Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 05:47 PM JST

PDB ID	:	7VN6
Title	:	Crystal structure of MBP-fused BIL1/BZR1 (21-90) in complex with double-stranded DNA contaning CGCACGTGCG
Authors	:	Nosaki, S.; Tanokura, M.; Miyakawa, T.
Deposited on	:	2021-10-10
Resolution	:	2.79 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

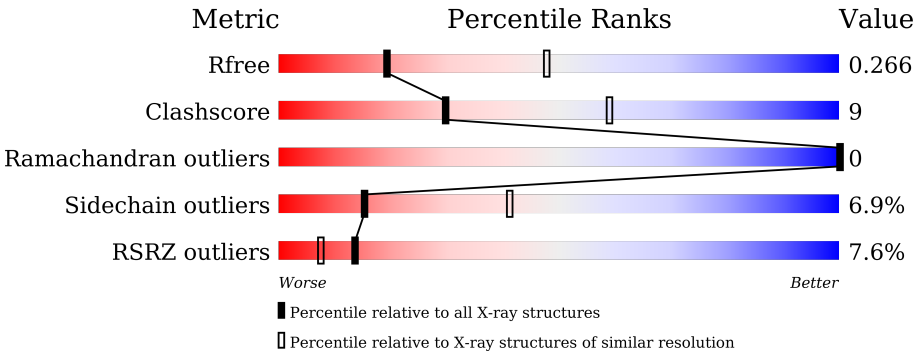
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	439	7% 78% 19% ·
1	B	439	10% 79% 18% ··
1	C	439	2% 83% 16% ··
1	D	439	13% 68% 27% · ·
2	E	15	80% 20%
2	F	15	93% 7%

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Mol	Chain	Length	Quality of chain
2	G	15	47% 53%
2	H	15	87% 13%
3	I	2	100%
3	K	2	100%
3	L	2	100%
3	M	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	102	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14924 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 Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	436	Total	C	N	O	S	0	0	0
			3394	2166	581	639	8			
1	D	436	Total	C	N	O	S	0	0	0
			3394	2166	581	639	8			
1	A	437	Total	C	N	O	S	0	0	0
			3402	2171	582	640	9			
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	-368	MET	-	initiating methionine	UNP A0A4P1LXE0
C	-286	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
C	-285	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	-196	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
C	-195	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
C	-129	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	-9	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
C	-6	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	-5	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
D	-368	MET	-	initiating methionine	UNP A0A4P1LXE0
D	-286	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
D	-285	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	-196	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
D	-195	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
D	-129	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	-9	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
D	-6	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	-5	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
A	-368	MET	-	initiating methionine	UNP A0A4P1LXE0
A	-286	ALA	ASP	engineered mutation	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-285	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	-196	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
A	-195	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
A	-129	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	-9	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
A	-6	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	-5	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
B	-368	MET	-	initiating methionine	UNP A0A4P1LXE0
B	-286	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
B	-285	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	-196	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
B	-195	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
B	-129	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	-9	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
B	-6	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	-5	ALA	ASP	engineered mutation	UNP A0A4P1LXE0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	15	Total	C	N	O	P	0	0	0
			305	146	58	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			305	146	58	87	14			
2	E	15	Total	C	N	O	P	0	0	0
			305	146	58	87	14			
2	F	15	Total	C	N	O	P	0	0	0
			305	146	58	87	14			

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

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

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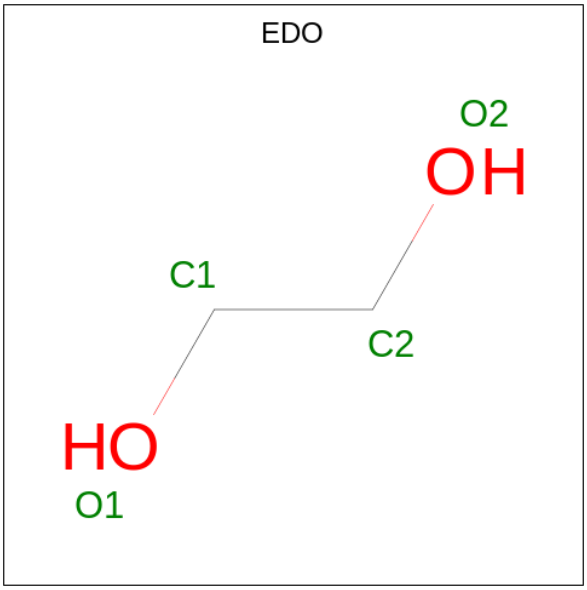
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	L	2	Total C O 23 12 11	0	0	0
3	M	2	Total C O 23 12 11	0	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



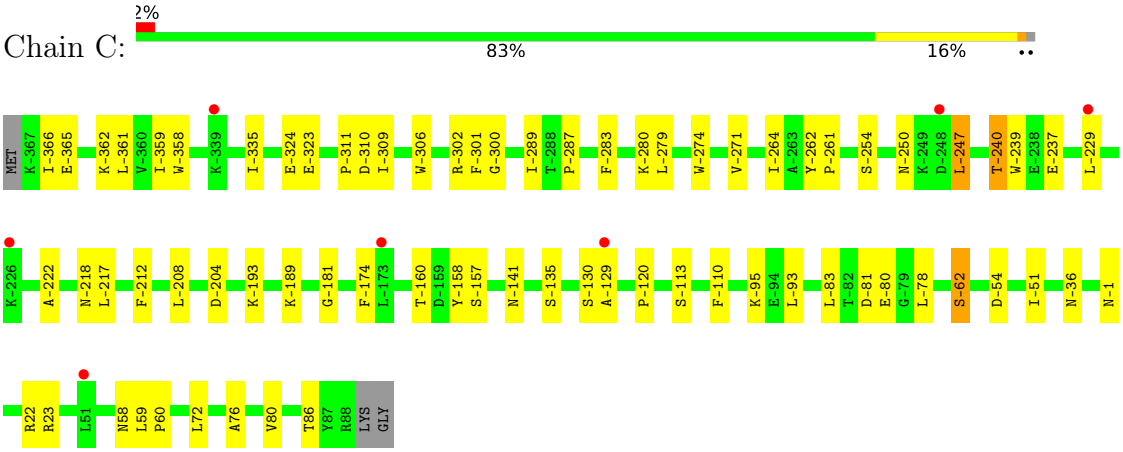
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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.

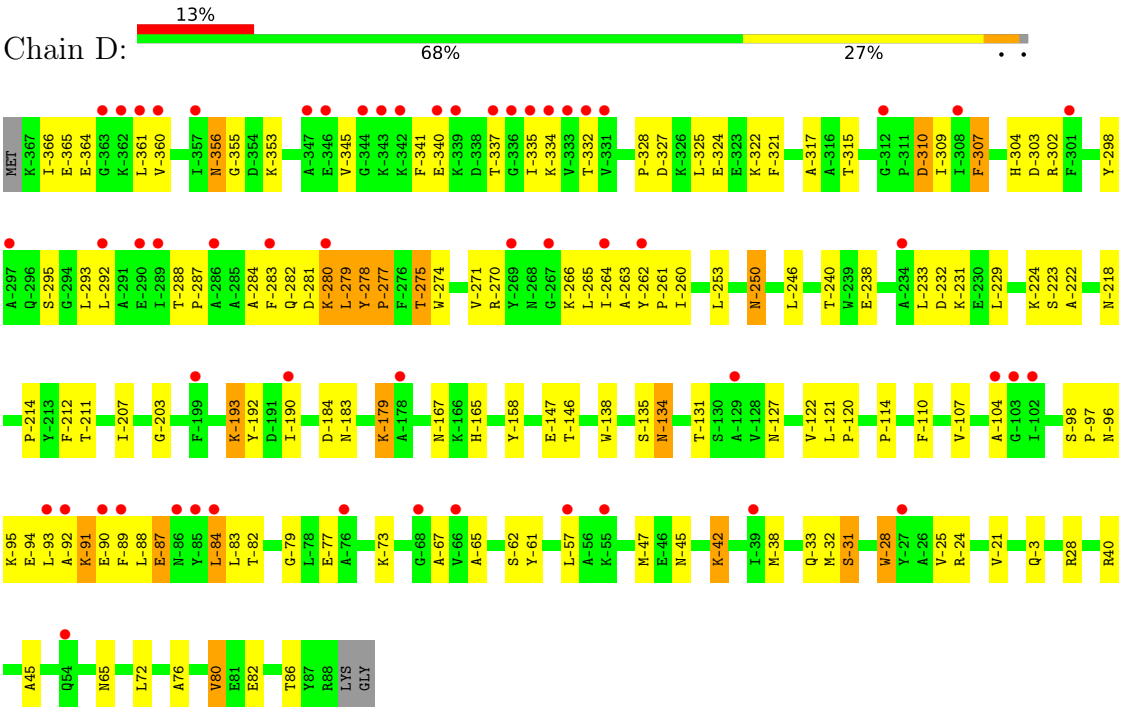
• Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1

Chain C:



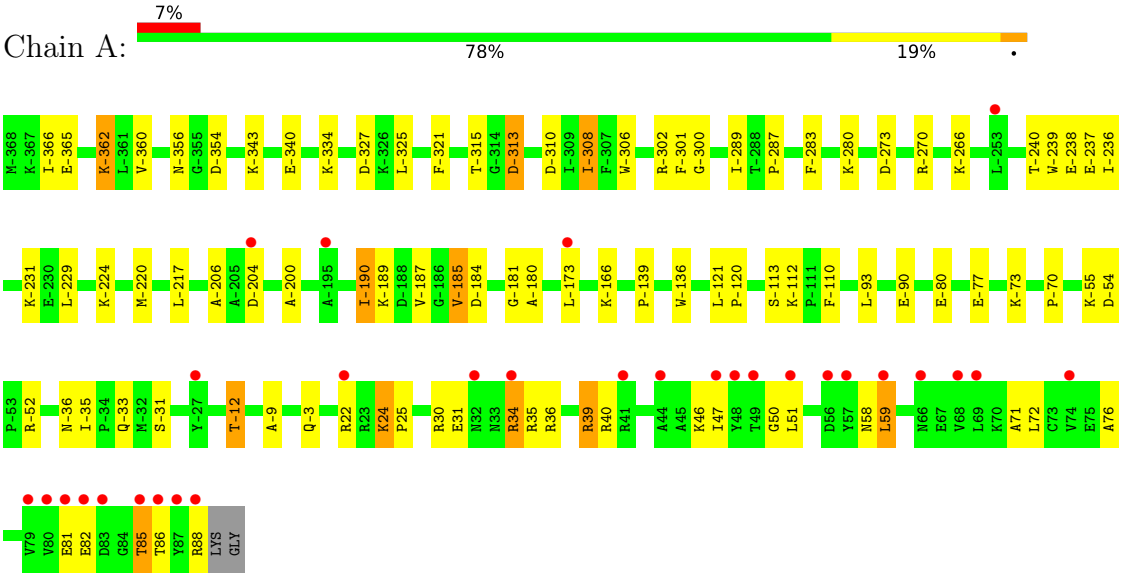
• Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1

Chain D:



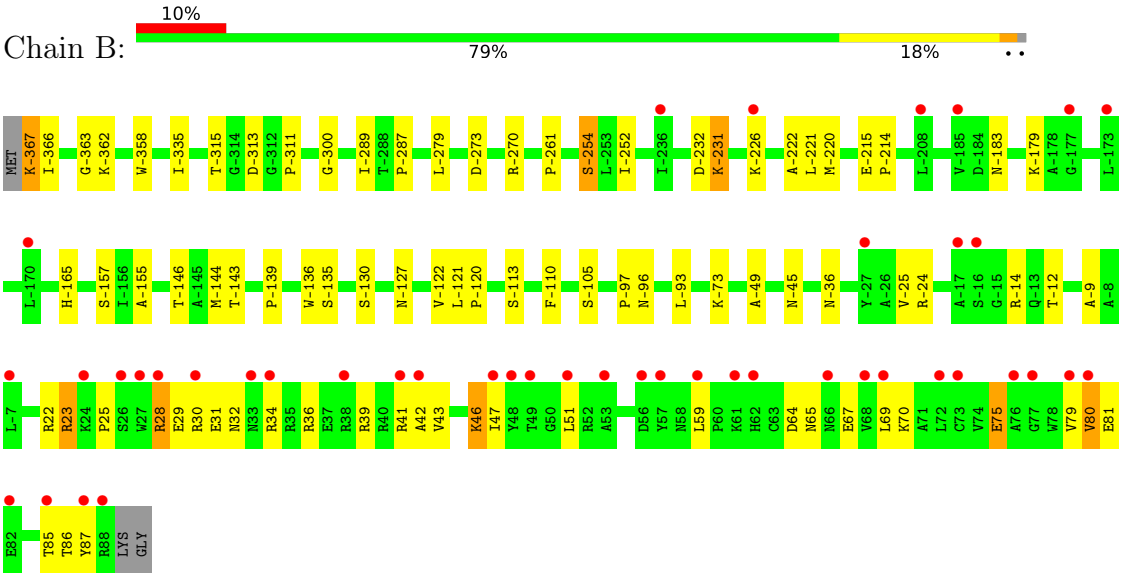
• Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1

Chain A:



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

Chain B:

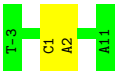


• Molecule 2: DNA (5'-D(*TP*TP*CP*GP*CP*AP*CP*GP*TP*GP*CP*GP*AP*AP*A)-3')

Chain G:

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

Chain H:

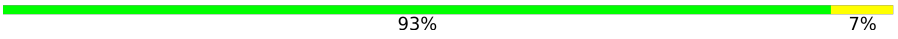


• Molecule 2: DNA (5'-D(*TP*TP*CP*GP*CP*AP*CP*GP*TP*GP*CP*GP*AP*AP*A)-3')

Chain E:

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

Chain F:

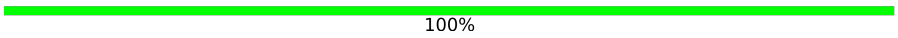


• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:

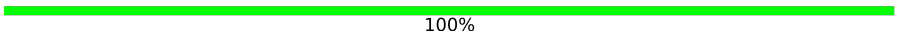
• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:



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

Chain L:



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

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.30Å 93.61Å 112.06Å 90.00° 100.87° 90.00°	Depositor
Resolution (Å)	42.75 – 2.79 42.75 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.75-2.79) 99.0 (42.75-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.216 , 0.266 0.216 , 0.266	Depositor DCC
R_{free} test set	2539 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14924	wwPDB-VP
Average B, all atoms (Å^2)	73.0	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 63.42 % 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 9.6958e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, GLC

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	0/3481	0.47	0/4723
1	B	0.30	0/3473	0.45	0/4713
1	C	0.40	0/3473	0.45	0/4713
1	D	0.38	0/3473	0.52	0/4713
2	E	0.54	0/342	0.92	0/526
2	F	0.55	0/342	0.93	0/526
2	G	0.62	0/342	0.96	0/526
2	H	0.58	0/342	0.91	0/526
All	All	0.39	0/15268	0.54	0/20966

There are no bond length outliers.

There are no bond angle outliers.

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	3402	0	3374	64	0
1	B	3394	0	3365	55	0
1	C	3394	0	3365	42	0
1	D	3394	0	3365	117	0
2	E	305	0	170	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	305	0	170	1	0
2	G	305	0	170	4	0
2	H	305	0	170	1	0
3	I	23	0	21	0	0
3	K	23	0	21	0	0
3	L	23	0	21	0	0
3	M	23	0	21	1	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
4	C	12	0	18	0	0
4	G	4	0	6	3	0
All	All	14924	0	14275	273	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 9.

