



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:02 PM UTC

PDB ID : 2J0Y / pdb_00002j0y
Title : L-ficolin complexed to b-1,3-D-glucan
Authors : Garlatti, V.; Gaboriaud, C.
Deposited on : 2006-08-08
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

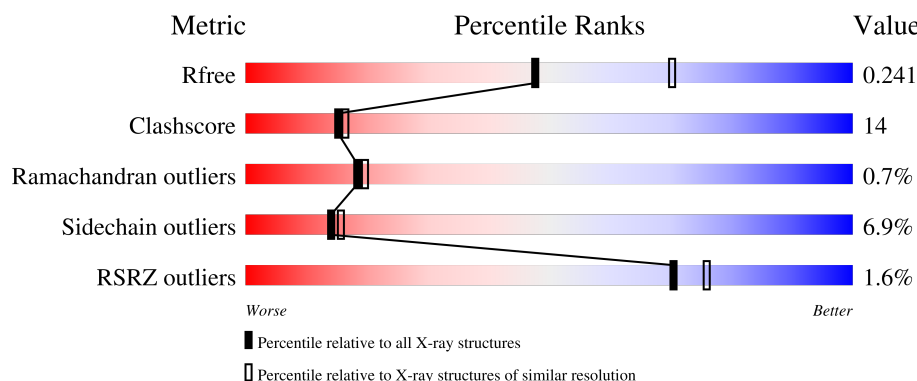
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	218	 3% 56% 28% 11%
1	B	218	 79% 19%
1	C	218	 73% 22%
1	D	218	 6% 60% 27% 6% 7%
1	E	218	 78% 19%

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Mol	Chain	Length	Quality of chain
1	F	218	 76% 19% . .
2	G	3	 67% 33%
2	I	3	 100%
3	H	4	 25% 75%
3	J	4	 100%

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
7	BGC	F	1289	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10651 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
1	A	193	Total	C	N	O	S	0	0	0
			1566	988	273	297	8			
1	B	218	Total	C	N	O	S	0	0	0
			1744	1096	307	332	9			
1	C	215	Total	C	N	O	S	0	0	0
			1723	1084	303	328	8			
1	D	202	Total	C	N	O	S	0	1	0
			1631	1024	288	310	9			
1	E	218	Total	C	N	O	S	0	0	0
			1744	1096	307	332	9			
1	F	215	Total	C	N	O	S	0	1	0
			1734	1093	304	329	8			

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 beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



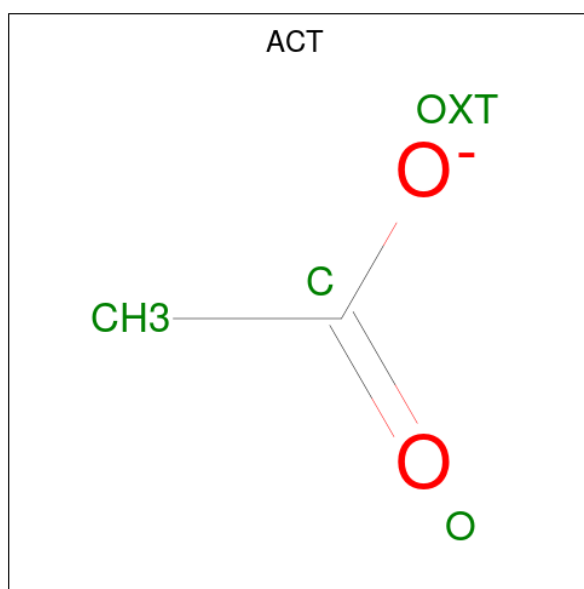
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	H	4	Total	C	O	0	0	0
			44	24	20			
3	J	4	Total	C	O	0	0	0
			44	24	20			

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

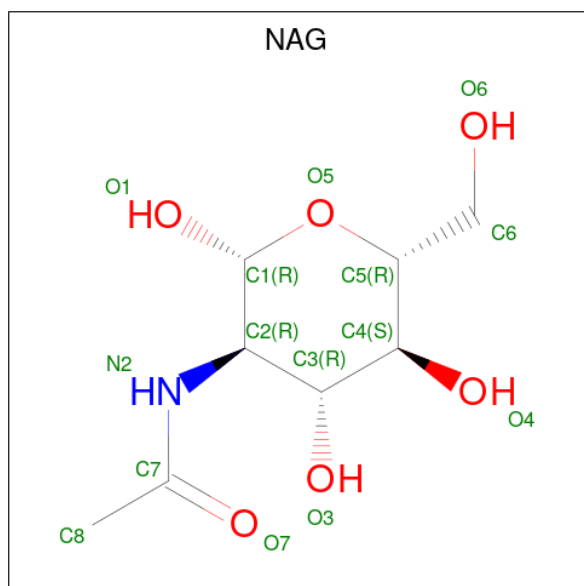


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

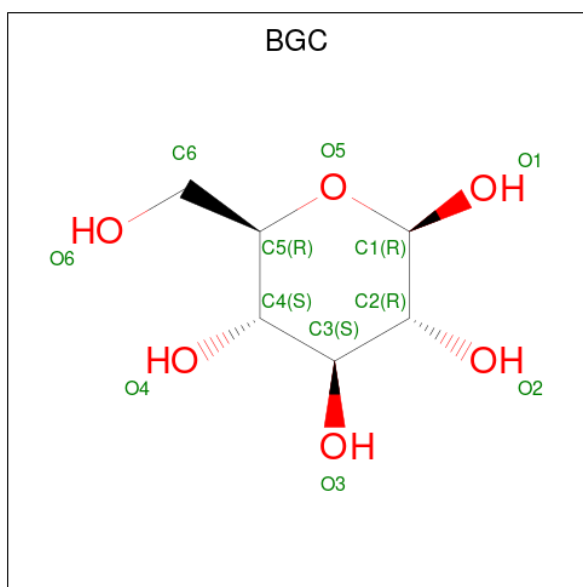
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	C	2	Total	Ca	0	0
			2	2		
5	E	1	Total	Ca	0	0
			1	1		
5	F	2	Total	Ca	0	0
			2	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



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

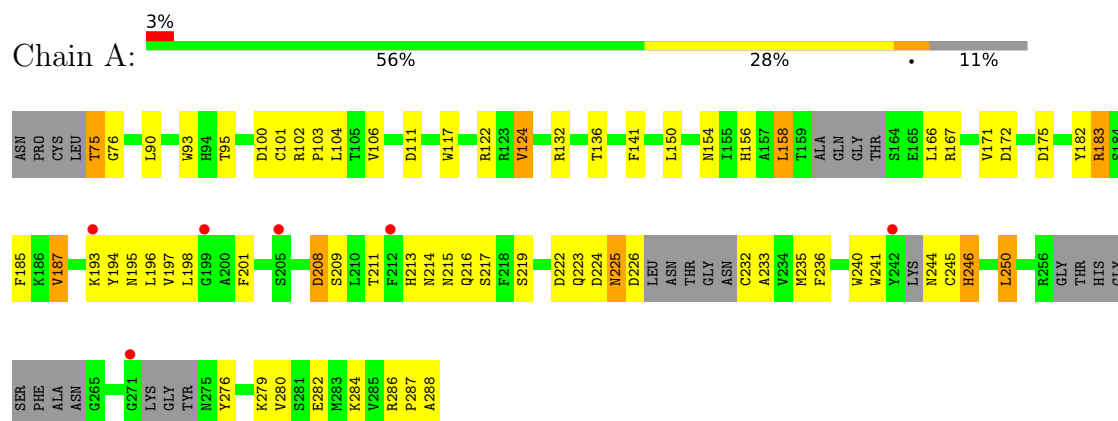
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	32	Total	O	0	0
			32	32		
8	B	61	Total	O	0	0
			61	61		
8	C	57	Total	O	0	0
			57	57		
8	D	24	Total	O	0	0
			24	24		
8	E	66	Total	O	0	0
			66	66		
8	F	54	Total	O	0	0
			54	54		

