



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:22 PM UTC

PDB ID : 3WDU / pdb_00003wdu
Title : The complex structure of PtLic16A with cellobiose
Authors : Cheng, Y.S.; Huang, C.H.; Chen, C.C.; Huang, T.Y.; Ko, T.P.; Huang, J.W.;
Wu, T.H.; Liu, J.R.; Guo, R.T.
Deposited on : 2013-06-25
Resolution : 2.25 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

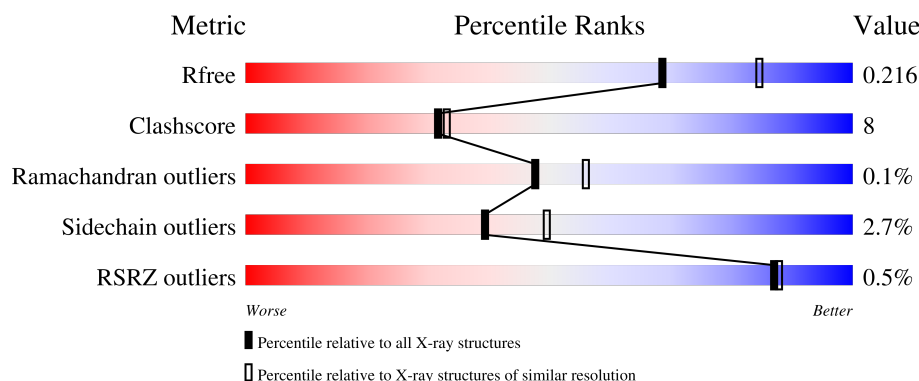
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

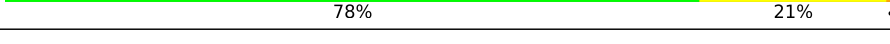
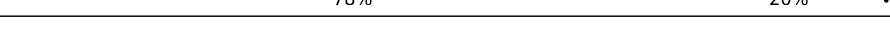
The reported resolution of this entry is 2.25 Å.

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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	297	
1	B	297	
1	C	297	
1	D	297	
2	E	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 50%50%
2	H	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10282 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 Beta-1,3-1,4-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2256	1420	386	439	11			
1	B	296	Total	C	N	O	S	0	0	0
			2256	1420	386	439	11			
1	C	297	Total	C	N	O	S	0	0	0
			2267	1429	387	440	11			
1	D	297	Total	C	N	O	S	0	0	0
			2267	1429	387	440	11			

There are 4 discrepancies between the modelled and reference sequences:

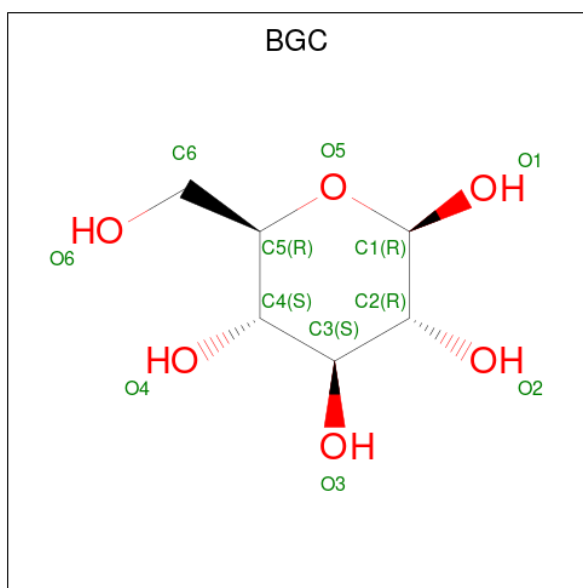
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PHE	-	expression tag	UNP E0XN39
B	0	PHE	-	expression tag	UNP E0XN39
C	0	PHE	-	expression tag	UNP E0XN39
D	0	PHE	-	expression tag	UNP E0XN39

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

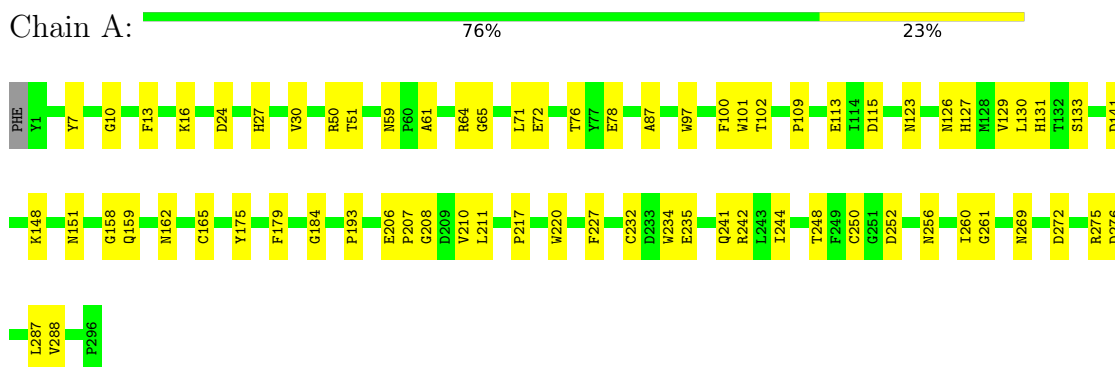
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	302	Total	O	0	0
			302	302		
4	B	293	Total	O	0	0
			293	293		
4	C	297	Total	O	0	0
			297	297		
4	D	228	Total	O	0	0
			228	228		

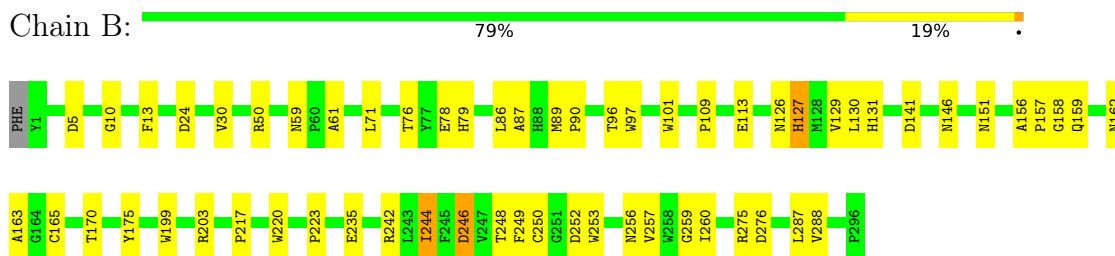
3 Residue-property plots

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.

