



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:58 AM UTC

PDB ID : 7VN4 / pdb_00007vn4
Title : Crystal structure of MBP-fused BIL1/BZR1 (21-90) in complex with double-stranded DNA containing TCCACGTGGA
Authors : Nosaki, S.; Tanokura, M.; Miyakawa, T.
Deposited on : 2021-10-10
Resolution : 2.10 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

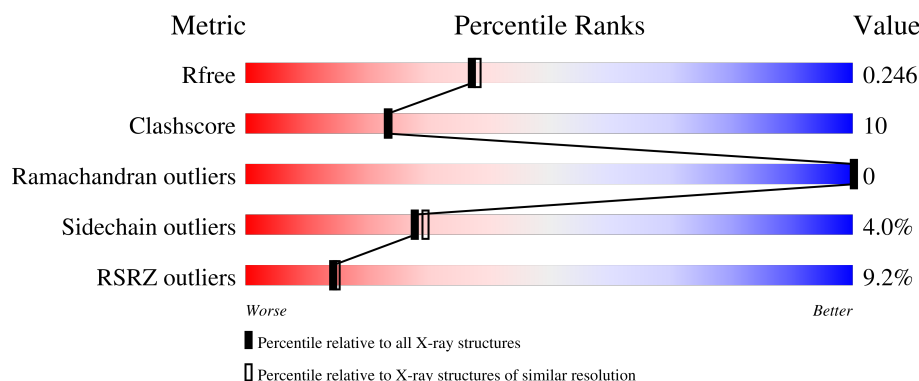
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



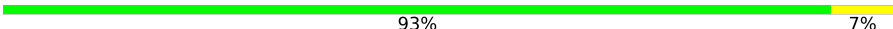
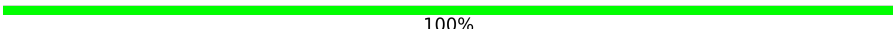
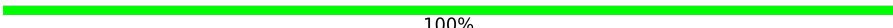
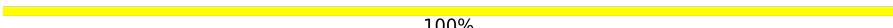
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	439	11% 79% 19% ..
1	B	439	25% 69% 24% 5% ..
1	C	439	% 88% 12%
1	D	439	% 86% 13%
2	E	15	67% 33%

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Mol	Chain	Length	Quality of chain
2	F	15	 67%33%
2	G	15	 80%20%
2	H	15	 93%7%
3	K	2	 100%
3	L	2	 50%50%
3	M	2	 100%
3	N	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15340 atoms, of which 6 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 Maltodextrin-binding protein, Protein BRASSINAZOLE-RESISTANT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	437	Total	C	N	O	S	0	0	0
			3402	2171	582	640	9			
1	D	437	Total	C	N	O	S	0	0	0
			3402	2171	582	640	9			
1	A	436	Total	C	N	O	S	0	0	0
			3394	2166	581	639	8			
1	B	436	Total	C	N	O	S	0	0	0
			3394	2166	581	639	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-348	MET	-	initiating methionine	UNP A0A4P1LXE0
C	-266	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
C	-265	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	-176	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
C	-175	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
C	-109	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	11	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
C	14	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	15	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
D	-348	MET	-	initiating methionine	UNP A0A4P1LXE0
D	-266	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
D	-265	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	-176	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
D	-175	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
D	-109	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	11	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
D	14	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	15	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
A	-348	MET	-	initiating methionine	UNP A0A4P1LXE0
A	-266	ALA	ASP	engineered mutation	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-265	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	-176	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
A	-175	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
A	-109	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	11	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
A	14	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	15	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
B	-348	MET	-	initiating methionine	UNP A0A4P1LXE0
B	-266	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
B	-265	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	-176	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
B	-175	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
B	-109	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	11	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
B	14	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	15	ALA	ASP	engineered mutation	UNP A0A4P1LXE0

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*TP*CP*CP*AP*CP*GP*TP*GP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	15	Total	C	N	O	P	0	0	0
			305	147	57	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			305	147	57	87	14			
2	E	15	Total	C	N	O	P	0	0	0
			305	147	57	87	14			
2	F	15	Total	C	N	O	P	0	0	0
			305	147	57	87	14			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



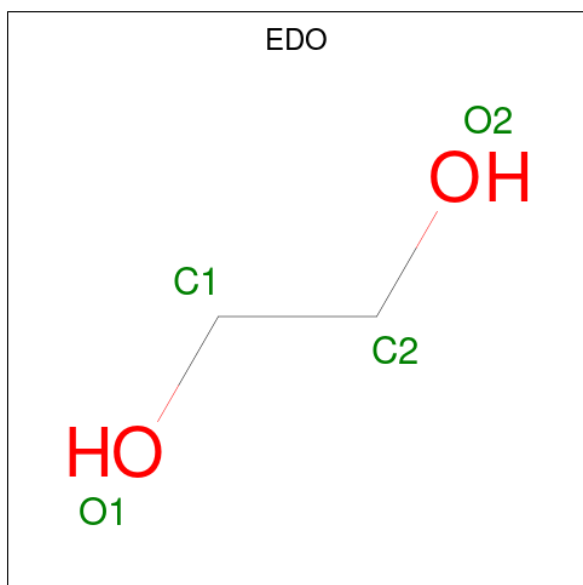
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	K	2	Total	C	O	0	0	0
			23	12	11			
3	L	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	M	2	Total	C	O	0	0	0
			23	12	11			
3	N	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	D	1	Total 10	C 2	H 6 O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0

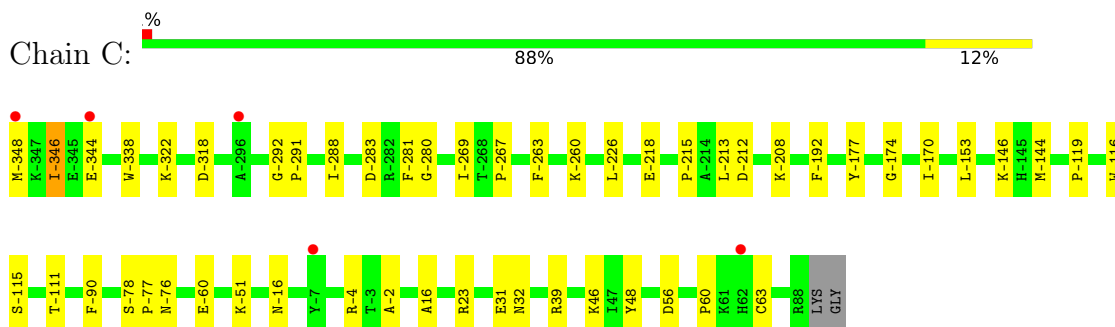
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	113	Total 113	O 113	0	0
5	D	109	Total 109	O 109	0	0
5	G	29	Total 29	O 29	0	0
5	H	26	Total 26	O 26	0	0
5	A	62	Total 62	O 62	0	0
5	B	55	Total 55	O 55	0	0
5	E	4	Total 4	O 4	0	0
5	F	4	Total 4	O 4	0	0

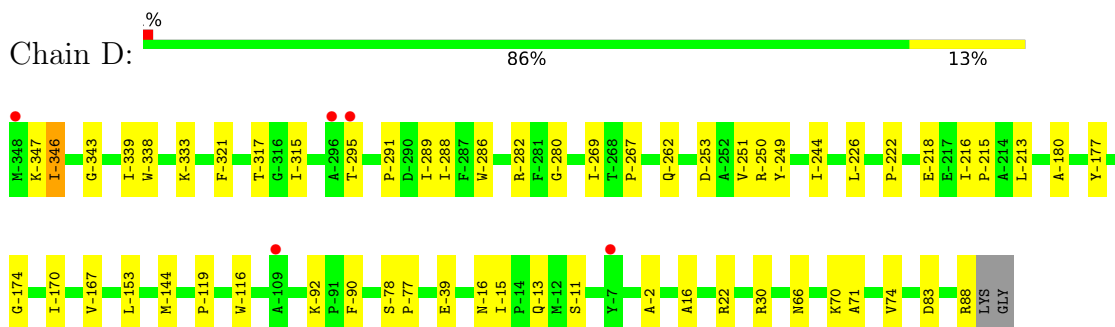
3 Residue-property plots [i](#)

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

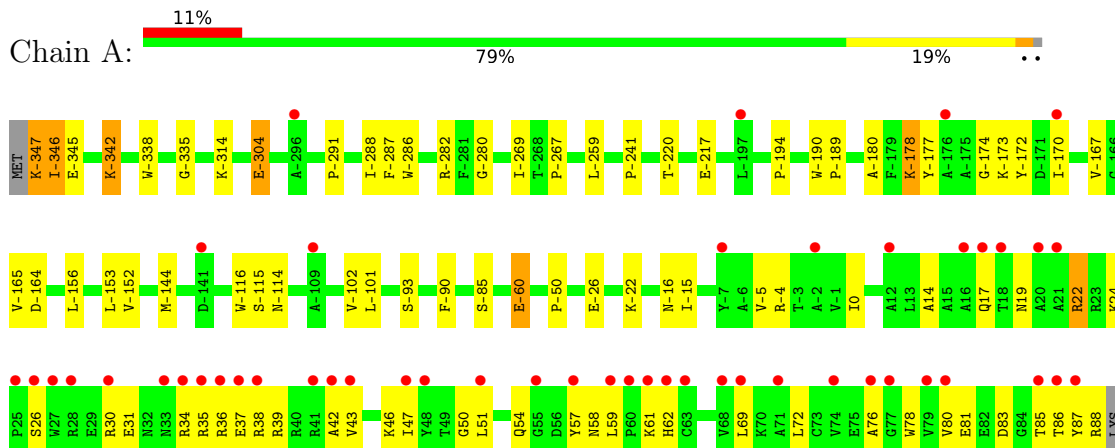
- Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1



- Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1



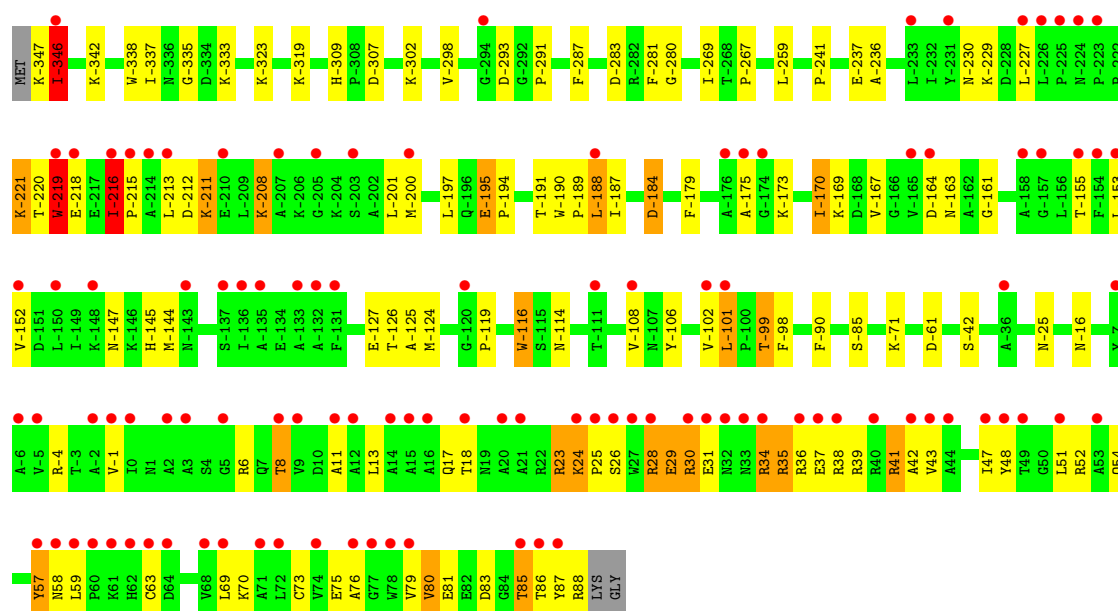
- Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1



GLY

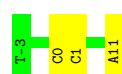
- Molecule 1: Maltodextrin-binding protein, Protein BRASSINAZOLE-RESISTANT 1

Chain B: 



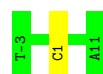
- Molecule 2: DNA (5'-D(*TP*TP*TP*CP*CP*AP*CP*GP*TP*GP*AP*AP*AP*AP*A)-3')

Chain G: 



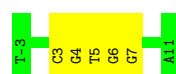
- Molecule 2: DNA (5'-D(*TP*TP*TP*CP*CP*AP*CP*GP*TP*GP*AP*AP*AP*AP*A)-3')

Chain H: 



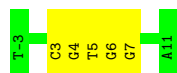
- Molecule 2: DNA (5'-D(*TP*TP*TP*CP*CP*AP*CP*GP*TP*GP*AP*AP*AP*AP*A)-3')

Chain E: 

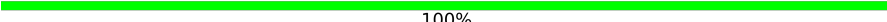


- Molecule 2: DNA (5'-D(*TP*TP*TP*CP*CP*AP*CP*GP*TP*GP*AP*AP*AP*AP*A)-3')

Chain F:  67% 33%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:  100%

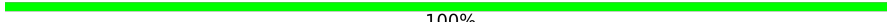


- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:  50% 50%

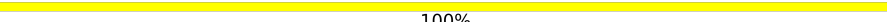


- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.62Å 93.65Å 112.49Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	43.05 – 2.10 43.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.05-2.10) 99.3 (43.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.218 , 0.245 0.218 , 0.246	Depositor DCC
R_{free} test set	6109 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15340	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 84.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7016e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GLC, EDO

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	0.33	0/3473	0.42	1/4713 (0.0%)
1	B	0.96	3/3473 (0.1%)	0.89	20/4713 (0.4%)
1	C	0.47	5/3481 (0.1%)	0.41	1/4723 (0.0%)
1	D	0.29	1/3481 (0.0%)	0.34	0/4723
2	E	0.68	0/342	0.73	0/526
2	F	0.21	0/342	0.45	0/526
2	G	0.25	0/342	0.53	0/526
2	H	0.54	0/342	0.66	1/526 (0.2%)
All	All	0.57	9/15276 (0.1%)	0.56	23/20976 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	-114	ASN	C-O	-6.20	1.17	1.24
1	C	31	GLU	C-O	-6.02	1.17	1.24
1	B	35	ARG	C-O	-5.77	1.16	1.23
1	C	-192	PHE	C-O	-5.73	1.16	1.24
1	D	-39	GLU	C-O	-5.68	1.17	1.24
1	C	-281	PHE	C-O	-5.42	1.17	1.24
1	B	-155	THR	C-O	-5.33	1.17	1.24
1	C	32	ASN	CG-OD1	-5.13	1.13	1.23
1	C	-283	ASP	C-O	-5.11	1.17	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	-101	LEU	CA-C-N	9.07	129.13	119.78
1	B	-101	LEU	C-N-CA	9.07	129.13	119.78
1	B	-195	GLU	CA-C-N	7.72	129.49	119.84
1	B	-195	GLU	C-N-CA	7.72	129.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	TYR	N-CA-C	7.71	122.27	113.02
1	B	-163	ASN	N-CA-C	7.57	120.80	110.35
1	C	-281	PHE	N-CA-C	7.37	119.31	111.28
1	B	-127	GLU	N-CA-C	6.96	118.94	111.36
1	B	-219	TRP	N-CA-C	-6.45	104.17	111.14
1	B	-216	ILE	N-CA-C	6.42	122.74	108.88
1	B	-125	ALA	N-CA-C	6.37	118.30	111.36
2	H	1	DC	C2'-C3'-O3'	6.30	120.95	111.50
1	B	-281	PHE	N-CA-C	6.20	118.83	111.33
1	B	-116	TRP	N-CA-C	5.87	117.68	111.28
1	B	-108	VAL	N-CA-C	5.67	116.73	109.30
1	B	-219	TRP	CA-CB-CG	5.66	124.34	113.60
1	B	-167	VAL	N-CA-C	5.37	116.32	108.53
1	B	-175	ALA	N-CA-C	5.33	118.75	111.39
1	B	-346	ILE	N-CA-C	5.31	117.51	109.12
1	A	58	ASN	N-CA-C	-5.11	104.37	111.52
1	B	-283	ASP	N-CA-C	5.04	117.43	111.33
1	B	35	ARG	CA-C-N	5.00	127.30	120.54
1	B	35	ARG	C-N-CA	5.00	127.30	120.54

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	3394	0	3365	107	0
1	B	3394	0	3365	134	0
1	C	3402	0	3374	34	0
1	D	3402	0	3374	39	0
2	E	305	0	171	3	0
2	F	305	0	171	9	0
2	G	305	0	171	2	0
2	H	305	0	171	0	0
3	K	23	0	21	0	0
3	L	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	23	0	21	0	0
3	N	23	0	21	1	0
4	A	8	0	12	1	0
4	B	4	0	6	0	0
4	C	12	0	18	1	0
4	D	4	6	6	0	0
5	A	62	0	0	3	0
5	B	55	0	0	7	0
5	C	113	0	0	2	0
5	D	109	0	0	4	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
5	G	29	0	0	1	0
5	H	26	0	0	0	0
All	All	15334	6	14288	297	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 10.