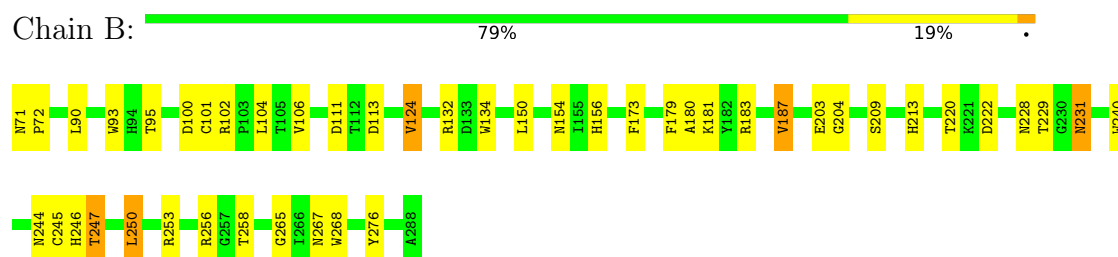
3 Residue-property plots

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

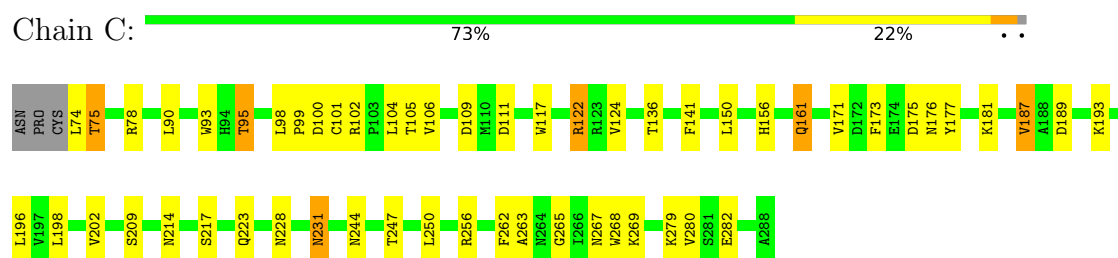
• Molecule 1: FICOLIN-2



• Molecule 1: FICOLIN-2

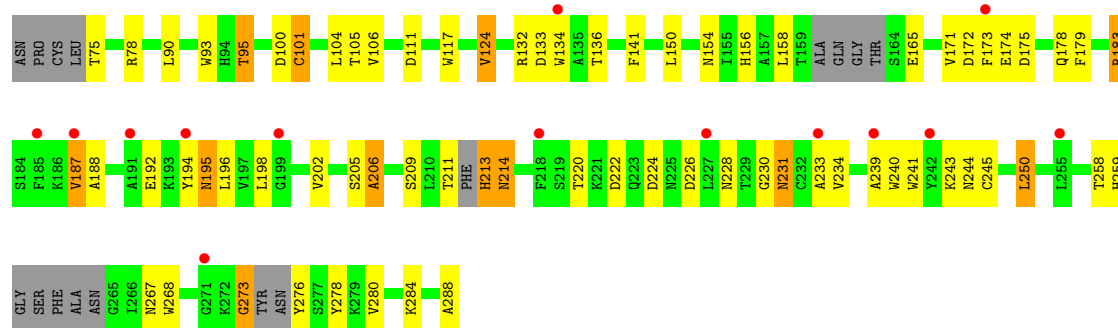


• Molecule 1: FICOLIN-2



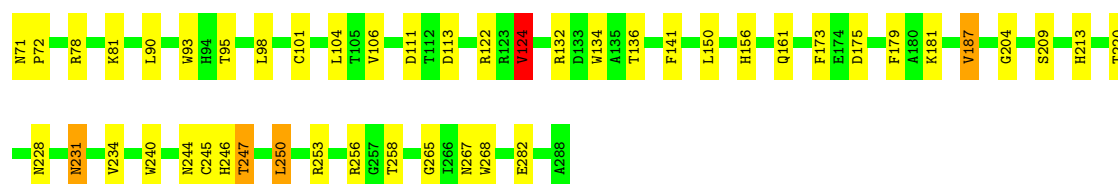
• Molecule 1: FICOLIN-2





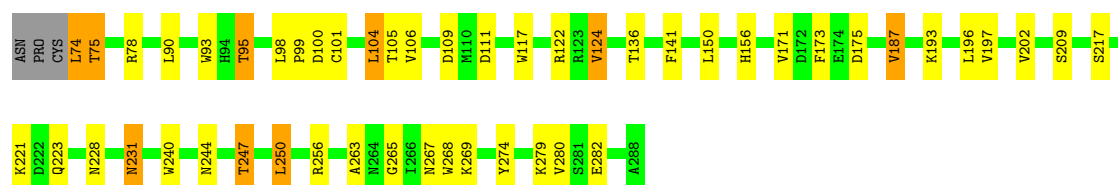
• Molecule 1: FICOLIN-2

Chain E: 78% 19%



• Molecule 1: FICOLIN-2

Chain F: 76% 19%



• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 67% 33%



• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



• Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain H: 25% 75%

BGC1
BGC2
BGC3
BGC4

- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain J:

100%

BGC1
BGC2
BGC3
BGC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.08Å 96.08Å 140.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.35 19.95 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.35) 98.8 (19.95-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.242 0.196 , 0.241	Depositor DCC
R_{free} test set	2990 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.470 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10651	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BGC, ACT, NAG, BMA

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	0.69	3/1605 (0.2%)	0.76	1/2164 (0.0%)
1	B	0.62	1/1792 (0.1%)	0.92	3/2425 (0.1%)
1	C	0.62	0/1770	0.82	1/2394 (0.0%)
1	D	0.75	3/1671 (0.2%)	0.75	0/2253
1	E	0.60	0/1792	0.88	1/2425 (0.0%)
1	F	0.62	0/1782	0.84	0/2410
All	All	0.65	7/10412 (0.1%)	0.83	6/14071 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	273	GLY	C-O	16.91	1.57	1.23
1	A	208	ASP	CG-OD1	10.62	1.45	1.25
1	B	222	ASP	C-N	8.22	1.45	1.33
1	D	213	HIS	CE1-NE2	6.49	1.39	1.32
1	A	208	ASP	CG-OD2	5.45	1.35	1.25
1	D	213	HIS	CG-ND1	5.25	1.44	1.38
1	A	246	HIS	C-O	5.09	1.30	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	HIS	N-CA-C	7.34	120.33	109.24
1	B	247	THR	N-CA-C	-7.09	104.11	114.39
1	E	247	THR	N-CA-C	-6.98	104.27	114.39
1	B	222	ASP	CA-C-N	-6.81	112.25	122.47
1	B	222	ASP	C-N-CA	-6.81	112.25	122.47
1	C	262	PHE	N-CA-C	5.51	117.22	108.67

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	1566	0	1441	58	0
1	B	1744	0	1611	31	1
1	C	1723	0	1595	38	0
1	D	1631	0	1510	67	1
1	E	1744	0	1611	35	0
1	F	1734	0	1603	32	0
2	G	39	0	34	1	0
2	I	39	0	34	0	0
3	H	44	0	37	6	0
3	J	44	0	37	7	0
4	B	4	0	3	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
6	C	14	0	13	0	0
6	F	14	0	13	0	0
7	F	11	0	10	8	0
8	A	32	0	0	12	0
8	B	61	0	0	7	0
8	C	57	0	0	6	0
8	D	24	0	0	25	0
8	E	66	0	0	10	0
8	F	54	0	0	3	0
All	All	10651	0	9552	270	1

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 14.