All (273) 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:-283:PHE:CD1	1:D:-87:GLU:HG2	1.75	1.21
1:D:-283:PHE:CE1	1:D:-87:GLU:HG2	1.86	1.10
1:D:-283:PHE:CD1	1:D:-87:GLU:CG	2.42	1.01
1:D:-262:TYR:CD1	1:D:-88:LEU:HD23	2.01	0.96
1:D:-335:ILE:HG12	1:D:-93:LEU:HD21	1.45	0.96
1:D:-262:TYR:CG	1:D:-88:LEU:HD23	2.01	0.95
1:D:-262:TYR:CD1	1:D:-88:LEU:CD2	2.50	0.93
1:D:-89:PHE:CZ	1:D:-84:LEU:HD12	2.07	0.88
1:D:-89:PHE:CZ	1:D:-84:LEU:CD1	2.60	0.85
1:D:-283:PHE:HD1	1:D:-87:GLU:CG	1.90	0.83
1:D:-270:ARG:HG3	1:D:-265:LEU:HD23	1.61	0.82
1:D:-283:PHE:CD1	1:D:-87:GLU:CD	2.53	0.82
1:C:-279:LEU:HD22	1:C:-274:TRP:CZ2	2.20	0.76
1:D:-89:PHE:CE1	1:D:-84:LEU:CD1	2.70	0.75
1:A:-365:GLU:H	1:A:-362:LYS:HE2	1.52	0.75
1:D:-77:GLU:HG2	1:D:-61:TYR:HE2	1.52	0.75
1:D:-89:PHE:CE1	1:D:-84:LEU:HD13	2.22	0.75
1:B:-289:ILE:HG22	1:B:-287:PRO:HD3	1.70	0.74
1:A:-239:TRP:CD1	1:A:-120:PRO:HB2	2.23	0.73
1:C:-324:GLU:HB2	1:C:-302:ARG:HD2	1.70	0.73
1:D:-283:PHE:HD1	1:D:-87:GLU:CD	1.93	0.71
1:D:-95:LYS:O	1:D:-91:LYS:HG2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ASN:HD21	4:G:101:EDO:H11	1.55	0.70
1:A:-289:ILE:HG22	1:A:-287:PRO:HD3	1.73	0.70
1:A:-340:GLU:HG3	1:A:-334:LYS:HA	1.74	0.70
1:D:-324:GLU:HG3	1:D:-302:ARG:HE	1.58	0.68
1:C:-366:ILE:HG21	1:C:-310:ASP:OD1	1.94	0.68
1:D:-232:ASP:HB3	1:D:-165:HIS:HD2	1.57	0.68
1:A:-240:THR:HG23	1:A:-237:GLU:HG2	1.77	0.67
1:C:-359:ILE:HG12	1:C:-309:ILE:HB	1.77	0.66
1:C:-204:ASP:O	1:C:-181:GLY:HA3	1.95	0.66
1:D:-366:ILE:HD12	1:D:-97:PRO:HD3	1.78	0.66
1:B:31:GLU:HA	1:B:34:ARG:HE	1.60	0.66
1:C:-240:THR:HG22	1:C:-237:GLU:H	1.59	0.66
1:D:-317:ALA:HB3	1:D:-293:LEU:HD23	1.78	0.66
1:A:76:ALA:HB1	1:B:75:GLU:HG2	1.78	0.66
1:A:59:LEU:HD21	1:A:71:ALA:HB2	1.78	0.66
1:D:40:ARG:HG3	1:D:40:ARG:HH11	1.62	0.65
1:A:-187:VAL:HB	1:A:-3:GLN:NE2	2.12	0.65
1:B:28:ARG:NH1	1:B:32:ASN:HD21	1.96	0.64
1:D:-284:ALA:O	1:D:-280:LYS:HG2	1.98	0.64
1:D:-262:TYR:CD1	1:D:-88:LEU:HD22	2.33	0.63
1:B:36:ARG:HE	1:B:39:ARG:HH11	1.46	0.63
1:D:-278:TYR:HB2	1:D:-275:THR:HG23	1.80	0.63
2:E:3:DC:H2"	2:E:4:DG:C8	2.35	0.62
1:D:-307:PHE:CE1	1:D:-104:ALA:HB2	2.35	0.61
1:B:-367:LYS:O	1:B:-367:LYS:HG2	2.00	0.61
1:A:-217:LEU:HD11	1:A:-173:LEU:HD11	1.83	0.60
1:D:-114:PRO:HB3	1:D:-42:LYS:HD3	1.82	0.59
1:A:-313:ASP:OD1	1:A:-313:ASP:N	2.35	0.59
1:D:-271:VAL:HG13	1:D:-271:VAL:O	2.01	0.59
1:D:-341:PHE:HZ	1:D:-90:GLU:HB3	1.67	0.59
1:A:-283:PHE:HA	1:A:-280:LYS:HD2	1.84	0.59
1:A:-187:VAL:HB	1:A:-3:GLN:HE21	1.67	0.59
1:D:-356:ASN:HD22	1:D:-355:GLY:H	1.51	0.59
1:A:31:GLU:OE2	1:A:34:ARG:NE	2.35	0.58
1:B:-279:LEU:HD23	1:B:-261:PRO:HG2	1.84	0.58
1:C:72:LEU:HD21	1:D:72:LEU:HG	1.85	0.58
1:D:-262:TYR:OH	1:D:-91:LYS:HE3	2.03	0.58
1:D:-271:VAL:O	1:D:-271:VAL:HG22	2.03	0.58
1:B:-363:GLY:H	1:B:-96:ASN:HD21	1.51	0.58
1:C:-289:ILE:HG22	1:C:-287:PRO:HD3	1.84	0.58
1:A:51:LEU:HD21	1:A:72:LEU:HD22	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD11	1:B:80:VAL:HG21	1.85	0.57
1:B:-120:PRO:O	1:B:-113:SER:OG	2.22	0.57
1:A:-229:LEU:HB3	1:A:-224:LYS:HB2	1.87	0.57
1:D:-77:GLU:HG2	1:D:-61:TYR:CE2	2.35	0.57
1:B:-220:MET:HB2	1:B:-146:THR:HG21	1.86	0.57
1:B:65:ASN:ND2	2:F:1:DC:O5'	2.38	0.57
1:D:-158:TYR:HH	1:D:-138:TRP:HE1	1.53	0.57
1:D:-184:ASP:HB2	1:D:-3:GLN:HB2	1.86	0.56
1:D:-95:LYS:O	1:D:-91:LYS:CG	2.51	0.56
1:B:-12:THR:HG23	1:B:-9:ALA:H	1.70	0.56
1:B:25:PRO:HG2	1:B:30:ARG:NH2	2.21	0.56
1:B:64:ASP:HB3	1:B:67:GLU:HG2	1.87	0.56
1:D:-246:LEU:HD21	1:D:-233:LEU:HD21	1.88	0.55
1:A:88:ARG:NH2	1:B:75:GLU:OE2	2.39	0.55
1:C:-271:VAL:HG21	1:C:-261:PRO:HD3	1.88	0.55
1:D:-283:PHE:HB3	1:D:-87:GLU:OE1	2.06	0.55
1:A:-136:TRP:HB2	1:A:-70:PRO:HG2	1.89	0.55
1:B:28:ARG:HH11	1:B:32:ASN:HD21	1.53	0.55
1:D:-240:THR:HG22	1:D:-238:GLU:H	1.71	0.54
1:B:25:PRO:HB2	1:B:30:ARG:HE	1.71	0.54
1:D:-295:SER:HB2	1:D:-293:LEU:CD1	2.37	0.54
1:D:-190:ILE:HD11	1:D:-33:GLN:HB2	1.89	0.54
1:C:-366:ILE:HG21	1:C:-310:ASP:CG	2.28	0.54
1:D:-287:PRO:HB2	1:D:-283:PHE:HB2	1.89	0.54
1:C:-217:LEU:HD23	1:C:-160:THR:HB	1.89	0.54
1:D:-94:GLU:HA	1:D:-91:LYS:HG3	1.90	0.54
1:C:-1:ASN:OD1	1:C:22:ARG:NH2	2.38	0.53
1:D:-89:PHE:CE1	1:D:-84:LEU:HD12	2.36	0.53
1:D:-89:PHE:HE1	1:D:-84:LEU:HD13	1.72	0.53
1:B:-215:GLU:OE1	1:B:-24:ARG:NH2	2.40	0.53
1:A:-139:PRO:HA	1:A:-136:TRP:CE2	2.44	0.53
1:D:45:ALA:HA	4:G:101:EDO:H12	1.91	0.53
1:C:-250:ASN:ND2	1:C:-247:LEU:HB2	2.23	0.53
1:B:-231:LYS:HD2	1:B:-165:HIS:HE1	1.74	0.53
1:B:-183:ASN:O	1:B:-179:LYS:HG3	2.09	0.52
1:A:36:ARG:NE	1:A:39:ARG:HH21	2.08	0.52
1:D:-224:LYS:HE3	1:D:-147:GLU:HA	1.91	0.52
1:D:-25:VAL:O	1:D:-21:VAL:HG23	2.09	0.52
1:D:-364:GLU:OE1	1:D:-97:PRO:HB2	2.10	0.52
1:A:-200:ALA:HB2	1:A:-110:PHE:HZ	1.74	0.52
1:D:-309:ILE:CD1	1:D:-88:LEU:HD13	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-240:THR:OG1	1:A:-238:GLU:OE1	2.27	0.52
1:A:47:ILE:HG21	1:B:69:LEU:HD21	1.92	0.51
1:C:76:ALA:HB2	1:D:76:ALA:HB2	1.93	0.51
1:D:-327:ASP:O	1:D:-322:LYS:HE3	2.10	0.51
1:A:-185:VAL:O	1:A:-180:ALA:HB3	2.10	0.51
1:D:-281:ASP:C	1:D:-279:LEU:H	2.14	0.51
1:A:-54:ASP:OD2	1:A:-52:ARG:NH2	2.42	0.51
1:A:-80:GLU:H	1:A:-80:GLU:CD	2.14	0.51
1:B:23:ARG:NH1	1:B:29:GLU:OE2	2.42	0.51
1:A:-190:ILE:HG22	1:A:-189:LYS:HG2	1.91	0.51
1:C:-250:ASN:HD22	1:C:-247:LEU:HB2	1.75	0.50
1:C:-301:PHE:HB3	1:C:-264:ILE:HD13	1.94	0.50
1:A:-321:PHE:CG	1:A:-308:ILE:HD12	2.47	0.50
1:D:-82:THR:HG23	1:D:-79:GLY:H	1.77	0.50
1:A:24:LYS:HD3	1:A:25:PRO:HD2	1.93	0.49
1:C:-120:PRO:O	1:C:-113:SER:OG	2.30	0.49
1:A:81:GLU:OE2	1:A:85:THR:OG1	2.27	0.49
1:B:25:PRO:HG2	1:B:30:ARG:HH21	1.76	0.49
1:D:-341:PHE:CZ	1:D:-90:GLU:HB3	2.46	0.49
1:D:-224:LYS:HD2	1:D:-224:LYS:N	2.28	0.49
1:B:31:GLU:OE1	1:B:34:ARG:NE	2.45	0.49
1:C:-54:ASP:HB3	1:C:-51:ILE:HG12	1.94	0.49
1:D:-28:TRP:CD1	3:M:2:GLC:H4	2.48	0.49
1:A:-190:ILE:HG23	1:A:-190:ILE:O	2.12	0.49
1:D:-309:ILE:HD13	1:D:-88:LEU:CD1	2.42	0.49
1:D:-278:TYR:O	1:D:-275:THR:HG23	2.13	0.49
1:D:-263:ALA:O	1:D:-261:PRO:HD3	2.12	0.49
1:D:-361:LEU:HD11	1:D:-92:ALA:HA	1.93	0.49
1:B:-300:GLY:HA3	1:B:-36:ASN:O	2.13	0.49
1:A:-77:GLU:O	1:A:-73:LYS:HG3	2.13	0.48
1:A:22:ARG:HH11	1:A:24:LYS:NZ	2.11	0.48
1:B:36:ARG:HH21	1:B:39:ARG:HD3	1.76	0.48
1:B:70:LYS:HD3	1:B:80:VAL:HG22	1.95	0.48
1:B:-220:MET:HE2	1:B:-155:ALA:HA	1.94	0.48
1:D:-295:SER:HB2	1:D:-293:LEU:HD11	1.94	0.48
1:B:-252:ILE:HB	1:B:-143:THR:HG22	1.96	0.48
1:D:-167:ASN:HB3	1:D:-165:HIS:CE1	2.49	0.48
1:A:-190:ILE:HG13	1:A:-33:GLN:HG2	1.95	0.48
