Full wwPDB X-ray Structure Validation Report (i)

Oct 7, 2023 – 06:34 PM EDT

PDB ID	:	6DMF
Title	:	Bacteroides ovatus mixed-linkage glucan utilization locus (MLGUL) SGBP-A with cellohexaose
Authors	:	Koropatkin, N.M.; Bahr, C.M.
Deposited on	:	2018-06-05
Resolution	:	2.40 Å(reported)

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

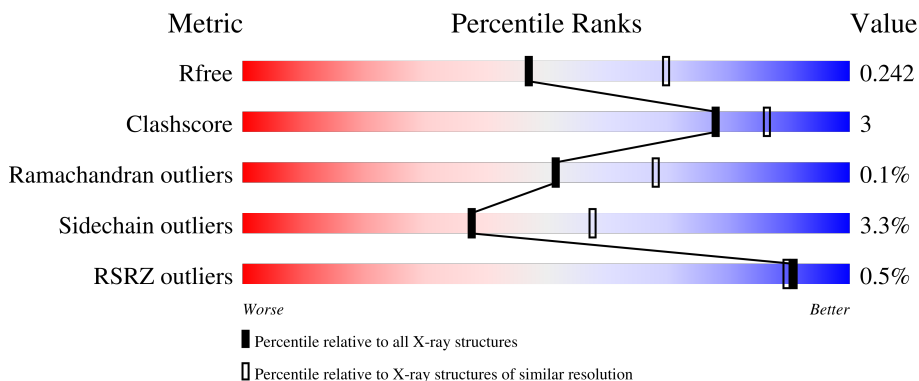|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.242
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		3.3%
RSRZ outliers		0.5%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	520	91% 7%
1	B	520	90% 9%
1	C	520	91% 8%
1	D	520	90% 9%
1	E	520	91% 8%

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Mol	Chain	Length	Quality of chain
1	F	520	92% 6%
1	G	520	% 90% 8%
1	H	520	% 89% 8%
1	I	520	90% 7%
1	J	520	% 89% 8%
2	K	5	60% 40%
3	L	6	17% 83%
3	M	6	33% 67%
3	N	6	67% 33%
3	O	6	33% 67%
3	P	6	50% 50%
3	Q	6	50% 50%
3	R	6	33% 67%
3	S	6	50% 50%
3	T	6	17% 83%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 42441 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 mixed-linkage glucan utilization locus (MLGUL) SGBP-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total 4072	C 2572	N 676	O 804	S 20	0	0	0
1	B	516	Total 4082	C 2579	N 680	O 803	S 20	0	0	0
1	C	512	Total 4061	C 2563	N 675	O 803	S 20	0	0	0
1	D	519	Total 4103	C 2592	N 683	O 808	S 20	0	0	0
1	E	517	Total 4097	C 2588	N 681	O 808	S 20	0	0	0
1	F	514	Total 4069	C 2571	N 677	O 801	S 20	0	0	0
1	G	512	Total 4041	C 2552	N 673	O 796	S 20	0	0	0
1	H	514	Total 4072	C 2574	N 677	O 801	S 20	0	0	0
1	I	510	Total 4035	C 2551	N 672	O 792	S 20	0	0	0
1	J	512	Total 4053	C 2561	N 674	O 798	S 20	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ILE	-	expression tag	UNP A7LY27
B	39	ILE	-	expression tag	UNP A7LY27
C	39	ILE	-	expression tag	UNP A7LY27
D	39	ILE	-	expression tag	UNP A7LY27
E	39	ILE	-	expression tag	UNP A7LY27
F	39	ILE	-	expression tag	UNP A7LY27
G	39	ILE	-	expression tag	UNP A7LY27
H	39	ILE	-	expression tag	UNP A7LY27
I	39	ILE	-	expression tag	UNP A7LY27

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Chain	Residue	Modelled	Actual	Comment	Reference
J	39	ILE	-	expression tag	UNP A7LY27

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1 -4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.
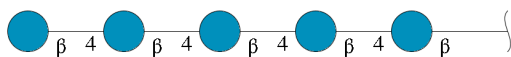
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	K	5	Total 56	C 30	O 26	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1 -4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-bet a-D-glucopyranose.
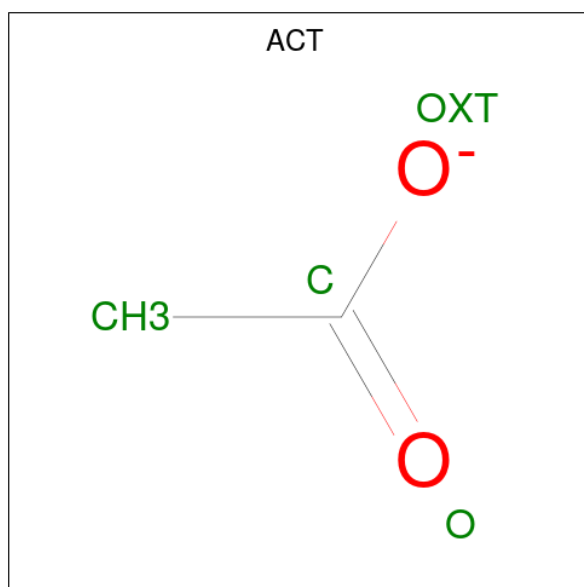
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	L	6	Total 67	C 36	O 31	0	0	0
3	M	6	Total 67	C 36	O 31	0	0	0
3	N	6	Total 67	C 36	O 31	0	0	0
3	O	6	Total 67	C 36	O 31	0	0	0
3	P	6	Total 67	C 36	O 31	0	0	0
3	Q	6	Total 67	C 36	O 31	0	0	0
3	R	6	Total 67	C 36	O 31	0	0	0
3	S	6	Total 67	C 36	O 31	0	0	0
3	T	6	Total 67	C 36	O 31	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 2		0	0
5	D	1	Total 4	C 2	O 2		0	0
5	E	1	Total 4	C 2	O 2		0	0
5	F	1	Total 4	C 2	O 2		0	0
5	H	1	Total 4	C 2	O 2		0	0
5	I	1	Total 4	C 2	O 2		0	0
5	J	1	Total 4	C 2	O 2		0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 7	C 4	O 3		0	0
6	A	1	Total 7	C 4	O 3		0	0
6	B	1	Total 7	C 4	O 3		0	0
6	B	1	Total 7	C 4	O 3		0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	J	1	Total 7	C 4	O 3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
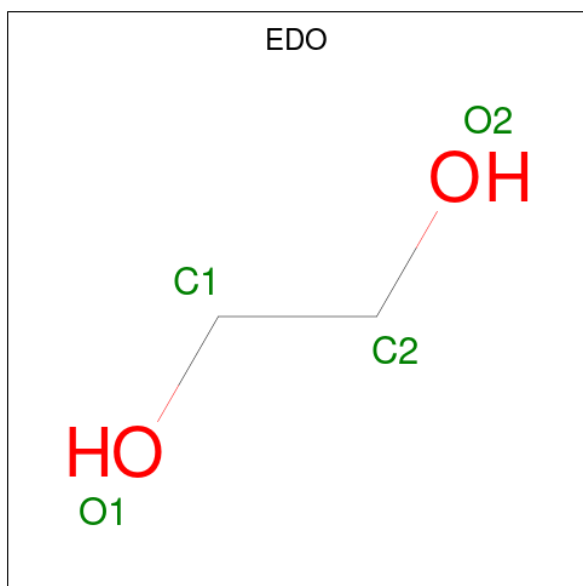
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	H	1	Total 4	C 2	O 2	0	0
7	I	1	Total 4	C 2	O 2	0	0

- Molecule 8 is water.

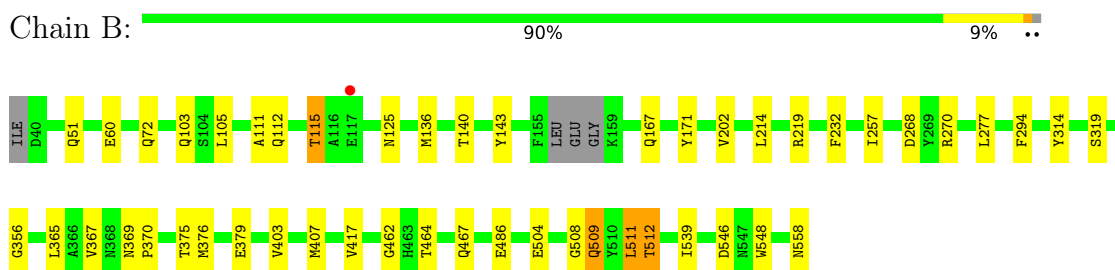| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	110	Total 110	O 110	0	0
8	B	129	Total 129	O 129	0	0
8	C	98	Total 98	O 98	0	0
8	D	88	Total 88	O 88	0	0
8	E	115	Total 115	O 115	0	0
8	F	59	Total 59	O 59	0	0
8	G	90	Total 90	O 90	0	0
8	H	87	Total 87	O 87	0	0
8	I	64	Total 64	O 64	0	0
8	J	104	Total 104	O 104	0	0

3 Residue-property plots ⓘ

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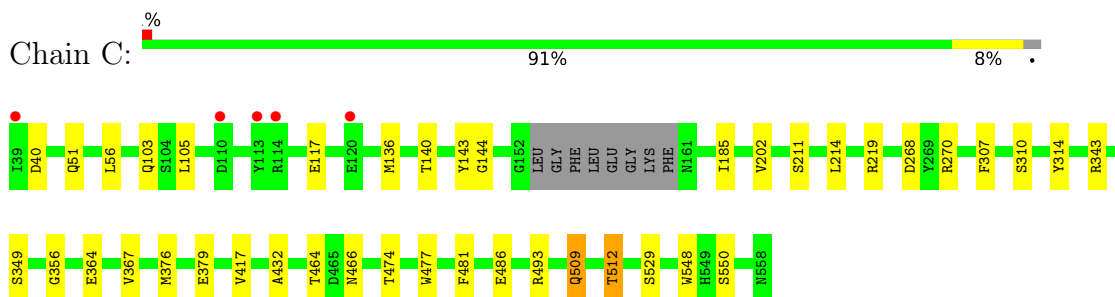
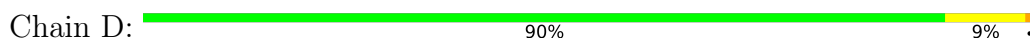- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain A:

- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain B:

- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain C:

- Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain D:

• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B
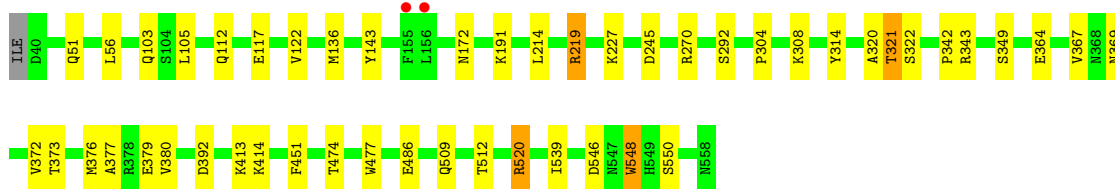
Chain E:

• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain F:

• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain G:

• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain H:

• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

Chain I:

90%　　　　7%

ILE D40 D55 L56 S57 E60 L105 Q112 Y113 R114 T115 A116 GLU ASP A119 N125 M136 G152 LEU GLY PHE LEU GLU GLY LYS F160 Y171 I185 V202 L214 R219 D245 L277 R305 K308 Y314 A320 T321 G356 Y357 D358

