	E	231	ASN
1	E	246	HIS
1	E	267	ASN
1	F	156	HIS
1	F	195	ASN
1	F	231	ASN
1	F	267	ASN

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](#)

9 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	$\# Z > 2$
2	NAG	G	1	1,2	14,14,15	0.83	0	17,19,21	1.85	5 (29%)
2	NAG	G	2	2	14,14,15	0.55	0	17,19,21	1.34	2 (11%)
2	MAN	G	3	2	11,11,12	0.87	1 (9%)	15,15,17	1.66	3 (20%)
2	MAN	G	4	2	11,11,12	0.62	0	15,15,17	1.08	1 (6%)
2	FUC	G	5	2	10,10,11	0.81	0	14,14,16	1.43	2 (14%)
3	NAG	H	1	1,3	14,14,15	0.85	1 (7%)	17,19,21	1.38	2 (11%)
3	NAG	H	2	3	14,14,15	0.71	0	17,19,21	1.27	1 (5%)
3	MAN	H	3	3,6	11,11,12	0.66	0	15,15,17	1.24	2 (13%)
3	FUC	H	4	3	10,10,11	0.90	0	14,14,16	2.98	6 (42%)

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
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	MAN	G	3	2	1/1/4/5	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	1/1/1/1
2	FUC	G	5	2	-	-	0/1/1/1
3	NAG	H	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	MAN	H	3	3,6	1/1/4/5	2/2/19/22	0/1/1/1
3	FUC	H	4	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-2.19	1.40	1.43
2	G	3	MAN	O5-C1	-2.06	1.40	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4	FUC	C2-C3-C4	-7.51	97.91	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4	FUC	C1-C2-C3	-4.52	104.12	109.67
2	G	1	NAG	O5-C1-C2	-4.40	104.35	111.29