All (270) 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:D:183:ARG:HG3	1:D:183:ARG:HH11	1.06	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ALA:HB1	8:D:2022:HOH:O	1.57	1.05
7:F:1289:BGC:H6C1	7:F:1289:BGC:H2	1.45	0.98
1:D:220:THR:HG22	8:D:2018:HOH:O	1.63	0.98
1:B:71:ASN:N	1:B:72:PRO:HD3	1.83	0.94
1:F:223:GLN:CD	3:J:1:BGC:H6C2	1.93	0.94
1:D:183:ARG:HH11	1:D:183:ARG:CG	1.80	0.94
1:E:124:VAL:HB	8:E:2010:HOH:O	1.67	0.93
1:D:214:ASN:HB2	8:D:2017:HOH:O	1.67	0.92
1:E:253:ARG:HD3	8:E:2050:HOH:O	1.69	0.90
1:E:71:ASN:N	1:E:72:PRO:HD3	1.89	0.88
1:C:75:THR:HA	8:C:2002:HOH:O	1.70	0.88
1:A:240:TRP:HD1	8:A:2022:HOH:O	1.55	0.87
1:A:224:ASP:O	1:A:225:ASN:ND2	2.08	0.86
1:A:214:ASN:ND2	1:A:215:ASN:N	2.24	0.86
1:D:198:LEU:H	1:D:214:ASN:HD21	1.24	0.85
1:D:239:ALA:HB1	8:D:2018:HOH:O	1.76	0.85
1:D:211:THR:HA	8:D:2017:HOH:O	1.76	0.84
1:E:228:ASN:HD22	1:E:244:ASN:ND2	1.75	0.84
1:A:214:ASN:HD22	1:A:215:ASN:H	1.24	0.84
1:A:183:ARG:HH11	1:A:183:ARG:HB2	1.43	0.84
1:D:183:ARG:HG3	1:D:183:ARG:NH1	1.85	0.83
1:A:201:PHE:CD1	8:A:2019:HOH:O	2.32	0.83
1:A:214:ASN:HD22	1:A:215:ASN:N	1.77	0.81
1:B:228:ASN:HD22	1:B:244:ASN:ND2	1.77	0.81
1:C:223:GLN:CD	3:H:1:BGC:H6C2	2.06	0.80
1:D:239:ALA:CB	8:D:2018:HOH:O	2.31	0.78
1:F:221:LYS:NZ	7:F:1289:BGC:H6C2	1.97	0.78
1:D:198:LEU:HB3	1:D:214:ASN:ND2	1.99	0.78
1:A:219:SER:OG	1:A:225:ASN:HB2	1.83	0.77
1:A:211:THR:HG22	8:A:2020:HOH:O	1.85	0.77
1:B:228:ASN:HD22	1:B:244:ASN:HD22	1.33	0.76
7:F:1289:BGC:H2	7:F:1289:BGC:C6	2.15	0.76
3:J:2:BGC:O4	3:J:3:BGC:O5	2.03	0.76
1:A:183:ARG:HB2	1:A:183:ARG:NH1	2.01	0.75
1:B:71:ASN:N	1:B:72:PRO:CD	2.49	0.75
1:E:228:ASN:HD22	1:E:244:ASN:HD22	1.34	0.74
3:H:2:BGC:O4	3:H:3:BGC:O5	2.05	0.74
1:D:178:GLN:C	8:D:2014:HOH:O	2.30	0.73
1:B:101:CYS:SG	8:B:2005:HOH:O	2.46	0.73
1:A:240:TRP:CD1	8:A:2022:HOH:O	2.34	0.71
1:A:201:PHE:HD1	8:A:2019:HOH:O	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:GLN:OE1	3:J:1:BGC:H6C2	1.91	0.70
1:C:198:LEU:H	1:C:214:ASN:ND2	1.88	0.70
1:D:205:SER:O	1:D:206:ALA:HB2	1.91	0.70
1:A:224:ASP:O	1:A:225:ASN:CG	2.35	0.70
1:D:172:ASP:HB3	8:D:2012:HOH:O	1.90	0.69
1:C:100:ASP:O	1:C:101:CYS:HB2	1.93	0.69
1:C:175:ASP:OD2	1:C:279:LYS:NZ	2.23	0.68
1:D:278:TYR:HD2	8:D:2012:HOH:O	1.77	0.68
7:F:1289:BGC:H6C1	7:F:1289:BGC:C2	2.20	0.67
1:C:223:GLN:OE1	3:H:1:BGC:H6C2	1.95	0.67
1:D:173:PHE:N	8:D:2013:HOH:O	2.28	0.67
1:D:134:TRP:HA	1:D:220:THR:HG21	1.77	0.66
1:C:231:ASN:HD22	1:C:231:ASN:C	2.03	0.66
1:F:231:ASN:C	1:F:231:ASN:HD22	2.04	0.66
1:A:214:ASN:ND2	1:A:215:ASN:H	1.92	0.65
1:D:209:SER:HB2	1:D:268:TRP:CE2	2.32	0.65
1:D:213:HIS:N	1:D:243:LYS:HZ2	1.94	0.65
1:E:124:VAL:CG2	8:E:2010:HOH:O	2.45	0.64
1:E:209:SER:HB2	1:E:268:TRP:CE2	2.32	0.64
1:E:71:ASN:N	1:E:72:PRO:CD	2.60	0.64
7:F:1289:BGC:C6	7:F:1289:BGC:C2	2.76	0.64
1:B:209:SER:HB2	1:B:268:TRP:CE2	2.33	0.63
1:D:211:THR:CA	8:D:2017:HOH:O	2.42	0.63
1:C:161:GLN:H	1:C:161:GLN:HE21	1.45	0.63
1:E:124:VAL:CB	8:E:2010:HOH:O	2.35	0.63
1:D:211:THR:C	8:D:2015:HOH:O	2.41	0.62
1:F:75:THR:HA	8:F:2003:HOH:O	1.99	0.62
1:A:111:ASP:HB2	8:A:2006:HOH:O	2.00	0.62
1:A:214:ASN:HB2	8:A:2023:HOH:O	1.99	0.61
1:D:240:TRP:CH2	1:D:250:LEU:HB2	2.36	0.61
1:F:221:LYS:HZ1	7:F:1289:BGC:H6C2	1.64	0.61
1:D:244:ASN:N	1:D:245:CYS:HA	2.15	0.61
1:C:75:THR:HG23	8:C:2001:HOH:O	1.99	0.61
1:D:258:THR:HG23	1:D:276:TYR:HD2	1.65	0.61
1:C:102:ARG:HG2	8:C:2008:HOH:O	2.00	0.60
1:E:228:ASN:ND2	1:E:244:ASN:ND2	2.48	0.60
3:J:3:BGC:O4	3:J:4:BGC:O5	2.15	0.60
1:A:183:ARG:HH11	1:A:183:ARG:CB	2.13	0.60
1:B:228:ASN:ND2	1:B:244:ASN:ND2	2.49	0.60
1:A:240:TRP:CH2	1:A:250:LEU:HB2	2.37	0.59
1:F:228:ASN:ND2	1:F:244:ASN:OD1	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:H	1:C:214:ASN:HD21	1.49	0.59
1:D:198:LEU:N	1:D:214:ASN:HD21	1.98	0.59
1:E:78:ARG:NH2	1:E:98:LEU:O	2.35	0.59
1:D:211:THR:C	8:D:2017:HOH:O	2.45	0.58
1:D:231:ASN:C	1:D:231:ASN:HD22	2.11	0.58
1:D:132:ARG:NH2	1:E:111:ASP:OD1	2.35	0.58
1:D:258:THR:HA	1:D:276:TYR:HA	1.86	0.58
1:A:100:ASP:O	1:A:101:CYS:HB2	2.03	0.58
1:C:181:LYS:HE2	8:C:2027:HOH:O	2.03	0.58
1:F:98:LEU:HB3	1:F:99:PRO:HD2	1.86	0.57
1:E:101:CYS:HB2	8:E:2003:HOH:O	2.03	0.57
1:F:99:PRO:HG2	8:F:2025:HOH:O	2.03	0.57
1:D:226:ASP:OD2	1:D:228:ASN:O	2.23	0.57
1:A:171:VAL:HB	1:A:280:VAL:HB	1.87	0.57
1:B:102:ARG:NH2	1:B:154:ASN:OD1	2.37	0.57
1:D:179:PHE:N	8:D:2014:HOH:O	2.38	0.57
1:A:222:ASP:O	1:A:223:GLN:HG2	2.04	0.56
1:D:273:GLY:HA2	8:D:2023:HOH:O	2.07	0.55
1:E:113:ASP:OD2	1:E:181:LYS:NZ	2.27	0.55
1:D:198:LEU:H	1:D:214:ASN:ND2	2.01	0.55
1:D:211:THR:O	1:D:213:HIS:N	2.40	0.55
1:B:244:ASN:N	1:B:245:CYS:HA	2.22	0.55
1:C:171:VAL:HB	1:C:280:VAL:HB	1.89	0.55
1:E:244:ASN:N	1:E:245:CYS:HA	2.22	0.55
1:C:263:ALA:HA	1:C:267:ASN:ND2	2.22	0.54
1:A:287:PRO:O	1:A:288:ALA:C	2.50	0.54
1:C:176:ASN:HB3	1:D:202:VAL:O	2.08	0.53
1:A:279:LYS:NZ	8:A:2032:HOH:O	2.32	0.53
1:D:171:VAL:HB	1:D:280:VAL:HB	1.89	0.53
1:D:268:TRP:NE1	8:D:2022:HOH:O	2.41	0.53
1:A:244:ASN:N	1:A:245:CYS:HA	2.23	0.53
1:E:81:LYS:HE3	8:E:2001:HOH:O	2.08	0.53
7:F:1289:BGC:H3	3:J:4:BGC:H3	1.91	0.53
1:A:132:ARG:NH2	1:B:111:ASP:OD1	2.39	0.53
1:B:231:ASN:C	1:B:231:ASN:HD22	2.17	0.53
3:H:2:BGC:HD	3:H:3:BGC:C1	2.20	0.53
1:E:231:ASN:C	1:E:231:ASN:HD22	2.17	0.53
1:E:265:GLY:H	1:E:267:ASN:HD21	1.57	0.52
1:D:205:SER:O	1:D:206:ALA:CB	2.57	0.52
1:B:258:THR:HG22	1:B:276:TYR:HD2	1.74	0.52
1:B:229:THR:CG2	8:B:2042:HOH:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:2:BGC:HD	3:J:3:BGC:C1	2.22	0.52
1:B:240:TRP:CH2	1:B:250:LEU:HB2	2.45	0.52
1:F:175:ASP:OD2	1:F:279:LYS:NZ	2.34	0.52
1:B:229:THR:HG21	8:B:2042:HOH:O	2.10	0.52
1:C:193:LYS:HB3	1:C:217:SER:HB3	1.90	0.51
1:D:154:ASN:O	1:D:158:LEU:HB2	2.11	0.51
1:C:247:THR:HG23	1:C:269:LYS:HB3	1.93	0.51
1:E:231:ASN:ND2	1:E:234:VAL:H	2.09	0.51
1:A:111:ASP:CB	8:A:2006:HOH:O	2.56	0.51
1:A:226:ASP:CG	8:A:2025:HOH:O	2.53	0.50
1:A:222:ASP:O	1:A:223:GLN:CG	2.59	0.50
3:J:2:BGC:O4	3:J:3:BGC:C1	2.59	0.50
1:B:101:CYS:CB	8:B:2005:HOH:O	2.60	0.50
3:H:2:BGC:O4	3:H:3:BGC:C1	2.59	0.50
1:B:102:ARG:HD3	8:B:2004:HOH:O	2.12	0.49
1:A:213:HIS:CE1	1:A:246:HIS:HA	2.46	0.49
1:D:259:HIS:HE1	1:D:267:ASN:HD21	1.60	0.49
1:F:263:ALA:HA	1:F:267:ASN:ND2	2.28	0.49
1:A:193:LYS:NZ	1:A:223:GLN:OE1	2.35	0.49
1:D:231:ASN:HD21	1:D:233:ALA:HB3	1.78	0.49
1:F:221:LYS:NZ	7:F:1289:BGC:C6	2.74	0.49
1:C:228:ASN:ND2	1:C:244:ASN:OD1	2.40	0.48
1:B:265:GLY:H	1:B:267:ASN:HD21	1.60	0.48
1:A:214:ASN:ND2	1:A:214:ASN:C	2.69	0.48
1:C:122:ARG:HD2	1:C:282:GLU:OE2	2.13	0.48
1:E:240:TRP:CH2	1:E:250:LEU:HB2	2.48	0.48
1:F:100:ASP:O	1:F:101:CYS:HB2	2.13	0.48
1:D:196:LEU:HB2	1:D:241:TRP:CD1	2.49	0.48
1:E:132:ARG:HH22	1:F:111:ASP:CG	2.21	0.48
1:B:93:TRP:HA	1:B:106:VAL:O	2.13	0.48
1:D:133:ASP:HB2	1:D:222:ASP:CG	2.39	0.48
1:B:156:HIS:HD2	1:B:187:VAL:O	1.96	0.48
1:F:240:TRP:CH2	1:F:250:LEU:HB2	2.49	0.48
1:E:93:TRP:HA	1:E:106:VAL:O	2.14	0.47
1:F:98:LEU:HB3	1:F:99:PRO:CD	2.44	0.47
1:B:101:CYS:HB2	8:B:2005:HOH:O	2.13	0.47
1:C:209:SER:HB2	1:C:268:TRP:CE2	2.49	0.47
1:D:156:HIS:HD2	1:D:187:VAL:O	1.97	0.47
1:A:214:ASN:CB	8:A:2023:HOH:O	2.61	0.47
1:C:247:THR:HG21	8:C:2029:HOH:O	2.14	0.47
1:D:231:ASN:N	8:D:2020:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:PHE:CE1	1:E:256:ARG:HA	2.50	0.47
1:F:269:LYS:HD2	1:F:274:TYR:CE2	2.49	0.47
1:A:93:TRP:HA	1:A:106:VAL:O	2.15	0.47
1:A:213:HIS:HE1	1:A:246:HIS:CB	2.27	0.47
1:D:165:GLU:HB3	1:D:288:ALA:HB2	1.95	0.47
1:E:81:LYS:NZ	8:E:2001:HOH:O	2.47	0.47
1:D:93:TRP:HA	1:D:106:VAL:O	2.15	0.47
1:E:156:HIS:HD2	1:E:187:VAL:O	1.96	0.47
1:A:213:HIS:HE1	1:A:246:HIS:HB2	1.80	0.47
1:D:100:ASP:O	1:D:101[B]:CYS:HB2	2.14	0.47
1:C:78:ARG:NH2	1:C:98:LEU:O	2.49	0.46
1:D:174:GLU:O	1:D:175:ASP:HB2	2.15	0.46
1:F:171:VAL:HB	1:F:280:VAL:HB	1.97	0.46
1:D:214:ASN:CG	8:D:2016:HOH:O	2.58	0.46
2:G:1:NAG:O3	2:G:2:NAG:O5	2.25	0.46
1:A:154:ASN:O	1:A:158:LEU:HB2	2.15	0.46
1:B:132:ARG:HH22	1:C:111:ASP:CG	2.23	0.46
1:C:95:THR:HA	1:C:105:THR:HA	1.96	0.46
1:C:209:SER:HB3	1:C:247:THR:HG22	1.98	0.46
1:C:98:LEU:HB3	1:C:99:PRO:HD2	1.97	0.46
1:B:113:ASP:OD2	1:B:181:LYS:NZ	2.37	0.46
1:A:156:HIS:HD2	1:A:187:VAL:O	1.99	0.46
1:D:171:VAL:C	8:D:2012:HOH:O	2.59	0.46
1:B:173:PHE:CE1	1:B:256:ARG:HA	2.51	0.45
1:C:156:HIS:HD2	1:C:187:VAL:O	1.99	0.45
1:A:75:THR:CG2	1:A:76:GLY:N	2.80	0.45
1:C:93:TRP:HA	1:C:106:VAL:O	2.16	0.45
1:F:136:THR:HG22	1:F:141:PHE:CD1	2.52	0.45
1:F:109:ASP:HB3	1:F:117:TRP:HB2	1.97	0.45
1:A:232:CYS:O	1:A:233:ALA:C	2.59	0.45
1:F:93:TRP:HA	1:F:106:VAL:O	2.16	0.45
1:F:78:ARG:NH2	1:F:98:LEU:O	2.50	0.45
1:C:109:ASP:HB3	1:C:117:TRP:HB2	1.98	0.45
1:E:81:LYS:CE	8:E:2001:HOH:O	2.62	0.45
1:F:209:SER:HB3	1:F:247:THR:HG22	1.99	0.45
1:E:209:SER:HB2	1:E:268:TRP:CD2	2.52	0.44
1:A:201:PHE:HB2	1:A:208:ASP:OD1	2.17	0.44
1:A:222:ASP:OD1	1:A:222:ASP:N	2.47	0.44
1:B:179:PHE:CE2	1:B:204:GLY:HA2	2.53	0.44
1:A:122:ARG:NH1	1:A:282:GLU:OE2	2.40	0.44
1:A:211:THR:O	1:A:214:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:O	1:A:287:PRO:C	2.61	0.44
1:E:124:VAL:HG23	8:E:2010:HOH:O	2.14	0.44
1:C:247:THR:CG2	8:C:2029:HOH:O	2.66	0.44
1:E:134:TRP:HA	1:E:220:THR:HG21	1.98	0.44
1:E:161:GLN:NE2	8:E:2024:HOH:O	2.50	0.44
1:F:104:LEU:HD13	1:F:106:VAL:CG1	2.48	0.44
1:F:74:LEU:HB3	8:F:2002:HOH:O	2.18	0.44
1:F:156:HIS:HD2	1:F:187:VAL:O	2.01	0.43
1:B:253:ARG:HD2	8:B:2049:HOH:O	2.17	0.43
1:E:122:ARG:HD2	1:E:282:GLU:OE2	2.18	0.43
1:C:171:VAL:HG22	1:C:177:TYR:CD2	2.53	0.43
1:F:95:THR:HA	1:F:105:THR:HA	1.99	0.43
1:F:173:PHE:CZ	1:F:256:ARG:HA	2.54	0.43
1:F:193:LYS:HB3	1:F:217:SER:HB3	1.99	0.43
1:D:188:ALA:HB1	1:D:192:GLU:OE2	2.19	0.43
1:A:196:LEU:HB2	1:A:241:TRP:CD1	2.53	0.43
1:D:78:ARG:HE	1:D:78:ARG:HB2	1.39	0.43
1:D:228:ASN:C	1:D:230:GLY:N	2.77	0.43
1:E:179:PHE:CE2	1:E:204:GLY:HA2	2.54	0.43
1:A:136:THR:HG22	1:A:141:PHE:CD1	2.54	0.42
1:A:172:ASP:HB2	1:A:276:TYR:CE1	2.54	0.42
1:B:246:HIS:CD2	1:B:246:HIS:C	2.97	0.42
1:F:209:SER:HB2	1:F:268:TRP:CE2	2.54	0.42
1:F:122:ARG:HD2	1:F:282:GLU:OE2	2.19	0.42
1:A:102:ARG:HA	1:A:103:PRO:HD3	1.92	0.42
1:A:124:VAL:HG23	1:A:280:VAL:HG22	2.01	0.42
1:A:166:LEU:HB2	1:A:185:PHE:CB	2.48	0.42
1:B:134:TRP:HA	1:B:220:THR:HG21	2.02	0.42
1:D:172:ASP:N	8:D:2012:HOH:O	2.52	0.42
1:A:117:TRP:HB3	1:A:284:LYS:HB2	2.02	0.42
1:A:232:CYS:O	1:A:235:MET:N	2.53	0.42
1:C:193:LYS:HE2	1:C:217:SER:OG	2.19	0.42
1:D:239:ALA:HB2	8:D:2018:HOH:O	2.10	0.42
1:A:217:SER:O	1:A:241:TRP:HA	2.19	0.42
1:C:173:PHE:CZ	1:C:256:ARG:HA	2.55	0.42
1:E:246:HIS:CD2	1:E:246:HIS:C	2.97	0.42
1:F:265:GLY:H	1:F:267:ASN:HD21	1.68	0.42
1:D:136:THR:HG22	1:D:141:PHE:CD1	2.55	0.42
1:A:194:TYR:O	1:A:195:ASN:C	2.63	0.42
1:A:182:TYR:CE2	1:A:198:LEU:HD21	2.56	0.41
1:D:224:ASP:HA	8:D:2019:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ASP:C	1:C:189:ASP:OD1	2.61	0.41
1:D:214:ASN:CB	8:D:2017:HOH:O	2.44	0.41
3:H:2:BGC:O4	3:H:2:BGC:O6	2.31	0.41
1:D:111:ASP:HB2	8:D:2004:HOH:O	2.21	0.41
1:D:183:ARG:CG	1:D:183:ARG:NH1	2.51	0.41
1:D:194:TYR:O	1:D:195:ASN:C	2.63	0.41
1:C:173:PHE:CE1	1:C:256:ARG:HA	2.55	0.41
1:D:278:TYR:CD2	8:D:2012:HOH:O	2.56	0.41
1:B:100:ASP:O	1:B:101:CYS:HB2	2.19	0.41
1:B:213:HIS:CE1	1:B:246:HIS:HA	2.56	0.41
1:D:231:ASN:ND2	1:D:234:VAL:H	2.19	0.41
1:D:133:ASP:HB2	1:D:222:ASP:OD2	2.21	0.41
1:C:136:THR:HG22	1:C:141:PHE:CD1	2.56	0.41
1:C:161:GLN:HE21	1:C:161:GLN:N	2.15	0.41
1:C:265:GLY:H	1:C:267:ASN:HD21	1.69	0.41
1:D:117:TRP:HB3	1:D:284:LYS:HB2	2.03	0.41
1:B:180:ALA:HA	1:B:204:GLY:HA3	2.03	0.41
1:E:136:THR:HG22	1:E:141:PHE:CD1	2.56	0.41
1:A:224:ASP:O	1:A:225:ASN:CB	2.69	0.40
1:A:236:PHE:CD1	1:A:246:HIS:NE2	2.76	0.40
1:A:167:ARG:NH1	8:A:2017:HOH:O	2.54	0.40
1:D:95:THR:HA	1:D:105:THR:HA	2.04	0.40
1:E:213:HIS:CE1	1:E:246:HIS:HA	2.56	0.40