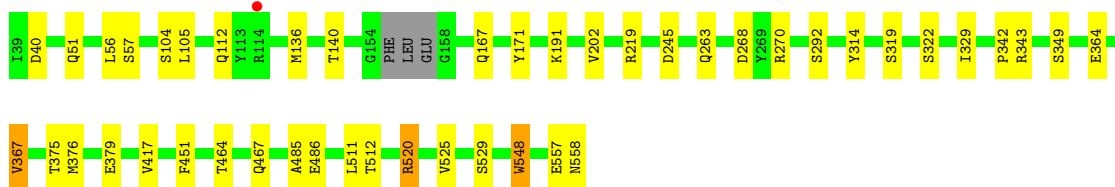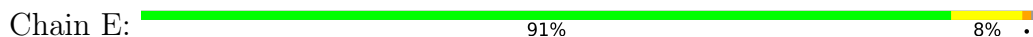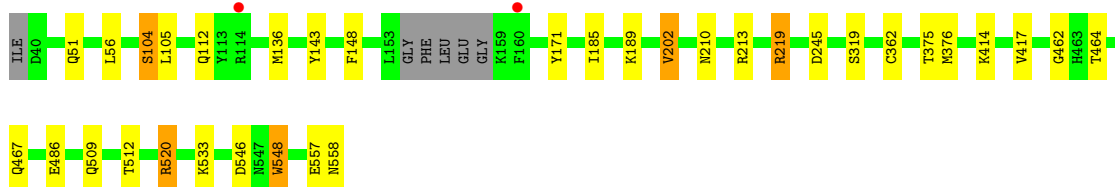V367 N368 N369 P370 T375 M376 V417 T444 T474 W477 G508 L511 T512 R520 W548 H549 S550 W554 E557 N558
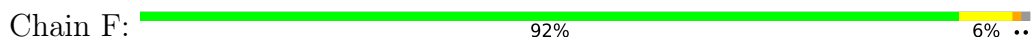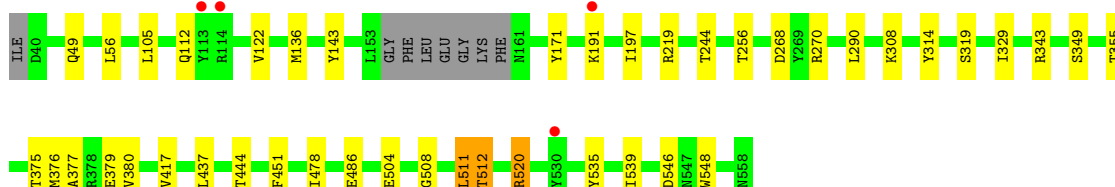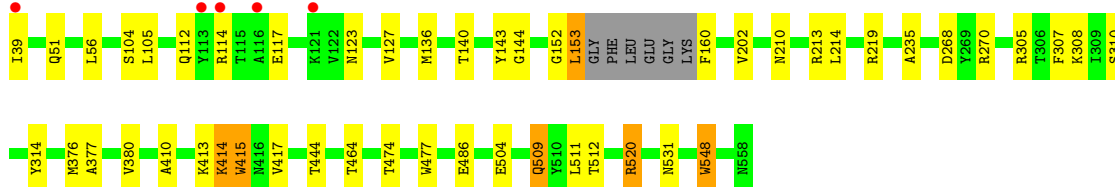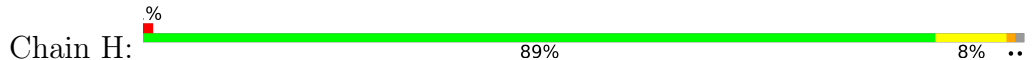
• Molecule 1: mixed-linkage glucan utilization locus (MLGUL) SGBP-B

%

Chain J:

89%　　　　8%

ILE D40 L56 E60 Q72 L105 Q112 Y113 R114 T115 A116 E117 I124 N125 M136 T140 Y143 G144 G152 LEU GLY PHE LEU GLU GLY LYS F160 Y171 N210 R213 L214 R219 D245 S248 L277 S292 T293 F294 Y314 V327

P342 R343 S349 M376 A377 R378 E379 V380 D392 V403 M407 K414 T474 W477 E486 G508 Q509 Y510 L511 T512 T515 R520 E540 W548 L552 E557 N558

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

Chain K:

60%　　　　40%

BGC1 BGC2 BGC3 BGC4 BGC5

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

Chain L:　17%　　　　83%

BGC1 BGC2 BGC3 BGC4 BGC5 BGC6

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

Chain M:　33%　　　　67%

BGC1 BGC2 BGC3 BGC4 BGC5 BGC6

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

Chain N:　67%　　　　33%

BGC1 BGC2 BGC3 BGC4 BGC5 BGC6

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

Chain O:

33% 67%

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

Chain P:

50% 50%

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

Chain Q:

50% 50%

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

Chain R:

33% 67%

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

Chain S:

50% 50%

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

Chain T:

17% 83%

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	228.84Å 228.84Å 246.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.60 – 2.40 49.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.60-2.40) 89.6 (49.55-2.40)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.190 , 0.242 0.191 , 0.242	Depositor DCC
R_{free} test set	14142 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.3	EDS
L-test for twinning [2]	$< \lvert L \rvert > = 0.53, < L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	42441	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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 57.57 % 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 2.3232e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: PEG, ACT, BGC, EDO, MG

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	0/4171	0.53	0/5671
1	B	0.36	0/4181	0.54	0/5684
1	C	0.35	0/4159	0.53	0/5655
1	D	0.35	0/4203	0.51	0/5715
1	E	0.37	0/4196	0.52	0/5703
1	F	0.33	0/4168	0.51	0/5668
1	G	0.34	0/4139	0.52	0/5631
1	H	0.37	0/4171	0.52	0/5672
1	I	0.34	0/4133	0.52	0/5619
1	J	0.36	0/4152	0.52	0/5646
All	All	0.35	0/41673	0.52	0/56664

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	F	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	219	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	270	ARG	Sidechain
1	F	219	ARG	Sidechain

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	4072	0	3860	19	0
1	B	4082	0	3870	28	0
1	C	4061	0	3851	28	0
1	D	4103	0	3890	27	0
1	E	4097	0	3890	21	0
1	F	4069	0	3854	17	0
1	G	4041	0	3822	24	0
1	H	4072	0	3863	30	0
1	I	4035	0	3824	25	0
1	J	4053	0	3837	24	0
2	K	56	0	48	0	0
3	L	67	0	57	0	0
3	M	67	0	57	0	0
3	N	67	0	57	0	0
3	O	67	0	57	1	0
3	P	67	0	57	0	0
3	Q	67	0	57	0	0
3	R	67	0	57	0	0
3	S	67	0	57	0	0
3	T	67	0	57	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
5	E	4	0	3	0	0
5	F	4	0	3	0	0
5	H	4	0	3	0	0
5	I	4	0	3	0	0
5	J	4	0	3	0	0
6	A	14	0	20	0	0
6	B	14	0	20	0	0
6	J	7	0	10	0	0
7	A	4	0	6	0	0
7	B	8	0	12	0	0
7	C	12	0	18	1	0
7	D	4	0	6	0	0
7	E	16	0	24	1	0
7	G	20	0	30	2	0
7	H	4	0	6	0	0
7	I	4	0	6	0	0
8	A	110	0	0	1	0
8	B	129	0	0	2	0
8	C	98	0	0	4	0
8	D	88	0	0	0	0
8	E	115	0	0	0	0
8	F	59	0	0	0	0
8	G	90	0	0	1	0
8	H	87	0	0	0	0
8	I	64	0	0	2	0
8	J	104	0	0	0	0
All	All	42441	0	39307	232	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 3.