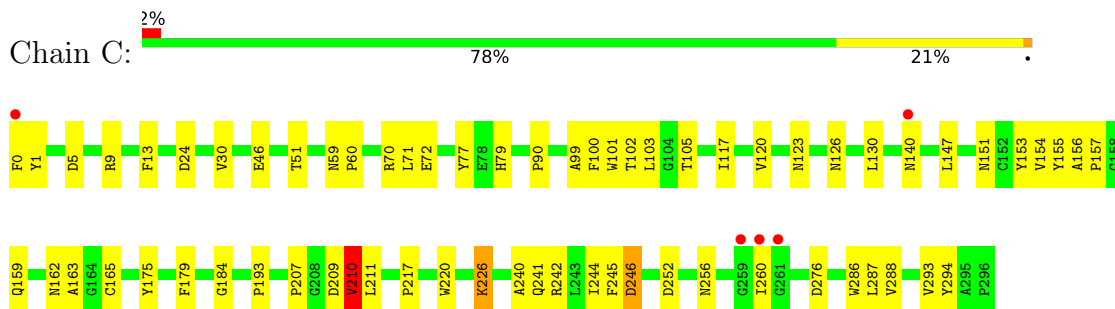
• Molecule 1: Beta-1,3-1,4-glucanase



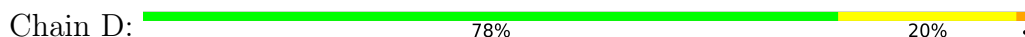
• Molecule 1: Beta-1,3-1,4-glucanase

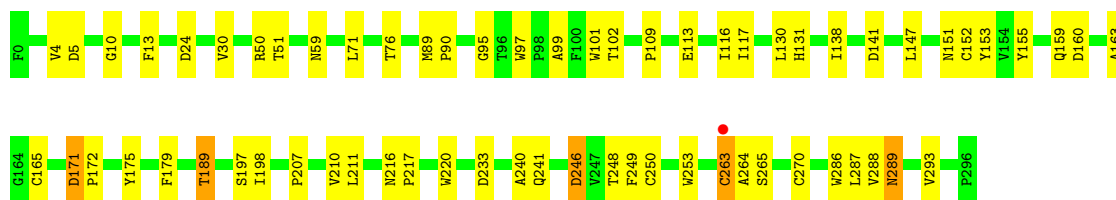


• Molecule 1: Beta-1,3-1,4-glucanase



• Molecule 1: Beta-1,3-1,4-glucanase





- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E:  100%



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:  50% 50%



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G:  50% 50%



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain H:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.14Å 172.56Å 166.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.25 25.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	92.8 (25.00-2.25) 92.7 (25.00-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.26Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.181 , 0.213 0.186 , 0.216	Depositor DCC
R_{free} test set	2837 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.778	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10282	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: BGC

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	0.37	0/2325	0.93	10/3168 (0.3%)
1	B	0.36	0/2325	0.97	11/3168 (0.3%)
1	C	0.36	0/2337	0.98	10/3184 (0.3%)
1	D	0.36	0/2337	0.96	13/3184 (0.4%)
All	All	0.36	0/9324	0.96	44/12704 (0.3%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	ALA	N-CA-C	-7.13	104.55	113.18
1	C	210	VAL	N-CA-C	6.76	123.41	109.34
1	B	288	VAL	N-CA-C	6.48	117.91	108.58
1	C	156	ALA	CA-C-N	6.38	127.82	119.84
1	C	156	ALA	C-N-CA	6.38	127.82	119.84
1	C	288	VAL	N-CA-C	6.32	117.68	108.58
1	B	156	ALA	CA-C-N	6.27	127.68	119.84
1	B	156	ALA	C-N-CA	6.27	127.68	119.84
1	A	65	GLY	N-CA-C	6.23	119.23	110.38
1	C	59	ASN	N-CA-C	6.14	118.37	110.39
1	B	276	ASP	N-CA-C	6.14	120.77	113.16
1	A	59	ASN	N-CA-C	5.99	118.17	110.39
1	D	263	CYS	N-CA-C	5.92	120.51	113.16
1	A	276	ASP	N-CA-C	5.87	120.45	113.28
1	A	100	PHE	N-CA-C	-5.75	99.03	108.41
1	D	288	VAL	N-CA-C	5.74	117.01	108.23
1	C	163	ALA	N-CA-C	-5.73	105.17	111.82
1	A	288	VAL	N-CA-C	5.62	116.83	108.23
1	C	100	PHE	N-CA-C	-5.60	99.28	108.41
1	A	87	ALA	N-CA-C	-5.59	106.59	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	GLY	N-CA-C	5.55	119.60	112.83
1	D	289	ASN	N-CA-C	-5.55	104.87	111.69
1	D	216	ASN	CA-C-N	5.53	125.37	119.28
1	D	216	ASN	C-N-CA	5.53	125.37	119.28
1	D	233	ASP	N-CA-C	-5.50	101.30	109.11
1	B	59	ASN	N-CA-C	5.48	117.87	110.31
1	D	171	ASP	CA-C-N	5.46	125.29	119.28
1	D	171	ASP	C-N-CA	5.46	125.29	119.28
1	A	208	GLY	N-CA-C	5.44	120.44	114.40
1	B	252	ASP	N-CA-C	5.43	117.90	111.33
1	C	276	ASP	N-CA-C	5.42	119.89	113.16
1	D	59	ASN	N-CA-C	5.38	117.73	110.31
1	B	244	ILE	N-CA-C	5.29	115.74	108.12
1	A	250	CYS	CB-CA-C	-5.29	110.46	116.54
1	B	87	ALA	N-CA-C	-5.25	106.72	113.23
1	C	252	ASP	N-CA-C	5.22	117.64	111.33
1	C	60	PRO	N-CA-C	-5.20	103.03	111.14
1	D	250	CYS	CB-CA-C	-5.19	110.57	116.54
1	B	163	ALA	N-CA-C	-5.16	105.35	111.69
1	A	252	ASP	N-CA-C	5.11	118.28	111.75
1	D	270	CYS	N-CA-C	5.08	117.21	111.11
1	D	163	ALA	N-CA-C	-5.07	105.45	111.69
1	B	250	CYS	CB-CA-C	-5.01	110.78	116.54
1	A	133	SER	N-CA-C	-5.00	103.45	110.35

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	2256	0	2043	41	0
1	B	2256	0	2043	34	0
1	C	2267	0	2052	35	0
1	D	2267	0	2052	35	0
2	E	23	0	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	23	0	21	1	0
2	G	23	0	21	1	0
2	H	23	0	21	0	0
3	A	12	0	12	0	0
3	B	12	0	12	1	0
4	A	302	0	0	5	0
4	B	293	0	0	4	0
4	C	297	0	0	2	0
4	D	228	0	0	0	0
All	All	10282	0	8298	142	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 8.