1:C:-358:TRP:CG	1:C:-311:PRO:HG3	2.48	0.48
1:B:-49:ALA:O	1:B:-45:ASN:ND2	2.46	0.48
1:D:-335:ILE:HG21	1:D:-93:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-309:ILE:HD13	1:D:-88:LEU:HD13	1.96	0.48
1:D:-203:GLY:O	1:D:-183:ASN:ND2	2.43	0.47
1:D:-231:LYS:HD2	1:D:-231:LYS:HA	1.77	0.47
1:A:-121:LEU:HB3	1:A:-113:SER:HB2	1.96	0.47
1:D:-365:GLU:HG2	1:D:-364:GLU:N	2.28	0.47
1:A:31:GLU:HA	1:A:34:ARG:HG3	1.96	0.47
1:D:-324:GLU:O	1:D:-298:TYR:OH	2.25	0.47
1:D:-253:LEU:HD13	1:D:-120:PRO:HD3	1.97	0.47
1:A:-239:TRP:CD1	1:A:-120:PRO:O	2.67	0.47
1:D:-253:LEU:HB2	1:D:-121:LEU:HA	1.97	0.47
1:D:40:ARG:HG3	1:D:40:ARG:NH1	2.28	0.47
2:G:-1:DC:H2"	2:G:0:DG:C8	2.50	0.47
1:D:-83:LEU:HD23	1:D:-83:LEU:HA	1.72	0.47
1:B:43:VAL:O	1:B:46:LYS:N	2.47	0.47
1:A:-185:VAL:O	1:A:-180:ALA:CB	2.63	0.47
1:D:28:ARG:NH2	1:A:-90:GLU:OE1	2.45	0.46
1:A:-204:ASP:OD2	1:A:-181:GLY:HA2	2.14	0.46
1:C:-218:ASN:ND2	1:C:-158:TYR:HB2	2.30	0.46
1:D:-302:ARG:HH22	1:D:-31:SER:HA	1.79	0.46
1:D:-270:ARG:HG3	1:D:-265:LEU:CD2	2.38	0.46
1:B:-73:LYS:HD2	1:B:-73:LYS:HA	1.53	0.46
1:A:-206:ALA:O	1:A:-112:LYS:HD2	2.15	0.46
1:A:-184:ASP:HB2	1:A:-3:GLN:HB2	1.97	0.46
1:B:41:ARG:HG2	1:B:41:ARG:HH11	1.81	0.46
1:B:-139:PRO:HA	1:B:-136:TRP:CE2	2.51	0.46
2:G:5:DT:H2"	2:G:6:DG:C8	2.51	0.46
1:B:-366:ILE:HD13	1:B:-97:PRO:HD3	1.98	0.46
1:C:-204:ASP:O	1:C:-181:GLY:CA	2.64	0.46
1:D:-250:ASN:ND2	1:D:-127:ASN:O	2.49	0.46
1:A:-121:LEU:HB3	1:A:-113:SER:CB	2.45	0.46
1:D:-28:TRP:CE3	1:D:-28:TRP:HA	2.50	0.45
2:H:1:DC:H2"	2:H:2:DA:C8	2.51	0.45
1:A:-306:TRP:HB3	1:A:-301:PHE:HE1	1.81	0.45
1:A:50:GLY:HA3	1:B:86:THR:HG22	1.97	0.45
1:B:-214:PRO:HB3	1:B:-25:VAL:HG12	1.97	0.45
1:D:-360:VAL:HG23	1:D:-332:THR:OG1	2.16	0.45
1:A:-360:VAL:N	1:A:-310:ASP:OD2	2.40	0.45
1:C:80:VAL:HG12	1:C:86:THR:OG1	2.16	0.45
1:A:-273:ASP:OD1	1:A:-270:ARG:NH1	2.41	0.45
1:C:-289:ILE:HD12	1:C:-262:TYR:CE2	2.51	0.45
1:C:-81:ASP:OD1	1:C:-62:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-303:ASP:HB2	1:D:-32:MET:HG3	1.97	0.45
1:C:-283:PHE:HA	1:C:-280:LYS:HD2	1.99	0.45
1:C:-279:LEU:HD23	1:C:-261:PRO:HG2	1.99	0.45
2:G:9:DA:H2"	2:G:10:DA:C8	2.52	0.45
1:D:-122:VAL:HA	1:D:-45:ASN:HD21	1.81	0.45
1:A:-184:ASP:HB3	1:A:-3:GLN:OE1	2.16	0.45
1:D:-214:PRO:HD3	1:D:-24:ARG:HG3	1.98	0.45
1:D:-134:ASN:N	1:D:-134:ASN:OD1	2.50	0.45
1:C:-239:TRP:HE3	1:C:-174:PHE:HE2	1.65	0.44
1:D:-274:TRP:CE3	1:D:-265:LEU:HD11	2.52	0.44
1:D:-278:TYR:HA	1:D:-277:PRO:HD2	1.74	0.44
1:D:-61:TYR:CE1	1:D:-57:LEU:HG	2.52	0.44
1:A:31:GLU:OE1	1:A:35:ARG:NH2	2.50	0.44
1:D:-98:SER:O	1:D:-95:LYS:NZ	2.32	0.44
1:A:-190:ILE:HD12	1:A:-190:ILE:HA	1.54	0.44
1:B:-363:GLY:H	1:B:-96:ASN:ND2	2.16	0.44
1:A:-239:TRP:O	1:A:-236:ILE:HG13	2.18	0.44
1:A:46:LYS:NZ	1:B:85:THR:HG22	2.33	0.44
1:C:-324:GLU:HG2	1:C:-323:GLU:HG3	2.00	0.44
1:D:-283:PHE:HB3	1:D:-87:GLU:CD	2.37	0.44
1:C:-365:GLU:HB2	1:C:-362:LYS:HD3	2.00	0.43
1:C:-335:ILE:HG13	1:C:-93:LEU:HD11	1.99	0.43
1:A:86:THR:OG1	1:B:47:ILE:HA	2.19	0.43
1:B:47:ILE:O	1:B:51:LEU:HG	2.18	0.43
1:D:-310:ASP:OD2	1:D:-96:ASN:ND2	2.50	0.43
1:B:-273:ASP:OD1	1:B:-270:ARG:NH1	2.35	0.43
1:C:-229:LEU:HD13	1:C:-222:ALA:HA	2.01	0.43
1:D:-193:LYS:HG3	1:D:-192:TYR:N	2.34	0.43
1:D:-356:ASN:HD22	1:D:-355:GLY:N	2.14	0.43
1:D:-232:ASP:HB3	1:D:-165:HIS:CD2	2.46	0.43
1:A:-120:PRO:O	1:A:-113:SER:OG	2.36	0.43
1:D:-321:PHE:CE2	1:D:-293:LEU:HD22	2.54	0.43
1:D:-223:SER:OG	1:D:-146:THR:OG1	2.36	0.43
1:B:-221:LEU:HD13	1:B:-144:MET:HE3	1.99	0.43
1:C:-80:GLU:CD	1:C:-80:GLU:H	2.22	0.43
1:A:30:ARG:HA	1:A:30:ARG:HD3	1.85	0.43
1:B:81:GLU:H	1:B:81:GLU:HG2	1.70	0.43
1:D:-278:TYR:CD1	1:D:-278:TYR:N	2.87	0.42
1:D:-183:ASN:O	1:D:-179:LYS:HG2	2.19	0.42
1:A:34:ARG:HD3	2:E:5:DT:OP2	2.19	0.42
1:C:-335:ILE:HG21	1:C:-93:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-340:GLU:HG3	1:D:-334:LYS:HA	2.00	0.42
1:A:-239:TRP:NE1	1:A:-120:PRO:HB2	2.34	0.42
1:C:59:LEU:HB3	1:C:60:PRO:CD	2.48	0.42
1:D:-229:LEU:HD13	1:D:-222:ALA:HA	2.01	0.42
1:A:-356:ASN:ND2	1:A:-354:ASP:OD1	2.45	0.42
1:A:-54:ASP:CG	1:A:-52:ARG:HE	2.22	0.42
1:C:-300:GLY:HA3	1:C:-36:ASN:O	2.19	0.42
1:D:65:ASN:ND2	4:G:101:EDO:H11	2.28	0.42
1:A:-300:GLY:HA3	1:A:-36:ASN:O	2.19	0.42
1:B:-358:TRP:CG	1:B:-311:PRO:HG3	2.55	0.42
1:C:-218:ASN:HB3	1:C:-212:PHE:CD1	2.54	0.42
1:D:-304:HIS:CE1	1:D:-107:VAL:HG23	2.54	0.42
1:D:82:GLU:CD	1:D:82:GLU:H	2.23	0.42
1:A:-12:THR:HG23	1:A:-9:ALA:H	1.85	0.42
1:C:-366:ILE:CG2	1:C:-310:ASP:OD2	2.68	0.42
1:D:-278:TYR:HD1	1:D:-65:ALA:O	2.03	0.42
1:B:-214:PRO:CB	1:B:-25:VAL:HG12	2.50	0.42
1:C:-130:SER:OG	1:C:-129:ALA:N	2.52	0.42
1:A:36:ARG:HA	1:A:36:ARG:HD3	1.82	0.42
1:D:-278:TYR:HB2	1:D:-275:THR:CG2	2.47	0.42
1:D:-57:LEU:HD23	1:D:-57:LEU:HA	1.88	0.42
1:D:-304:HIS:NE2	1:D:-38:MET:O	2.48	0.41
1:D:-67:ALA:HB2	1:D:-47:MET:SD	2.60	0.41
1:D:80:VAL:HG13	1:D:86:THR:HG23	2.01	0.41
1:C:-83:LEU:HD23	1:C:-78:LEU:HD11	2.03	0.41
1:D:-360:VAL:HG12	1:D:-310:ASP:OD1	2.20	0.41
1:B:36:ARG:HE	1:B:39:ARG:NH1	2.15	0.41
1:D:-218:ASN:HB3	1:D:-212:PHE:CD1	2.55	0.41
1:D:-122:VAL:HA	1:D:-45:ASN:ND2	2.36	0.41
1:A:-93:LEU:HD23	1:A:-93:LEU:HA	1.90	0.41
1:B:-232:ASP:OD1	1:B:-222:ALA:N	2.43	0.41
1:B:-122:VAL:HG12	1:B:-121:LEU:O	2.21	0.41
1:D:-278:TYR:CD1	1:D:-65:ALA:O	2.73	0.41
1:A:47:ILE:HD11	1:B:80:VAL:CG2	2.50	0.41
1:B:-335:ILE:HG13	1:B:-93:LEU:HD22	2.03	0.41
1:C:-361:LEU:HD23	1:C:-361:LEU:HA	1.95	0.41
1:D:-135:SER:O	1:D:-131:THR:HG23	2.21	0.41
1:D:-211:THR:HG22	1:D:-207:ILE:HD12	2.02	0.40
1:C:-306:TRP:CD1	1:C:-302:ARG:HG3	2.56	0.40
1:C:-189:LYS:HA	1:C:-189:LYS:HD2	1.89	0.40
2:G:1:DC:H2"	2:G:2:DA:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-254:SER:OG	1:B:-45:ASN:ND2	2.54	0.40
1:B:39:ARG:HA	1:B:42:ALA:HB3	2.03	0.40
1:B:70:LYS:HD3	1:B:80:VAL:CG2	2.50	0.40
1:D:-328:PRO:HG2	1:D:-325:LEU:HB3	2.03	0.40
1:D:-270:ARG:CG	1:D:-265:LEU:HD23	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/439 (99%)	424 (98%)	11 (2%)	0	100	100
1	B	434/439 (99%)	421 (97%)	13 (3%)	0	100	100
1	C	434/439 (99%)	422 (97%)	12 (3%)	0	100	100
1	D	434/439 (99%)	411 (95%)	23 (5%)	0	100	100
All	All	1737/1756 (99%)	1678 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/345 (100%)	317 (92%)	27 (8%)	12	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	343/345 (99%)	320 (93%)	23 (7%)	16 43
1	C	343/345 (99%)	330 (96%)	13 (4%)	33 67
1	D	343/345 (99%)	311 (91%)	32 (9%)	9 26
All	All	1373/1380 (100%)	1278 (93%)	95 (7%)	15 41