All (297) 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:A:-342:LYS:HE2	1:A:-314:LYS:HB3	1.21	1.13
1:A:-164:ASP:HB2	1:A:17:GLN:HG3	1.16	1.13
1:D:-346:ILE:HD13	1:D:-77:PRO:HD3	1.29	1.12
1:C:-269:ILE:HG22	1:C:-267:PRO:HD3	1.35	1.08
1:A:76:ALA:HB1	1:B:75:GLU:HG2	1.42	1.01
1:B:-219:TRP:HZ2	1:B:-188:LEU:HB2	1.23	1.00
1:B:-219:TRP:CZ2	1:B:-188:LEU:HB2	1.98	0.98
1:A:-342:LYS:HE2	1:A:-314:LYS:CB	1.95	0.96
1:B:57:TYR:HB2	1:B:59:LEU:HD23	1.48	0.94
1:A:-346:ILE:HD13	1:A:-346:ILE:H	1.34	0.92
1:B:41:ARG:HH22	2:F:3:DC:H2'	1.31	0.91
1:B:34:ARG:O	1:B:38:ARG:HD3	1.70	0.90
1:D:-346:ILE:CD1	1:D:-77:PRO:HD3	2.03	0.88
1:A:-342:LYS:CE	1:A:-314:LYS:HB3	2.02	0.88
1:B:-219:TRP:NE1	1:B:-188:LEU:HD13	1.88	0.88
1:B:-216:ILE:HD13	1:B:-124:MET:HE1	1.56	0.88
1:B:18:THR:HG23	5:B:215:HOH:O	1.74	0.85
1:B:-197:LEU:HD11	1:B:-144:MET:HE3	1.55	0.85
1:A:-164:ASP:HB2	1:A:17:GLN:CG	2.06	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-216:ILE:CD1	1:B:-124:MET:HE1	2.09	0.82
1:A:80:VAL:HG22	1:A:86:THR:HG23	1.61	0.81
1:A:34:ARG:O	1:A:38:ARG:HG3	1.78	0.81
1:C:-346:ILE:HD13	1:C:-77:PRO:HD3	1.62	0.81
1:B:-221:LYS:O	1:B:-99:THR:HG22	1.80	0.81
1:B:41:ARG:NH2	2:F:3:DC:H2'	1.96	0.81
1:B:43:VAL:O	1:B:47:ILE:HG13	1.80	0.80
1:C:-346:ILE:HD13	1:C:-78:SER:HA	1.62	0.80
1:D:-269:ILE:HG22	1:D:-267:PRO:HD3	1.61	0.80
1:B:-219:TRP:CZ2	1:B:-188:LEU:HD22	2.16	0.80
1:B:-201:LEU:HD13	1:B:-124:MET:HE3	1.61	0.80
1:A:-194:PRO:HB3	1:A:-5:VAL:HG12	1.63	0.79
1:D:-346:ILE:HD13	1:D:-78:SER:HA	1.64	0.78
1:A:87:TYR:HA	1:B:54:GLN:HE22	1.48	0.78
1:B:-190:TRP:HA	1:B:-187:ILE:HD12	1.65	0.78
1:C:-346:ILE:CD1	1:C:-77:PRO:HD3	2.13	0.78
1:A:76:ALA:HB1	1:B:75:GLU:CG	2.15	0.77
1:A:37:GLU:HG3	2:E:5:DT:O4	1.85	0.77
1:A:-164:ASP:OD2	1:A:14:ALA:HA	1.85	0.76
1:B:-219:TRP:CE2	1:B:-188:LEU:HD22	2.20	0.76
1:B:-219:TRP:HE1	1:B:-188:LEU:HD13	1.47	0.76
1:B:-219:TRP:HD1	1:B:-98:PHE:HB2	1.51	0.75
1:B:34:ARG:O	1:B:38:ARG:CD	2.35	0.74
1:B:-197:LEU:HD11	1:B:-144:MET:CE	2.17	0.74
1:A:-153:LEU:HD12	1:A:-144:MET:HE1	1.71	0.73
1:B:37:GLU:O	1:B:41:ARG:HG3	1.89	0.72
1:D:-253:ASP:OD1	1:D:-250:ARG:NH2	2.22	0.72
1:B:-219:TRP:CD1	1:B:-98:PHE:HB2	2.24	0.72
1:D:88:ARG:HG2	5:D:235:HOH:O	1.88	0.71
1:B:29:GLU:HA	1:B:29:GLU:OE1	1.89	0.71
1:A:35:ARG:HG2	1:A:38:ARG:HH21	1.55	0.71
1:B:-323:LYS:NZ	5:B:201:HOH:O	2.24	0.69
1:B:-280:GLY:HA3	1:B:-16:ASN:O	1.92	0.69
1:A:-170:ILE:HD11	1:A:-15:ILE:HD12	1.74	0.69
1:A:54:GLN:NE2	1:B:87:TYR:HA	2.07	0.69
1:A:-220:THR:HG22	1:A:-217:GLU:OE1	1.93	0.68
1:B:8:THR:HG23	1:B:11:ALA:H	1.59	0.68
1:B:28:ARG:HG3	1:B:28:ARG:HH21	1.57	0.68
1:B:34:ARG:O	1:B:34:ARG:HG2	1.92	0.68
1:D:-280:GLY:HA3	1:D:-16:ASN:O	1.94	0.68
1:B:-188:LEU:HD12	1:B:-188:LEU:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLU:HA	1:A:34:ARG:CD	2.25	0.67
1:A:43:VAL:O	1:A:47:ILE:HG13	1.94	0.67
1:B:-101:LEU:H	1:B:-25:ASN:HD21	1.43	0.67
1:A:31:GLU:HA	1:A:34:ARG:HD2	1.76	0.67
1:B:-319:LYS:NZ	5:B:203:HOH:O	2.28	0.67
1:B:37:GLU:HG3	2:F:5:DT:O4	1.95	0.67
1:A:51:LEU:HD21	1:A:72:LEU:HD22	1.77	0.67
1:A:-286:TRP:CD1	1:A:-282:ARG:HG3	2.30	0.66
1:C:-4:ARG:HD3	5:C:282:HOH:O	1.94	0.66
1:C:-60:GLU:H	1:C:-60:GLU:CD	2.03	0.65
1:A:88:ARG:NH2	1:B:75:GLU:OE2	2.29	0.65
1:C:46:LYS:HD2	1:D:83:ASP:O	1.97	0.64
1:B:34:ARG:HG3	2:F:4:DG:OP2	1.96	0.64
1:A:-280:GLY:HA3	1:A:-16:ASN:O	1.97	0.64
1:C:-153:LEU:CD1	1:C:-144:MET:HE1	2.28	0.64
1:B:-194:PRO:HG3	1:B:-4:ARG:HB2	1.78	0.64
1:B:-269:ILE:HG22	1:B:-267:PRO:HD3	1.80	0.64
1:A:46:LYS:HE3	1:B:85:THR:HG23	1.80	0.63
1:B:-184:ASP:HB3	1:B:-161:GLY:HA2	1.78	0.63
1:A:-167:VAL:O	1:A:17:GLN:NE2	2.30	0.63
1:A:31:GLU:HG2	1:A:35:ARG:HE	1.61	0.63
1:A:87:TYR:HA	1:B:54:GLN:NE2	2.13	0.63
1:C:-280:GLY:HA3	1:C:-16:ASN:O	2.00	0.62
1:A:50:GLY:O	1:A:54:GLN:HB2	1.99	0.61
1:A:-342:LYS:CE	1:A:-314:LYS:H	2.13	0.61
1:A:69:LEU:HD23	1:B:47:ILE:CD1	2.30	0.61
1:A:30:ARG:O	1:A:34:ARG:HG3	2.01	0.60
1:A:-153:LEU:CD1	1:A:-144:MET:HE1	2.31	0.60
1:A:-259:LEU:HD23	1:A:-241:PRO:HG2	1.82	0.60
1:C:-212:ASP:OD2	1:C:-208:LYS:HE3	2.02	0.60
1:D:-170:ILE:HG23	1:D:-13:GLN:HG2	1.84	0.59
1:C:-348:MET:HE2	1:C:-292:GLY:O	2.02	0.59
1:A:24:LYS:HE3	1:A:24:LYS:HA	1.84	0.59
1:B:28:ARG:HH21	1:B:28:ARG:CG	2.15	0.59
1:A:76:ALA:HB2	1:B:76:ALA:HB2	1.85	0.59
1:A:-304:GLU:HG2	1:A:-286:TRP:CH2	2.38	0.59
1:A:-220:THR:HG23	1:A:-217:GLU:H	1.68	0.59
1:A:59:LEU:HD23	1:A:59:LEU:H	1.65	0.58
1:A:-165:VAL:HG22	1:A:17:GLN:HG2	1.84	0.58
1:A:47:ILE:CD1	1:B:69:LEU:HD23	2.32	0.58
1:B:34:ARG:O	1:B:38:ARG:NE	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-322:LYS:NZ	1:C:-318:ASP:OD2	2.36	0.58
1:D:-249:TYR:HB3	1:D:-244:ILE:HD13	1.85	0.58
1:A:-115:SER:OG	1:A:-50:PRO:HD3	2.04	0.58
1:A:31:GLU:O	1:A:35:ARG:HG3	2.04	0.58
1:B:-220:THR:N	5:B:207:HOH:O	2.37	0.57
1:C:-115:SER:O	1:C:-111:THR:HG23	2.04	0.57
1:A:-345:GLU:OE2	1:A:-342:LYS:HG3	2.04	0.57
1:A:-194:PRO:CB	1:A:-5:VAL:HG12	2.33	0.57
1:C:-153:LEU:HD12	1:C:-144:MET:HE1	1.86	0.57
1:A:-177:TYR:OH	1:A:-174:GLY:HA2	2.05	0.57
1:A:-164:ASP:CB	1:A:17:GLN:HG3	2.11	0.56
1:A:-347:LYS:N	1:A:-347:LYS:HD3	2.20	0.56
1:A:76:ALA:CB	1:B:75:GLU:HG2	2.27	0.56
1:A:-178:LYS:NZ	1:A:-177:TYR:H	2.04	0.56
1:B:48:TYR:HA	1:B:51:LEU:HD12	1.87	0.56
1:D:-170:ILE:CG2	1:D:-13:GLN:HG2	2.35	0.56
1:A:69:LEU:HD23	1:B:47:ILE:HD12	1.86	0.56
1:B:41:ARG:HH22	2:F:3:DC:C2'	2.13	0.56
1:A:-269:ILE:HG22	1:A:-267:PRO:HD3	1.87	0.56
1:B:37:GLU:O	1:B:41:ARG:CG	2.53	0.56
1:B:-230:ASN:CG	1:B:-227:LEU:HD13	2.31	0.56
1:B:-164:ASP:HB2	1:B:17:GLN:HB2	1.88	0.56
1:B:41:ARG:CZ	2:F:3:DC:H6	2.18	0.56
1:C:-212:ASP:CG	1:C:-208:LYS:HE3	2.31	0.55
1:A:61:LYS:HE3	1:A:62:HIS:CE1	2.41	0.55
1:C:60:PRO:HG2	1:C:63:CYS:HB3	1.89	0.55
1:B:28:ARG:CZ	1:B:28:ARG:HB3	2.36	0.55
1:D:30:ARG:HG3	5:D:306:HOH:O	2.06	0.55
1:A:-4:ARG:O	1:A:0:ILE:HD12	2.07	0.55
1:A:57:TYR:HB2	1:A:59:LEU:HD22	1.90	0.54
1:D:-321:PHE:O	1:D:-317:THR:OG1	2.26	0.54
1:B:36:ARG:HB3	1:B:37:GLU:OE1	2.08	0.54
1:A:47:ILE:HD12	1:B:69:LEU:HD23	1.89	0.54
1:B:70:LYS:HE2	1:B:80:VAL:HG22	1.90	0.53
1:C:-346:ILE:HD13	1:C:-77:PRO:CD	2.34	0.53
1:A:31:GLU:HA	1:A:34:ARG:NE	2.23	0.53
1:B:-221:LYS:O	1:B:-99:THR:CG2	2.54	0.53
1:B:-190:TRP:N	1:B:-189:PRO:HD2	2.23	0.53
1:A:76:ALA:HB1	1:B:75:GLU:OE1	2.08	0.53
1:B:-119:PRO:HA	1:B:-116:TRP:CE2	2.44	0.53
2:G:11:DA:H5''	5:G:122:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TYR:O	1:B:52:ARG:HG3	2.08	0.53
1:A:-102:VAL:HG22	1:A:-26:GLU:HG2	1.91	0.52
1:B:-188:LEU:HD12	1:B:-188:LEU:C	2.34	0.52
1:B:-101:LEU:HD13	1:B:-25:ASN:ND2	2.25	0.52
1:A:39:ARG:O	1:A:42:ALA:N	2.41	0.52
1:C:-263:PHE:HA	1:C:-260:LYS:HD2	1.91	0.52
1:D:-346:ILE:HD13	1:D:-77:PRO:CD	2.20	0.52
1:B:24:LYS:HD2	1:B:25:PRO:HD2	1.92	0.52
1:D:71:ALA:O	1:D:74:VAL:HG22	2.09	0.52
1:C:-346:ILE:HD12	1:C:-77:PRO:HD3	1.91	0.51
1:A:78:TRP:HE3	1:A:86:THR:HG22	1.76	0.51