All (142) 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:C:0:PHE:N	4:C:539:HOH:O	1.92	0.99
1:C:210:VAL:HG13	1:C:211:LEU:HG	1.63	0.80
1:D:189:THR:HB	1:D:198:ILE:HG12	1.62	0.80
1:C:154:VAL:HG23	1:C:155:TYR:CD2	2.17	0.79
1:C:130:LEU:HB2	1:C:165:CYS:SG	2.26	0.75
1:B:113:GLU:HB3	1:B:131:HIS:HB2	1.75	0.68
1:D:113:GLU:HB3	1:D:131:HIS:HB2	1.77	0.67
1:C:151:ASN:H	1:C:159:GLN:HE22	1.40	0.66
1:A:151:ASN:H	1:A:159:GLN:HE22	1.46	0.64
1:A:130:LEU:HB2	1:A:165:CYS:SG	2.38	0.63
1:A:113:GLU:HB3	1:A:131:HIS:HB2	1.79	0.63
1:A:193:PRO:HB3	1:A:235:GLU:OE1	2.00	0.62
1:A:210:VAL:HG13	1:A:211:LEU:HG	1.82	0.60
1:D:210:VAL:HG13	1:D:211:LEU:HG	1.84	0.60
1:C:207:PRO:C	1:C:209:ASP:H	2.12	0.58
3:B:301:BGC:O1	4:B:469:HOH:O	2.17	0.58
1:C:13:PHE:CD2	1:C:51:THR:HG21	2.38	0.58
1:B:170:THR:OG1	1:C:140:ASN:HB2	2.05	0.57
1:C:226:LYS:HE2	4:C:606:HOH:O	2.05	0.57
1:C:1:TYR:HB3	1:C:294:TYR:HB3	1.86	0.56
1:B:146:ASN:OD1	1:C:147:LEU:HD23	2.06	0.56
1:D:10:GLY:O	1:D:13:PHE:HB3	2.06	0.55
1:D:71:LEU:N	1:D:71:LEU:HD12	2.21	0.55
1:D:4:VAL:HG22	1:D:293:VAL:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ILE:CD1	1:D:189:THR:HG21	2.36	0.55
1:A:123:ASN:ND2	1:A:127:HIS:HE1	2.04	0.54
1:D:130:LEU:HB2	1:D:165:CYS:SG	2.48	0.54
1:D:207:PRO:HG2	1:D:210:VAL:HB	1.88	0.54
1:A:27:HIS:HA	4:A:551:HOH:O	2.09	0.53
1:D:152:CYS:HA	1:D:165:CYS:H	1.74	0.53
1:D:138:ILE:HD11	1:D:147:LEU:HD11	1.91	0.53
1:D:152:CYS:HA	1:D:165:CYS:N	2.24	0.52
1:A:64:ARG:HG2	4:A:542:HOH:O	2.08	0.52
1:B:126:ASN:HB2	1:B:175:TYR:HB2	1.91	0.52
1:C:105:THR:HG23	1:C:240:ALA:O	2.10	0.52
1:B:130:LEU:HB2	1:B:165:CYS:SG	2.50	0.52
1:A:7:TYR:HA	1:A:16:LYS:HE2	1.93	0.51
1:C:154:VAL:HG12	1:C:162:ASN:OD1	2.11	0.51
1:A:158:GLY:HA3	1:B:256:ASN:HD21	1.75	0.51
1:B:101:TRP:N	1:B:101:TRP:CD1	2.78	0.51
1:B:127:HIS:O	1:B:127:HIS:CD2	2.64	0.51
1:C:103:LEU:HD23	1:C:242:ARG:NH2	2.26	0.51
1:A:10:GLY:O	1:A:13:PHE:HB3	2.12	0.50
1:A:97:TRP:HB3	1:A:248:THR:HG23	1.93	0.50
1:C:153:TYR:CE2	1:C:155:TYR:HB2	2.46	0.50
1:A:97:TRP:HB3	1:A:248:THR:CG2	2.42	0.50
1:A:256:ASN:HD21	1:B:158:GLY:HA3	1.76	0.50
1:C:72:GLU:HG2	1:C:244:ILE:HG12	1.92	0.50
1:C:77:TYR:CD1	1:C:293:VAL:HG11	2.47	0.49
1:B:71:LEU:O	1:B:244:ILE:HA	2.12	0.49
1:D:89:MET:HE1	1:D:175:TYR:CE1	2.47	0.49
1:B:76:THR:HG22	1:B:242:ARG:HB3	1.95	0.49
1:C:71:LEU:O	1:C:244:ILE:HA	2.13	0.49
1:C:120:VAL:H	1:C:123:ASN:ND2	2.10	0.48
1:B:260:ILE:C	1:B:260:ILE:HD12	2.38	0.48
1:B:24:ASP:HB2	1:B:30:VAL:CG1	2.43	0.48
1:B:10:GLY:O	1:B:13:PHE:HB3	2.13	0.48
1:C:101:TRP:CD1	1:C:101:TRP:N	2.81	0.48
1:D:13:PHE:CD2	1:D:51:THR:HG21	2.49	0.47
1:B:217:PRO:HA	1:B:220:TRP:CD2	2.49	0.47
1:C:179:PHE:CE1	1:C:184:GLY:HA2	2.49	0.47
1:C:162:ASN:HD22	2:G:1:BGC:H1	1.79	0.47
1:A:260:ILE:HD12	1:A:260:ILE:C	2.39	0.46
1:A:260:ILE:HD12	1:A:261:GLY:N	2.30	0.46
1:D:97:TRP:HB3	1:D:248:THR:HG23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:THR:HG22	1:A:242:ARG:HB3	1.98	0.46
1:A:141:ASP:HA	4:A:503:HOH:O	2.15	0.46
1:A:71:LEU:HD12	1:A:71:LEU:N	2.30	0.46
1:B:151:ASN:H	1:B:159:GLN:HE22	1.64	0.46
1:D:246:ASP:C	1:D:246:ASP:OD1	2.58	0.46
1:C:154:VAL:HG23	1:C:155:TYR:CE2	2.50	0.46
1:C:207:PRO:C	1:C:209:ASP:N	2.74	0.46
1:A:260:ILE:HG23	4:A:506:HOH:O	2.15	0.45
1:D:24:ASP:HB2	1:D:30:VAL:CG1	2.47	0.45
1:D:116:ILE:HD13	1:D:189:THR:HG21	1.99	0.45
1:D:138:ILE:HD11	1:D:147:LEU:CD1	2.47	0.45
1:A:13:PHE:CD2	1:A:51:THR:HG21	2.52	0.45
1:C:102:THR:HB	1:C:241:GLN:HB3	1.97	0.45
1:D:50:ARG:HG2	1:D:289:ASN:HD22	1.82	0.45
1:B:96:THR:HG22	1:B:249:PHE:CE1	2.51	0.45
1:A:101:TRP:CD1	1:A:101:TRP:N	2.85	0.45
1:C:126:ASN:HB2	1:C:175:TYR:HB2	1.98	0.45
1:C:246:ASP:OD1	1:C:246:ASP:C	2.60	0.45
1:B:246:ASP:OD1	1:B:246:ASP:C	2.60	0.44
1:B:71:LEU:HD12	1:B:71:LEU:N	2.33	0.44
1:B:242:ARG:HD3	4:B:582:HOH:O	2.18	0.44
1:C:70:ARG:HA	1:C:245:PHE:O	2.16	0.44
1:D:153:TYR:CZ	1:D:155:TYR:HB2	2.53	0.44
1:A:71:LEU:O	1:A:244:ILE:HA	2.18	0.44
1:B:79:HIS:HE1	1:B:235:GLU:OE1	2.01	0.44
1:A:287:LEU:HD12	1:A:287:LEU:HA	1.87	0.44
1:A:72:GLU:HG2	1:A:244:ILE:HG12	2.00	0.44
1:A:269:ASN:ND2	1:A:272:ASP:H	2.16	0.44
1:A:126:ASN:HB2	1:A:175:TYR:HB2	2.00	0.43
1:D:90:PRO:HD3	1:D:286:TRP:CD2	2.53	0.43
1:D:101:TRP:CD1	1:D:101:TRP:N	2.85	0.43
1:B:50:ARG:HB3	1:B:287:LEU:HG	2.00	0.43
1:D:99:ALA:HA	1:D:117:ILE:O	2.18	0.43
1:A:61:ALA:HB3	1:A:275:ARG:HA	1.99	0.43
1:C:24:ASP:HB2	1:C:30:VAL:CG1	2.49	0.43
1:A:211:LEU:HA	4:A:532:HOH:O	2.17	0.43
1:B:127:HIS:O	1:B:127:HIS:HD2	2.01	0.43
1:A:207:PRO:HG2	1:A:210:VAL:HB	2.00	0.43
1:A:232:CYS:HB3	1:A:234:TRP:CE2	2.53	0.43
1:B:253:TRP:O	1:B:257:VAL:HG22	2.19	0.43
1:A:130:LEU:HG	1:A:227:PHE:CD1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PHE:CE1	1:A:184:GLY:HA2	2.55	0.42
1:A:217:PRO:HA	1:A:220:TRP:CD2	2.54	0.42
1:B:97:TRP:HB3	1:B:248:THR:HG23	2.00	0.42
1:A:131:HIS:HE1	1:A:162:ASN:O	2.03	0.42
1:D:102:THR:HB	1:D:241:GLN:HB3	2.00	0.42
1:D:287:LEU:HD12	1:D:287:LEU:HA	1.84	0.42
1:B:199:TRP:CD1	1:B:223:PRO:HA	2.54	0.42
1:D:151:ASN:HB3	1:D:159:GLN:HE22	1.85	0.42
1:D:217:PRO:HA	1:D:220:TRP:CD2	2.55	0.42
1:A:101:TRP:HB3	1:A:115:ASP:HA	2.01	0.42
1:C:287:LEU:HD12	1:C:287:LEU:HA	1.89	0.42
1:A:24:ASP:HB2	1:A:30:VAL:CG1	2.50	0.41
1:A:123:ASN:ND2	1:A:127:HIS:CE1	2.86	0.41
1:B:86:LEU:O	1:B:203:ARG:NH2	2.53	0.41
1:C:9:ARG:HD3	1:C:46:GLU:OE2	2.20	0.41
1:C:99:ALA:HA	1:C:117:ILE:O	2.20	0.41
1:A:50:ARG:HB3	1:A:287:LEU:HG	2.02	0.41
1:D:50:ARG:HG2	1:D:289:ASN:ND2	2.36	0.41
1:D:253:TRP:CD1	1:D:253:TRP:C	2.98	0.41
1:B:141:ASP:HA	4:B:686:HOH:O	2.20	0.41
1:B:162:ASN:O	2:F:1:BGC:H5	2.20	0.41
1:C:79:HIS:NE2	1:C:193:PRO:HG3	2.34	0.41
1:D:189:THR:HA	1:D:197:SER:O	2.20	0.41
1:D:171:ASP:HA	1:D:172:PRO:HD3	1.79	0.41
1:B:256:ASN:ND2	4:B:446:HOH:O	2.53	0.41
1:D:76:THR:HB	1:D:240:ALA:HB1	2.02	0.41
1:B:127:HIS:CD2	1:B:127:HIS:C	2.99	0.41
1:C:217:PRO:HA	1:C:220:TRP:CD2	2.54	0.41
1:D:95:GLY:O	1:D:249:PHE:HA	2.20	0.41
1:A:206:GLU:HB2	1:A:210:VAL:HG11	2.03	0.41
1:B:97:TRP:HB3	1:B:248:THR:CG2	2.50	0.41
1:D:89:MET:HG2	1:D:179:PHE:CD1	2.56	0.41
1:B:89:MET:O	1:B:90:PRO:C	2.63	0.41
1:A:102:THR:HB	1:A:241:GLN:HB3	2.03	0.40
1:C:90:PRO:HD3	1:C:286:TRP:CD2	2.57	0.40
1:B:61:ALA:HB3	1:B:275:ARG:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/297 (99%)	282 (96%)	12 (4%)	0	100	100
1	B	294/297 (99%)	281 (96%)	13 (4%)	0	100	100
1	C	295/297 (99%)	282 (96%)	12 (4%)	1 (0%)	36	40
1	D	295/297 (99%)	285 (97%)	10 (3%)	0	100	100
All	All	1178/1188 (99%)	1130 (96%)	47 (4%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	210	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	229/230 (100%)	225 (98%)	4 (2%)	53	65
1	B	229/230 (100%)	222 (97%)	7 (3%)	35	44
1	C	230/230 (100%)	224 (97%)	6 (3%)	40	50
1	D	230/230 (100%)	222 (96%)	8 (4%)	32	39
All	All	918/920 (100%)	893 (97%)	25 (3%)	39	49