2	G	1	NAG	C3-C4-C5	-3.85	103.37	110.24
3	H	4	FUC	O5-C5-C4	3.81	116.35	109.52
2	G	3	MAN	O5-C1-C2	-3.60	105.21	110.77
3	H	2	NAG	C4-C3-C2	3.60	116.29	111.02
3	H	1	NAG	O5-C1-C2	-3.34	106.02	111.29
2	G	3	MAN	C3-C4-C5	3.29	116.11	110.24
2	G	5	FUC	C1-C2-C3	3.24	113.65	109.67
2	G	2	NAG	C2-N2-C7	3.04	127.23	122.90
2	G	2	NAG	C1-O5-C5	2.96	116.20	112.19
2	G	1	NAG	O5-C5-C6	2.78	111.56	107.20
3	H	4	FUC	O2-C2-C3	2.41	114.97	110.14
3	H	1	NAG	C4-C3-C2	2.33	114.43	111.02
2	G	3	MAN	C2-C3-C4	2.26	114.81	110.89
3	H	4	FUC	C1-O5-C5	2.25	117.88	112.78
2	G	1	NAG	C8-C7-N2	2.21	119.85	116.10
3	H	3	MAN	C1-O5-C5	-2.17	109.25	112.19
3	H	3	MAN	C2-C3-C4	-2.16	107.15	110.89
2	G	4	MAN	C1-O5-C5	2.15	115.11	112.19
2	G	5	FUC	O5-C5-C6	2.10	111.85	107.33
2	G	1	NAG	C4-C3-C2	2.09	114.08	111.02
3	H	4	FUC	O4-C4-C3	-2.00	105.72	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	3	MAN	C1
2	G	3	MAN	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	3	MAN	O5-C5-C6-O6
2	G	3	MAN	O5-C5-C6-O6
3	H	3	MAN	C4-C5-C6-O6
2	G	3	MAN	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6

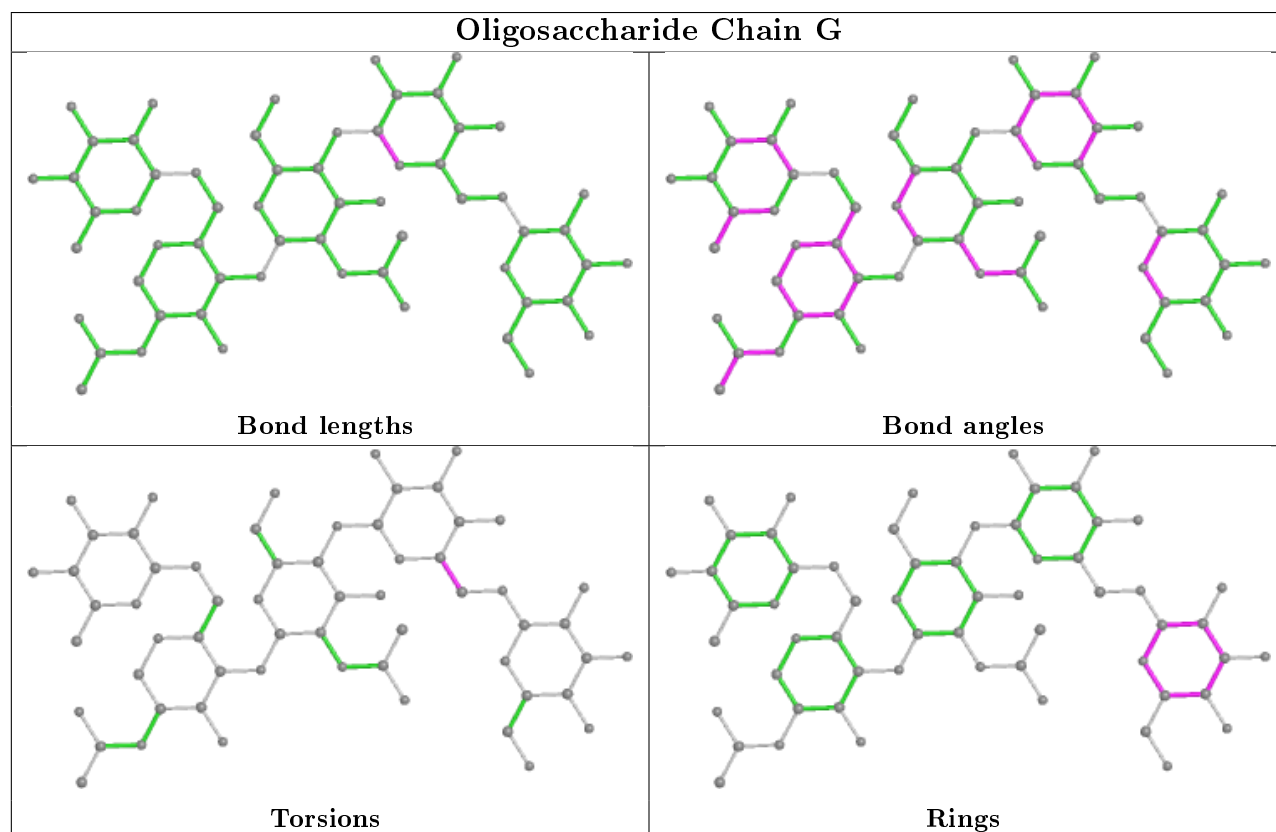
All (1) ring outliers are listed below:

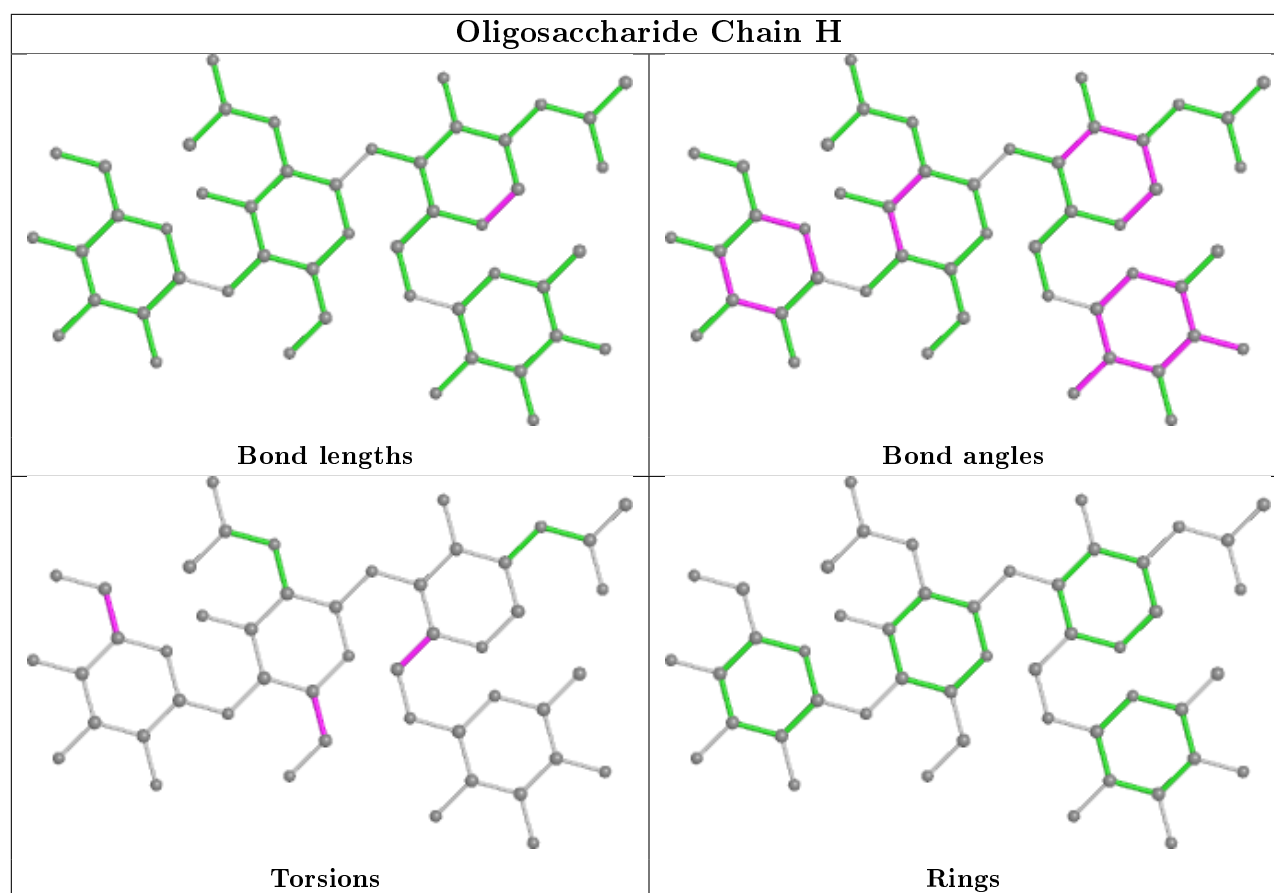
Mol	Chain	Res	Type	Atoms
2	G	4	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	3	MAN	1	0
2	G	4	MAN	1	0