1:B:-307:ASP:O	1:B:-302:LYS:HE2	2.11	0.51
1:A:-180:ALA:O	1:A:-167:VAL:HA	2.11	0.51
1:B:-230:ASN:ND2	1:B:-227:LEU:HD13	2.26	0.51
1:C:-226:LEU:HD21	1:C:-213:LEU:HD11	1.93	0.50
1:D:-286:TRP:CD1	1:D:-282:ARG:HG3	2.45	0.50
1:A:30:ARG:HB2	1:A:34:ARG:HH21	1.76	0.50
1:A:78:TRP:CE3	1:A:86:THR:HG22	2.45	0.50
2:E:3:DC:H2"	2:E:4:DG:C8	2.46	0.50
1:B:-101:LEU:HD13	1:B:-25:ASN:CG	2.36	0.50
1:A:-60:GLU:CD	1:A:-60:GLU:H	2.17	0.50
1:B:-212:ASP:HB3	1:B:-145:HIS:ND1	2.27	0.49
1:B:-219:TRP:HD1	1:B:-98:PHE:CB	2.24	0.49
1:B:-194:PRO:HA	1:B:-191:THR:HG22	1.93	0.49
1:B:-213:LEU:HD12	1:B:-213:LEU:O	2.13	0.49
1:A:-165:VAL:H	1:A:17:GLN:HE21	1.61	0.49
1:B:6:ARG:HH11	1:B:6:ARG:HG2	1.77	0.49
1:A:76:ALA:HB1	1:B:75:GLU:CD	2.38	0.49
1:B:-195:GLU:OE1	1:B:-194:PRO:HD2	2.13	0.49
1:B:-164:ASP:HB2	1:B:17:GLN:OE1	2.13	0.48
1:D:66:ASN:O	1:D:70:LYS:HG3	2.13	0.48
1:B:23:ARG:NH1	1:B:23:ARG:HG3	2.28	0.48
1:B:-219:TRP:CZ2	1:B:-188:LEU:CD2	2.93	0.48
1:C:-153:LEU:HD11	1:C:-144:MET:HE1	1.95	0.48
1:D:-343:GLY:O	1:D:-315:ILE:HG23	2.13	0.48
1:B:-302:LYS:O	1:B:-298:VAL:HG22	2.14	0.47
1:B:-184:ASP:HB3	1:B:-161:GLY:CA	2.44	0.47
1:D:-346:ILE:H	1:D:-346:ILE:HG13	1.37	0.47
1:A:-114:ASN:HB3	4:A:102:EDO:H22	1.95	0.47
1:C:-208:LYS:NZ	1:C:-146:LYS:O	2.47	0.47
1:B:29:GLU:OE1	1:B:29:GLU:CA	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-119:PRO:HA	1:D:-116:TRP:CE2	2.49	0.47
1:D:-11:SER:HB3	5:D:224:HOH:O	2.14	0.47
1:A:-220:THR:HG22	1:A:-217:GLU:CG	2.45	0.47
1:B:81:GLU:HG3	1:B:83:ASP:H	1.80	0.47
1:C:-212:ASP:O	1:C:-208:LYS:HG2	2.14	0.47
2:G:0:DC:H2"	2:G:1:DC:C6	2.50	0.47
1:C:-344:GLU:HA	1:C:-76:ASN:OD1	2.15	0.46
1:D:-346:ILE:O	1:D:-346:ILE:HD12	2.15	0.46
1:D:-153:LEU:CD1	1:D:-144:MET:HE1	2.45	0.46
1:A:-346:ILE:HD13	1:A:-346:ILE:N	2.17	0.46
1:D:-180:ALA:O	1:D:-167:VAL:HA	2.16	0.46
1:A:-177:TYR:CZ	1:A:-174:GLY:HA2	2.51	0.46
1:A:47:ILE:HA	1:B:86:THR:OG1	2.15	0.46
1:B:-259:LEU:HD23	1:B:-241:PRO:HG2	1.98	0.46
1:B:28:ARG:CG	1:B:28:ARG:NH2	2.75	0.46
1:D:-218:GLU:O	1:D:-215:PRO:HD2	2.15	0.46
1:A:54:GLN:HE21	1:B:87:TYR:HA	1.78	0.46
1:A:86:THR:OG1	1:B:47:ILE:HA	2.16	0.46
1:A:-156:LEU:O	1:A:-152:VAL:HG23	2.17	0.45
1:C:-177:TYR:OH	1:C:-174:GLY:HA2	2.16	0.45
1:C:-212:ASP:OD1	1:C:-208:LYS:HE3	2.17	0.45
1:D:-333:LYS:NZ	3:N:1:GLC:O2	2.41	0.45
1:B:-208:LYS:HA	1:B:-208:LYS:HD3	1.60	0.45
1:A:31:GLU:CG	1:A:35:ARG:HE	2.29	0.44
1:B:-335:GLY:N	5:B:218:HOH:O	2.50	0.44
1:B:-333:LYS:HE2	1:B:-237:GLU:OE2	2.16	0.44
1:B:30:ARG:HD2	1:B:30:ARG:HA	1.72	0.44
1:A:81:GLU:HG3	1:A:83:ASP:H	1.83	0.44
1:B:-236:ALA:HA	5:B:212:HOH:O	2.17	0.44
1:A:69:LEU:HD23	1:B:47:ILE:HD13	1.97	0.44
1:D:-249:TYR:CB	1:D:-244:ILE:HD13	2.47	0.44
1:D:-92:LYS:HD2	5:D:241:HOH:O	2.16	0.44
1:D:22:ARG:HE	1:D:22:ARG:HB2	1.56	0.44
1:B:-216:ILE:HD11	1:B:-124:MET:HE1	1.95	0.44
1:A:-347:LYS:HD3	1:A:-347:LYS:H3	1.80	0.44
1:A:-170:ILE:HD13	1:A:-170:ILE:HA	1.84	0.44
1:D:-2:ALA:HB2	1:D:16:ALA:HB2	1.99	0.44
1:B:-147:ASN:HB2	1:B:-145:HIS:HD2	1.82	0.44
1:B:-338:TRP:CD2	1:B:-291:PRO:HG3	2.53	0.44
1:D:-170:ILE:CD1	1:D:-15:ILE:HD12	2.48	0.44
1:B:-319:LYS:HB2	1:B:-319:LYS:HE3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:NH1	2:F:3:DC:C6	2.85	0.44
1:C:-346:ILE:H	1:C:-346:ILE:HG13	1.46	0.44
1:C:-115:SER:OG	1:C:-51:LYS:HD3	2.17	0.44
1:A:-173:LYS:HG2	1:A:-172:TYR:N	2.33	0.44
1:A:-346:ILE:H	1:A:-346:ILE:CD1	2.06	0.43
1:A:-342:LYS:HE3	1:A:-314:LYS:H	1.83	0.43
1:A:-116:TRP:HB2	1:A:-50:PRO:HG2	2.00	0.43
1:B:-200:MET:HB2	1:B:-126:THR:HG21	2.00	0.43
1:B:-346:ILE:H	1:B:-346:ILE:HG13	1.51	0.43
1:B:24:LYS:HA	1:B:24:LYS:HD3	1.66	0.43
1:D:-226:LEU:HD21	1:D:-222:PRO:HD3	2.01	0.43
1:A:-165:VAL:N	1:A:17:GLN:HE21	2.16	0.43
1:A:47:ILE:HD13	1:B:69:LEU:HD23	1.98	0.43
1:C:-2:ALA:HB2	1:C:16:ALA:HB2	2.00	0.43
1:A:-338:TRP:CG	1:A:-291:PRO:HG3	2.53	0.43
1:A:-335:GLY:O	5:A:201:HOH:O	2.21	0.43
1:A:31:GLU:HG2	1:A:35:ARG:HH11	1.84	0.43
1:B:-218:GLU:O	1:B:-215:PRO:HD2	2.18	0.43
1:C:-338:TRP:CD2	1:C:-291:PRO:HG3	2.54	0.43
1:A:35:ARG:O	1:A:39:ARG:N	2.49	0.43
1:C:39:ARG:HD3	5:C:311:HOH:O	2.18	0.42
1:D:-267:PRO:HG2	1:D:-262:GLN:HG3	2.01	0.42
1:B:-216:ILE:HA	1:B:-213:LEU:HB3	2.01	0.42
2:F:6:DG:H2"	2:F:7:DG:C8	2.54	0.42
1:D:-226:LEU:HD11	1:D:-213:LEU:HD21	2.00	0.42
1:B:26:SER:OG	1:B:28:ARG:HB2	2.19	0.42
1:D:-339:ILE:HG12	1:D:-289:ILE:HB	2.01	0.42
1:D:-338:TRP:CG	1:D:-291:PRO:HG3	2.54	0.42
2:E:6:DG:H2"	2:E:7:DG:C8	2.54	0.42
1:B:-293:ASP:OD1	1:B:-293:ASP:N	2.53	0.42
1:A:30:ARG:C	1:A:34:ARG:HE	2.27	0.42
1:B:13:LEU:HD23	1:B:13:LEU:HA	1.85	0.42
1:D:-177:TYR:OH	1:D:-174:GLY:HA2	2.20	0.42
1:A:-170:ILE:CD1	1:A:-15:ILE:HD12	2.47	0.42
1:A:-347:LYS:N	1:A:-347:LYS:CD	2.83	0.42
1:A:37:GLU:OE1	1:A:37:GLU:HA	2.18	0.41
1:B:-191:THR:HG21	1:B:-1:VAL:HG21	2.01	0.41
1:B:35:ARG:O	1:B:39:ARG:N	2.51	0.41
1:B:39:ARG:O	1:B:42:ALA:N	2.52	0.41
1:A:19:ASN:O	1:A:22:ARG:HG2	2.20	0.41
1:B:-287:PHE:HA	1:B:-85:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LYS:CD	1:B:25:PRO:HD2	2.50	0.41
1:B:80:VAL:HB	1:B:86:THR:HG23	2.02	0.41
1:A:-287:PHE:HA	1:A:-85:SER:O	2.21	0.41
1:B:-338:TRP:CG	1:B:-291:PRO:HG3	2.56	0.41
1:B:-164:ASP:CB	1:B:17:GLN:OE1	2.68	0.41
1:B:23:ARG:HG3	1:B:23:ARG:HH11	1.85	0.41
1:B:23:ARG:HH11	1:B:23:ARG:CG	2.33	0.41
1:A:72:LEU:HD21	1:B:73:CYS:SG	2.61	0.41
1:B:-212:ASP:OD2	1:B:-145:HIS:ND1	2.54	0.41
1:B:-179:PHE:CD2	1:B:-170:ILE:HA	2.55	0.41
1:B:-71:LYS:NZ	5:B:210:HOH:O	2.42	0.41
1:B:-61:ASP:OD1	1:B:-42:SER:OG	2.38	0.41
1:D:-251:VAL:O	1:D:-244:ILE:HG12	2.20	0.41
1:A:-22:LYS:HE2	5:A:262:HOH:O	2.20	0.41
1:A:22:ARG:O	1:A:22:ARG:HG3	2.19	0.41
1:C:-119:PRO:HA	1:C:-116:TRP:CE2	2.56	0.41
1:D:-216:ILE:N	1:D:-215:PRO:CD	2.83	0.41
1:A:-282:ARG:NH2	5:A:209:HOH:O	2.45	0.41
1:B:-337:ILE:O	1:B:-309:HIS:HA	2.20	0.41
1:B:-211:LYS:HD3	1:B:-145:HIS:HE1	1.86	0.41
1:B:59:LEU:HD13	1:B:63:CYS:SG	2.60	0.41
1:B:24:LYS:CD	1:B:25:PRO:CD	2.99	0.41
1:A:-101:LEU:HB2	1:A:-93:SER:HB2	2.02	0.40
1:C:-218:GLU:O	1:C:-215:PRO:HD2	2.21	0.40
1:A:-220:THR:HG22	1:A:-217:GLU:HG2	2.02	0.40
1:A:-220:THR:O	1:A:-217:GLU:HG2	2.21	0.40
1:A:-102:VAL:HG12	1:A:-101:LEU:O	2.21	0.40
1:B:28:ARG:CZ	1:B:28:ARG:CB	2.97	0.40
1:C:48:TYR:HB2	4:C:103:EDO:H12	2.04	0.40
1:A:-190:TRP:N	1:A:-189:PRO:CD	2.85	0.40
1:B:-229:LYS:HD2	1:B:-106:TYR:C	2.47	0.40
1:B:37:GLU:HG2	2:F:5:DT:H71	2.03	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	434/439 (99%)	430 (99%)	4 (1%)	0	100	100
1	B	434/439 (99%)	427 (98%)	7 (2%)	0	100	100
1	C	435/439 (99%)	431 (99%)	4 (1%)	0	100	100
1	D	435/439 (99%)	430 (99%)	5 (1%)	0	100	100
All	All	1738/1756 (99%)	1718 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	343/345 (99%)	331 (96%)	12 (4%)	32	35
1	B	343/345 (99%)	311 (91%)	32 (9%)	8	6
1	C	344/345 (100%)	338 (98%)	6 (2%)	53	62
1	D	344/345 (100%)	339 (98%)	5 (2%)	57	65
All	All	1374/1380 (100%)	1319 (96%)	55 (4%)	28	29