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	109	PRO
1	A	129	VAL
1	A	148	LYS
1	B	5	ASP
1	B	78	GLU
1	B	109	PRO
1	B	127	HIS
1	B	129	VAL
1	B	157	PRO
1	B	246	ASP
1	C	5	ASP
1	C	157	PRO
1	C	226	LYS
1	C	246	ASP
1	C	256	ASN
1	C	260	ILE
1	D	5	ASP
1	D	109	PRO
1	D	141	ASP
1	D	160	ASP
1	D	189	THR
1	D	246	ASP
1	D	263	CYS
1	D	265	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	79	HIS
1	A	123	ASN
1	A	127	HIS
1	A	140	ASN
1	A	146	ASN
1	A	159	GLN
1	A	194	ASN
1	A	256	ASN
1	A	269	ASN
1	A	289	ASN
1	B	75	ASN
1	B	79	HIS
1	B	127	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	159	GLN
1	B	194	ASN
1	B	241	GLN
1	B	256	ASN
1	C	59	ASN
1	C	75	ASN
1	C	123	ASN
1	C	127	HIS
1	C	159	GLN
1	C	194	ASN
1	D	59	ASN
1	D	75	ASN
1	D	127	HIS
1	D	146	ASN
1	D	159	GLN
1	D	194	ASN
1	D	289	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 ⓘ

8 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	BGC	E	1	2	12,12,12	0.51	0	17,17,17	0.81	0
2	BGC	E	2	2	11,11,12	0.29	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	F	1	2	12,12,12	0.51	0	17,17,17	0.82	0
2	BGC	F	2	2	11,11,12	0.30	0	15,15,17	0.74	0
2	BGC	G	1	2	12,12,12	0.50	0	17,17,17	0.83	0
2	BGC	G	2	2	11,11,12	0.29	0	15,15,17	0.74	0
2	BGC	H	1	2	12,12,12	0.51	0	17,17,17	0.79	0
2	BGC	H	2	2	11,11,12	0.30	0	15,15,17	0.63	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
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	BGC	F	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	BGC	H	2	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