All (1) 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:B:183:ARG:NH1	1:D:288:ALA:O[3_455]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/218 (83%)	162 (90%)	17 (9%)	2 (1%)	11	11
1	B	216/218 (99%)	205 (95%)	10 (5%)	1 (0%)	24	27
1	C	213/218 (98%)	199 (93%)	13 (6%)	1 (0%)	24	27
1	D	193/218 (88%)	171 (89%)	19 (10%)	3 (2%)	7	6
1	E	216/218 (99%)	203 (94%)	12 (6%)	1 (0%)	24	27
1	F	214/218 (98%)	201 (94%)	12 (6%)	1 (0%)	24	27
All	All	1233/1308 (94%)	1141 (92%)	83 (7%)	9 (1%)	18	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	D	206	ALA
1	D	195	ASN
1	A	124	VAL
1	B	124	VAL
1	C	124	VAL
1	D	124	VAL
1	E	124	VAL
1	F	124	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/183 (90%)	152 (92%)	13 (8%)	11	12
1	B	183/183 (100%)	173 (94%)	10 (6%)	19	24
1	C	180/183 (98%)	167 (93%)	13 (7%)	13	14
1	D	172/183 (94%)	159 (92%)	13 (8%)	12	13
1	E	183/183 (100%)	172 (94%)	11 (6%)	17	21
1	F	181/183 (99%)	167 (92%)	14 (8%)	12	13
All	All	1064/1098 (97%)	990 (93%)	74 (7%)	14	15