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	-254	SER
1	C	-247	LEU
1	C	-240	THR
1	C	-208	LEU
1	C	-193	LYS
1	C	-157	SER
1	C	-141	ASN
1	C	-135	SER
1	C	-110	PHE
1	C	-95	LYS
1	C	-62	SER
1	C	23	ARG
1	C	58	ASN
1	D	-356	ASN
1	D	-353	LYS
1	D	-345	VAL
1	D	-337	THR
1	D	-315	THR
1	D	-310	ASP
1	D	-307	PHE
1	D	-292	LEU
1	D	-288	THR
1	D	-282	GLN
1	D	-280	LYS
1	D	-279	LEU
1	D	-278	TYR
1	D	-277	PRO
1	D	-275	THR
1	D	-266	LYS
1	D	-264	ILE
1	D	-260	ILE
1	D	-250	ASN
1	D	-193	LYS

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Mol	Chain	Res	Type
1	D	-179	LYS
1	D	-134	ASN
1	D	-110	PHE
1	D	-91	LYS
1	D	-87	GLU
1	D	-84	LEU
1	D	-73	LYS
1	D	-62	SER
1	D	-42	LYS
1	D	-31	SER
1	D	-28	TRP
1	D	80	VAL
1	A	-366	ILE
1	A	-362	LYS
1	A	-343	LYS
1	A	-327	ASP
1	A	-325	LEU
1	A	-315	THR
1	A	-313	ASP
1	A	-308	ILE
1	A	-302	ARG
1	A	-266	LYS
1	A	-231	LYS
1	A	-220	MET
1	A	-190	ILE
1	A	-185	VAL
1	A	-166	LYS
1	A	-55	LYS
1	A	-35	ILE
1	A	-31	SER
1	A	-12	THR
1	A	24	LYS
1	A	34	ARG
1	A	39	ARG
1	A	40	ARG
1	A	58	ASN
1	A	59	LEU
1	A	82	GLU
1	A	85	THR
1	B	-367	LYS
1	B	-362	LYS
1	B	-315	THR

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Mol	Chain	Res	Type
1	B	-313	ASP
1	B	-254	SER
1	B	-231	LYS
1	B	-226	LYS
1	B	-157	SER
1	B	-135	SER
1	B	-130	SER
1	B	-127	ASN
1	B	-110	PHE
1	B	-105	SER
1	B	-14	ARG
1	B	22	ARG
1	B	23	ARG
1	B	28	ARG
1	B	46	LYS
1	B	59	LEU
1	B	75	GLU
1	B	79	VAL
1	B	80	VAL
1	B	87	TYR

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

Mol	Chain	Res	Type
1	D	-356	ASN
1	D	-282	GLN
1	D	-165	HIS
1	D	-127	ASN
1	D	-86	ASN
1	D	65	ASN
1	B	-165	HIS
1	B	-96	ASN
1	B	32	ASN
1	B	66	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	I	1	3	12,12,12	0.51	0	17,17,17	0.70	0
3	GLC	I	2	3	11,11,12	0.61	0	15,15,17	0.85	0
3	GLC	K	1	3	12,12,12	0.51	0	17,17,17	0.45	0
3	GLC	K	2	3	11,11,12	0.70	0	15,15,17	0.76	0
3	GLC	L	1	3	12,12,12	0.56	0	17,17,17	0.65	0
3	GLC	L	2	3	11,11,12	0.61	0	15,15,17	0.72	0
3	GLC	M	1	3	12,12,12	0.54	0	17,17,17	0.62	0
3	GLC	M	2	3	11,11,12	0.66	0	15,15,17	0.79	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	GLC	I	1	3	-	1/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1
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

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
3	I	1	GLC	C4-C5-C6-O6

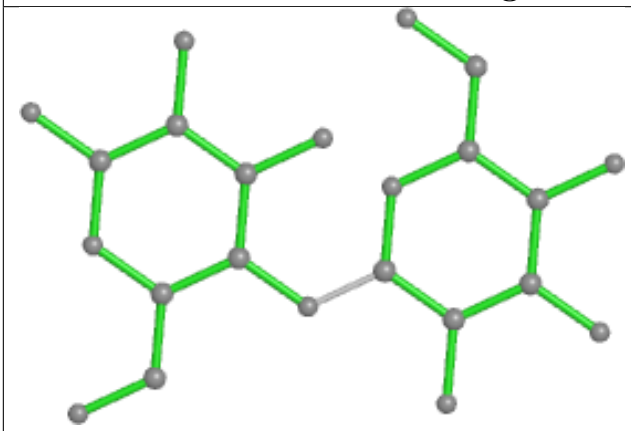
There are no ring outliers.

1 monomer is involved in 1 short contact:

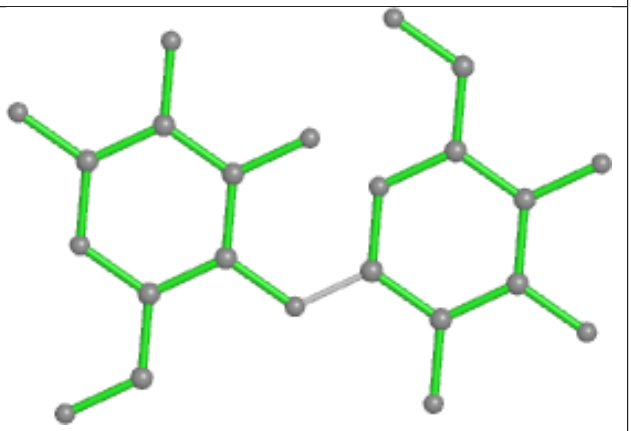
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	GLC	1	0