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	-346	ILE
1	C	-288	ILE
1	C	-170	ILE
1	C	-90	PHE
1	C	23	ARG
1	C	56	ASP
1	D	-347	LYS
1	D	-346	ILE

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Mol	Chain	Res	Type
1	D	-295	THR
1	D	-288	ILE
1	D	-90	PHE
1	A	-347	LYS
1	A	-346	ILE
1	A	-342	LYS
1	A	-304	GLU
1	A	-288	ILE
1	A	-178	LYS
1	A	-90	PHE
1	A	-60	GLU
1	A	22	ARG
1	A	26	SER
1	A	36	ARG
1	A	85	THR
1	B	-347	LYS
1	B	-346	ILE
1	B	-342	LYS
1	B	-221	LYS
1	B	-219	TRP
1	B	-216	ILE
1	B	-211	LYS
1	B	-208	LYS
1	B	-188	LEU
1	B	-184	ASP
1	B	-173	LYS
1	B	-170	ILE
1	B	-169	LYS
1	B	-153	LEU
1	B	-152	VAL
1	B	-102	VAL
1	B	-99	THR
1	B	-90	PHE
1	B	8	THR
1	B	23	ARG
1	B	24	LYS
1	B	28	ARG
1	B	29	GLU
1	B	30	ARG
1	B	31	GLU
1	B	34	ARG
1	B	41	ARG

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Mol	Chain	Res	Type
1	B	58	ASN
1	B	79	VAL
1	B	80	VAL
1	B	85	THR
1	B	88	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	-107	ASN
1	C	62	HIS
1	D	-107	ASN
1	A	-143	ASN
1	A	54	GLN
1	B	-309	HIS
1	B	-107	ASN
1	B	-25	ASN
1	B	33	ASN
1	B	54	GLN

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
3	GLC	K	1	3	12,12,12	0.53	0	17,17,17	0.60	0
3	GLC	K	2	3	11,11,12	0.61	0	15,15,17	0.61	0
3	GLC	L	1	3	12,12,12	0.57	0	17,17,17	0.67	0
3	GLC	L	2	3	11,11,12	0.55	0	15,15,17	0.78	1 (6%)
3	GLC	M	1	3	12,12,12	0.53	0	17,17,17	0.51	0
3	GLC	M	2	3	11,11,12	0.60	0	15,15,17	0.71	0
3	GLC	N	1	3	12,12,12	0.51	0	17,17,17	0.57	0
3	GLC	N	2	3	11,11,12	0.57	0	15,15,17	0.80	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
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1
3	GLC	M	1	3	-	0/2/22/22	0/1/1/1
3	GLC	M	2	3	-	0/2/19/22	0/1/1/1
3	GLC	N	1	3	-	1/2/22/22	0/1/1/1
3	GLC	N	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2	GLC	C1-O5-C5	2.14	115.06	112.19
3	N	2	GLC	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

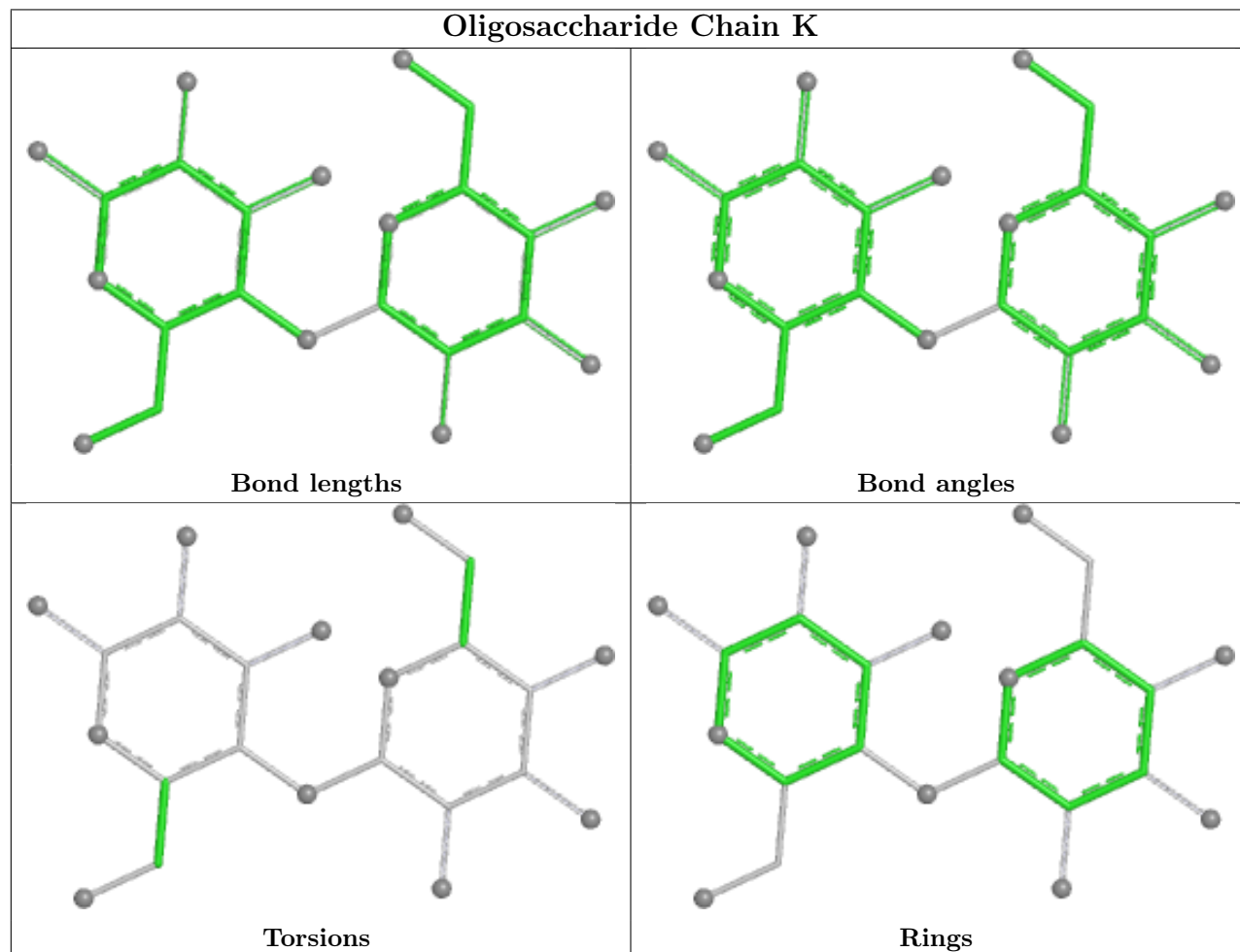
Mol	Chain	Res	Type	Atoms
3	N	1	GLC	C4-C5-C6-O6