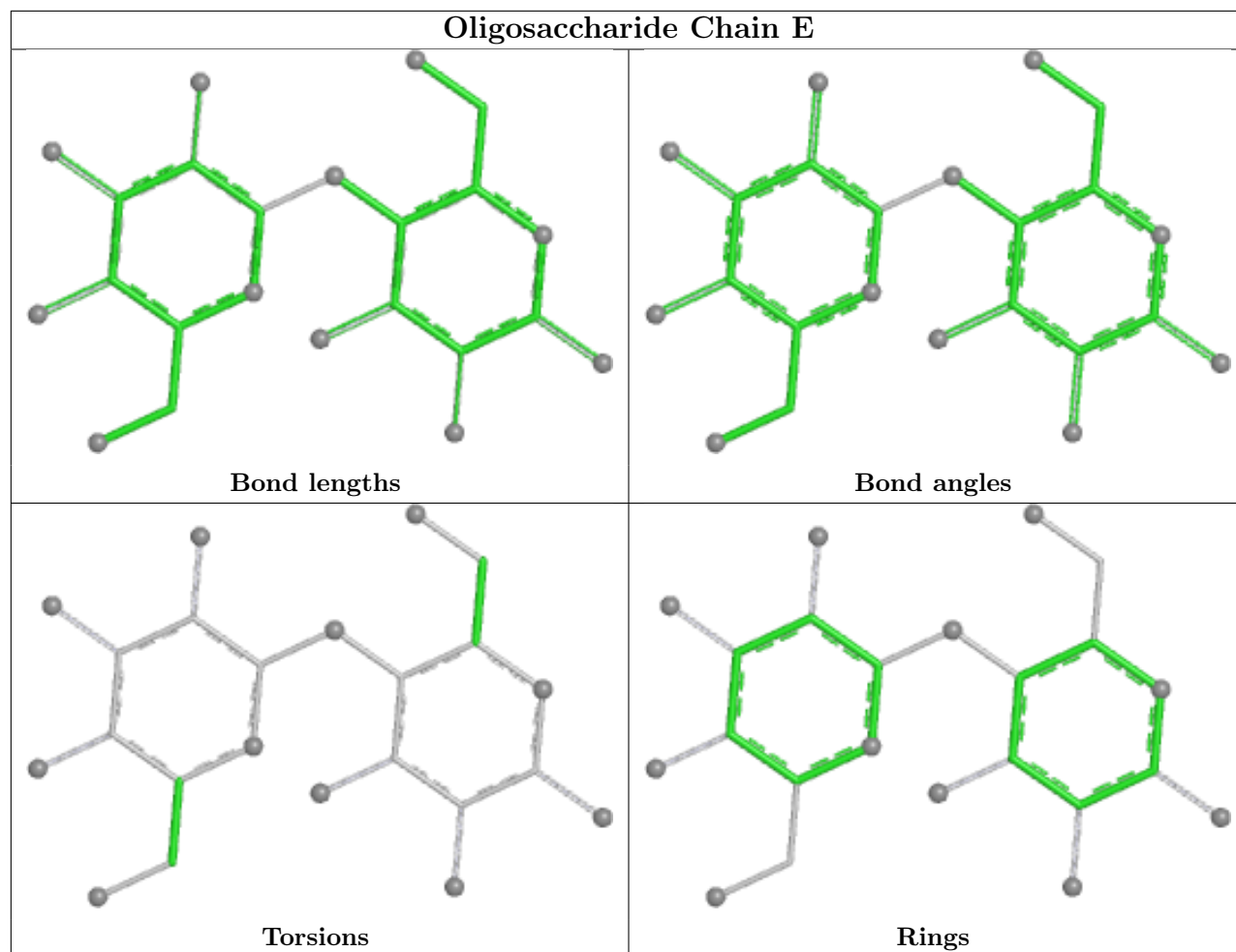
Mol	Chain	Res	Type	Atoms
2	H	2	BGC	O5-C5-C6-O6

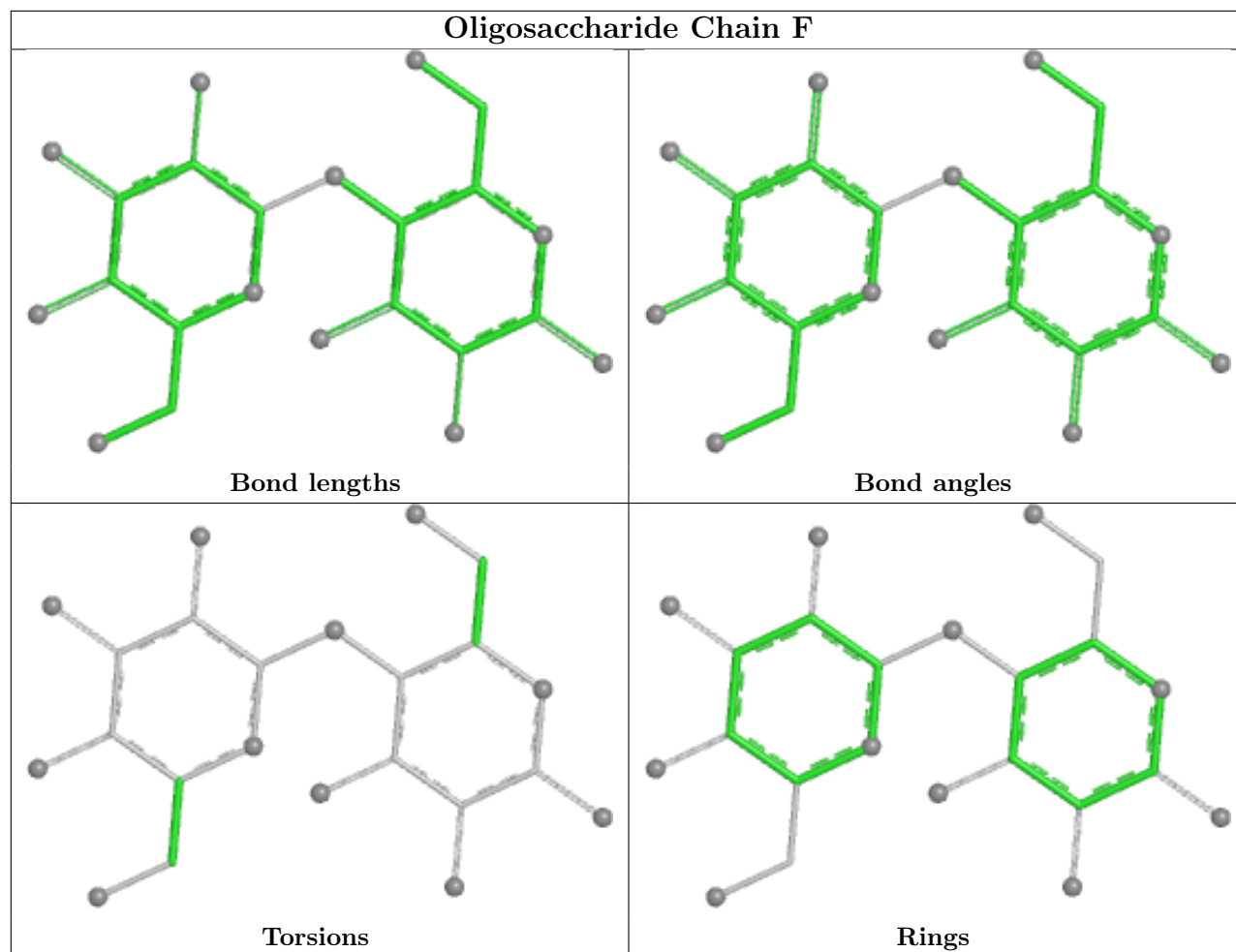
There are no ring outliers.