3	H	2	NAG	1	0
2	G	3	MAN	1	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](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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$
5	BM3	F	400	-	15,15,15	3.09	6 (40%)	21,21,21	3.77	8 (38%)
5	BM3	E	400	-	15,15,15	2.63	3 (20%)	21,21,21	3.93	13 (61%)
5	BM3	B	400	-	15,15,15	3.15	6 (40%)	21,21,21	4.49	11 (52%)
6	MAN	F	402	3	11,11,12	1.39	1 (9%)	15,15,17	1.07	1 (6%)
5	BM3	C	400	-	15,15,15	2.64	4 (26%)	21,21,21	4.52	9 (42%)

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
5	BM3	F	400	-	-	4/6/26/26	0/1/1/1
5	BM3	E	400	-	-	4/6/26/26	0/1/1/1
5	BM3	B	400	-	-	4/6/26/26	0/1/1/1
6	MAN	F	402	3	-	0/2/19/22	0/1/1/1
5	BM3	C	400	-	-	4/6/26/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	400	BM3	O6-C6	9.35	1.81	1.42
5	E	400	BM3	C1-C2	-8.68	1.42	1.52
5	C	400	BM3	O6-C6	8.27	1.77	1.42
5	B	400	BM3	O6-C6	7.85	1.75	1.42
5	B	400	BM3	C1-C2	-6.37	1.45	1.52
5	F	400	BM3	O1-C1	4.53	1.54	1.39
5	C	400	BM3	C1-C2	-4.15	1.48	1.52
5	B	400	BM3	C4-C3	3.67	1.61	1.52
6	F	402	MAN	C2-C3	3.45	1.57	1.52
5	B	400	BM3	C2-N2	-3.39	1.40	1.45
5	F	400	BM3	C2-N2	2.93	1.50	1.45
5	E	400	BM3	O1-C1	2.72	1.48	1.39
5	B	400	BM3	C4-C5	2.61	1.58	1.53
5	F	400	BM3	C7-N2	2.59	1.43	1.34
5	B	400	BM3	O5-C5	2.59	1.50	1.44
5	C	400	BM3	C2-N2	2.27	1.49	1.45