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	90	LEU
1	A	95	THR
1	A	104	LEU
1	A	150	LEU
1	A	158	LEU
1	A	175	ASP
1	A	183	ARG
1	A	187	VAL
1	A	197	VAL
1	A	209	SER
1	A	216	GLN
1	A	250	LEU
1	B	90	LEU
1	B	95	THR
1	B	104	LEU
1	B	124	VAL
1	B	150	LEU
1	B	187	VAL
1	B	203	GLU
1	B	231	ASN
1	B	247	THR
1	B	250	LEU
1	C	74	LEU
1	C	75	THR
1	C	90	LEU
1	C	95	THR
1	C	104	LEU
1	C	122	ARG
1	C	150	LEU
1	C	161	GLN
1	C	187	VAL
1	C	196	LEU
1	C	202	VAL
1	C	231	ASN
1	C	250	LEU
1	D	75	THR
1	D	90	LEU
1	D	95	THR
1	D	101[A]	CYS
1	D	101[B]	CYS
1	D	104	LEU

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Mol	Chain	Res	Type
1	D	124	VAL
1	D	150	LEU
1	D	183	ARG
1	D	187	VAL
1	D	214	ASN
1	D	231	ASN
1	D	250	LEU
1	E	90	LEU
1	E	95	THR
1	E	104	LEU
1	E	124	VAL
1	E	150	LEU
1	E	175	ASP
1	E	187	VAL
1	E	231	ASN
1	E	247	THR
1	E	250	LEU
1	E	258	THR
1	F	74	LEU
1	F	75	THR
1	F	90	LEU
1	F	95	THR
1	F	104	LEU
1	F	124	VAL
1	F	150	LEU
1	F	187	VAL
1	F	196	LEU
1	F	197	VAL
1	F	202	VAL
1	F	231	ASN
1	F	247	THR
1	F	250	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	139	GLN
1	A	156	HIS
1	A	176	ASN
1	A	195	ASN
1	A	213	HIS

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Mol	Chain	Res	Type
1	A	214	ASN
1	A	225	ASN
1	A	244	ASN
1	B	88	HIS
1	B	139	GLN
1	B	156	HIS
1	B	161	GLN
1	B	225	ASN
1	B	231	ASN
1	B	244	ASN
1	B	246	HIS
1	B	267	ASN
1	C	88	HIS
1	C	94	HIS
1	C	139	GLN
1	C	156	HIS
1	C	161	GLN
1	C	214	ASN
1	C	216	GLN
1	C	231	ASN
1	C	267	ASN
1	C	275	ASN
1	D	94	HIS
1	D	139	GLN
1	D	156	HIS
1	D	195	ASN
1	D	214	ASN
1	D	228	ASN
1	D	231	ASN
1	D	267	ASN
1	E	88	HIS
1	E	139	GLN
1	E	156	HIS
1	E	161	GLN
1	E	223	GLN
1	E	225	ASN
1	E	231	ASN
1	E	244	ASN
1	E	246	HIS
1	E	267	ASN
1	F	139	GLN
1	F	156	HIS

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Mol	Chain	Res	Type
1	F	195	ASN
1	F	216	GLN
1	F	231	ASN
1	F	267	ASN
1	F	275	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 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	2,1	14,14,15	0.83	0	17,19,21	1.15	1 (5%)
2	NAG	G	2	2	14,14,15	0.63	0	17,19,21	0.89	0
2	BMA	G	3	2	11,11,12	0.76	0	15,15,17	1.02	1 (6%)
3	BGC	H	1	3	11,11,12	0.80	0	15,15,17	1.42	4 (26%)
3	BGC	H	2	3	11,11,12	0.68	0	15,15,17	2.42	6 (40%)
3	BGC	H	3	3	11,11,12	0.59	0	15,15,17	1.46	2 (13%)
3	BGC	H	4	3	11,11,12	0.60	0	15,15,17	1.81	5 (33%)
2	NAG	I	1	2,1	14,14,15	0.76	0	17,19,21	1.28	2 (11%)
2	NAG	I	2	2	14,14,15	0.55	0	17,19,21	0.97	1 (5%)
2	BMA	I	3	2	11,11,12	0.42	0	15,15,17	2.05	3 (20%)
3	BGC	J	1	3	11,11,12	0.75	0	15,15,17	1.55	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	J	2	3	11,11,12	0.68	0	15,15,17	2.33	5 (33%)
3	BGC	J	3	3	11,11,12	0.58	0	15,15,17	1.16	2 (13%)
3	BGC	J	4	3	11,11,12	0.62	0	15,15,17	1.58	2 (13%)