All (232) 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:143:TYR:O	1:D:520:ARG:NH1	1.60	1.31
1:H:51:GLN:NE2	1:H:104:SER:OG	1.87	1.07
1:G:143:TYR:O	1:G:520:ARG:NH1	2.05	0.89
1:G:268:ASP:OD1	1:G:270:ARG:HD3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:520:ARG:NH1	8:I:701:HOH:O	2.00	0.78
1:D:219:ARG:NH2	1:D:486:GLU:OE2	2.21	0.74
1:A:520:ARG:NH2	1:A:546:ASP:OD1	2.21	0.73
1:A:367:VAL:HG21	1:E:464:THR:HG21	1.72	0.71
1:F:362:CYS:SG	1:F:376:MET:CE	2.79	0.70
1:F:520:ARG:NH2	1:F:546:ASP:OD1	2.27	0.68
1:G:314:TYR:HB2	1:G:376:MET:HE1	1.75	0.67
1:D:364:GLU:O	1:D:367:VAL:HG12	1.96	0.65
1:I:115:THR:HG22	1:I:125:ASN:HB2	1.78	0.64
1:F:362:CYS:SG	1:F:376:MET:HE3	2.38	0.64
1:H:144:GLY:H	1:H:520:ARG:HH12	1.46	0.64
1:C:185:ILE:HG23	1:C:202:VAL:CG1	2.29	0.63
1:H:105:LEU:HD21	1:H:136:MET:CE	2.29	0.63
1:B:51:GLN:HE22	1:B:103:GLN:HB3	1.64	0.62
1:H:219:ARG:HH22	1:H:486:GLU:CD	2.01	0.62
1:E:51:GLN:NE2	1:E:104:SER:OG	2.28	0.61
1:B:512:THR:HB	8:B:753:HOH:O	2.00	0.61
1:C:432:ALA:HB2	8:C:791:HOH:O	2.00	0.61
1:I:320:ALA:O	1:I:321:THR:OG1	2.11	0.60
1:I:314:TYR:HB2	1:I:376:MET:HE1	1.83	0.60
1:D:105:LEU:HD21	1:D:136:MET:CE	2.32	0.60
1:A:367:VAL:HG21	1:E:464:THR:CG2	2.31	0.59
1:B:219:ARG:NH2	1:B:486:GLU:OE2	2.36	0.59
1:G:512:THR:HB	8:G:706:HOH:O	2.02	0.58
1:J:219:ARG:NH2	1:J:486:GLU:OE2	2.36	0.58
1:B:268:ASP:OD1	1:B:270:ARG:HD3	2.04	0.58
1:F:143:TYR:O	1:F:520:ARG:NH1	2.37	0.58
1:I:185:ILE:HG23	1:I:202:VAL:CG1	2.34	0.58
1:I:105:LEU:HD21	1:I:136:MET:CE	2.34	0.58
1:J:115:THR:HG22	1:J:125:ASN:HB2	1.85	0.57
1:D:376:MET:HE3	1:D:379:GLU:HB2	1.85	0.57
1:G:219:ARG:HH22	1:G:486:GLU:CD	2.08	0.57
1:H:219:ARG:NH2	1:H:486:GLU:OE2	2.38	0.56
1:G:314:TYR:HB2	1:G:376:MET:CE	2.36	0.56
1:B:105:LEU:HD21	1:B:136:MET:CE	2.36	0.55
1:A:219:ARG:NH2	1:A:486:GLU:OE2	2.39	0.55
1:G:376:MET:HE1	1:G:379:GLU:HG2	1.89	0.55
1:D:51:GLN:HE22	1:D:103:GLN:HE21	1.54	0.54
1:E:171:TYR:OH	1:E:219:ARG:HD2	2.08	0.54
1:E:292:SER:HA	1:E:342:PRO:HB2	1.88	0.54
1:J:105:LEU:HD21	1:J:136:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:105:LEU:HD21	1:I:136:MET:HE2	1.89	0.54
1:C:51:GLN:HE22	1:C:103:GLN:HB3	1.71	0.54
1:G:520:ARG:NH2	1:G:546:ASP:OD1	2.41	0.54
1:H:51:GLN:NE2	1:H:104:SER:CB	2.71	0.54
1:H:51:GLN:NE2	1:H:104:SER:HG	2.04	0.54
1:J:219:ARG:HH22	1:J:486:GLU:CD	2.10	0.53
1:E:376:MET:HE1	1:E:379:GLU:HG2	1.90	0.53
1:B:376:MET:HE1	1:B:379:GLU:HG2	1.90	0.53
1:F:136:MET:HE3	1:F:148:PHE:CD1	2.44	0.53
1:D:219:ARG:HH22	1:D:486:GLU:CD	2.12	0.53
1:G:219:ARG:NH2	1:G:486:GLU:OE2	2.42	0.53
1:B:512:THR:HG21	1:D:245:ASP:HB3	1.90	0.53
1:B:356:GLY:HA3	1:B:376:MET:O	2.09	0.53
1:I:512:THR:HB	8:I:710:HOH:O	2.08	0.53
1:J:140:THR:O	1:J:143:TYR:O	2.27	0.53
1:C:219:ARG:HH22	1:C:486:GLU:CD	2.13	0.52
1:H:305:ARG:HA	1:H:308:LYS:HD2	1.91	0.52
1:B:112:GLN:NE2	8:B:704:HOH:O	2.43	0.52
1:H:520:ARG:O	1:H:548:TRP:HB2	2.08	0.52
1:J:171:TYR:OH	1:J:219:ARG:HD2	2.09	0.52
1:A:171:TYR:OH	1:A:219:ARG:HD2	2.10	0.52
1:A:140:THR:O	1:A:143:TYR:O	2.28	0.52
1:B:214:LEU:HG	1:B:232:PHE:CE2	2.45	0.51
1:B:111:ALA:O	1:B:115:THR:HB	2.11	0.51
1:A:314:TYR:HB3	1:A:327:VAL:HB	1.92	0.51
1:C:219:ARG:HA	1:C:493:ARG:HD3	1.92	0.51
1:D:51:GLN:NE2	1:D:103:GLN:NE2	2.58	0.51
1:B:219:ARG:HH22	1:B:486:GLU:CD	2.13	0.51
1:C:343:ARG:HD2	1:C:349:SER:HA	1.93	0.51
1:F:520:ARG:O	1:F:548:TRP:HB2	2.10	0.51
1:A:115:THR:HG22	1:A:125:ASN:HB2	1.92	0.51
1:G:377:ALA:O	1:G:380:VAL:HG22	2.11	0.50
1:I:474:THR:O	1:I:477:TRP:HB3	2.11	0.50
1:A:225:PRO:O	8:A:701:HOH:O	2.19	0.50
1:I:305:ARG:HA	1:I:308:LYS:HD2	1.92	0.50
1:E:364:GLU:O	1:E:367:VAL:HG13	2.12	0.50
1:H:123:ASN:O	1:H:127:VAL:HG23	2.11	0.50
1:D:320:ALA:O	1:D:321:THR:CB	2.60	0.50
1:I:60:GLU:OE2	1:I:277:LEU:HD11	2.11	0.50
1:I:314:TYR:HB2	1:I:376:MET:CE	2.42	0.50
1:G:329:ILE:HD13	1:G:376:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:362:CYS:SG	1:F:376:MET:HE1	2.52	0.50
1:J:314:TYR:HB2	1:J:376:MET:CE	2.42	0.50
1:C:51:GLN:HE22	1:C:103:GLN:CB	2.25	0.49
1:J:210:ASN:HA	1:J:213:ARG:HD3	1.93	0.49
1:D:343:ARG:HD2	1:D:349:SER:HA	1.93	0.49
1:D:520:ARG:NH2	1:D:546:ASP:OD1	2.44	0.49
1:F:245:ASP:HB3	1:I:512:THR:HG21	1.93	0.49
1:C:417:VAL:O	1:C:417:VAL:CG1	2.60	0.49
1:B:60:GLU:HA	1:B:277:LEU:HD21	1.95	0.49
1:E:105:LEU:HD21	1:E:136:MET:CE	2.42	0.49
1:C:219:ARG:NH2	1:C:486:GLU:OE2	2.45	0.49
1:B:115:THR:HG22	1:B:125:ASN:OD1	2.13	0.49
1:B:314:TYR:HB2	1:B:376:MET:CE	2.43	0.49
1:C:105:LEU:HD21	1:C:136:MET:CE	2.42	0.49
1:I:417:VAL:CG1	1:I:417:VAL:O	2.60	0.49
1:H:39:ILE:HG23	1:H:114:ARG:HH12	1.77	0.49
1:J:115:THR:HG21	1:J:124:ILE:HG23	1.95	0.49
1:H:140:THR:O	1:H:143:TYR:O	2.30	0.49
1:C:144:GLY:HA3	8:C:780:HOH:O	2.12	0.48
1:A:314:TYR:HB2	1:A:376:MET:HE1	1.94	0.48
1:G:244:THR:O	1:J:512:THR:HB	2.12	0.48
1:J:60:GLU:HA	1:J:277:LEU:HD21	1.94	0.48
1:B:171:TYR:OH	1:B:219:ARG:HD2	2.14	0.48
1:D:376:MET:HE3	1:D:379:GLU:CB	2.43	0.48
1:G:105:LEU:HD21	1:G:136:MET:CE	2.43	0.48
1:I:171:TYR:OH	1:I:219:ARG:HD2	2.14	0.48
1:H:144:GLY:N	1:H:520:ARG:HH12	2.11	0.48
1:C:211:SER:O	1:C:214:LEU:HB2	2.14	0.48
1:G:343:ARG:HD2	1:G:349:SER:HA	1.95	0.48
1:H:51:GLN:HE22	1:H:104:SER:CB	2.27	0.48
1:I:508:GLY:HA2	1:I:511:LEU:HD22	1.96	0.48
1:J:474:THR:O	1:J:477:TRP:HB3	2.14	0.48
1:C:512:THR:HG21	1:E:245:ASP:HB3	1.96	0.48
1:D:314:TYR:CE2	1:D:372:VAL:HG13	2.49	0.48
1:A:314:TYR:HB2	1:A:376:MET:CE	2.44	0.47
1:C:493:ARG:HD3	8:C:775:HOH:O	2.14	0.47
1:F:105:LEU:HD21	1:F:136:MET:CE	2.45	0.47
1:I:520:ARG:O	1:I:548:TRP:HB2	2.13	0.47
1:J:403:VAL:O	1:J:407:MET:HG2	2.13	0.47
1:G:329:ILE:HD13	1:G:376:MET:CE	2.44	0.47
1:E:268:ASP:OD2	1:E:270:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ASN:OD1	1:D:227:LYS:HE3	2.15	0.47
1:E:343:ARG:HD2	1:E:349:SER:HA	1.96	0.47
1:F:185:ILE:HG23	1:F:202:VAL:HG13	1.96	0.47
1:F:464:THR:HG23	1:G:504:GLU:OE1	2.14	0.47
1:J:508:GLY:HA2	1:J:511:LEU:HD22	1.96	0.47
1:C:417:VAL:O	1:C:417:VAL:HG12	2.15	0.46
1:J:377:ALA:O	1:J:380:VAL:HG22	2.15	0.46
1:H:308:LYS:HE3	1:H:444:THR:O	2.15	0.46
1:F:51:GLN:NE2	1:F:104:SER:OG	2.49	0.46
1:J:314:TYR:HB3	1:J:327:VAL:HB	1.96	0.46
1:D:474:THR:O	1:D:477:TRP:HB3	2.16	0.46
1:A:369:ASN:HA	1:A:370:PRO:HD3	1.81	0.46
1:H:377:ALA:O	1:H:380:VAL:HG22	2.16	0.46
1:A:320:ALA:O	1:A:321:THR:CB	2.63	0.46
1:C:140:THR:O	1:C:143:TYR:O	2.34	0.45
1:E:219:ARG:NH2	1:E:486:GLU:OE2	2.48	0.45
1:G:171:TYR:OH	1:G:219:ARG:HD2	2.16	0.45
1:I:60:GLU:HA	1:I:277:LEU:HD21	1.99	0.45
1:B:508:GLY:HA2	1:B:511:LEU:HD22	1.97	0.45
1:B:512:THR:CG2	1:D:245:ASP:HB3	2.47	0.45
1:F:219:ARG:NH2	1:F:486:GLU:OE2	2.50	0.45
1:B:72:GLN:HA	1:B:294:PHE:HB2	1.98	0.45
1:B:539:ILE:CD1	1:B:546:ASP:HB2	2.47	0.44
1:C:364:GLU:O	1:C:367:VAL:HG13	2.17	0.44
1:E:464:THR:HG22	1:E:467:GLN:H	1.80	0.44
1:I:219:ARG:HD3	1:I:554:TRP:CE2	2.51	0.44
1:G:49:GLN:HE21	1:G:197:ILE:HD12	1.82	0.44
1:D:292:SER:HA	1:D:342:PRO:HB2	1.99	0.44
1:D:51:GLN:NE2	1:D:103:GLN:HE21	2.16	0.44
1:H:152:GLY:HA2	1:H:153:LEU:HG	1.99	0.44
1:J:343:ARG:HD2	1:J:349:SER:HA	1.99	0.44
1:C:268:ASP:OD1	1:C:270:ARG:HD3	2.17	0.44
1:C:356:GLY:HA3	1:C:376:MET:O	2.18	0.44
1:H:268:ASP:CG	1:H:270:ARG:HH11	2.19	0.44
1:E:520:ARG:O	1:E:548:TRP:HB2	2.17	0.44
1:G:308:LYS:HE3	1:G:444:THR:O	2.18	0.44
1:A:403:VAL:O	1:A:407:MET:HG2	2.18	0.44
1:B:314:TYR:HB2	1:B:376:MET:HE1	2.00	0.44
1:H:474:THR:O	1:H:477:TRP:HB3	2.18	0.44
1:I:356:GLY:HA3	1:I:376:MET:O	2.18	0.43
1:A:377:ALA:O	1:A:380:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:TYR:OH	1:F:219:ARG:HD2	2.18	0.43
1:H:413:LYS:O	1:H:414:LYS:HB2	2.17	0.43
1:C:314:TYR:HB2	1:C:376:MET:HE2	2.00	0.43
1:G:508:GLY:HA2	1:G:511:LEU:HD22	2.01	0.43
1:D:377:ALA:O	1:D:380:VAL:HG22	2.18	0.43
1:H:268:ASP:OD2	1:H:270:ARG:NH1	2.51	0.43
1:D:105:LEU:HD21	1:D:136:MET:HE1	2.00	0.43
1:B:462:GLY:HA3	1:B:467:GLN:HB3	2.00	0.43
1:C:307:PHE:HA	1:C:310:SER:O	2.19	0.43
1:C:481:PHE:HB3	7:C:611:EDO:H21	2.00	0.43
1:D:413:LYS:O	1:D:414:LYS:HB2	2.18	0.43
1:B:369:ASN:HA	1:B:370:PRO:HD3	1.76	0.43
1:G:535:TYR:O	1:G:539:ILE:HG12	2.19	0.43
1:B:403:VAL:O	1:B:407:MET:HG2	2.19	0.43
1:A:256:THR:HA	1:A:391:SER:OG	2.19	0.42
1:F:210:ASN:HA	1:F:213:ARG:HD3	2.00	0.42
1:A:356:GLY:HA3	1:A:376:MET:O	2.18	0.42
1:I:308:LYS:HE3	1:I:444:THR:O	2.19	0.42
1:B:51:GLN:HE22	1:B:103:GLN:CB	2.32	0.42
1:F:462:GLY:HA3	1:F:467:GLN:HB3	2.01	0.42
1:G:478:ILE:HG22	7:G:608:EDO:H12	2.01	0.42
1:H:314:TYR:HB2	1:H:376:MET:CE	2.49	0.42
1:A:219:ARG:HH22	1:A:486:GLU:CD	2.21	0.42
1:B:509:GLN:HG2	1:D:451:PHE:CE2	2.54	0.42
1:D:520:ARG:O	1:D:548:TRP:HB2	2.20	0.42
1:E:314:TYR:HB2	1:E:376:MET:HE2	2.02	0.42
1:D:539:ILE:CD1	1:D:546:ASP:HB2	2.50	0.42
1:E:263:GLN:OE1	3:O:1:BGC:H6C1	2.19	0.42
1:C:474:THR:O	1:C:477:TRP:HB3	2.20	0.42
1:G:437:LEU:HD11	7:G:608:EDO:H21	2.02	0.42
1:H:410:ALA:HB1	1:H:415:TRP:CD1	2.54	0.42
1:I:369:ASN:HA	1:I:370:PRO:HD3	1.79	0.42
1:D:304:PRO:O	1:D:308:LYS:HD2	2.21	0.41
1:E:140:THR:O	1:E:167:GLN:NE2	2.53	0.41
1:E:485:ALA:HB2	7:E:610:EDO:H22	2.02	0.41
1:J:314:TYR:HB2	1:J:376:MET:HE2	2.02	0.41
1:H:210:ASN:HA	1:H:213:ARG:HD3	2.01	0.41
1:C:477:TRP:HB2	8:C:784:HOH:O	2.20	0.41
1:B:140:THR:O	1:B:167:GLN:NE2	2.53	0.41
1:D:320:ALA:O	1:D:321:THR:HB	2.21	0.41
1:E:417:VAL:O	1:E:417:VAL:CG1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:LEU:HD21	1:H:136:MET:HE1	2.02	0.41
1:J:72:GLN:HA	1:J:294:PHE:HB2	2.02	0.41
1:J:520:ARG:O	1:J:548:TRP:HB2	2.20	0.41
1:B:539:ILE:HD12	1:B:546:ASP:HB2	2.03	0.41
1:I:368:ASN:HD22	1:I:368:ASN:HA	1.59	0.41
1:H:509:GLN:HE21	1:H:509:GLN:HB2	1.71	0.41
1:C:509:GLN:HG2	1:E:451:PHE:CE2	2.56	0.41
1:A:462:GLY:HA3	1:A:467:GLN:HB3	2.03	0.41
1:C:376:MET:HE1	1:C:379:GLU:HG2	2.03	0.41
1:C:464:THR:HG22	1:C:466:ASN:N	2.36	0.41
1:E:329:ILE:HD13	1:E:376:MET:CE	2.51	0.41
1:G:451:PHE:CE2	1:J:509:GLN:HG2	2.56	0.41
1:I:358:ASP:OD1	1:I:375:THR:HG22	2.21	0.41
1:C:464:THR:HG22	1:C:466:ASN:H	1.86	0.41
1:H:307:PHE:HA	1:H:310:SER:O	2.20	0.40
1:I:55:ASP:OD1	1:I:57:SER:HB3	2.21	0.40
1:J:292:SER:HA	1:J:342:PRO:HB2	2.03	0.40
1:J:144:GLY:HA2	1:J:552:LEU:HD22	2.03	0.40
1:J:376:MET:HE1	1:J:379:GLU:HG2	2.03	0.40
1:H:144:GLY:N	1:H:520:ARG:NH1	2.69	0.40
1:H:314:TYR:HB2	1:H:376:MET:HE2	2.04	0.40
1:F:417:VAL:O	1:F:417:VAL:CG1	2.69	0.40
1:H:214:LEU:CD1	1:H:235:ALA:HB3	2.52	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	509/520 (98%)	487 (96%)	21 (4%)	1 (0%)	47	62
1	B	512/520 (98%)	492 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	508/520 (98%)	489 (96%)	19 (4%)	0	100	100
1	D	517/520 (99%)	500 (97%)	16 (3%)	1 (0%)	47	62
1	E	513/520 (99%)	493 (96%)	20 (4%)	0	100	100
1	F	510/520 (98%)	489 (96%)	20 (4%)	1 (0%)	47	62
1	G	508/520 (98%)	489 (96%)	19 (4%)	0	100	100
1	H	510/520 (98%)	483 (95%)	27 (5%)	0	100	100
1	I	504/520 (97%)	489 (97%)	14 (3%)	1 (0%)	47	62
1	J	508/520 (98%)	493 (97%)	14 (3%)	1 (0%)	47	62
All	All	5099/5200 (98%)	4904 (96%)	190 (4%)	5 (0%)	51	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	321	THR
1	F	189	LYS
1	A	321	THR
1	I	321	THR
1	J	144	GLY