5	F	400	BM3	C3-C2	-2.21	1.49	1.53
5	C	400	BM3	C4-C5	2.19	1.57	1.53
5	F	400	BM3	C1-C2	-2.08	1.50	1.52
5	E	400	BM3	C4-C5	2.01	1.57	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	400	BM3	C1-C2-N2	12.74	125.49	110.73
5	F	400	BM3	C1-C2-N2	11.37	123.90	110.73
5	C	400	BM3	C3-C2-N2	10.61	130.66	110.62
5	E	400	BM3	C1-C2-N2	10.19	122.54	110.73
5	C	400	BM3	O1-C1-C2	9.68	129.33	109.22
5	C	400	BM3	C1-C2-N2	8.21	120.24	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	400	BM3	O1-C1-C2	7.40	124.59	109.22
5	F	400	BM3	O1-C1-C2	7.37	124.53	109.22
5	B	400	BM3	C1-C2-C3	-7.34	100.53	110.54
5	B	400	BM3	O1-C1-C2	7.25	124.28	109.22
5	E	400	BM3	C4-C3-C2	-6.98	100.12	110.34
5	B	400	BM3	C1-O5-C5	-6.89	100.66	113.66
5	C	400	BM3	C4-C3-C2	-6.86	100.29	110.34
5	E	400	BM3	C3-C2-N2	6.28	122.48	110.62
5	C	400	BM3	C1-O5-C5	-5.73	102.86	113.66
5	B	400	BM3	C4-C3-C2	-5.28	102.61	110.34
5	F	400	BM3	C3-C2-N2	5.10	120.26	110.62
5	E	400	BM3	C1-O5-C5	-4.75	104.70	113.66
5	F	400	BM3	O5-C1-C2	4.71	114.25	109.52
5	B	400	BM3	C3-C2-N2	4.54	119.18	110.62
5	F	400	BM3	C2-N2-C7	4.52	134.18	123.18
5	C	400	BM3	C1-C2-C3	-4.43	104.50	110.54
5	C	400	BM3	O5-C1-C2	-4.35	105.15	109.52
5	F	400	BM3	C4-C3-C2	-3.68	104.96	110.34
5	B	400	BM3	C3-C4-C5	3.56	116.59	110.24
5	F	400	BM3	C1-O5-C5	-3.54	106.98	113.66
5	C	400	BM3	C2-N2-C7	3.35	131.32	123.18