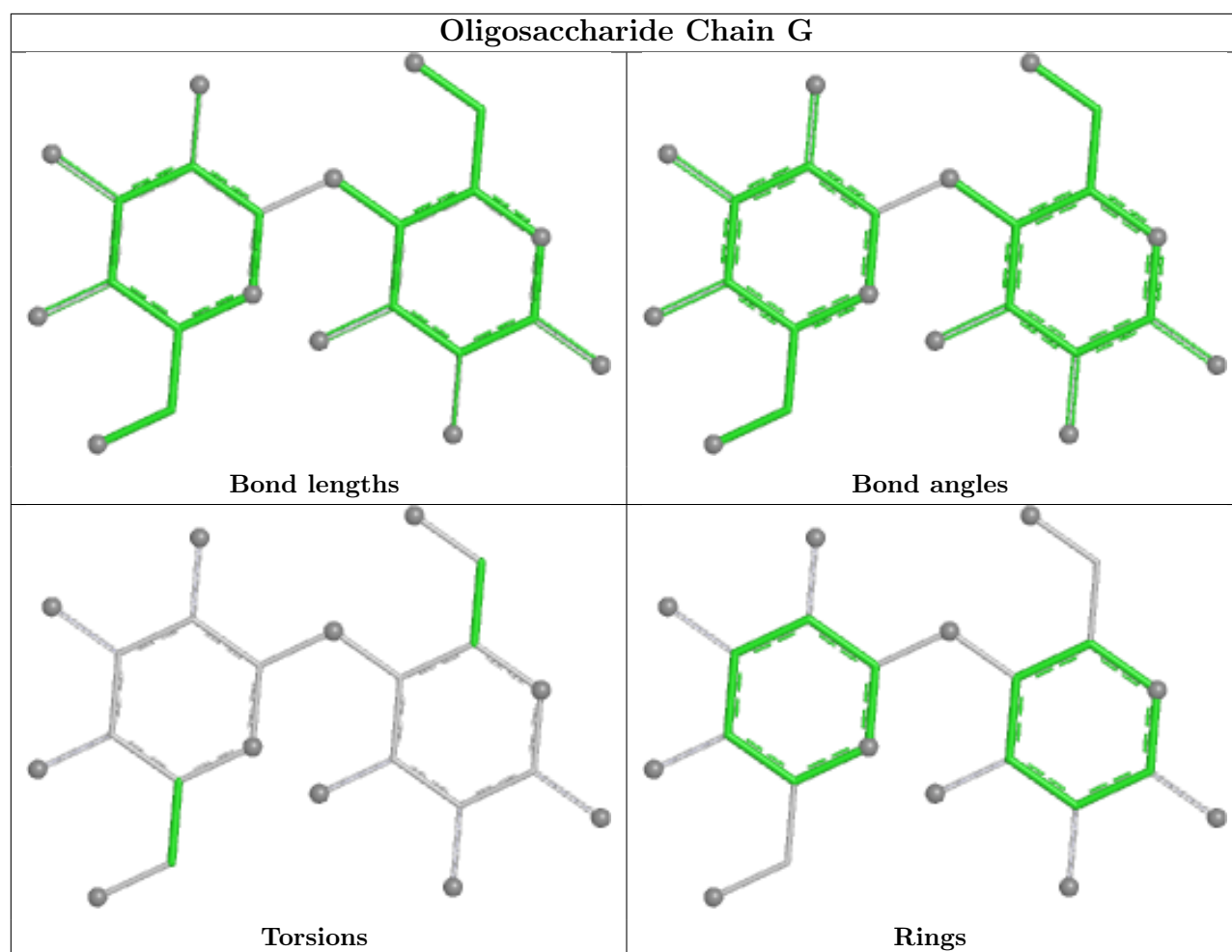
2 monomers are involved in 2 short contacts:

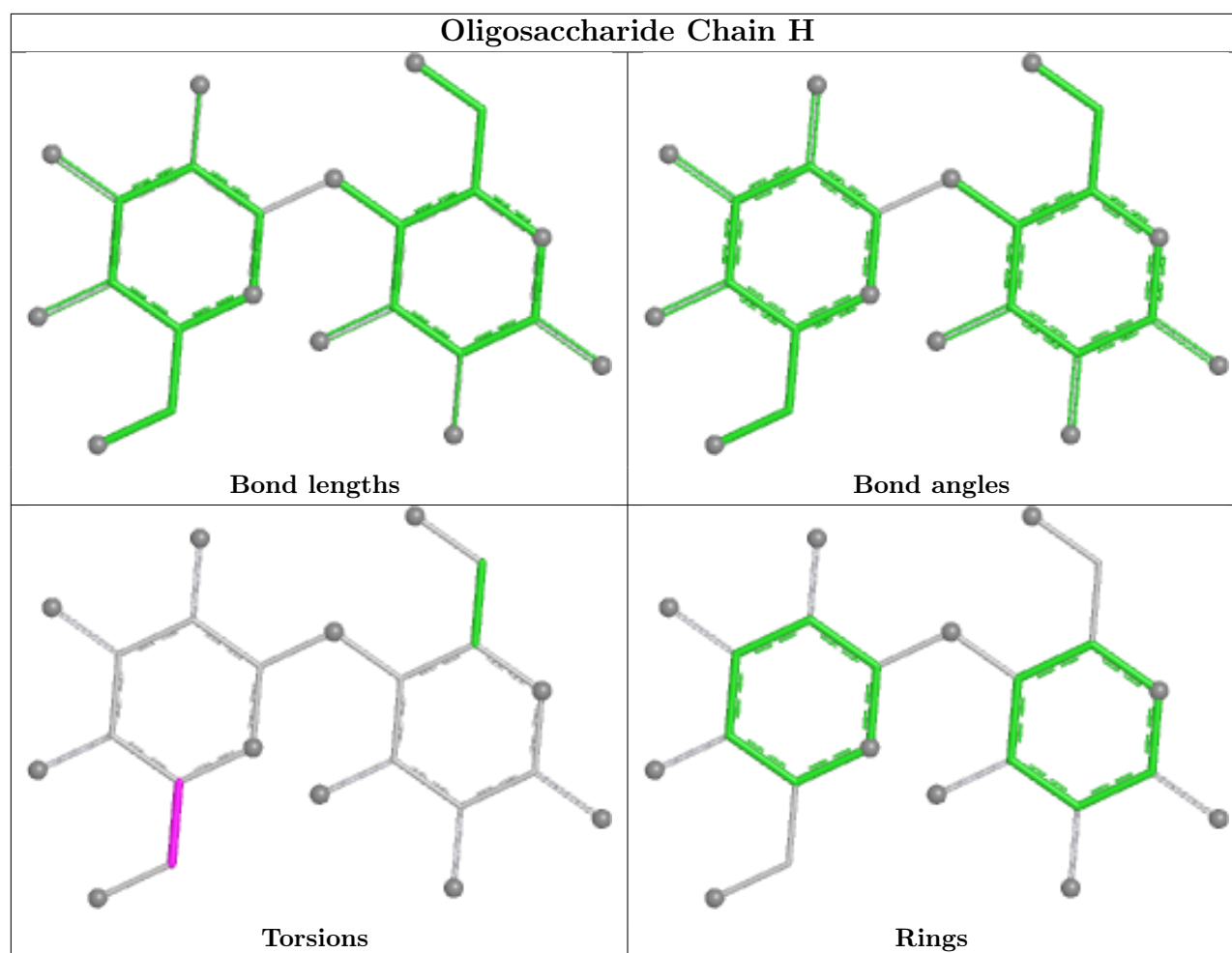
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	BGC	1	0
2	F	1	BGC	1	0