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	436/441 (99%)	419 (96%)	17 (4%)	32	50
1	B	435/441 (99%)	419 (96%)	16 (4%)	34	53
1	C	435/441 (99%)	427 (98%)	8 (2%)	59	76
1	D	437/441 (99%)	422 (97%)	15 (3%)	37	56
1	E	438/441 (99%)	420 (96%)	18 (4%)	30	48
1	F	434/441 (98%)	420 (97%)	14 (3%)	39	59
1	G	430/441 (98%)	416 (97%)	14 (3%)	38	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	435/441 (99%)	418 (96%)	17 (4%)	32	50
1	I	430/441 (98%)	418 (97%)	12 (3%)	43	63
1	J	432/441 (98%)	418 (97%)	14 (3%)	39	59
All	All	4342/4410 (98%)	4197 (97%)	145 (3%)	38	57

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	117	GLU
1	A	143	TYR
1	A	160	PHE
1	A	214	LEU
1	A	365	LEU
1	A	367	VAL
1	A	369	ASN
1	A	373	THR
1	A	375	THR
1	A	390	LYS
1	A	392	ASP
1	A	509	GLN
1	A	511	LEU
1	A	512	THR
1	A	529	SER
1	A	548	TRP
1	B	115	THR
1	B	143	TYR
1	B	202	VAL
1	B	257	ILE
1	B	319	SER
1	B	365	LEU
1	B	367	VAL
1	B	375	THR
1	B	417	VAL
1	B	464	THR
1	B	504	GLU
1	B	509	GLN
1	B	511	LEU
1	B	512	THR
1	B	548	TRP
1	B	558	ASN

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Mol	Chain	Res	Type
1	C	40	ASP
1	C	56	LEU
1	C	117	GLU
1	C	509	GLN
1	C	512	THR
1	C	529	SER
1	C	548	TRP
1	C	550	SER
1	D	56	LEU
1	D	112	GLN
1	D	117	GLU
1	D	122	VAL
1	D	191	LYS
1	D	214	LEU
1	D	322	SER
1	D	369	ASN
1	D	373	THR
1	D	392	ASP
1	D	509	GLN
1	D	512	THR
1	D	520	ARG
1	D	548	TRP
1	D	550	SER
1	E	40	ASP
1	E	56	LEU
1	E	57	SER
1	E	112	GLN
1	E	191	LYS
1	E	202	VAL
1	E	319	SER
1	E	322	SER
1	E	367	VAL
1	E	375	THR
1	E	511	LEU
1	E	512	THR
1	E	520	ARG
1	E	525	VAL
1	E	529	SER
1	E	548	TRP
1	E	557	GLU
1	E	558	ASN
1	F	56	LEU

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Mol	Chain	Res	Type
1	F	104	SER
1	F	112	GLN
1	F	202	VAL
1	F	319	SER
1	F	375	THR
1	F	414	LYS
1	F	509	GLN
1	F	512	THR
1	F	520	ARG
1	F	533	LYS
1	F	548	TRP
1	F	557	GLU
1	F	558	ASN
1	G	56	LEU
1	G	112	GLN
1	G	122	VAL
1	G	191	LYS
1	G	256	THR
1	G	290	LEU
1	G	319	SER
1	G	355	THR
1	G	375	THR
1	G	417	VAL
1	G	511	LEU
1	G	512	THR
1	G	520	ARG
1	G	548	TRP
1	H	56	LEU
1	H	112	GLN
1	H	117	GLU
1	H	153	LEU
1	H	160	PHE
1	H	202	VAL
1	H	414	LYS
1	H	415	TRP
1	H	417	VAL
1	H	464	THR
1	H	504	GLU
1	H	509	GLN
1	H	511	LEU
1	H	512	THR
1	H	520	ARG

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Mol	Chain	Res	Type
1	H	531	ASN
1	H	548	TRP
1	I	56	LEU
1	I	112	GLN
1	I	202	VAL
1	I	214	LEU
1	I	245	ASP
1	I	367	VAL
1	I	368	ASN
1	I	511	LEU
1	I	512	THR
1	I	548	TRP
1	I	550	SER
1	I	557	GLU
1	J	56	LEU
1	J	112	GLN
1	J	143	TYR
1	J	214	LEU
1	J	245	ASP
1	J	248	SER
1	J	392	ASP
1	J	414	LYS
1	J	509	GLN
1	J	511	LEU
1	J	515	THR
1	J	540	GLU
1	J	548	TRP
1	J	557	GLU

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

Mol	Chain	Res	Type
1	A	369	ASN
1	A	440	ASN
1	B	51	GLN
1	B	440	ASN
1	B	536	ASN
1	C	51	GLN
1	C	103	GLN
1	D	103	GLN
1	D	536	ASN
1	E	51	GLN

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Mol	Chain	Res	Type
1	E	509	GLN
1	E	536	ASN
1	F	51	GLN
1	F	161	ASN
1	F	331	GLN
1	F	440	ASN
1	F	456	GLN
1	F	531	ASN
1	F	558	ASN
1	G	44	GLN
1	G	112	GLN
1	G	125	ASN
1	G	161	ASN
1	G	536	ASN
1	H	51	GLN
1	H	509	GLN
1	H	531	ASN
1	I	368	ASN
1	J	112	GLN
1	J	125	ASN
1	J	536	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