5	B	400	BM3	O3-C3-C2	2.88	115.47	109.66
5	E	400	BM3	O3-C3-C2	2.82	115.35	109.66
5	F	400	BM3	C1-C2-C3	-2.81	106.71	110.54
5	B	400	BM3	C6-C5-C4	-2.67	106.76	113.00
5	B	400	BM3	O7-C7-C8	-2.64	117.15	122.06
5	E	400	BM3	O1-C1-O5	2.63	118.27	110.38
6	F	402	MAN	O5-C5-C6	-2.47	103.33	107.20
5	E	400	BM3	O6-C6-C5	-2.46	102.85	111.29
5	E	400	BM3	C8-C7-N2	-2.28	112.23	116.10
5	C	400	BM3	O3-C3-C4	2.25	115.56	110.35
5	E	400	BM3	C2-N2-C7	2.22	128.57	123.18
5	E	400	BM3	C6-C5-C4	-2.12	108.04	113.00
5	B	400	BM3	O6-C6-C5	-2.12	104.03	111.29
5	E	400	BM3	O4-C4-C3	2.04	115.06	110.35
5	E	400	BM3	O7-C7-N2	2.01	125.65	121.95

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	400	BM3	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	E	400	BM3	C8-C7-N2-C2
5	C	400	BM3	O7-C7-N2-C2
5	C	400	BM3	C8-C7-N2-C2
5	F	400	BM3	O7-C7-N2-C2
5	F	400	BM3	C8-C7-N2-C2
5	B	400	BM3	O7-C7-N2-C2
5	B	400	BM3	C8-C7-N2-C2
5	E	400	BM3	C4-C5-C6-O6
5	E	400	BM3	O5-C5-C6-O6
5	C	400	BM3	O5-C5-C6-O6
5	B	400	BM3	O5-C5-C6-O6
5	F	400	BM3	O5-C5-C6-O6
5	F	400	BM3	C4-C5-C6-O6
5	B	400	BM3	C4-C5-C6-O6
5	C	400	BM3	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	400	BM3	4	0
5	E	400	BM3	3	0
5	B	400	BM3	17	0
6	F	402	MAN	1	0
5	C	400	BM3	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	224:ASP	C	225:ASN	N	1.20