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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
3	BGC	H	1	3	-	0/2/19/22	0/1/1/1
3	BGC	H	2	3	-	1/2/19/22	0/1/1/1
3	BGC	H	3	3	-	2/2/19/22	0/1/1/1
3	BGC	H	4	3	-	1/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	BMA	I	3	2	-	2/2/19/22	0/1/1/1
3	BGC	J	1	3	-	0/2/19/22	0/1/1/1
3	BGC	J	2	3	-	1/2/19/22	0/1/1/1
3	BGC	J	3	3	-	1/2/19/22	0/1/1/1
3	BGC	J	4	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	BMA	C1-O5-C5	6.28	120.60	112.19
3	H	2	BGC	C1-O5-C5	5.64	119.75	112.19
3	J	2	BGC	C1-O5-C5	5.34	119.34	112.19
3	H	2	BGC	C2-C3-C4	-5.14	101.82	110.86
3	J	2	BGC	C2-C3-C4	-4.21	103.46	110.86
3	H	4	BGC	C3-C4-C5	3.78	117.08	110.23
3	J	2	BGC	O2-C2-C1	3.71	117.72	109.22
3	J	4	BGC	C3-C4-C5	3.11	115.87	110.23
3	J	4	BGC	C6-C5-C4	-3.05	105.53	113.02
3	J	2	BGC	O5-C5-C6	2.96	113.42	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	BMA	C3-C4-C5	2.88	115.45	110.23
3	H	3	BGC	C2-C3-C4	-2.83	105.88	110.86
3	H	2	BGC	O2-C2-C1	2.78	115.58	109.22
3	J	1	BGC	O3-C3-C2	-2.78	104.39	110.05
3	H	2	BGC	C3-C4-C5	-2.70	105.34	110.23
3	H	4	BGC	C2-C3-C4	2.62	115.46	110.86
3	H	3	BGC	O3-C3-C2	-2.51	104.93	110.05
2	I	1	NAG	O5-C1-C2	-2.46	107.49	111.29
3	H	2	BGC	O5-C5-C6	2.45	112.42	107.66
2	I	3	BMA	O5-C5-C4	2.43	116.74	110.83
2	G	1	NAG	O5-C5-C4	-2.39	105.01	110.83
3	H	1	BGC	O2-C2-C3	2.37	115.07	110.15
2	I	1	NAG	C1-O5-C5	2.34	115.32	112.19
3	J	1	BGC	C1-O5-C5	2.34	115.32	112.19
3	H	1	BGC	C1-O5-C5	2.34	115.32	112.19
3	H	4	BGC	C1-C2-C3	2.31	113.01	109.64
3	J	1	BGC	C2-C3-C4	-2.23	106.95	110.86
3	H	4	BGC	C6-C5-C4	-2.17	107.69	113.02
3	J	1	BGC	C3-C4-C5	2.14	114.12	110.23
3	H	4	BGC	O5-C5-C4	2.14	116.02	110.83
2	I	2	NAG	O4-C4-C3	-2.13	105.35	110.38
3	H	1	BGC	C2-C3-C4	-2.08	107.21	110.86
3	J	3	BGC	O5-C5-C6	2.06	111.67	107.66
2	G	3	BMA	C1-C2-C3	2.05	112.63	109.64
3	J	2	BGC	C6-C5-C4	-2.05	107.99	113.02
3	J	3	BGC	O3-C3-C2	-2.04	105.88	110.05
3	H	2	BGC	C6-C5-C4	-2.01	108.09	113.02
3	H	1	BGC	O3-C3-C2	-2.01	105.96	110.05

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	3	BMA	O5-C5-C6-O6
3	J	4	BGC	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	J	4	BGC	C4-C5-C6-O6
2	I	3	BMA	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
3	H	3	BGC	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6

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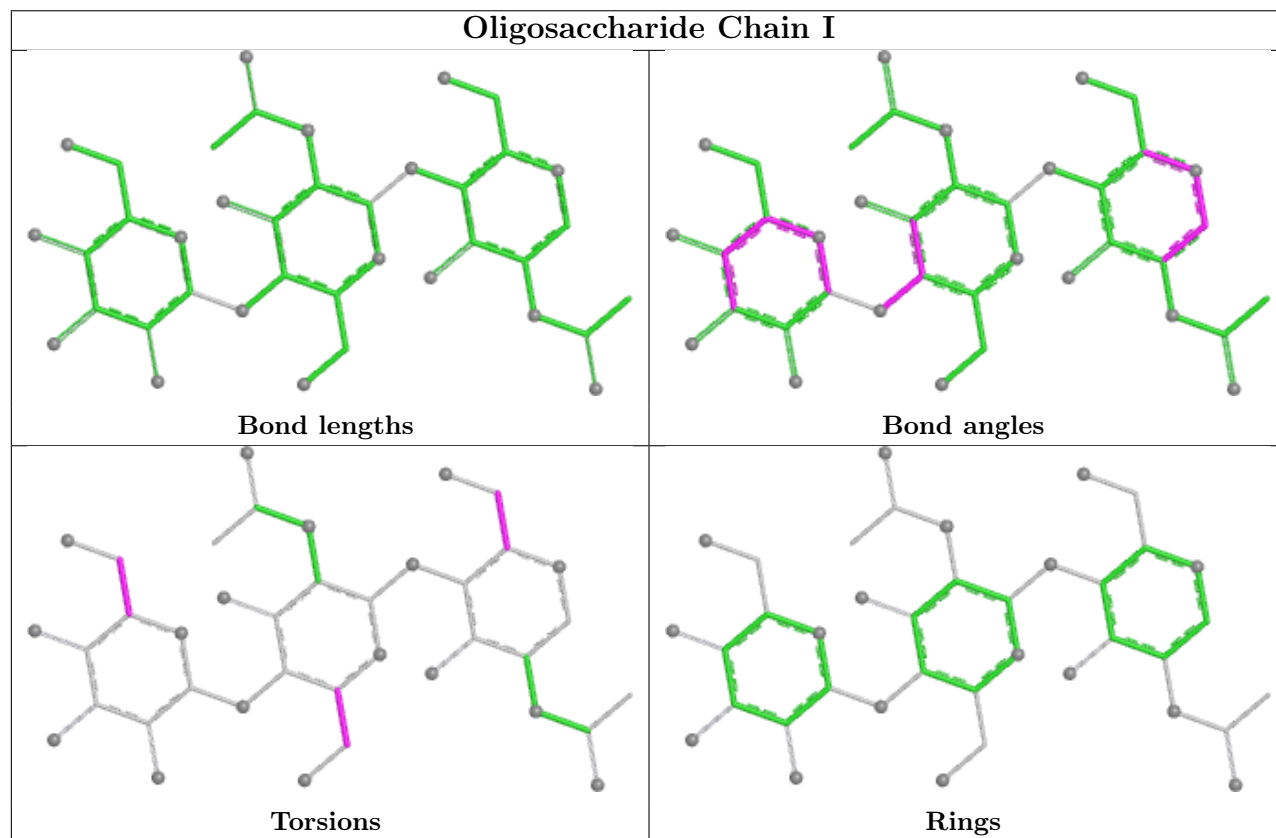
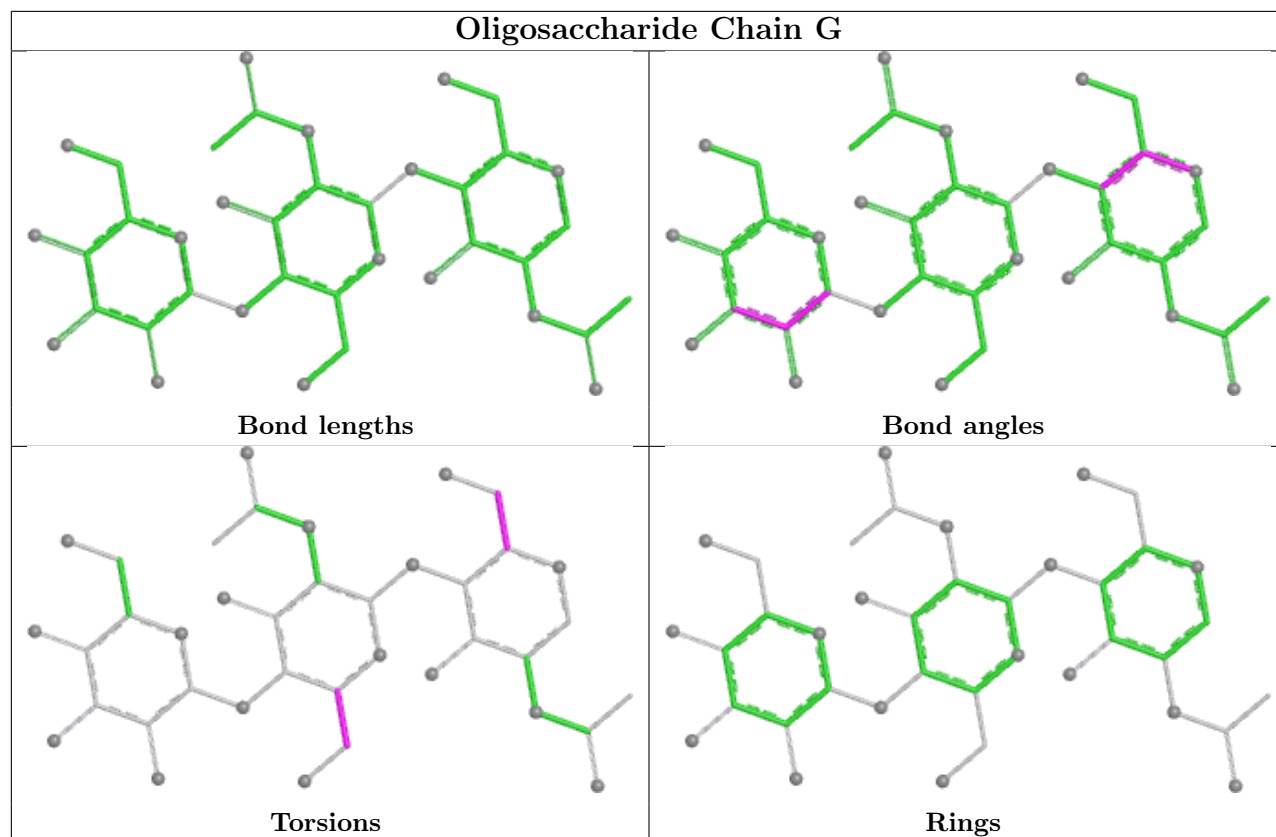
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C4-C5-C6-O6
3	J	2	BGC	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	J	3	BGC	O5-C5-C6-O6
3	H	4	BGC	O5-C5-C6-O6
3	H	2	BGC	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	H	3	BGC	C4-C5-C6-O6