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](#)

2 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	$\# Z > 2$
3	BGC	B	301	-	12,12,12	0.35	0	17,17,17	0.36	0
3	BGC	A	301	-	12,12,12	0.36	0	17,17,17	0.34	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	BGC	B	301	-	-	0/2/22/22	0/1/1/1
3	BGC	A	301	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	BGC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	296/297 (99%)	-0.47	0	100 100	7, 15, 25, 33	0
1	B	296/297 (99%)	-0.43	0	100 100	7, 16, 26, 36	0
1	C	297/297 (100%)	-0.26	5 (1%)	69 70	9, 17, 32, 44	0
1	D	297/297 (100%)	-0.20	1 (0%)	90 90	12, 22, 37, 42	0
All	All	1186/1188 (99%)	-0.34	6 (0%)	87 88	7, 17, 32, 44	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	259	GLY	4.3
1	D	263	CYS	4.2
1	C	260	ILE	3.5
1	C	261	GLY	2.5
1	C	140	ASN	2.1
1	C	0	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.

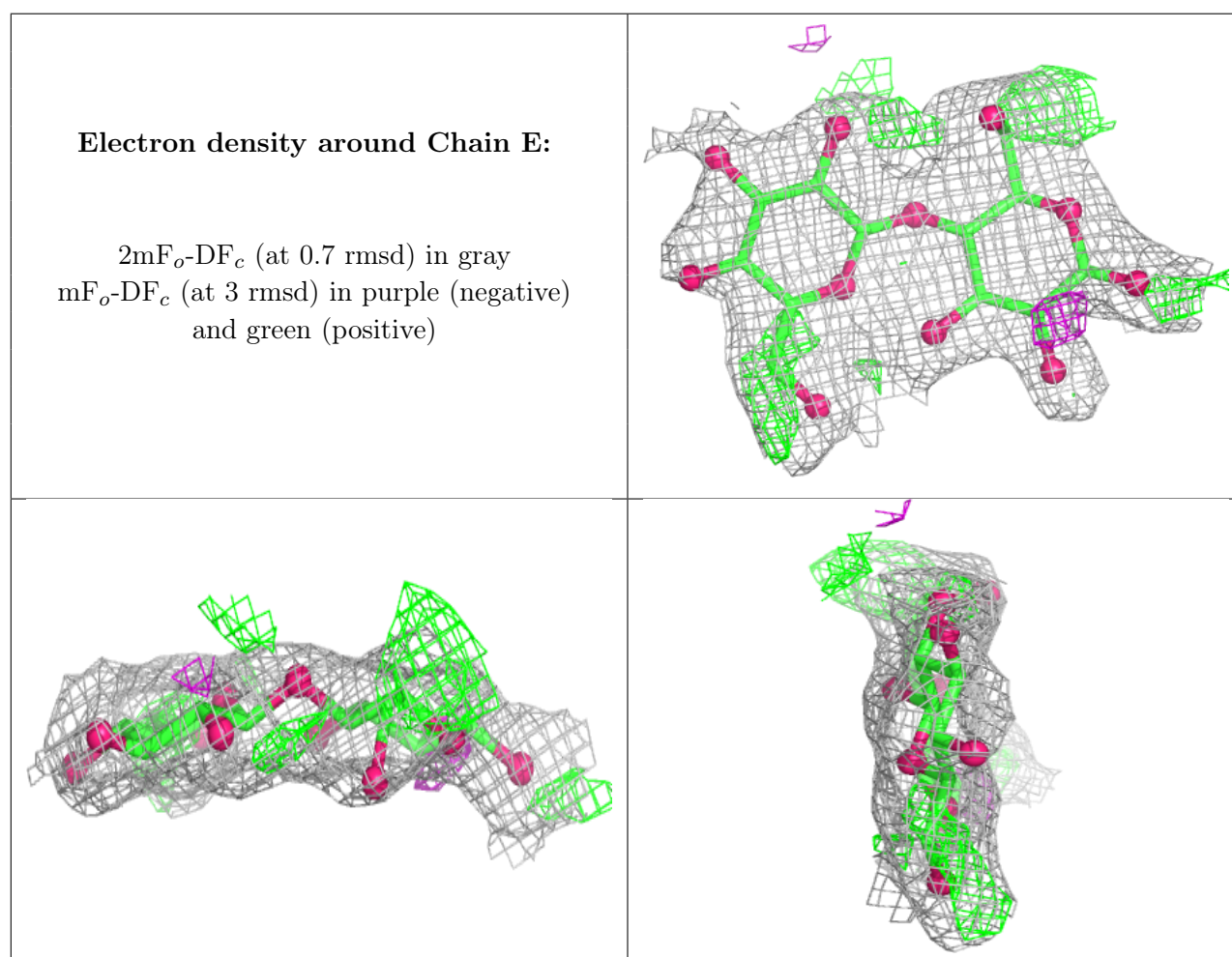
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	H	2	11/12	0.53	0.25	74,75,75,77	0

Continued on next page...

Continued from previous page...