1	A	224:ASP	C	225:ASN	N	1.14
1	C	223:GLN	C	224:ASP	N	1.07

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, 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	212/218 (97%)	0.27	13 (6%) 21 17	33, 39, 50, 55	0
1	B	217/218 (99%)	-0.16	0 100 100	34, 39, 46, 54	0
1	C	216/218 (99%)	-0.06	0 100 100	34, 39, 50, 74	0
1	D	214/218 (98%)	0.59	30 (14%) 2 2	34, 39, 49, 59	0
1	E	218/218 (100%)	-0.16	0 100 100	32, 39, 47, 60	0
1	F	212/218 (97%)	-0.09	1 (0%) 91 90	34, 39, 47, 54	0
All	All	1289/1308 (98%)	0.06	44 (3%) 45 39	32, 39, 48, 74	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	219	SER	7.6
1	D	242	TYR	5.8
1	A	161	GLN	5.0
1	A	242	TYR	5.0
1	D	239	ALA	4.9
1	D	240	TRP	4.9
1	D	231	ASN	4.7
1	D	161	GLN	4.4
1	D	98	LEU	4.0
1	D	248	SER	3.8
1	D	99	PRO	3.7
1	D	89	PHE	3.7
1	A	247	THR	3.5
1	D	232	CYS	3.4
1	D	247	THR	3.4
1	D	268	TRP	3.2
1	D	246	HIS	3.2
1	A	273	GLY	3.0
1	D	194	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	131	TYR	2.9
1	D	218	PHE	2.8
1	D	217	SER	2.7
1	A	219	SER	2.7
1	D	190	GLU	2.6
1	F	218	PHE	2.6
1	D	234	VAL	2.6
1	D	220	THR	2.5
1	D	245	CYS	2.5
1	A	218	PHE	2.4
1	D	160	ALA	2.4
1	D	115	GLY	2.3
1	D	104	LEU	2.3
1	A	238	GLY	2.3
1	A	220	THR	2.2
1	A	240	TRP	2.2
1	A	248	SER	2.2
1	A	232	CYS	2.2
1	A	157	ALA	2.2
1	D	278	TYR	2.2
1	D	271	GLY	2.1
1	D	191	ALA	2.1