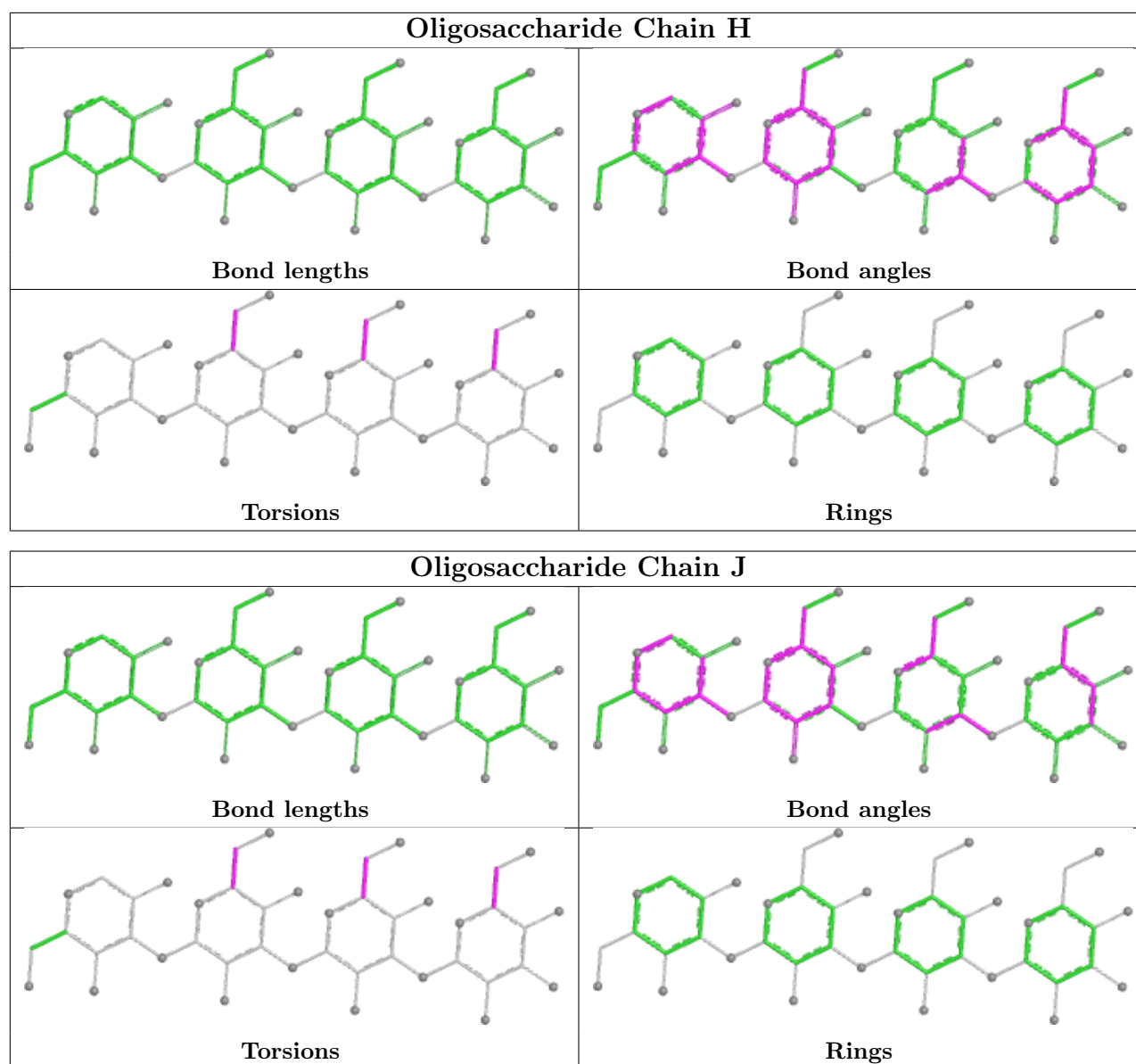
There are no ring outliers.

9 monomers are involved in 14 short contacts:

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

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





5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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
6	NAG	F	1296	1	14,14,15	0.63	0	17,19,21	1.05	2 (11%)
6	NAG	C	1295	1	14,14,15	0.64	0	17,19,21	0.70	0
4	ACT	B	1289	-	3,3,3	0.76	0	3,3,3	1.30	0
7	BGC	F	1289	-	11,11,12	0.53	0	15,15,17	1.20	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1296	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1295	1	-	0/6/23/26	0/1/1/1
7	BGC	F	1289	-	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1296	NAG	C4-C3-C2	2.31	114.40	111.02
7	F	1289	BGC	O4-C4-C5	2.19	114.73	109.32
6	F	1296	NAG	C2-N2-C7	-2.12	120.06	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	1289	BGC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1289	BGC	8	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, 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	193/218 (88%)	0.05	6 (3%)	51	58	42, 46, 56, 59	0
1	B	218/218 (100%)	-1.03	0	100	100	38, 45, 54, 62	0
1	C	215/218 (98%)	-0.86	0	100	100	39, 45, 56, 67	0
1	D	202/218 (92%)	0.34	14 (6%)	23	26	26, 45, 50, 53	1 (0%)
1	E	218/218 (100%)	-1.11	0	100	100	38, 45, 54, 61	0
1	F	215/218 (98%)	-0.95	0	100	100	22, 45, 55, 68	1 (0%)
All	All	1261/1308 (96%)	-0.62	20 (1%)	70	76	22, 45, 54, 68	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	187	VAL	3.8
1	D	271	GLY	3.0
1	A	242	TYR	3.0
1	D	199	GLY	3.0
1	D	191	ALA	2.8
1	D	242	TYR	2.5
1	D	227	LEU	2.4
1	A	199	GLY	2.4
1	A	271	GLY	2.4
1	D	194	TYR	2.3
1	D	239	ALA	2.2
1	D	255	LEU	2.2
1	A	212	PHE	2.2
1	D	173	PHE	2.2
1	D	185	PHE	2.2
1	A	205	SER	2.2
1	A	193	LYS	2.1
1	D	134	TRP	2.1
1	D	233	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	218	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