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

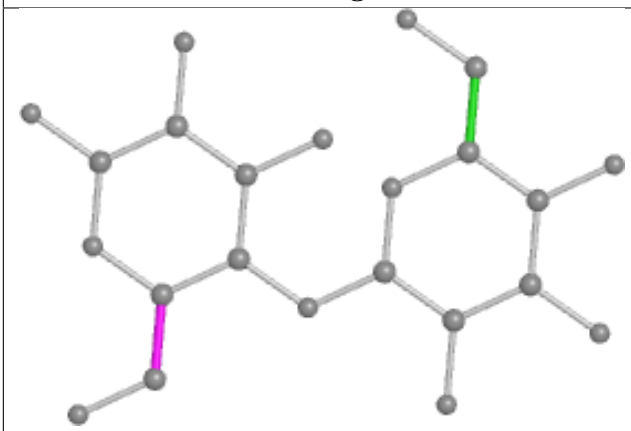
Oligosaccharide Chain I



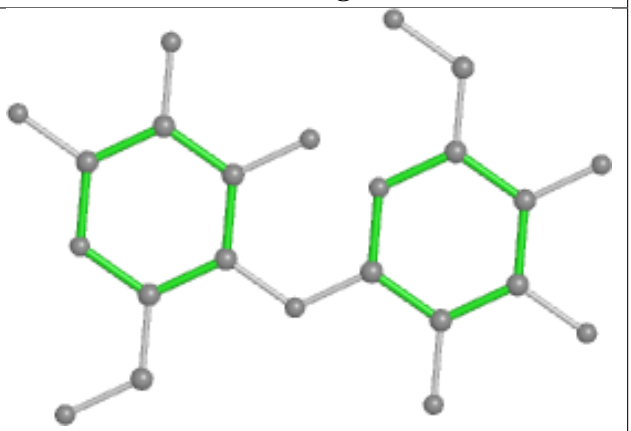
Bond lengths



Bond angles

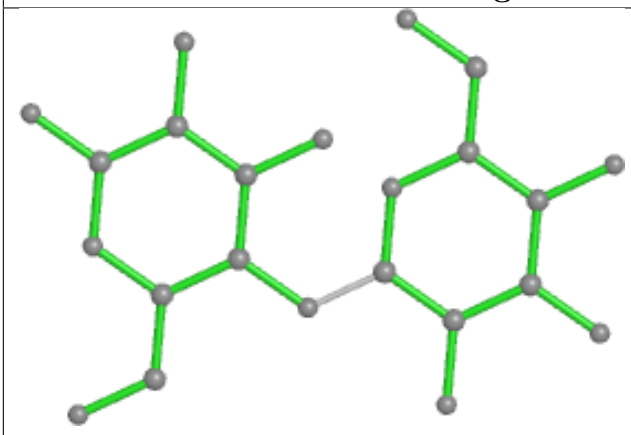


Torsions

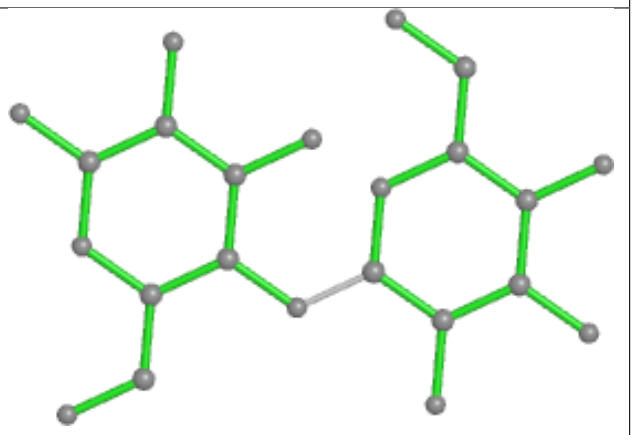


Rings

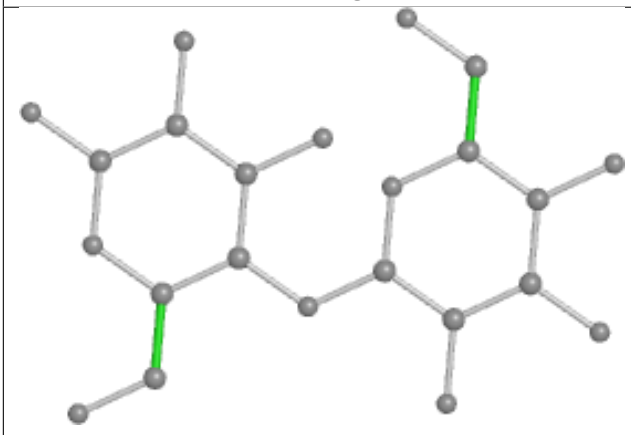
Oligosaccharide Chain K



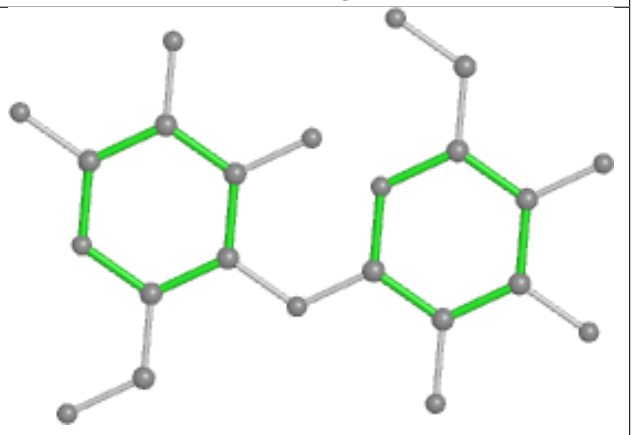
Bond lengths



Bond angles

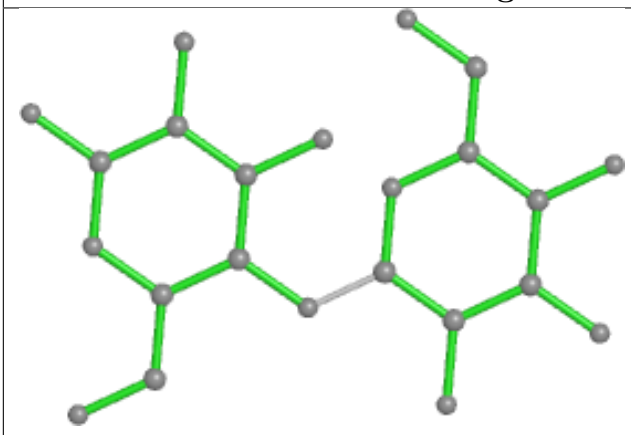


Torsions

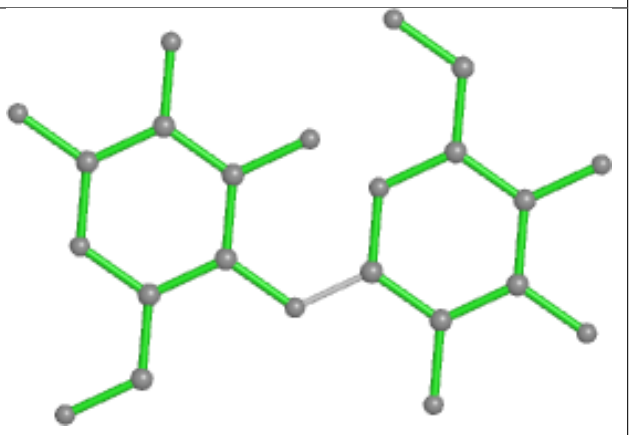


Rings

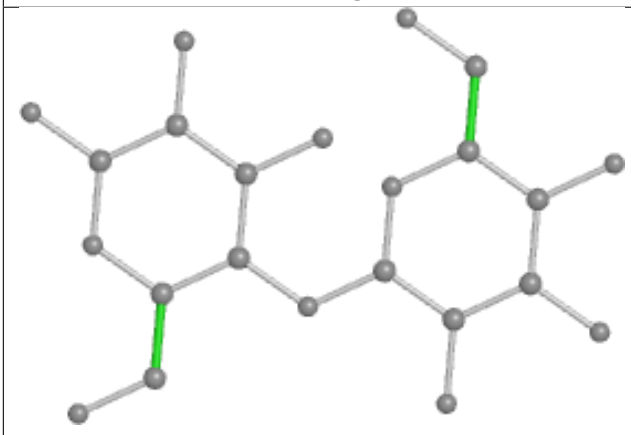
Oligosaccharide Chain L



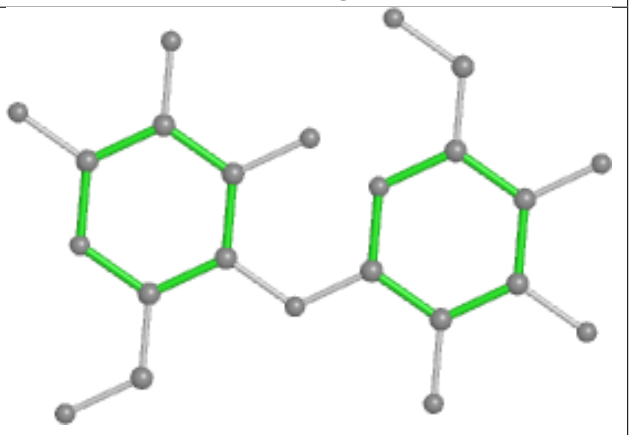
Bond lengths



Bond angles

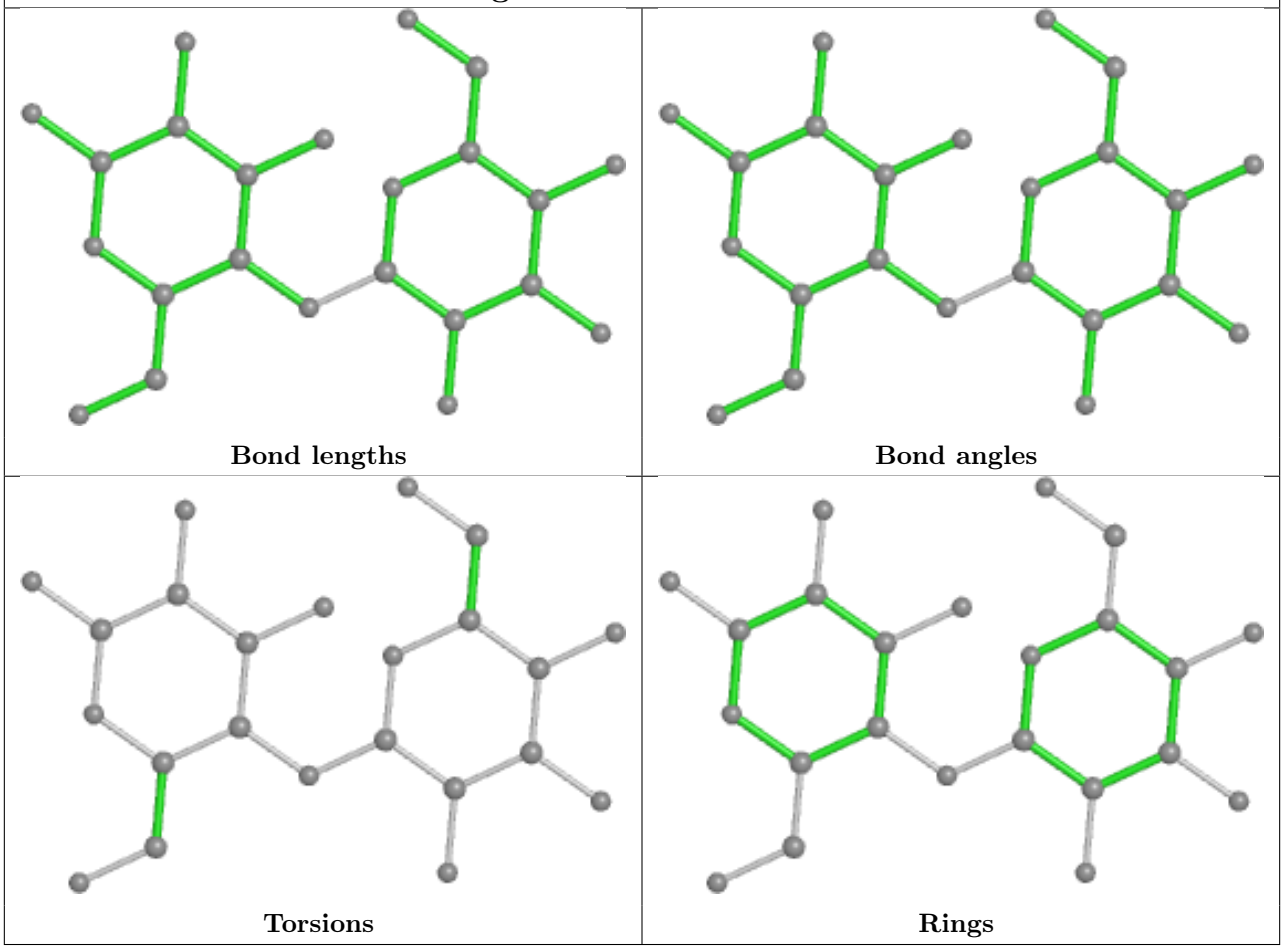


Torsions



Rings

Oligosaccharide Chain M



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	C	102	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	B	101	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	G	101	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	C	103	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	C	101	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	A	102	-	3,3,3	0.48	0	2,2,2	0.29	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	0.47	0	2,2,2	0.27	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	C	102	-	-	1/1/1/1	-
4	EDO	B	101	-	-	0/1/1/1	-
4	EDO	G	101	-	-	0/1/1/1	-
4	EDO	C	103	-	-	0/1/1/1	-
4	EDO	C	101	-	-	0/1/1/1	-
4	EDO	A	102	-	-	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 (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	102	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	101	EDO	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	437/439 (99%)	0.28	30 (6%) 16 10	29, 63, 119, 142	0
1	B	436/439 (99%)	0.29	44 (10%) 7 4	29, 59, 124, 146	0
1	C	436/439 (99%)	0.02	7 (1%) 72 66	32, 63, 98, 136	0
1	D	436/439 (99%)	0.67	56 (12%) 3 2	36, 89, 144, 186	0
2	E	15/15 (100%)	0.02	0 100 100	88, 108, 118, 118	0
2	F	15/15 (100%)	0.23	0 100 100	78, 113, 127, 133	0
2	G	15/15 (100%)	-0.46	0 100 100	40, 44, 80, 89	0
2	H	15/15 (100%)	-0.38	0 100 100	37, 48, 71, 82	0
All	All	1805/1816 (99%)	0.30	137 (7%) 13 7	29, 68, 126, 186	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	76	ALA	6.2
1	D	-290	GLU	6.1
1	B	42	ALA	6.1
1	D	-262	TYR	5.7
1	B	69	LEU	5.7
1	A	79	VAL	5.4
1	A	51	LEU	5.3
1	D	-363	GLY	5.2
1	D	-283	PHE	5.0
1	D	-339	LYS	5.0
1	B	85	THR	5.0
1	A	48	TYR	4.9
1	B	-173	LEU	4.8
1	D	-346	GLU	4.7
1	A	87	TYR	4.6
1	A	85	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	34	ARG	4.4
1	D	-190	ILE	4.4
1	B	88	ARG	4.2
1	D	-129	ALA	4.2
1	B	87	TYR	4.2
1	C	-129	ALA	4.1
1	D	-68	GLY	4.0
1	A	47	ILE	4.0