1	D	269	LYS	2.1
1	D	100	ASP	2.1
1	A	162	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

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

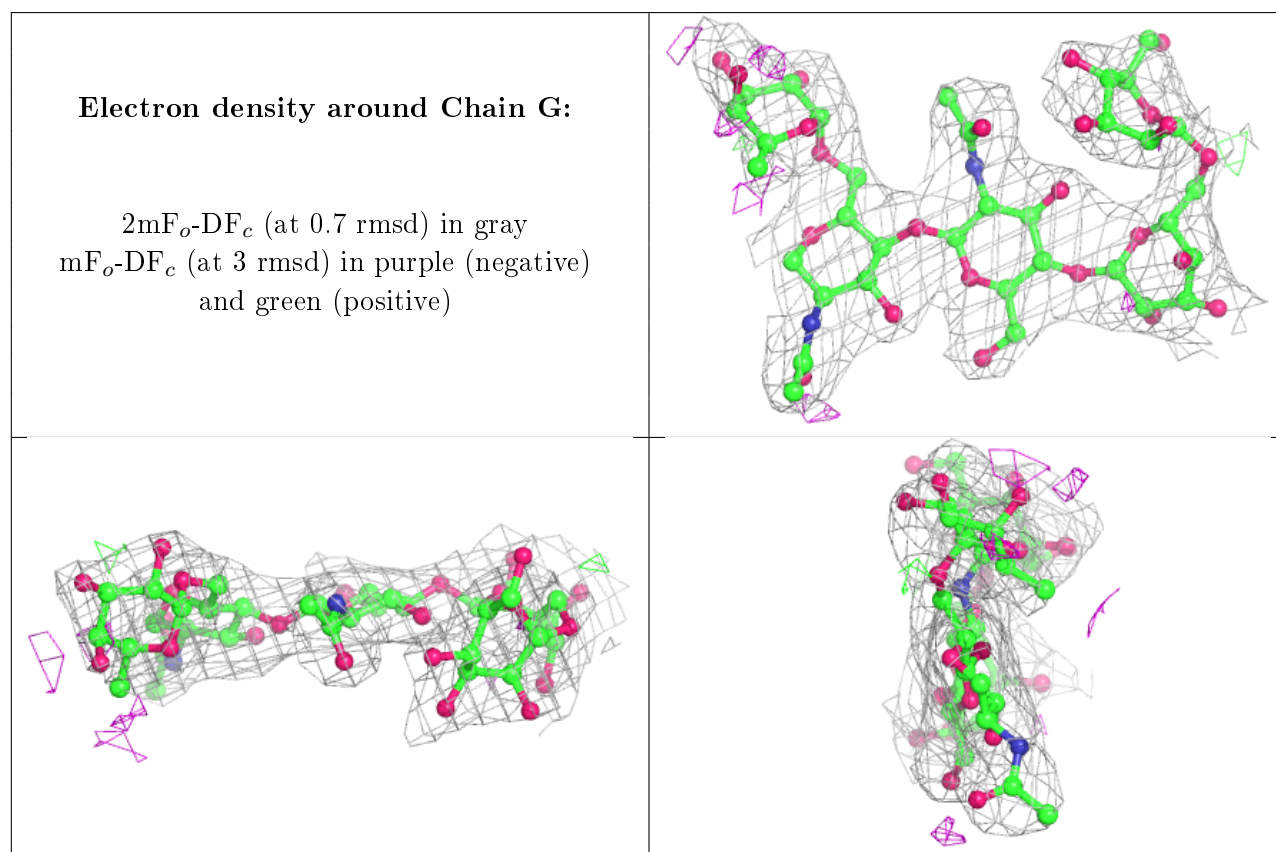
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	H	4	10/11	0.64	0.86	61,63,65,65	0
3	NAG	H	2	14/15	0.79	0.41	59,63,67,70	0
3	MAN	H	3	11/12	0.81	0.27	72,73,74,74	0

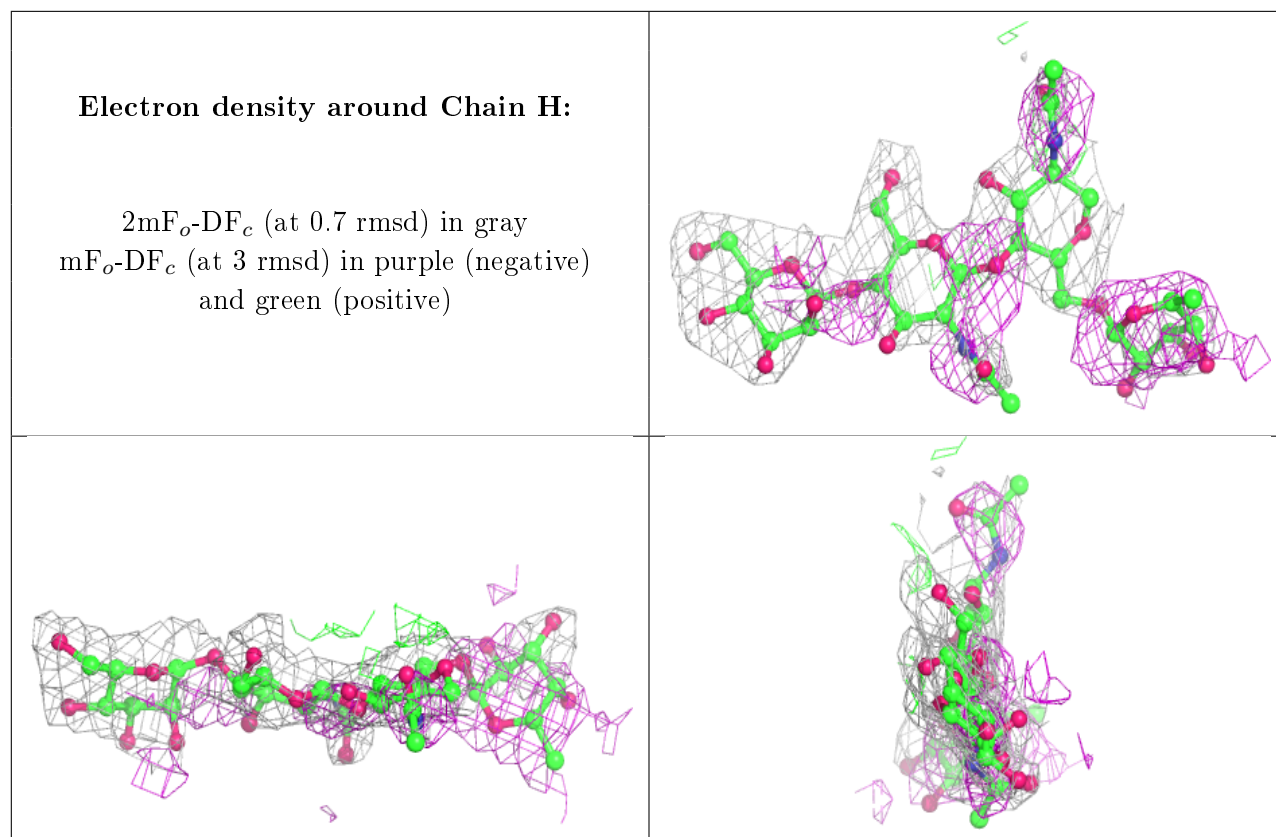
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	H	1	14/15	0.81	0.38	49,53,59,59	0
2	MAN	G	4	11/12	0.85	0.24	88,90,91,91	0
2	MAN	G	3	11/12	0.88	0.18	68,71,80,85	0
2	FUC	G	5	10/11	0.91	0.25	52,53,53,54	0
2	NAG	G	2	14/15	0.96	0.20	48,53,57,63	0
2	NAG	G	1	14/15	0.97	0.17	37,40,49,51	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.





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(Å ²)	Q<0.9
4	CA	F	500	1/1	0.66	0.13	46,46,46,46	0
5	BM3	E	400	15/15	0.73	0.37	27,34,43,45	11
4	CA	A	500	1/1	0.77	0.11	75,75,75,75	0
5	BM3	B	400	15/15	0.81	0.39	32,36,44,48	8
5	BM3	C	400	15/15	0.82	0.24	28,33,41,42	0
4	CA	D	500	1/1	0.88	0.09	70,70,70,70	0
5	BM3	F	400	15/15	0.89	0.24	29,33,41,42	11
6	MAN	F	402	11/12	0.90	0.23	20,20,20,20	0
4	CA	B	500	1/1	0.94	0.09	27,27,27,27	0
4	CA	C	500	1/1	0.95	0.09	38,38,38,38	0
4	CA	E	500	1/1	0.96	0.07	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.