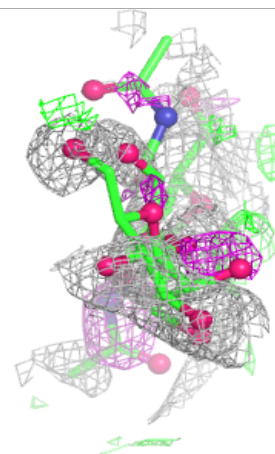
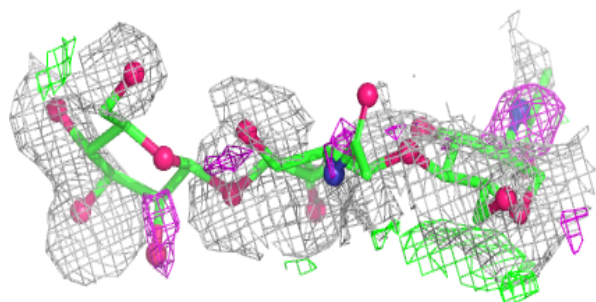
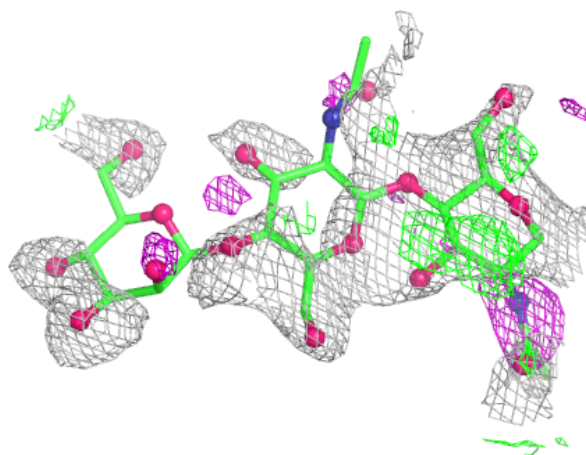
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	G	3	11/12	0.93	0.09	63,65,66,66	0
2	NAG	G	1	14/15	0.94	0.08	45,47,50,50	0
2	NAG	G	2	14/15	0.96	0.07	52,53,55,59	0
3	BGC	H	2	11/12	0.96	0.05	47,50,53,55	0
3	BGC	J	2	11/12	0.96	0.06	50,52,54,55	0
3	BGC	H	4	11/12	0.97	0.06	54,57,59,61	0
3	BGC	J	3	11/12	0.97	0.04	50,52,54,55	0
3	BGC	J	4	11/12	0.97	0.05	55,56,57,59	0
3	BGC	J	1	11/12	0.98	0.05	47,51,52,53	0
2	NAG	I	2	14/15	0.98	0.05	40,41,44,49	0
3	BGC	H	3	11/12	0.98	0.04	52,53,55,56	0
2	BMA	I	3	11/12	0.98	0.04	54,58,60,61	0
3	BGC	H	1	11/12	0.99	0.05	47,51,52,55	0
2	NAG	I	1	14/15	0.99	0.04	36,38,40,41	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.

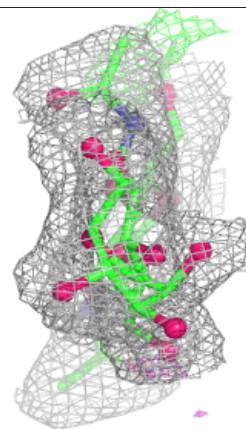
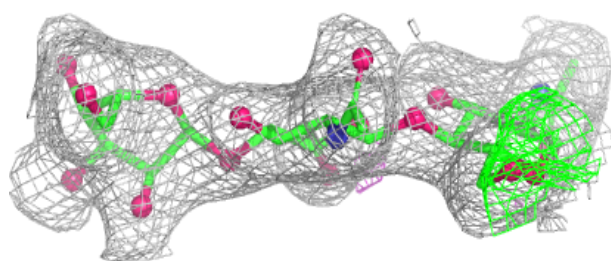
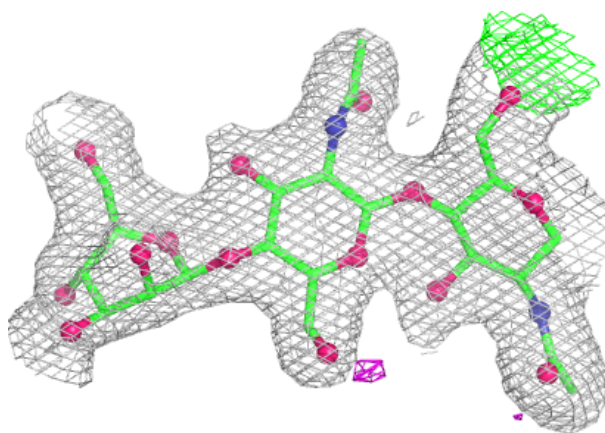
Electron density around Chain G:

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

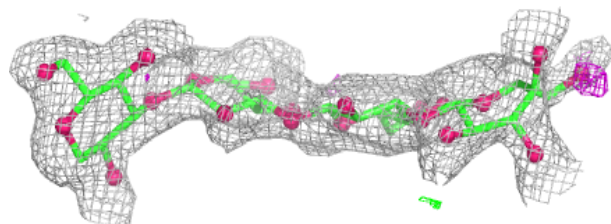
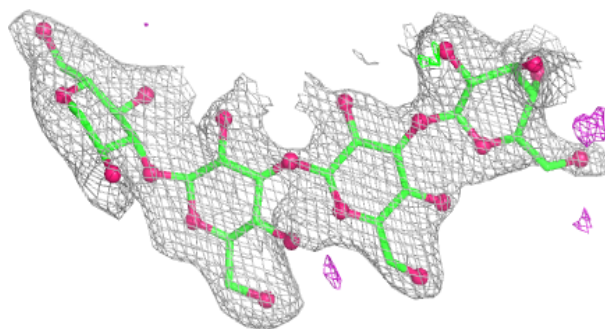


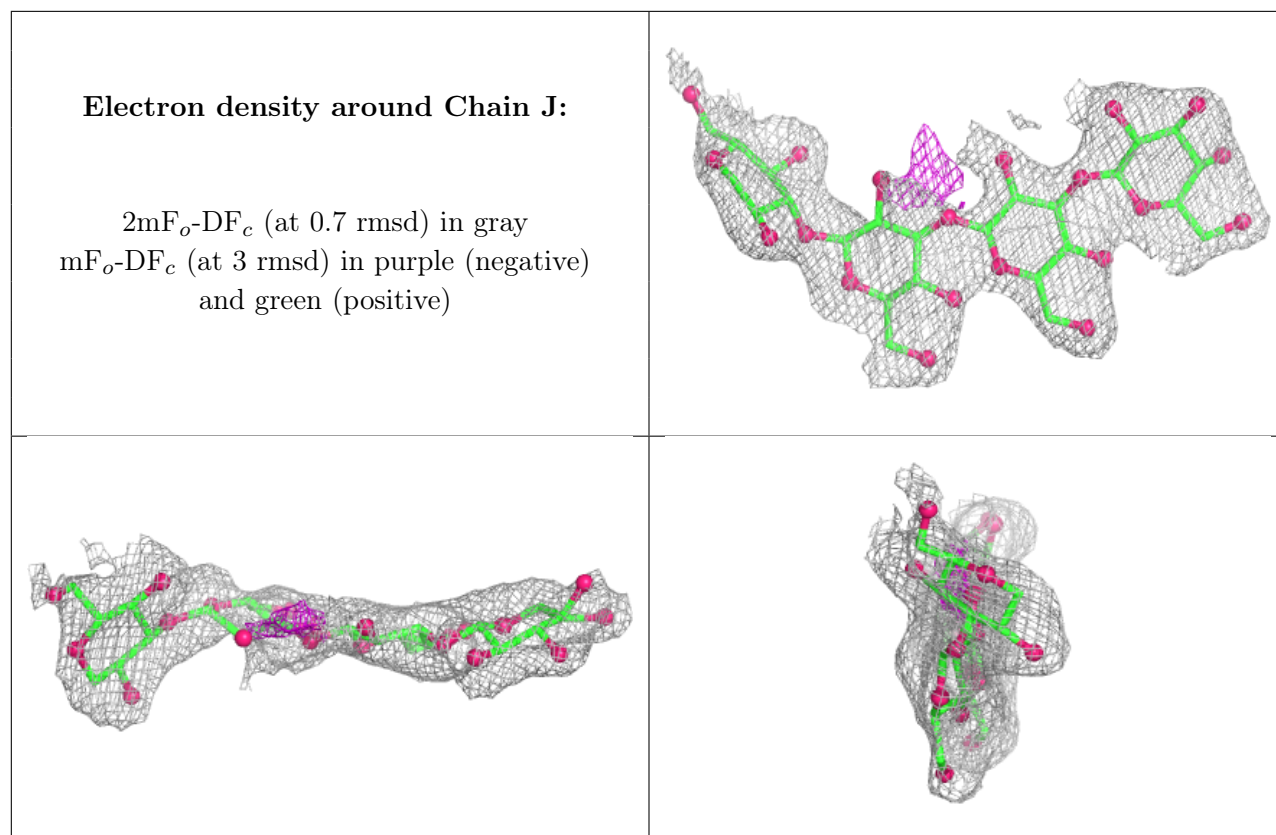
Electron density around Chain I:

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

**Electron density around Chain H:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	F	1296	14/15	0.95	0.05	62,65,68,68	0
6	NAG	C	1295	14/15	0.97	0.04	61,65,67,67	0
7	BGC	F	1289	11/12	0.97	0.07	70,76,77,78	0
5	CA	F	1294	1/1	0.98	0.03	38,38,38,38	0
4	ACT	B	1289	4/4	0.98	0.05	56,57,58,58	0
5	CA	C	1294	1/1	0.99	0.03	46,46,46,46	0
5	CA	B	1290	1/1	0.99	0.07	27,27,27,27	0
5	CA	F	1295	1/1	0.99	0.03	48,48,48,48	0
5	CA	E	1289	1/1	1.00	0.04	28,28,28,28	0
5	CA	C	1293	1/1	1.00	0.03	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.