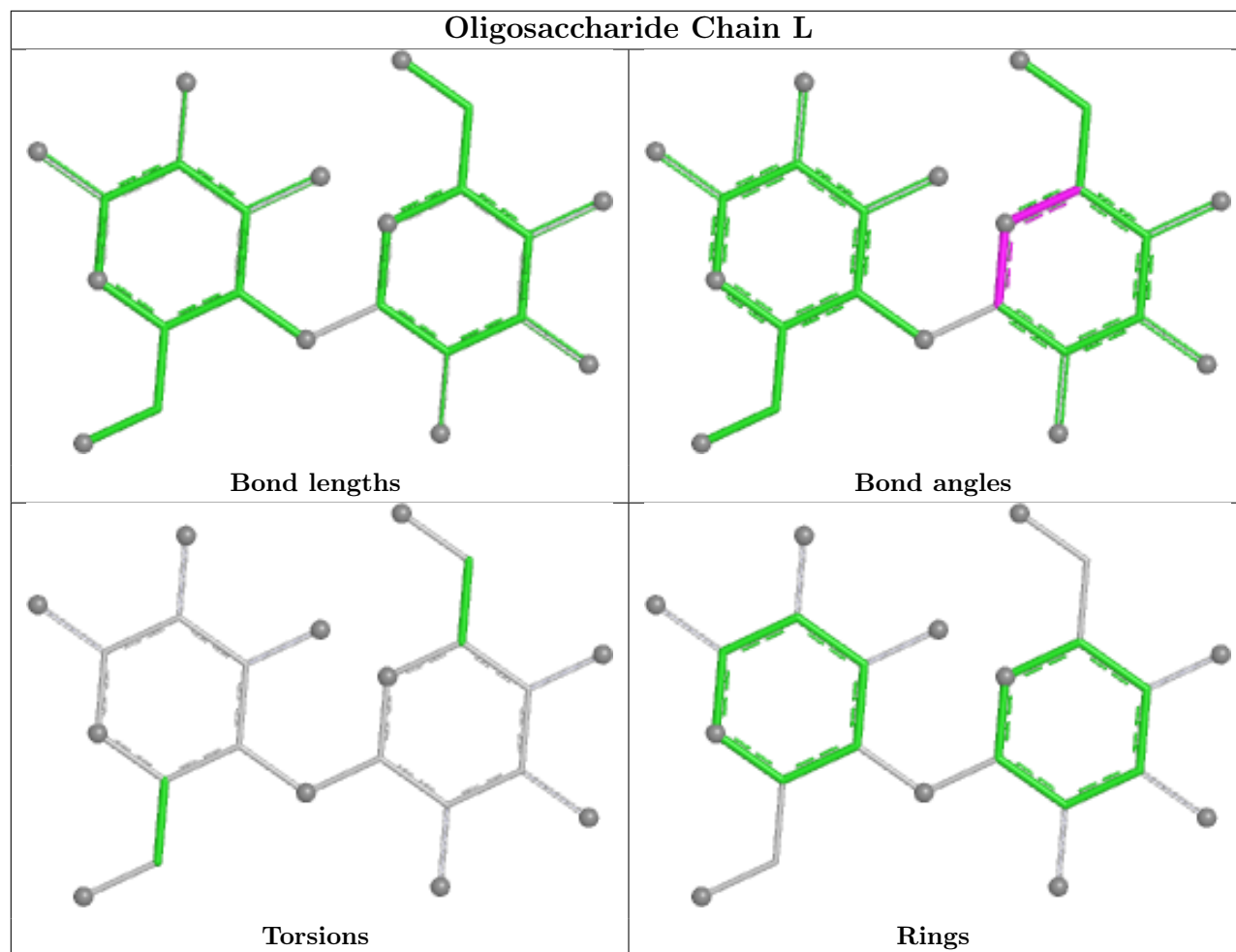
There are no ring outliers.

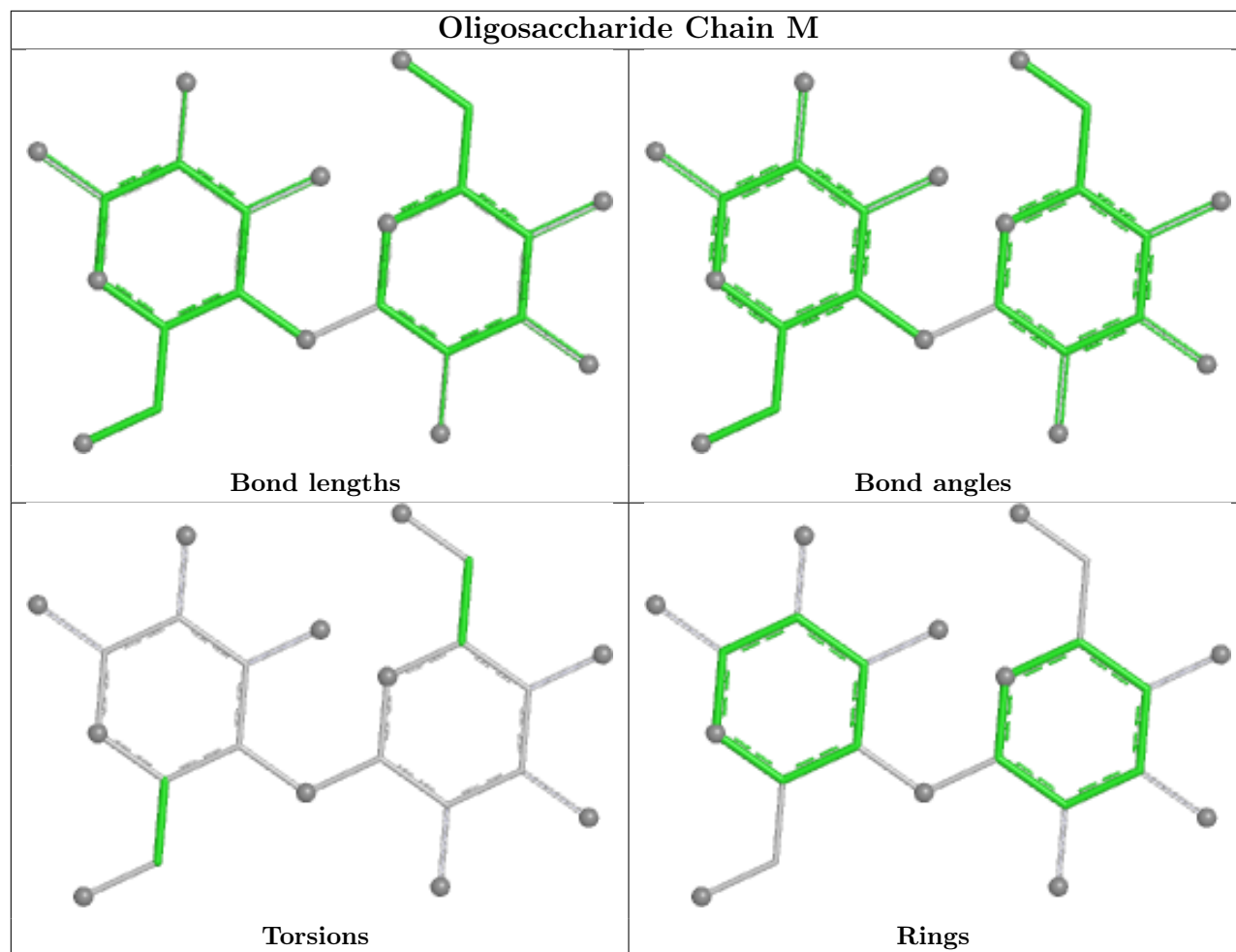
1 monomer is involved in 1 short contact:

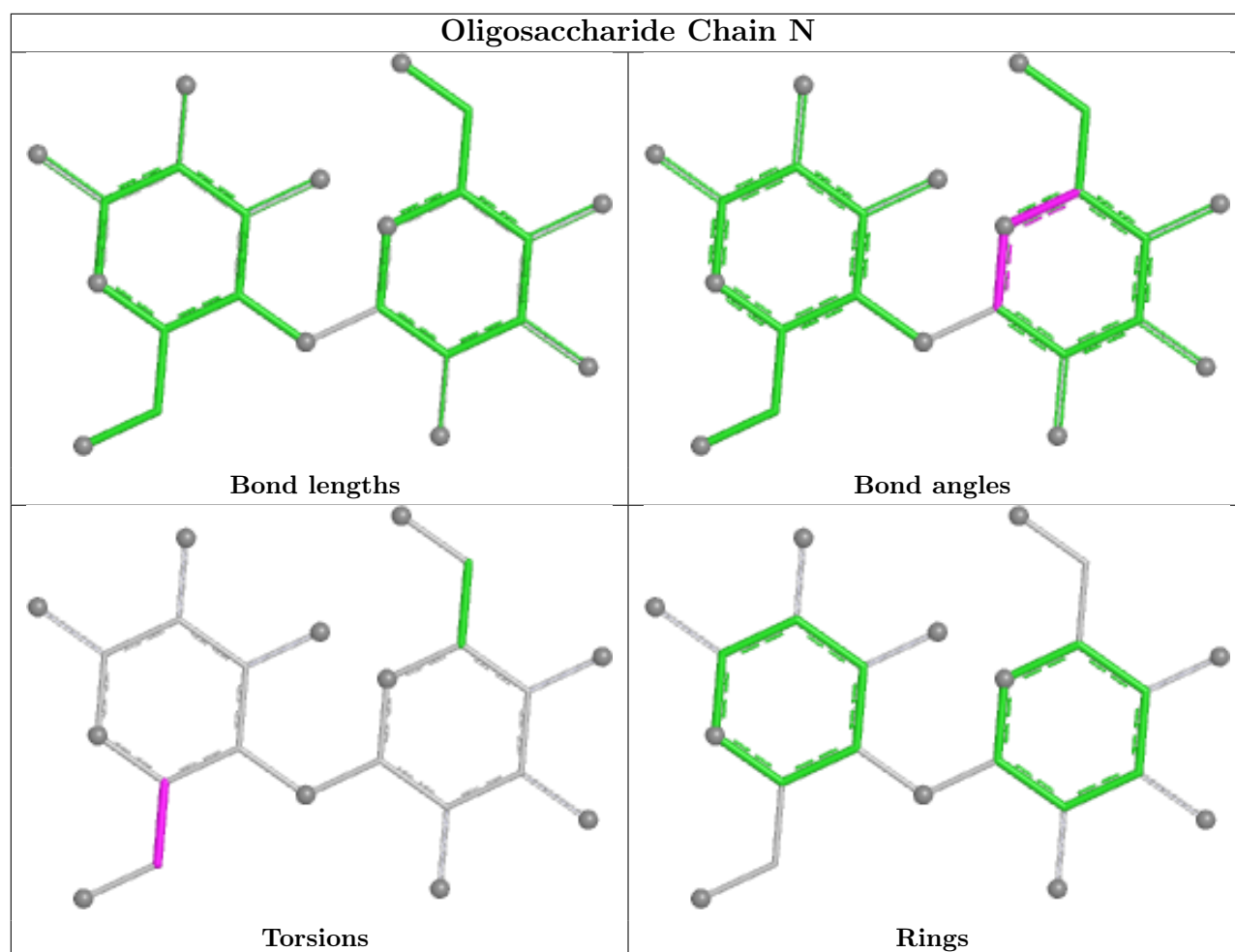
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	GLC	1	0