1	D	-333	VAL	4.0
1	B	68	VAL	4.0
1	B	59	LEU	3.8
1	D	-292	LEU	3.8
1	D	-92	ALA	3.7
1	D	-343	LYS	3.7
1	D	-340	GLU	3.7
1	D	-104	ALA	3.6
1	D	-286	ALA	3.6
1	B	79	VAL	3.6
1	D	-84	LEU	3.6
1	A	80	VAL	3.5
1	C	-339	LYS	3.5
1	D	-234	ALA	3.4
1	C	-173	LEU	3.4
1	B	27	TRP	3.3
1	D	-342	LYS	3.3
1	D	-334	LYS	3.3
1	B	-185	VAL	3.3
1	D	-347	ALA	3.2
1	D	-102	ILE	3.2
1	A	57	TYR	3.2
1	B	73	CYS	3.2
1	B	77	GLY	3.2
1	D	-361	LEU	3.2
1	D	-332	THR	3.1
1	D	-85	TYR	3.1
1	B	80	VAL	3.1
1	B	49	THR	3.1
1	D	-289	ILE	3.1
1	D	-89	PHE	3.1
1	A	74	VAL	3.1
1	B	53	ALA	3.1
1	D	-103	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	41	ARG	3.0
1	D	-337	THR	3.0
1	D	-76	ALA	3.0
1	A	86	THR	2.9
1	B	48	TYR	2.9
1	D	-57	LEU	2.9
1	B	-27	TYR	2.9
1	A	34	ARG	2.9
1	B	-208	LEU	2.9
1	A	88	ARG	2.9
1	A	32	ASN	2.9
1	D	-362	LYS	2.8
1	D	-297	ALA	2.8
1	D	-55	LYS	2.8
1	A	59	LEU	2.8
1	D	-199	PHE	2.8
1	B	56	ASP	2.8
1	A	83	ASP	2.8
1	A	69	LEU	2.8
1	B	38	ARG	2.8
1	D	-280	LYS	2.7
1	B	-177	GLY	2.7
1	B	26	SER	2.7
1	D	-336	GLY	2.7
1	C	-226	LYS	2.7
1	D	-90	GLU	2.7
1	A	41	ARG	2.6
1	D	-39	ILE	2.6
1	D	-27	TYR	2.5
1	A	44	ALA	2.5
1	B	57	TYR	2.5
1	D	-93	LEU	2.5
1	A	-253	LEU	2.5
1	A	82	GLU	2.5
1	A	22	ARG	2.5
1	B	-7	LEU	2.5
1	A	-204	ASP	2.5
1	B	51	LEU	2.4
1	B	72	LEU	2.4
1	B	82	GLU	2.4
1	D	-308	ILE	2.4
1	D	-86	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	-170	LEU	2.4
1	B	-236	ILE	2.4
1	D	-66	VAL	2.4
1	B	-226	LYS	2.4
1	A	81	GLU	2.4
1	B	66	ASN	2.3
1	B	28	ARG	2.3
1	D	-264	ILE	2.3
1	B	33	ASN	2.3
1	B	24	LYS	2.3
1	A	68	VAL	2.3
1	C	-229	LEU	2.3
1	B	-17	ALA	2.3
1	A	-195	ALA	2.2
1	D	-267	GLY	2.2
1	D	-357	ILE	2.2
1	B	47	ILE	2.2
1	B	62	HIS	2.2
1	D	-312	GLY	2.2
1	A	49	THR	2.2
1	A	56	ASP	2.2
1	D	-335	ILE	2.1
1	A	-173	LEU	2.1
1	A	66	ASN	2.1
1	B	-16	SER	2.1
1	D	-301	PHE	2.1
1	D	54	GLN	2.1
1	D	-331	VAL	2.1
1	B	30	ARG	2.1
1	D	-344	GLY	2.0
1	D	-269	TYR	2.0
1	A	-27	TYR	2.0
1	D	-178	ALA	2.0
1	D	-360	VAL	2.0
1	B	61	LYS	2.0
1	C	-248	ASP	2.0
1	C	51	LEU	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)

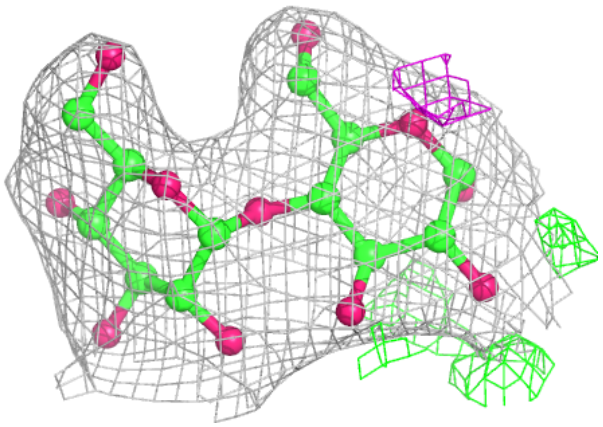
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

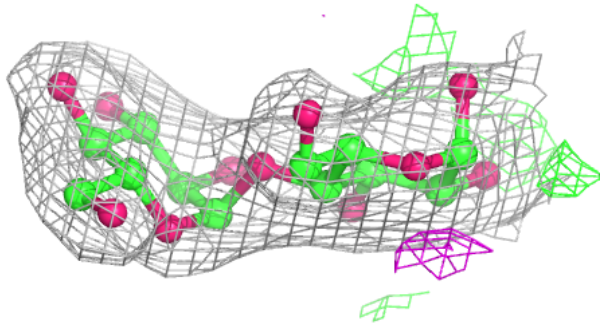
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	M	2	11/12	0.93	0.20	48,62,75,75	0
3	GLC	I	2	11/12	0.95	0.16	28,41,48,50	0
3	GLC	K	1	12/12	0.97	0.17	32,42,50,59	0
3	GLC	K	2	11/12	0.97	0.17	29,37,45,45	0
3	GLC	L	1	12/12	0.97	0.18	34,38,52,60	0
3	GLC	M	1	12/12	0.97	0.18	43,54,68,74	0
3	GLC	I	1	12/12	0.97	0.18	29,35,51,54	0
3	GLC	L	2	11/12	0.98	0.17	31,37,42,53	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 I:

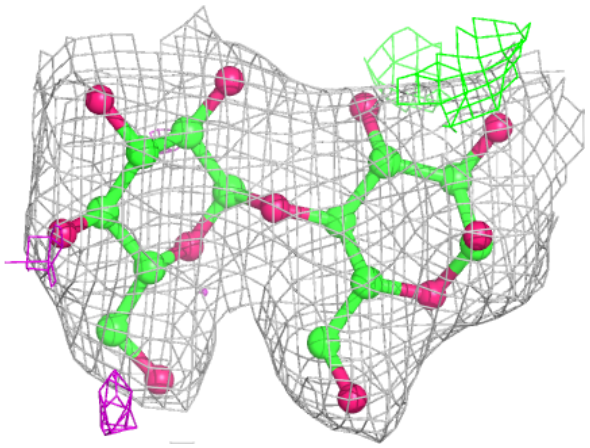
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