59 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BGC	K	1	2	12,12,12	0.45	0	17,17,17	0.64	0
2	BGC	K	2	2	11,11,12	0.29	0	15,15,17	0.88	0
2	BGC	K	3	2	11,11,12	0.56	0	15,15,17	1.10	1 (6%)
2	BGC	K	4	2	11,11,12	0.56	0	15,15,17	0.83	0
2	BGC	K	5	2	11,11,12	0.58	0	15,15,17	1.26	1 (6%)
3	BGC	L	1	3	12,12,12	0.54	0	17,17,17	1.06	1 (5%)
3	BGC	L	2	3	11,11,12	0.31	0	15,15,17	0.88	0
3	BGC	L	3	3	11,11,12	0.57	0	15,15,17	1.96	2 (13%)
3	BGC	L	4	3	11,11,12	0.45	0	15,15,17	1.02	2 (13%)
3	BGC	L	5	3	11,11,12	0.36	0	15,15,17	1.10	2 (13%)
3	BGC	L	6	3	11,11,12	0.66	0	15,15,17	1.24	2 (13%)
3	BGC	M	1	3	12,12,12	0.50	0	17,17,17	0.87	0
3	BGC	M	2	3	11,11,12	0.29	0	15,15,17	0.83	0
3	BGC	M	3	3	11,11,12	0.64	0	15,15,17	0.88	1 (6%)
3	BGC	M	4	3	11,11,12	0.38	0	15,15,17	0.89	2 (13%)
3	BGC	M	5	3	11,11,12	0.38	0	15,15,17	0.83	1 (6%)
3	BGC	M	6	3	11,11,12	0.44	0	15,15,17	1.11	1 (6%)
3	BGC	N	1	3	12,12,12	0.48	0	17,17,17	0.90	1 (5%)
3	BGC	N	2	3	11,11,12	0.33	0	15,15,17	1.14	1 (6%)
3	BGC	N	3	3	11,11,12	0.43	0	15,15,17	0.97	0
3	BGC	N	4	3	11,11,12	0.31	0	15,15,17	0.79	0
3	BGC	N	5	3	11,11,12	0.51	0	15,15,17	0.86	0
3	BGC	N	6	3	11,11,12	0.40	0	15,15,17	1.04	0
3	BGC	O	1	3	12,12,12	0.56	0	17,17,17	0.96	0
3	BGC	O	2	3	11,11,12	0.40	0	15,15,17	1.14	2 (13%)
3	BGC	O	3	3	11,11,12	0.36	0	15,15,17	0.77	1 (6%)
3	BGC	O	4	3	11,11,12	0.38	0	15,15,17	0.69	0
3	BGC	O	5	3	11,11,12	0.48	0	15,15,17	1.26	3 (20%)
3	BGC	O	6	3	11,11,12	0.33	0	15,15,17	0.65	0
3	BGC	P	1	3	12,12,12	0.53	0	17,17,17	0.89	0
3	BGC	P	2	3	11,11,12	0.40	0	15,15,17	0.61	0
3	BGC	P	3	3	11,11,12	0.30	0	15,15,17	0.90	1 (6%)
3	BGC	P	4	3	11,11,12	0.51	0	15,15,17	0.85	1 (6%)
3	BGC	P	5	3	11,11,12	0.39	0	15,15,17	1.17	1 (6%)
3	BGC	P	6	3	11,11,12	0.40	0	15,15,17	0.77	0
3	BGC	Q	1	3	12,12,12	0.47	0	17,17,17	0.59	0
3	BGC	Q	2	3	11,11,12	0.39	0	15,15,17	0.78	0
3	BGC	Q	3	3	11,11,12	0.25	0	15,15,17	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	BGC	Q	4	3	11,11,12	0.31	0	15,15,17	0.89	0
3	BGC	Q	5	3	11,11,12	0.41	0	15,15,17	1.29	1 (6%)
3	BGC	Q	6	3	11,11,12	0.42	0	15,15,17	1.01	1 (6%)
3	BGC	R	1	3	12,12,12	0.55	0	17,17,17	1.03	0
3	BGC	R	2	3	11,11,12	0.69	0	15,15,17	0.74	0
3	BGC	R	3	3	11,11,12	0.49	0	15,15,17	0.79	1 (6%)
3	BGC	R	4	3	11,11,12	0.38	0	15,15,17	0.81	1 (6%)
3	BGC	R	5	3	11,11,12	0.39	0	15,15,17	1.39	1 (6%)
3	BGC	R	6	3	11,11,12	0.33	0	15,15,17	0.90	1 (6%)
3	BGC	S	1	3	12,12,12	0.46	0	17,17,17	0.85	1 (5%)
3	BGC	S	2	3	11,11,12	0.37	0	15,15,17	1.71	2 (13%)
3	BGC	S	3	3	11,11,12	0.40	0	15,15,17	0.51	0
3	BGC	S	4	3	11,11,12	0.25	0	15,15,17	0.90	0
3	BGC	S	5	3	11,11,12	0.49	0	15,15,17	0.83	0
3	BGC	S	6	3	11,11,12	0.35	0	15,15,17	1.11	2 (13%)
3	BGC	T	1	3	12,12,12	0.47	0	17,17,17	0.81	1 (5%)
3	BGC	T	2	3	11,11,12	0.26	0	15,15,17	1.28	2 (13%)
3	BGC	T	3	3	11,11,12	0.61	0	15,15,17	0.70	0
3	BGC	T	4	3	11,11,12	0.36	0	15,15,17	0.87	1 (6%)
3	BGC	T	5	3	11,11,12	0.29	0	15,15,17	1.27	3 (20%)
3	BGC	T	6	3	11,11,12	0.36	0	15,15,17	0.96	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
2	BGC	K	1	2	-	1/2/22/22	0/1/1/1
2	BGC	K	2	2	-	0/2/19/22	0/1/1/1
2	BGC	K	3	2	-	0/2/19/22	0/1/1/1
2	BGC	K	4	2	-	0/2/19/22	0/1/1/1
2	BGC	K	5	2	-	2/2/19/22	0/1/1/1
3	BGC	L	1	3	-	0/2/22/22	0/1/1/1
3	BGC	L	2	3	-	0/2/19/22	0/1/1/1
3	BGC	L	3	3	-	1/2/19/22	0/1/1/1
3	BGC	L	4	3	-	1/2/19/22	0/1/1/1
3	BGC	L	5	3	-	2/2/19/22	0/1/1/1
3	BGC	L	6	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	M	1	3	-	2/2/22/22	0/1/1/1
3	BGC	M	2	3	-	2/2/19/22	0/1/1/1
3	BGC	M	3	3	-	0/2/19/22	0/1/1/1
3	BGC	M	4	3	-	1/2/19/22	0/1/1/1
3	BGC	M	5	3	-	2/2/19/22	0/1/1/1
3	BGC	M	6	3	-	2/2/19/22	0/1/1/1
3	BGC	N	1	3	-	2/2/22/22	0/1/1/1
3	BGC	N	2	3	-	0/2/19/22	0/1/1/1
3	BGC	N	3	3	-	0/2/19/22	0/1/1/1
3	BGC	N	4	3	-	0/2/19/22	0/1/1/1
3	BGC	N	5	3	-	2/2/19/22	0/1/1/1
3	BGC	N	6	3	-	2/2/19/22	0/1/1/1
3	BGC	O	1	3	-	2/2/22/22	0/1/1/1
3	BGC	O	2	3	-	0/2/19/22	0/1/1/1
3	BGC	O	3	3	-	0/2/19/22	0/1/1/1
3	BGC	O	4	3	-	1/2/19/22	0/1/1/1
3	BGC	O	5	3	-	0/2/19/22	0/1/1/1
3	BGC	O	6	3	-	0/2/19/22	0/1/1/1
3	BGC	P	1	3	-	2/2/22/22	0/1/1/1
3	BGC	P	2	3	-	0/2/19/22	0/1/1/1
3	BGC	P	3	3	-	2/2/19/22	0/1/1/1
3	BGC	P	4	3	-	0/2/19/22	0/1/1/1
3	BGC	P	5	3	-	2/2/19/22	0/1/1/1
3	BGC	P	6	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	1	3	-	0/2/22/22	0/1/1/1
3	BGC	Q	2	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	3	3	-	2/2/19/22	0/1/1/1
3	BGC	Q	4	3	-	0/2/19/22	0/1/1/1
3	BGC	Q	5	3	-	1/2/19/22	0/1/1/1
3	BGC	Q	6	3	-	1/2/19/22	0/1/1/1
3	BGC	R	1	3	-	0/2/22/22	0/1/1/1
3	BGC	R	2	3	-	0/2/19/22	0/1/1/1
3	BGC	R	3	3	-	2/2/19/22	0/1/1/1
3	BGC	R	4	3	-	0/2/19/22	0/1/1/1
3	BGC	R	5	3	-	2/2/19/22	0/1/1/1
3	BGC	R	6	3	-	2/2/19/22	0/1/1/1
3	BGC	S	1	3	-	2/2/22/22	0/1/1/1
3	BGC	S	2	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	S	3	3	-	0/2/19/22	0/1/1/1
3	BGC	S	4	3	-	0/2/19/22	0/1/1/1
3	BGC	S	5	3	-	1/2/19/22	0/1/1/1
3	BGC	S	6	3	-	2/2/19/22	0/1/1/1
3	BGC	T	1	3	-	1/2/22/22	0/1/1/1
3	BGC	T	2	3	-	0/2/19/22	0/1/1/1
3	BGC	T	3	3	-	0/2/19/22	0/1/1/1
3	BGC	T	4	3	-	0/2/19/22	0/1/1/1
3	BGC	T	5	3	-	2/2/19/22	0/1/1/1
3	BGC	T	6	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	3	BGC	C1-O5-C5	5.75	119.98	112.19
3	S	2	BGC	C1-O5-C5	5.28	119.35	112.19
3	R	5	BGC	C1-O5-C5	3.90	117.48	112.19
3	M	6	BGC	O5-C5-C6	3.40	112.53	107.20
3	T	2	BGC	C1-O5-C5	3.37	116.75	112.19
3	Q	5	BGC	C1-O5-C5	3.35	116.73	112.19
3	O	2	BGC	C1-C2-C3	3.32	113.74	109.67
3	L	6	BGC	O5-C5-C6	3.27	112.34	107.20
3	L	3	BGC	O5-C5-C6	-3.21	102.17	107.20
2	K	5	BGC	C1-O5-C5	3.10	116.39	112.19
3	P	5	BGC	C1-O5-C5	3.02	116.28	112.19
2	K	3	BGC	C1-C2-C3	3.00	113.35	109.67
3	O	5	BGC	C1-O5-C5	2.81	116.00	112.19
3	L	1	BGC	O5-C1-C2	-2.76	105.36	110.28
3	T	5	BGC	O5-C5-C6	2.71	111.45	107.20
3	P	4	BGC	C1-C2-C3	2.67	112.95	109.67
3	S	6	BGC	O5-C5-C6	2.59	111.26	107.20
3	T	6	BGC	O5-C5-C6	2.52	111.15	107.20
3	Q	6	BGC	O5-C5-C6	2.49	111.10	107.20
3	T	2	BGC	C6-C5-C4	-2.39	107.41	113.00
3	L	5	BGC	C1-O5-C5	2.38	115.41	112.19
3	N	2	BGC	C1-O5-C5	2.36	115.39	112.19
3	T	4	BGC	O5-C5-C6	2.33	110.86	107.20
3	S	1	BGC	C4-C3-C2	-2.32	106.77	110.82
3	T	5	BGC	C6-C5-C4	-2.28	107.66	113.00
3	N	1	BGC	O5-C1-C2	-2.25	106.27	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	4	BGC	O5-C5-C6	2.23	110.70	107.20
3	M	4	BGC	O5-C5-C6	2.23	110.70	107.20
3	O	5	BGC	C6-C5-C4	-2.23	107.78	113.00
3	O	5	BGC	O5-C5-C6	2.20	110.65	107.20
3	O	3	BGC	C1-O5-C5	2.19	115.16	112.19
3	R	3	BGC	O5-C1-C2	-2.18	107.41	110.77
3	L	5	BGC	O5-C5-C6	2.17	110.61	107.20
3	T	5	BGC	C1-O5-C5	2.16	115.11	112.19
3	L	4	BGC	O5-C1-C2	-2.15	107.45	110.77
3	L	6	BGC	C1-C2-C3	2.13	112.29	109.67
3	S	2	BGC	C6-C5-C4	-2.13	108.01	113.00
3	R	6	BGC	O5-C5-C6	2.12	110.53	107.20
3	M	4	BGC	C1-C2-C3	2.11	112.26	109.67
3	Q	3	BGC	C6-C5-C4	-2.10	108.09	113.00
3	T	1	BGC	C4-C3-C2	-2.09	107.17	110.82
3	M	3	BGC	O5-C5-C6	2.09	110.47	107.20
3	S	6	BGC	C1-C2-C3	2.06	112.20	109.67
3	R	4	BGC	C1-C2-C3	2.06	112.20	109.67
3	O	2	BGC	C1-O5-C5	2.05	114.98	112.19
3	P	3	BGC	O2-C2-C1	2.02	113.28	109.15
3	M	5	BGC	O5-C5-C6	2.00	110.35	107.20

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	6	BGC	O5-C5-C6-O6
3	M	5	BGC	O5-C5-C6-O6
2	K	5	BGC	O5-C5-C6-O6
3	P	3	BGC	O5-C5-C6-O6
3	S	6	BGC	O5-C5-C6-O6
3	N	1	BGC	C4-C5-C6-O6
3	R	6	BGC	C4-C5-C6-O6
3	N	1	BGC	O5-C5-C6-O6
3	M	5	BGC	C4-C5-C6-O6
3	S	2	BGC	O5-C5-C6-O6
3	N	5	BGC	O5-C5-C6-O6
3	O	1	BGC	O5-C5-C6-O6
3	S	1	BGC	O5-C5-C6-O6
3	S	6	BGC	C4-C5-C6-O6
3	M	1	BGC	C4-C5-C6-O6
3	O	1	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	R	3	BGC	C4-C5-C6-O6
3	N	5	BGC	C4-C5-C6-O6
2	K	5	BGC	C4-C5-C6-O6
3	S	1	BGC	C4-C5-C6-O6
3	L	5	BGC	O5-C5-C6-O6
3	R	5	BGC	C4-C5-C6-O6
3	S	2	BGC	C4-C5-C6-O6
3	M	6	BGC	O5-C5-C6-O6
3	T	5	BGC	O5-C5-C6-O6
3	M	1	BGC	O5-C5-C6-O6
3	P	5	BGC	C4-C5-C6-O6
3	M	2	BGC	O5-C5-C6-O6
3	R	3	BGC	O5-C5-C6-O6
3	P	3	BGC	C4-C5-C6-O6
3	Q	3	BGC	O5-C5-C6-O6
3	S	5	BGC	O5-C5-C6-O6
3	N	6	BGC	O5-C5-C6-O6
3	N	6	BGC	C4-C5-C6-O6
3	R	5	BGC	O5-C5-C6-O6
3	T	1	BGC	O5-C5-C6-O6
3	P	1	BGC	C4-C5-C6-O6
3	Q	6	BGC	O5-C5-C6-O6
3	L	3	BGC	O5-C5-C6-O6
3	M	4	BGC	O5-C5-C6-O6
3	L	5	BGC	C4-C5-C6-O6
3	M	6	BGC	C4-C5-C6-O6
3	T	5	BGC	C4-C5-C6-O6
3	Q	5	BGC	C4-C5-C6-O6
3	T	6	BGC	O5-C5-C6-O6
3	P	5	BGC	O5-C5-C6-O6
3	L	6	BGC	O5-C5-C6-O6
2	K	1	BGC	C4-C5-C6-O6
3	O	4	BGC	C4-C5-C6-O6
3	P	1	BGC	O5-C5-C6-O6
3	L	4	BGC	O5-C5-C6-O6
3	M	2	BGC	C4-C5-C6-O6
3	Q	3	BGC	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	O	1	BGC	1	0