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](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	B	101	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	D	101	-	3,3,3	0.42	0	2,2,2	0.66	0
4	EDO	C	102	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	A	102	-	3,3,3	0.42	0	2,2,2	0.40	0
4	EDO	C	101	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	C	103	-	3,3,3	0.43	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	101	-	3,3,3	0.42	0	2,2,2	0.36	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
4	EDO	B	101	-	-	0/1/1/1	-
4	EDO	D	101	-	-	1/1/1/1	-
4	EDO	C	102	-	-	0/1/1/1	-
4	EDO	A	102	-	-	1/1/1/1	-
4	EDO	C	101	-	-	0/1/1/1	-
4	EDO	C	103	-	-	0/1/1/1	-
4	EDO	A	101	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	102	EDO	O1-C1-C2-O2
4	D	101	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	102	EDO	1	0
4	C	103	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	436/439 (99%)	0.73	49 (11%) 10 10	24, 44, 94, 118	0
1	B	436/439 (99%)	1.13	108 (24%) 2 2	25, 56, 96, 118	0
1	C	437/439 (99%)	-0.00	5 (1%) 78 80	22, 36, 56, 69	0
1	D	437/439 (99%)	0.05	5 (1%) 78 80	25, 37, 56, 64	0
2	E	15/15 (100%)	0.90	0 100 100	68, 79, 96, 100	0
2	F	15/15 (100%)	0.78	0 100 100	60, 72, 94, 96	0
2	G	15/15 (100%)	-0.51	0 100 100	29, 33, 39, 40	0
2	H	15/15 (100%)	-0.51	0 100 100	27, 34, 39, 42	0
All	All	1806/1816 (99%)	0.46	167 (9%) 14 15	22, 41, 88, 118	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	TRP	5.8
1	B	-153	LEU	4.7
1	A	27	TRP	4.5
1	B	79	VAL	4.4
1	B	59	LEU	4.2
1	B	9	VAL	4.2
1	B	26	SER	4.1
1	A	28	ARG	4.1
1	B	-214	ALA	4.1
1	B	43	VAL	4.1
1	A	33	ASN	4.0
1	A	47	ILE	3.9
1	B	42	ALA	3.9
1	B	21	ALA	3.8
1	A	57	TYR	3.8
1	B	-226	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	-7	TYR	3.7
1	B	57	TYR	3.6
1	B	25	PRO	3.6
1	B	-7	TYR	3.5
1	B	-2	ALA	3.4
1	B	51	LEU	3.4
1	B	-205	GLY	3.4
1	B	-157	GLY	3.4
1	B	-137	SER	3.4
1	A	59	LEU	3.4
1	B	-227	LEU	3.4
1	A	36	ARG	3.4
1	B	38	ARG	3.4
1	B	-219	TRP	3.4
1	B	-215	PRO	3.4
1	B	33	ASN	3.3
1	A	38	ARG	3.3
1	B	62	HIS	3.2
1	B	68	VAL	3.2
1	B	-135	ALA	3.2
1	A	74	VAL	3.1
1	A	26	SER	3.1
1	B	8	THR	3.1
1	B	-132	ALA	3.1
1	C	62	HIS	3.1
1	B	-207	ALA	3.1
1	A	43	VAL	3.1
1	A	-197	LEU	3.1
1	B	-175	ALA	3.0
1	A	25	PRO	3.0
1	B	61	LYS	3.0
1	B	-216	ILE	3.0
1	B	85	THR	3.0
1	A	51	LEU	3.0
1	B	-143	ASN	3.0
1	B	-294	GLY	3.0
1	A	76	ALA	2.9
1	B	3	ALA	2.9
1	B	53	ALA	2.9
1	B	28	ARG	2.9
1	A	34	ARG	2.8
1	B	69	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	-111	THR	2.8
1	A	-2	ALA	2.8
1	A	42	ALA	2.8
1	A	62	HIS	2.8
1	B	-231	TYR	2.8
1	D	-109	ALA	2.8
1	B	-158	ALA	2.8
1	B	12	ALA	2.8
1	B	20	ALA	2.8
1	B	48	TYR	2.8
1	A	20	ALA	2.7
1	B	87	TYR	2.7
1	B	-108	VAL	2.7
1	A	-170	ILE	2.7
1	B	34	ARG	2.7
1	B	60	PRO	2.7
1	B	-36	ALA	2.6
1	B	15	ALA	2.6
1	B	49	THR	2.6
1	A	69	LEU	2.6
1	D	-7	TYR	2.6
1	A	85	THR	2.6
1	B	11	ALA	2.6
1	B	18	THR	2.6
1	B	0	ILE	2.5
1	B	47	ILE	2.5
1	B	-224	ASN	2.5
1	B	14	ALA	2.5
1	B	44	ALA	2.5
1	B	78	TRP	2.5
1	B	-200	MET	2.5
1	B	-136	ILE	2.5
1	A	87	TYR	2.5
1	A	30	ARG	2.5
1	D	-295	THR	2.5
1	A	37	GLU	2.5
1	D	-348	MET	2.5
1	A	61	LYS	2.5
1	B	-188	LEU	2.5
1	A	35	ARG	2.5
1	B	74	VAL	2.4
1	B	-164	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	-203	SER	2.4
1	B	-150	LEU	2.4
1	A	79	VAL	2.4
1	B	-5	VAL	2.4
1	A	-176	ALA	2.4
1	B	-176	ALA	2.4
1	B	77	GLY	2.4
1	B	-346	ILE	2.4
1	B	37	GLU	2.4
1	B	5	GLY	2.4
1	A	41	ARG	2.4
1	A	80	VAL	2.4
1	B	-152	VAL	2.4
1	C	-7	TYR	2.3
1	A	21	ALA	2.3
1	B	-6	ALA	2.3
1	B	-131	PHE	2.3
1	B	36	ARG	2.3
1	B	63	CYS	2.3
1	A	16	ALA	2.3
1	B	2	ALA	2.3
1	B	32	ASN	2.3
1	C	-348	MET	2.3
1	C	-344	GLU	2.3
1	B	31	GLU	2.3
1	B	-213	LEU	2.3
1	B	-174	GLY	2.3
1	B	-218	GLU	2.3
1	D	-296	ALA	2.3
1	B	76	ALA	2.3
1	B	-101	LEU	2.3
1	B	72	LEU	2.3
1	A	48	TYR	2.3
1	A	18	THR	2.2
1	B	-225	PRO	2.2
1	B	-155	THR	2.2
1	B	30	ARG	2.2
1	B	-133	ALA	2.2
1	B	71	ALA	2.2
1	A	77	GLY	2.2
1	A	-109	ALA	2.2
1	B	24	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	86	THR	2.2
1	A	68	VAL	2.2
1	B	-210	GLU	2.2
1	C	-296	ALA	2.2
1	A	-296	ALA	2.2
1	A	71	ALA	2.2
1	B	58	ASN	2.2
1	A	60	PRO	2.1
1	B	-165	VAL	2.1
1	A	-141	ASP	2.1
1	B	40	ARG	2.1
1	B	16	ALA	2.1
1	B	-154	PHE	2.1
1	B	-102	VAL	2.1
1	B	64	ASP	2.1
1	B	-1	VAL	2.1
1	B	-233	LEU	2.0
1	A	17	GLN	2.0
1	A	63	CYS	2.0
1	B	-223	PRO	2.0
1	B	86	THR	2.0
1	A	12	ALA	2.0
1	B	-148	LYS	2.0
1	A	55	GLY	2.0
1	B	-120	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

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

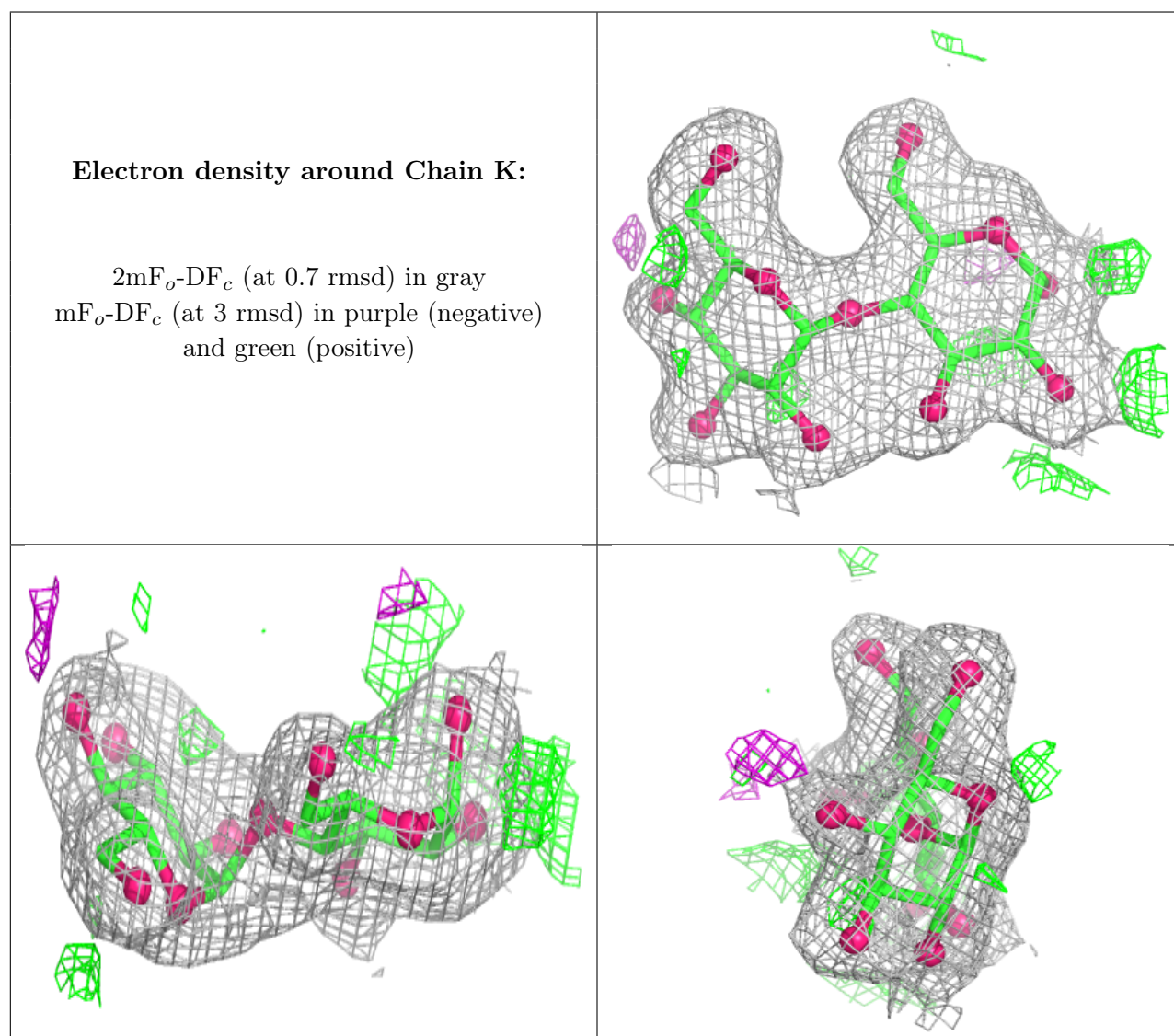
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	K	1	12/12	0.93	0.09	32,35,38,42	0
3	GLC	L	1	12/12	0.95	0.06	37,42,45,46	0
3	GLC	K	2	11/12	0.96	0.06	28,36,41,42	0