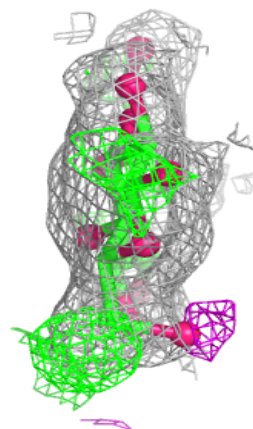
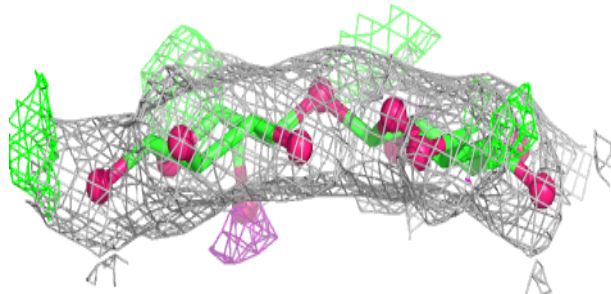
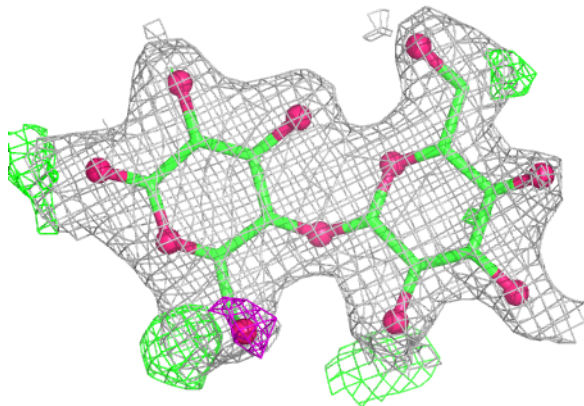
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	H	1	12/12	0.59	0.25	69,73,74,75	0
2	BGC	E	2	11/12	0.77	0.15	32,37,40,41	0
2	BGC	G	1	12/12	0.77	0.17	40,43,46,47	0
2	BGC	E	1	12/12	0.79	0.16	38,40,41,42	0
2	BGC	F	2	11/12	0.81	0.11	29,32,33,34	0
2	BGC	F	1	12/12	0.82	0.13	30,32,34,39	0
2	BGC	G	2	11/12	0.87	0.09	32,35,37,37	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.



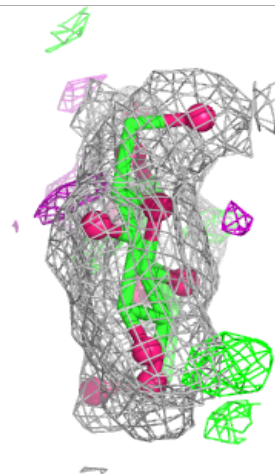
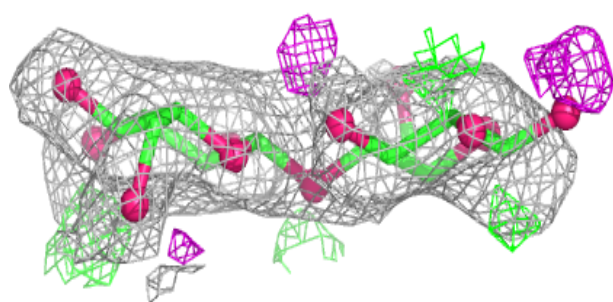
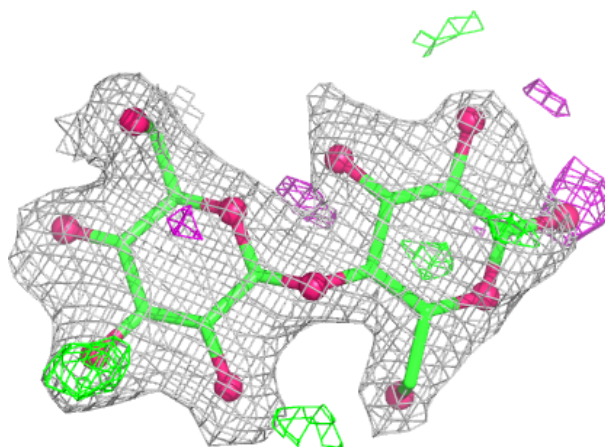
Electron density around Chain F:

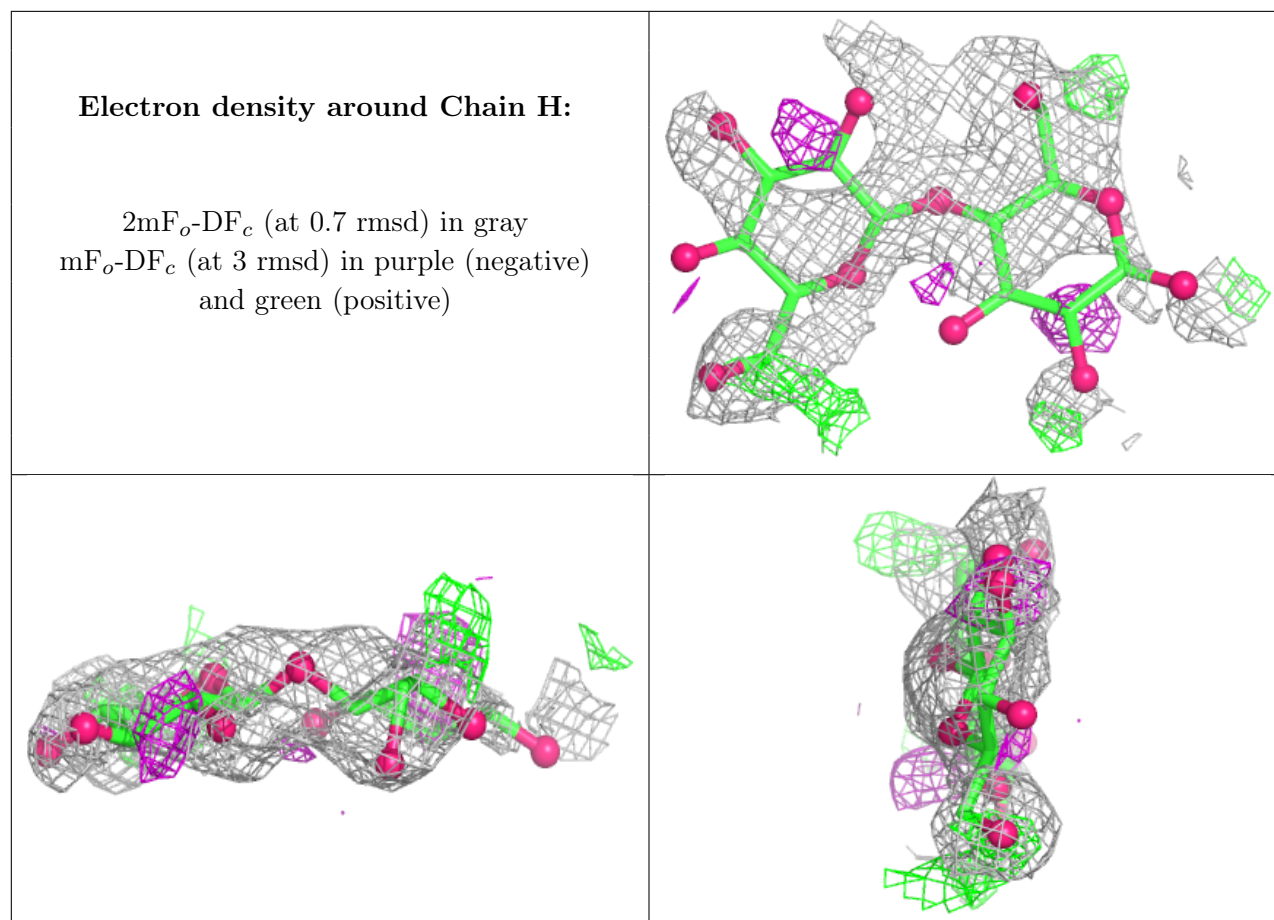
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





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
3	BGC	A	301	12/12	0.73	0.16	45,48,49,49	0
3	BGC	B	301	12/12	0.76	0.13	43,50,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.