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

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain P

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain Q

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain R

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain S

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain T
Bond lengths
Bond angles
Torsions
Rings

5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 10 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	ACT	A	607	-	3,3,3	0.73	0	3,3,3	0.66	0
7	EDO	B	612	-	3,3,3	0.45	0	2,2,2	0.25	0
7	EDO	G	609	-	3,3,3	0.50	0	2,2,2	0.19	0
7	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.22	0
7	EDO	G	608	-	3,3,3	0.77	0	2,2,2	0.83	0
5	ACT	I	608	-	3,3,3	0.77	0	3,3,3	0.64	0
6	PEG	J	609	-	6,6,6	0.44	0	5,5,5	0.28	0
7	EDO	H	609	-	3,3,3	0.45	0	2,2,2	0.26	0
6	PEG	A	608	-	6,6,6	0.58	0	5,5,5	0.77	0
5	ACT	J	608	-	3,3,3	0.77	0	3,3,3	0.83	0
7	EDO	E	612	-	3,3,3	0.52	0	2,2,2	0.21	0
7	EDO	E	609	-	3,3,3	0.53	0	2,2,2	0.17	0
5	ACT	C	608	-	3,3,3	0.72	0	3,3,3	0.79	0
7	EDO	G	612	-	3,3,3	0.48	0	2,2,2	0.34	0
7	EDO	E	610	-	3,3,3	0.55	0	2,2,2	0.38	0
7	EDO	C	611	-	3,3,3	0.50	0	2,2,2	0.12	0
6	PEG	B	610	-	6,6,6	0.48	0	5,5,5	0.19	0
5	ACT	D	608	-	3,3,3	0.72	0	3,3,3	0.89	0
5	ACT	E	608	-	3,3,3	0.76	0	3,3,3	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PEG	A	609	-	6,6,6	0.48	0	5,5,5	0.17	0
6	PEG	B	609	-	6,6,6	0.53	0	5,5,5	0.29	0
7	EDO	I	609	-	3,3,3	0.52	0	2,2,2	0.21	0
5	ACT	B	608	-	3,3,3	0.87	0	3,3,3	0.49	0
7	EDO	C	609	-	3,3,3	0.49	0	2,2,2	0.21	0
7	EDO	G	611	-	3,3,3	0.48	0	2,2,2	0.23	0
5	ACT	H	608	-	3,3,3	0.77	0	3,3,3	0.74	0
7	EDO	C	610	-	3,3,3	0.45	0	2,2,2	0.25	0
7	EDO	E	611	-	3,3,3	0.50	0	2,2,2	0.15	0
7	EDO	D	609	-	3,3,3	0.45	0	2,2,2	0.23	0
7	EDO	G	610	-	3,3,3	0.49	0	2,2,2	0.27	0
7	EDO	B	611	-	3,3,3	0.47	0	2,2,2	0.19	0
5	ACT	F	608	-	3,3,3	0.75	0	3,3,3	0.80	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
7	EDO	B	612	-	-	0/1/1/1	-
7	EDO	G	609	-	-	1/1/1/1	-
7	EDO	A	610	-	-	1/1/1/1	-
7	EDO	G	608	-	-	0/1/1/1	-
6	PEG	J	609	-	-	2/4/4/4	-
7	EDO	H	609	-	-	1/1/1/1	-
6	PEG	A	608	-	-	2/4/4/4	-
7	EDO	E	612	-	-	1/1/1/1	-
7	EDO	E	609	-	-	0/1/1/1	-
7	EDO	G	612	-	-	0/1/1/1	-
7	EDO	E	610	-	-	1/1/1/1	-
7	EDO	C	611	-	-	1/1/1/1	-
6	PEG	B	610	-	-	2/4/4/4	-
6	PEG	A	609	-	-	2/4/4/4	-
6	PEG	B	609	-	-	2/4/4/4	-
7	EDO	I	609	-	-	1/1/1/1	-
7	EDO	C	609	-	-	0/1/1/1	-
7	EDO	G	611	-	-	1/1/1/1	-
7	EDO	C	610	-	-	1/1/1/1	-
7	EDO	E	611	-	-	0/1/1/1	-
7	EDO	D	609	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	G	610	-	-	0/1/1/1	-
7	EDO	B	611	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	609	PEG	O1-C1-C2-O2
6	A	608	PEG	O2-C3-C4-O4
6	A	609	PEG	O2-C3-C4-O4
7	A	610	EDO	O1-C1-C2-O2
7	B	611	EDO	O1-C1-C2-O2
7	C	611	EDO	O1-C1-C2-O2
7	E	610	EDO	O1-C1-C2-O2
7	E	612	EDO	O1-C1-C2-O2
7	G	609	EDO	O1-C1-C2-O2
7	G	611	EDO	O1-C1-C2-O2
7	I	609	EDO	O1-C1-C2-O2
6	A	609	PEG	O1-C1-C2-O2
6	B	610	PEG	O1-C1-C2-O2
7	D	609	EDO	O1-C1-C2-O2
7	C	610	EDO	O1-C1-C2-O2
6	B	610	PEG	C4-C3-O2-C2
6	B	609	PEG	O1-C1-C2-O2
7	H	609	EDO	O1-C1-C2-O2
6	A	608	PEG	C1-C2-O2-C3
6	J	609	PEG	C4-C3-O2-C2
6	B	609	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	608	EDO	2	0
7	E	610	EDO	1	0
7	C	611	EDO	1	0

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

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	513/520 (98%)	-0.62	3 (0%)	89	88	19, 30, 53, 79	0
1	B	516/520 (99%)	-0.70	1 (0%)	95	94	16, 27, 46, 78	0
1	C	512/520 (98%)	-0.57	5 (0%)	82	80	19, 32, 58, 87	0
1	D	519/520 (99%)	-0.59	2 (0%)	92	91	18, 34, 55, 79	0
1	E	517/520 (99%)	-0.63	1 (0%)	95	94	19, 31, 52, 75	0
1	F	514/520 (98%)	-0.52	2 (0%)	92	91	20, 39, 63, 81	0
1	G	512/520 (98%)	-0.61	4 (0%)	86	84	21, 32, 56, 72	0
1	H	514/520 (98%)	-0.53	5 (0%)	82	80	20, 35, 56, 76	0
1	I	510/520 (98%)	-0.55	2 (0%)	92	91	24, 39, 59, 70	0
1	J	512/520 (98%)	-0.59	3 (0%)	89	88	19, 34, 58, 85	0
All	All	5139/5200 (98%)	-0.59	28 (0%)	91	89	16, 33, 58, 87	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	160	PHE	3.7
1	C	39	ILE	3.4
1	C	114	ARG	3.1
1	D	155	PHE	2.9
1	A	114	ARG	2.9
1	E	114	ARG	2.9
1	J	160	PHE	2.9
1	I	114	ARG	2.8
1	H	116	ALA	2.7
1	H	113	TYR	2.6
1	B	117	GLU	2.4
1	C	113	TYR	2.4
1	J	117	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	39	ILE	2.3
1	J	114	ARG	2.3
1	G	114	ARG	2.3
1	C	120	GLU	2.3
1	G	530	TYR	2.2
1	A	117	GLU	2.2
1	G	113	TYR	2.2
1	G	191	LYS	2.2
1	H	114	ARG	2.2
1	H	121	LYS	2.1
1	I	368	ASN	2.1
1	F	114	ARG	2.1
1	D	156	LEU	2.1
1	A	530	TYR	2.0
1	C	110	ASP	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(Å^2)	Q<0.9
3	BGC	L	1	12/12	0.81	0.21	53,58,62,65	0
3	BGC	O	1	12/12	0.83	0.21	53,63,71,75	0
3	BGC	N	1	12/12	0.87	0.17	54,62,64,71	0
3	BGC	S	1	12/12	0.87	0.17	51,62,72,74	0
3	BGC	M	1	12/12	0.88	0.23	54,68,73,74	0
3	BGC	T	1	12/12	0.88	0.15	53,57,64,68	0
3	BGC	Q	1	12/12	0.89	0.13	56,59,64,65	0
3	BGC	R	2	11/12	0.89	0.13	49,53,57,57	0
3	BGC	R	1	12/12	0.90	0.16	57,63,66,66	0
2	BGC	K	1	12/12	0.90	0.16	50,59,66,66	0
3	BGC	M	2	11/12	0.91	0.14	44,47,58,64	0
3	BGC	N	2	11/12	0.91	0.14	53,55,58,60	0
3	BGC	P	6	11/12	0.92	0.18	63,68,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	BGC	P	1	12/12	0.92	0.14	61,67,71,76	0
3	BGC	P	2	11/12	0.93	0.11	49,57,60,61	0
3	BGC	P	3	11/12	0.93	0.15	60,62,68,74	0
3	BGC	L	6	11/12	0.93	0.13	42,47,51,53	0
3	BGC	M	3	11/12	0.93	0.11	40,43,45,47	0
3	BGC	P	5	11/12	0.94	0.12	56,60,66,70	0
3	BGC	N	6	11/12	0.94	0.11	53,58,63,65	0
3	BGC	M	6	11/12	0.94	0.11	44,48,52,62	0
3	BGC	Q	2	11/12	0.94	0.10	44,46,49,54	0
3	BGC	Q	6	11/12	0.94	0.12	41,44,49,51	0
3	BGC	L	2	11/12	0.94	0.11	40,43,50,57	0
3	BGC	L	3	11/12	0.94	0.11	33,35,42,43	0
3	BGC	N	3	11/12	0.94	0.09	46,50,52,54	0
3	BGC	S	2	11/12	0.94	0.10	42,45,51,60	0
3	BGC	P	4	11/12	0.94	0.11	52,56,59,59	0
3	BGC	T	2	11/12	0.94	0.12	41,48,52,62	0
3	BGC	T	5	11/12	0.94	0.11	36,39,46,48	0
3	BGC	N	5	11/12	0.95	0.10	50,54,63,65	0
3	BGC	L	5	11/12	0.95	0.12	34,38,42,46	0
3	BGC	R	3	11/12	0.95	0.13	46,47,57,59	0
3	BGC	R	6	11/12	0.95	0.12	50,54,60,60	0
2	BGC	K	5	11/12	0.95	0.10	38,42,48,50	0
3	BGC	O	2	11/12	0.95	0.14	43,51,57,58	0
3	BGC	S	5	11/12	0.95	0.13	39,43,46,49	0
3	BGC	O	3	11/12	0.95	0.10	40,41,48,48	0
2	BGC	K	3	11/12	0.95	0.11	37,45,53,58	0
3	BGC	T	4	11/12	0.95	0.10	32,34,36,36	0
3	BGC	N	4	11/12	0.95	0.10	46,52,57,58	0
3	BGC	T	6	11/12	0.95	0.18	45,49,57,64	0
2	BGC	K	2	11/12	0.96	0.09	47,49,53,55	0
3	BGC	S	3	11/12	0.96	0.08	39,42,47,50	0
3	BGC	S	4	11/12	0.96	0.10	36,38,42,45	0
3	BGC	M	4	11/12	0.96	0.10	33,39,41,42	0
3	BGC	Q	3	11/12	0.96	0.12	37,41,48,59	0
3	BGC	R	4	11/12	0.96	0.10	45,48,55,62	0
3	BGC	R	5	11/12	0.96	0.10	46,49,52,60	0
3	BGC	Q	5	11/12	0.96	0.10	37,39,44,47	0
3	BGC	O	6	11/12	0.96	0.11	38,40,43,45	0
3	BGC	L	4	11/12	0.97	0.11	32,33,35,35	0
3	BGC	S	6	11/12	0.97	0.12	41,44,47,52	0
3	BGC	M	5	11/12	0.97	0.09	39,42,43,45	0
2	BGC	K	4	11/12	0.97	0.07	35,36,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	BGC	T	3	11/12	0.97	0.08	36,39,42,49	0
3	BGC	O	4	11/12	0.97	0.10	33,36,40,42	0
3	BGC	O	5	11/12	0.97	0.09	36,40,47,51	0
3	BGC	Q	4	11/12	0.97	0.08	32,37,41,42	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.
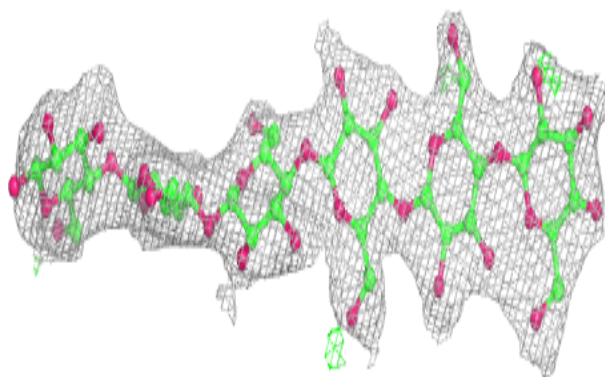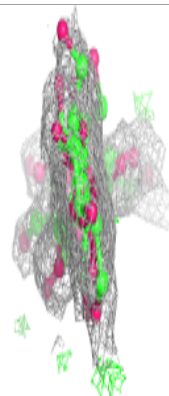

Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
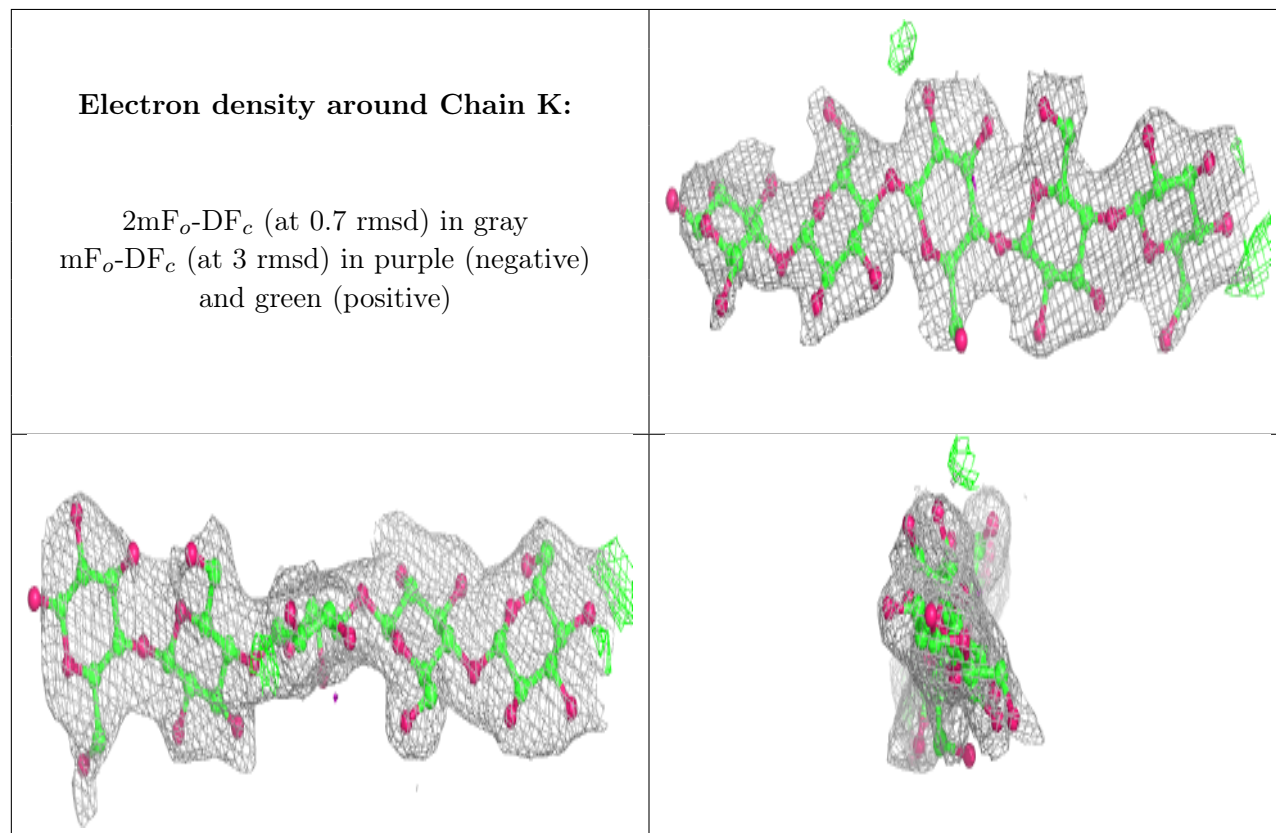
Electron density around Chain L:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
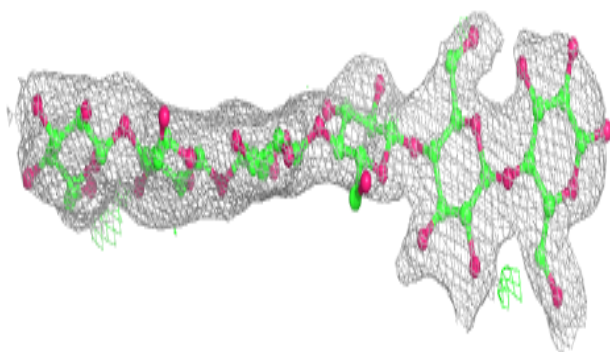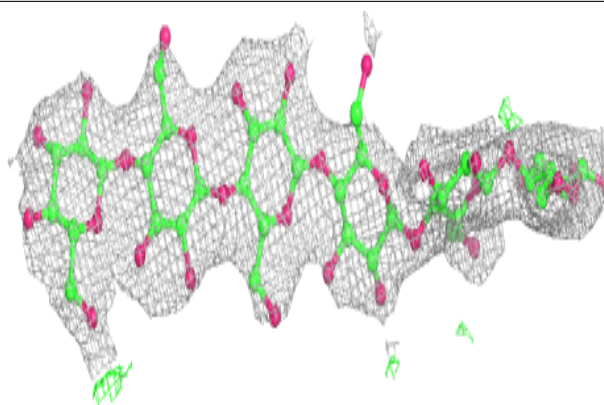and green (positive)
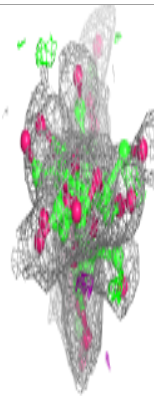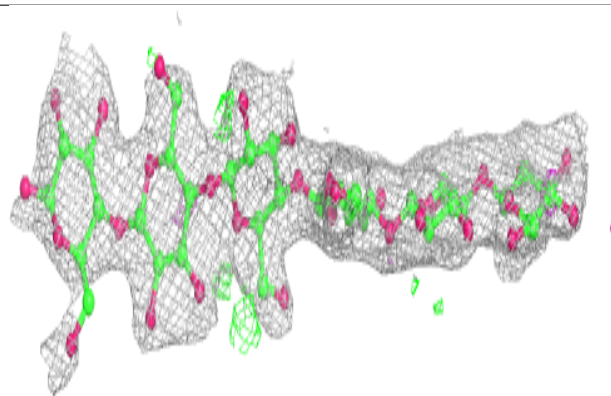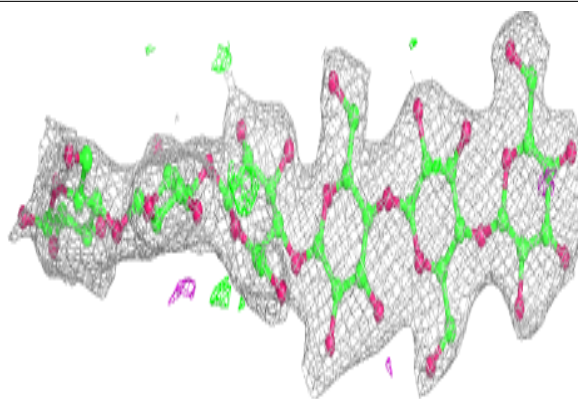
Electron density around Chain M:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
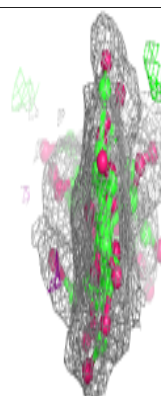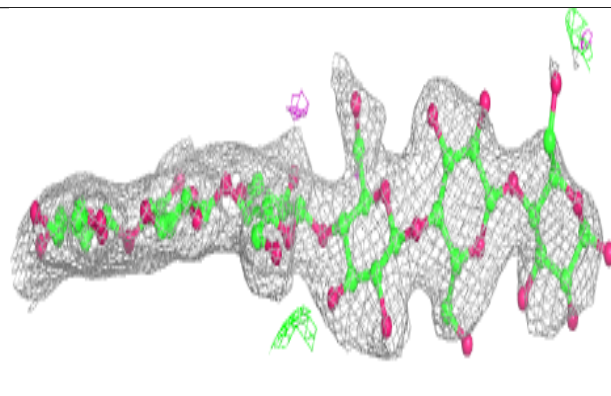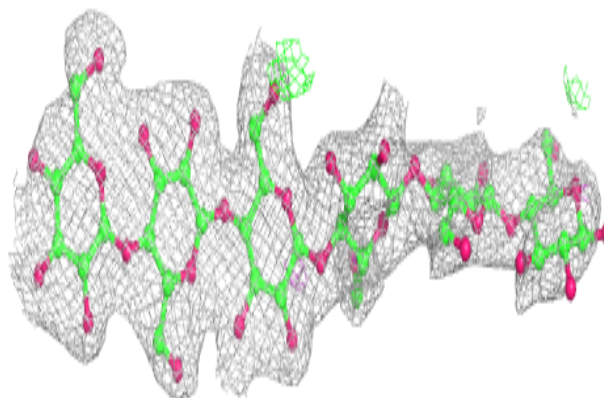
Electron density around Chain N:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
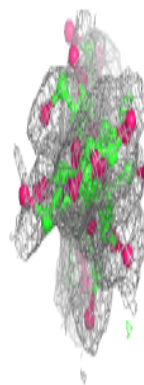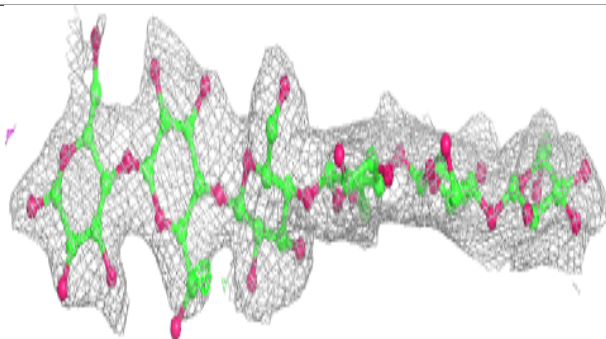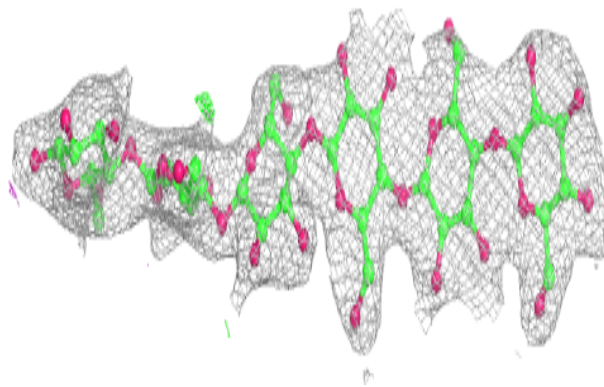
Electron density around Chain O:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
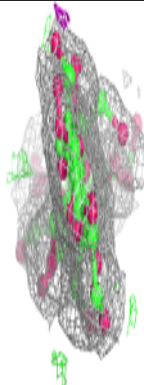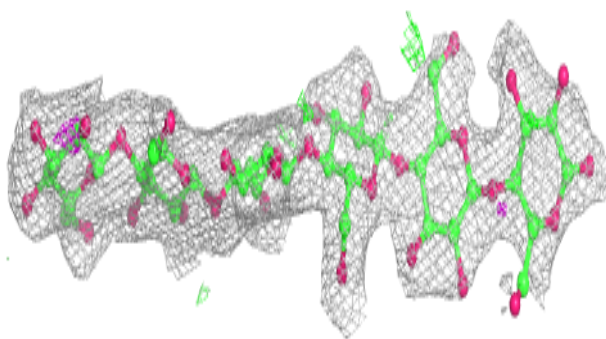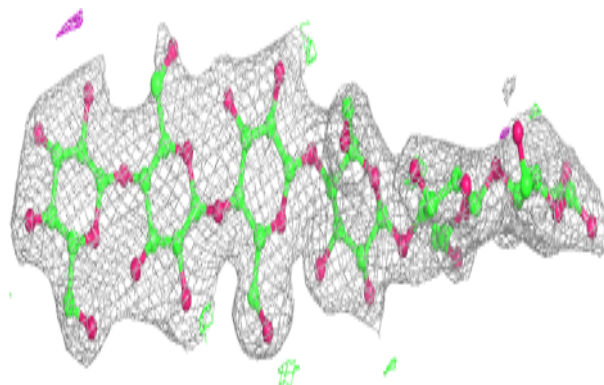
Electron density around Chain P:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
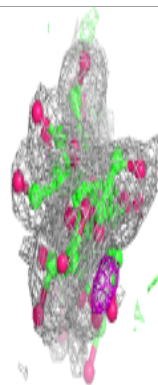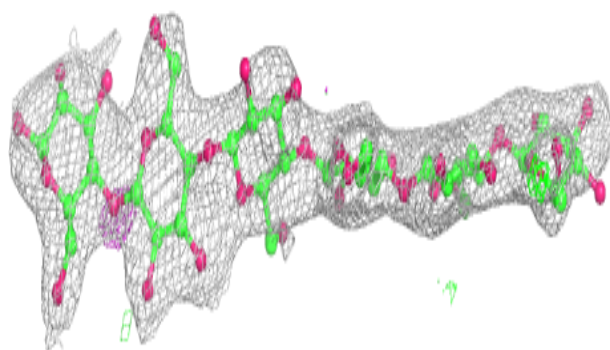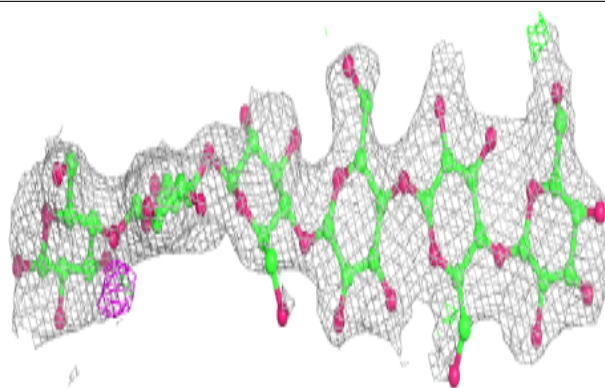
Electron density around Chain Q:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
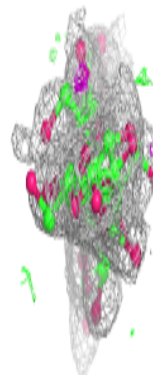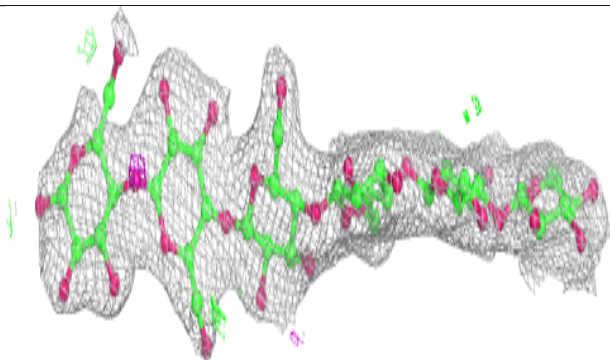$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
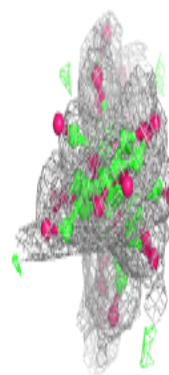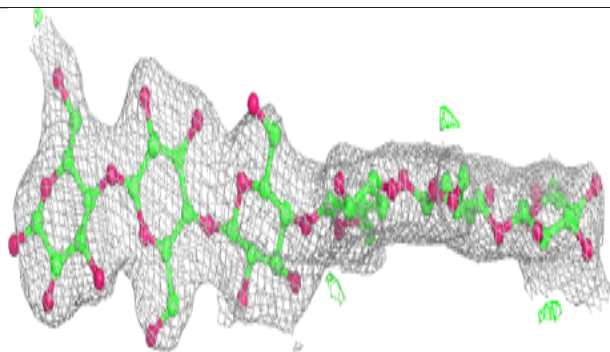
Electron density around Chain R:

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 S:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

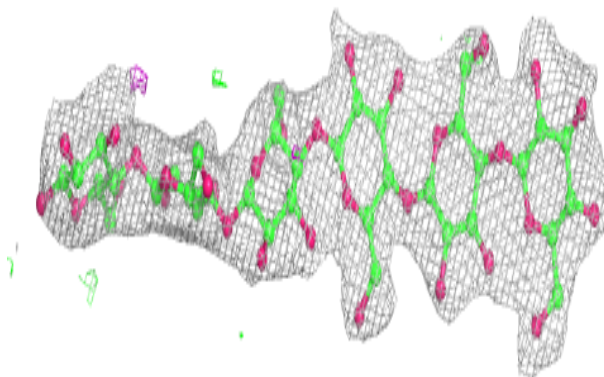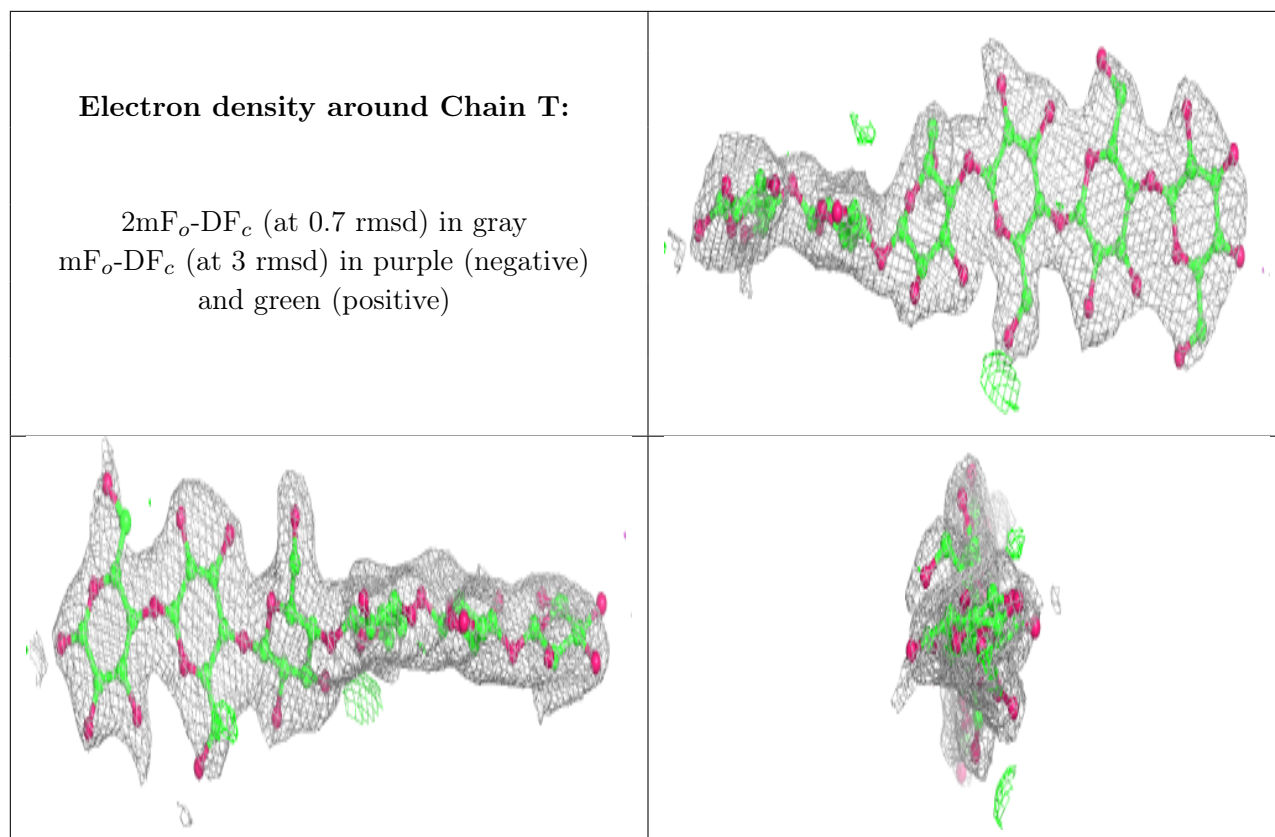**Electron density around Chain T:**

$2mF_o$-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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	G	610	4/4	0.73	0.17	54,57,57,58	0
5	ACT	H	608	4/4	0.78	0.16	66,69,70,74	0
7	EDO	E	609	4/4	0.79	0.19	52,55,56,56	0
7	EDO	G	611	4/4	0.79	0.16	54,55,56,57	0
6	PEG	B	609	7/7	0.82	0.21	49,53,61,62	0
7	EDO	D	609	4/4	0.84	0.17	56,63,63,65	0
6	PEG	A	609	7/7	0.85	0.15	52,57,64,66	0
5	ACT	I	608	4/4	0.86	0.20	52,53,56,57	0
6	PEG	B	610	7/7	0.86	0.12	56,57,60,61	0
5	ACT	E	608	4/4	0.86	0.23	42,51,53,64	0
7	EDO	C	609	4/4	0.87	0.18	51,53,53,53	0
7	EDO	H	609	4/4	0.87	0.16	52,54,55,57	0
5	ACT	D	608	4/4	0.88	0.21	53,53,54,57	0
7	EDO	E	612	4/4	0.88	0.15	65,67,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
7	EDO	G	612	4/4	0.88	0.21	44,46,50,51	0
7	EDO	G	608	4/4	0.88	0.23	41,47,50,52	0
5	ACT	J	608	4/4	0.89	0.14	48,49,54,58	0
5	ACT	B	608	4/4	0.89	0.17	38,42,43,50	0
5	ACT	F	608	4/4	0.89	0.14	51,55,57,57	0
7	EDO	G	609	4/4	0.89	0.11	50,57,58,59	0
7	EDO	C	610	4/4	0.91	0.16	47,50,51,51	0
7	EDO	E	610	4/4	0.91	0.20	43,47,50,52	0
6	PEG	J	609	7/7	0.91	0.12	52,52,56,56	0
6	PEG	A	608	7/7	0.92	0.30	36,45,58,62	0
7	EDO	I	609	4/4	0.92	0.12	54,57,58,59	0
7	EDO	B	612	4/4	0.93	0.11	54,54,55,55	0
5	ACT	A	607	4/4	0.93	0.17	54,56,58,60	0
5	ACT	C	608	4/4	0.94	0.16	47,51,54,55	0
7	EDO	E	611	4/4	0.94	0.12	48,49,52,53	0
4	MG	F	607	1/1	0.95	0.06	52,52,52,52	0
4	MG	C	607	1/1	0.95	0.10	50,50,50,50	0
4	MG	I	607	1/1	0.96	0.05	55,55,55,55	0
4	MG	D	607	1/1	0.96	0.09	44,44,44,44	0
4	MG	G	607	1/1	0.96	0.06	53,53,53,53	0
7	EDO	A	610	4/4	0.97	0.14	46,47,51,52	0
4	MG	A	606	1/1	0.97	0.12	45,45,45,45	0
7	EDO	C	611	4/4	0.97	0.15	36,37,38,38	0
4	MG	E	607	1/1	0.98	0.12	54,54,54,54	0
4	MG	H	607	1/1	0.98	0.08	51,51,51,51	0
4	MG	B	607	1/1	0.99	0.09	48,48,48,48	0
7	EDO	B	611	4/4	0.99	0.12	36,37,37,39	0
4	MG	J	607	1/1	0.99	0.08	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.