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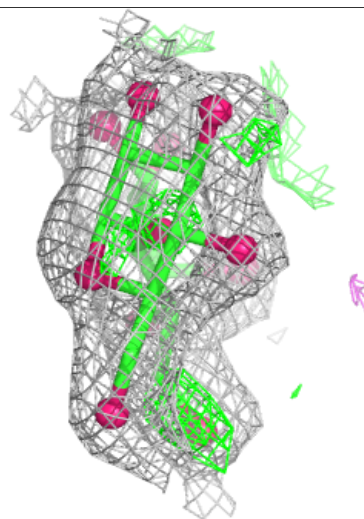
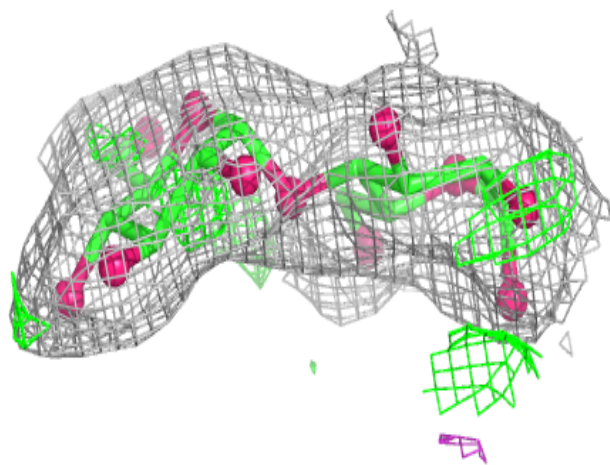
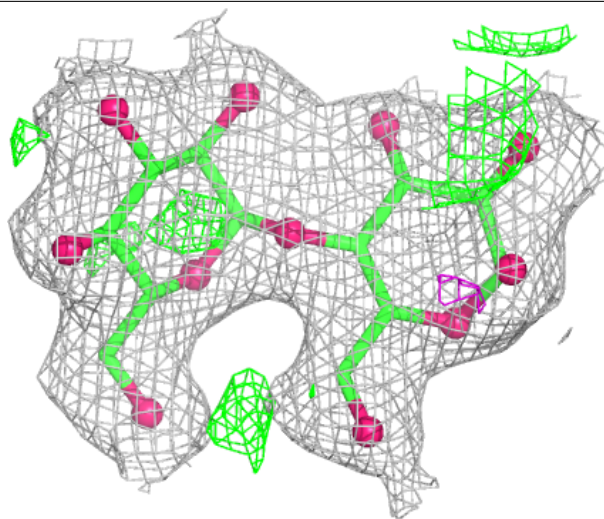
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	L	2	11/12	0.96	0.06	34,39,43,43	0
3	GLC	M	1	12/12	-	-	25,29,30,31	0
3	GLC	M	2	11/12	-	-	21,24,26,28	0
3	GLC	N	1	12/12	-	-	24,28,31,32	0
3	GLC	N	2	11/12	-	-	22,25,28,32	0

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.



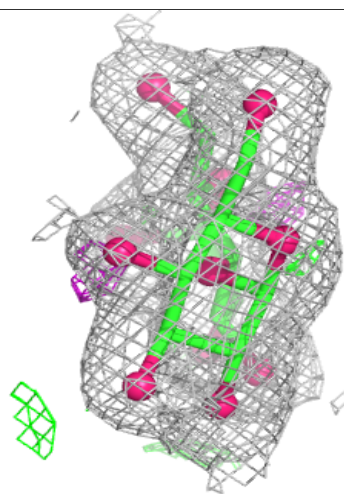
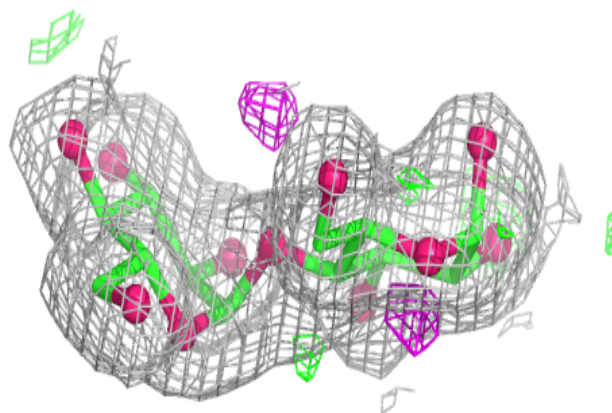
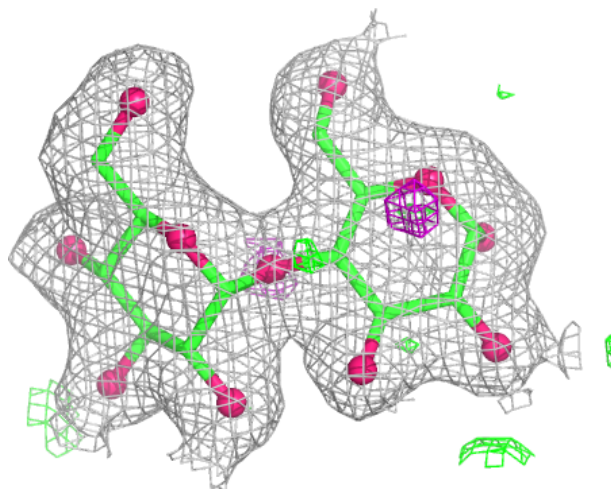
Electron density around Chain L:

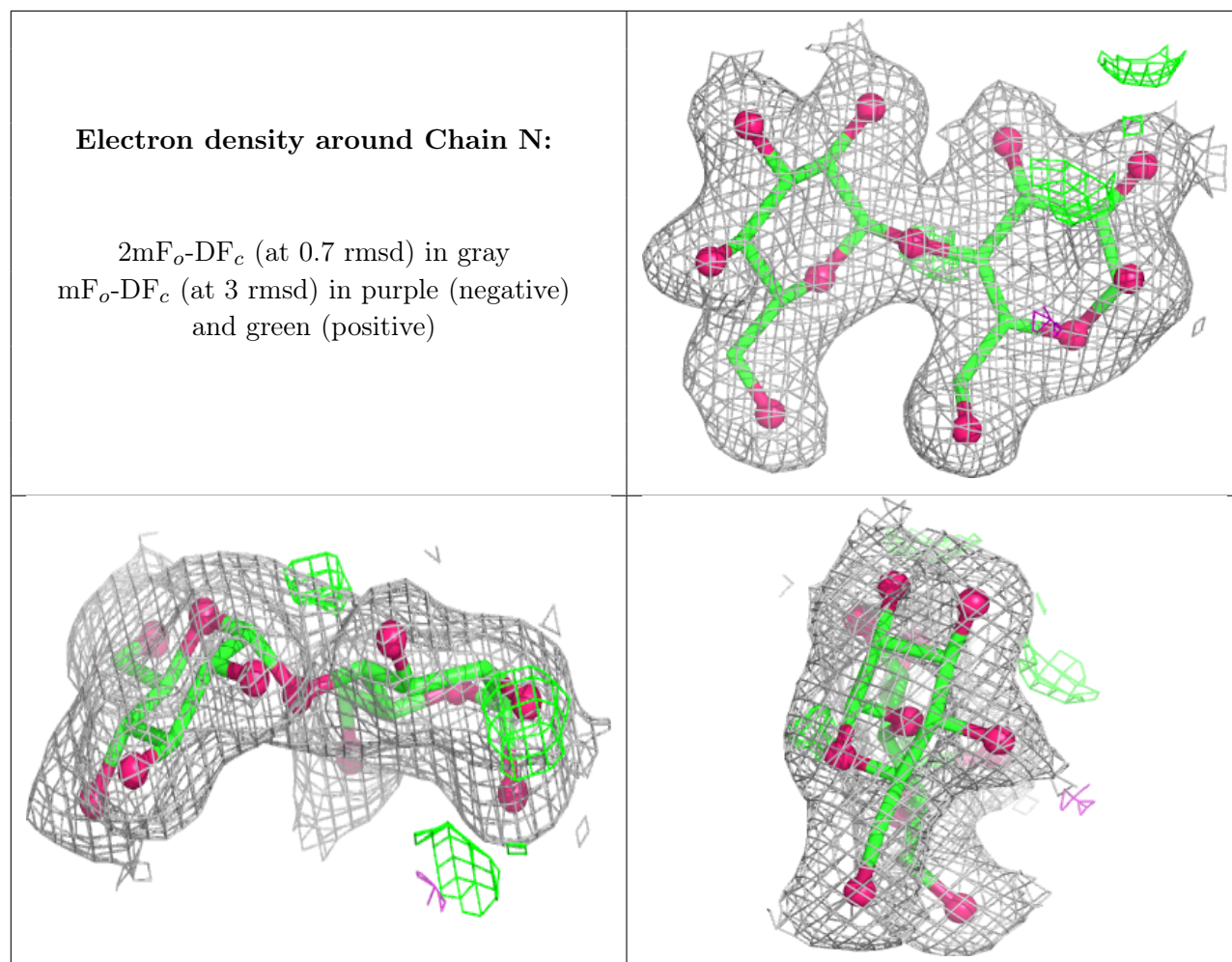
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain M:

$2mF_o-DF_c$ (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
4	EDO	C	103	4/4	0.83	0.16	41,45,46,46	0
4	EDO	A	102	4/4	0.83	0.29	40,51,51,51	0
4	EDO	D	101	4/4	0.88	0.13	34,41,46,46	0
4	EDO	C	102	4/4	0.89	0.14	38,45,49,54	0
4	EDO	A	101	4/4	0.93	0.10	36,37,37,40	0
4	EDO	C	101	4/4	0.95	0.08	32,32,36,36	0
4	EDO	B	101	4/4	0.97	0.06	32,41,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.