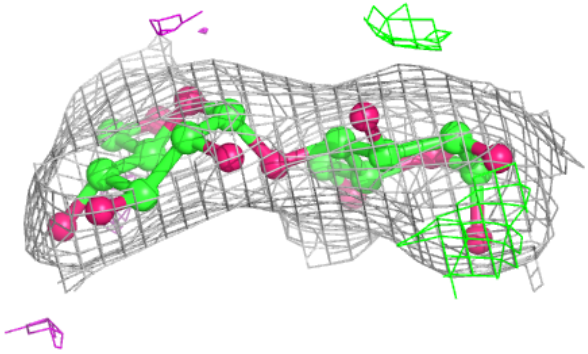


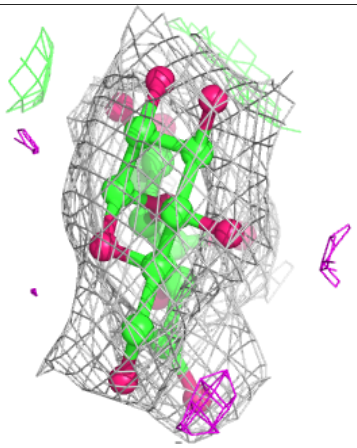


Electron density around Chain K:

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

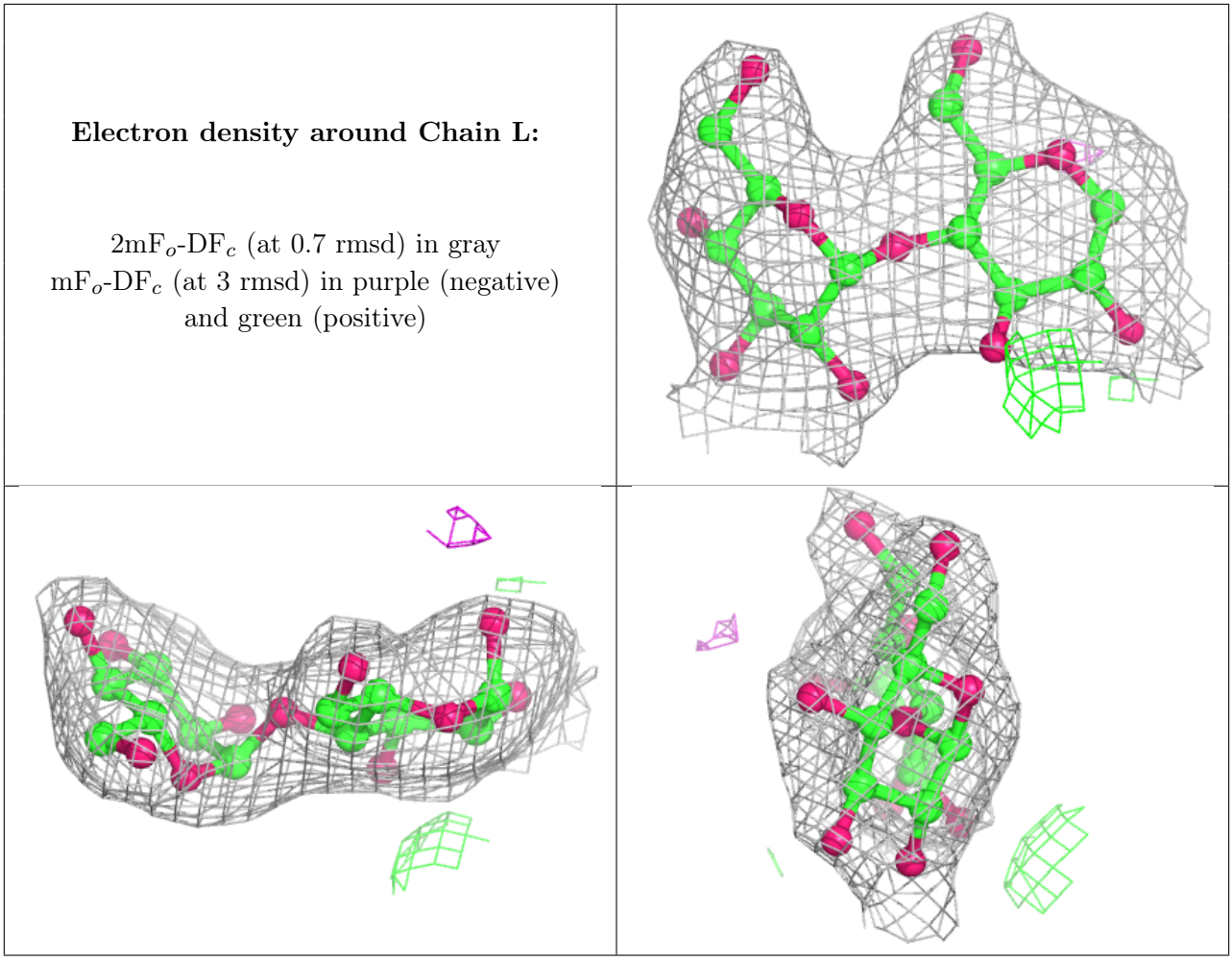






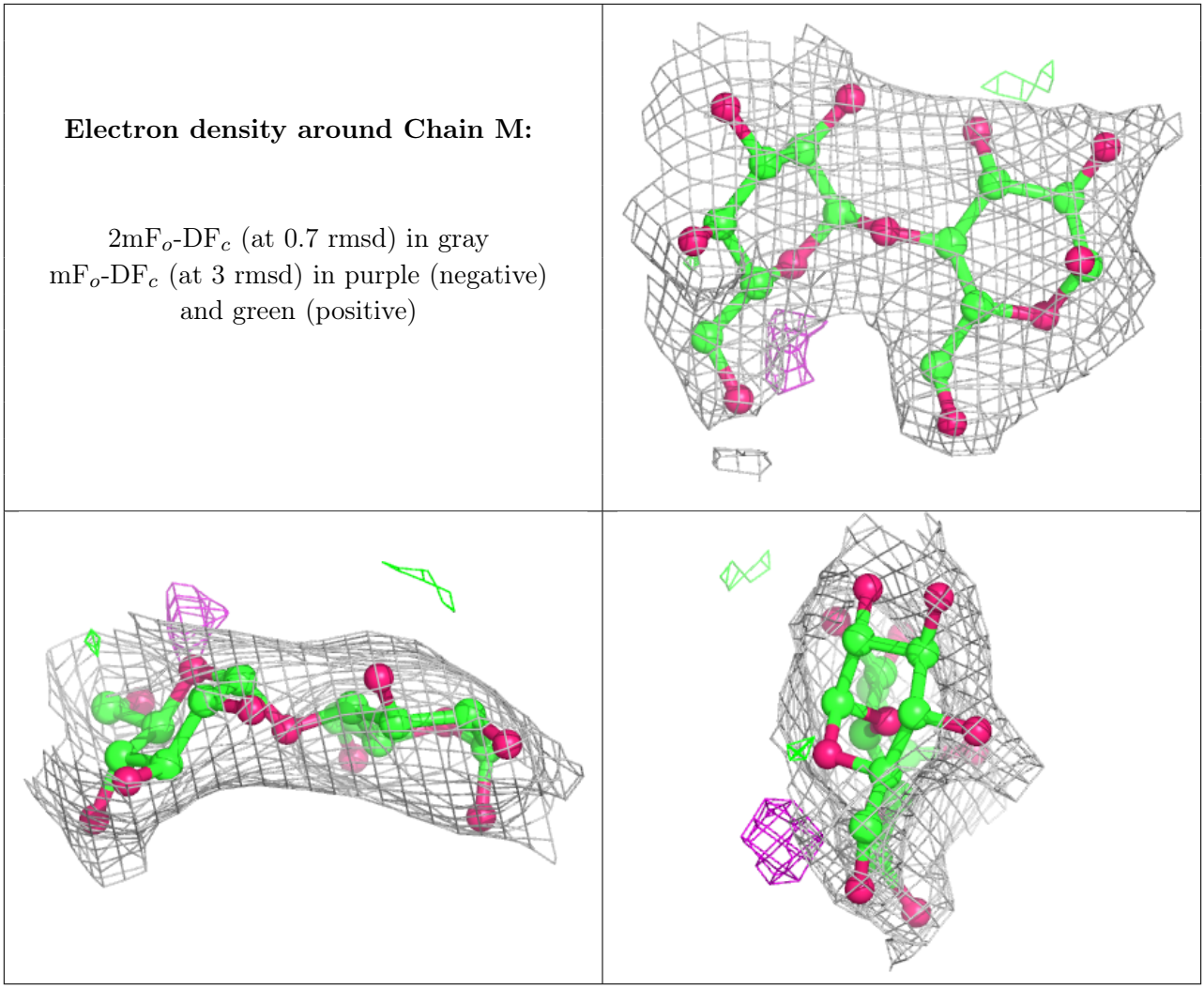
Electron density around Chain L:

$2mF_o$-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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	102	4/4	0.70	0.43	52,54,62,66	0
4	EDO	G	101	4/4	0.89	0.56	54,61,64,67	0
4	EDO	C	102	4/4	0.89	0.43	57,57,62,69	0
4	EDO	C	103	4/4	0.94	0.42	50,55,63,70	0
4	EDO	B	101	4/4	0.94	0.26	32,46,53,58	0
4	EDO	C	101	4/4	0.95	0.23	44,49,50,59	0
4	EDO	A	101	4/4	0.98	0.21	35,41,44,69	0

6.5 Other polymers (i)

There are no such residues in this entry.