



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:46 PM UTC

PDB ID : 4WJV / pdb_00004wjv
Title : Crystal structure of Rsa4 in complex with the Nsa2 binding peptide
Authors : Holdermann, I.; Paternoga, H.; Bassler, J.; Hurt, E.; Sinning, I.
Deposited on : 2014-10-01
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

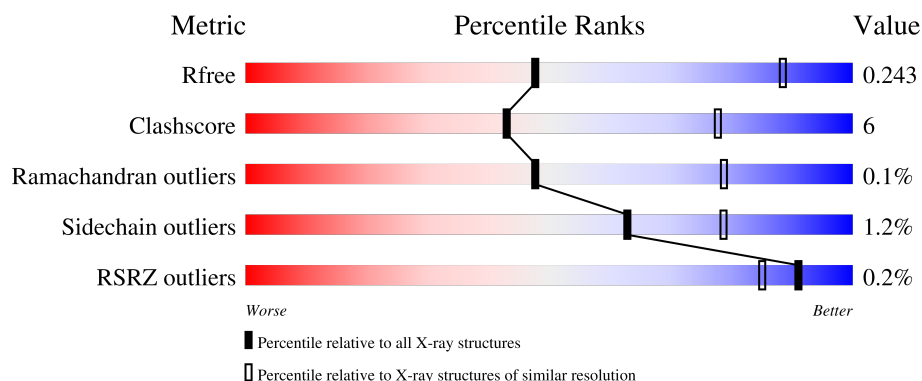
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



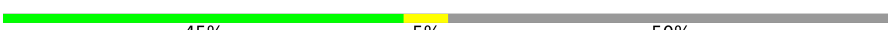
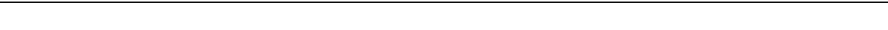
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	381	 77% 22% ..
1	B	381	 77% 22% .
1	C	381	 77% 22% ..
1	D	381	 79% 20% ..
2	E	381	 85% 12% .

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Mol	Chain	Length	Quality of chain
2	F	381	 85% 11% .
2	G	381	 85% 12% .
2	H	381	 86% 10% .
3	I	22	 45% 5% 50%
3	J	22	 36% 14% 50%
3	K	22	 55% 45%
3	L	22	 45% 5% 50%
4	M	2	 100%
4	N	2	 100%
4	O	2	 50% 50%
4	P	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	D	602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23675 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 Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2958	1854	534	550	20			
1	B	378	Total	C	N	O	S	0	0	0
			2958	1854	534	550	20			
1	C	378	Total	C	N	O	S	0	0	0
			2958	1854	534	550	20			
1	D	378	Total	C	N	O	S	0	0	0
			2958	1854	534	550	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	MET	-	initiating methionine	UNP P25382
A	136	GLY	-	expression tag	UNP P25382
B	135	MET	-	initiating methionine	UNP P25382
B	136	GLY	-	expression tag	UNP P25382
C	135	MET	-	initiating methionine	UNP P25382
C	136	GLY	-	expression tag	UNP P25382
D	135	MET	-	initiating methionine	UNP P25382
D	136	GLY	-	expression tag	UNP P25382

- Molecule 2 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	369	Total	C	N	O	S	0	0	0
			2834	1825	461	542	6			
2	F	368	Total	C	N	O	S	0	0	0
			2826	1819	460	541	6			
2	G	369	Total	C	N	O	S	0	0	0
			2834	1825	461	542	6			
2	H	369	Total	C	N	O	S	0	0	0
			2834	1825	461	542	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP P0AEX9
E	2	LYS	-	expression tag	UNP P0AEX9
E	3	HIS	-	expression tag	UNP P0AEX9
E	4	HIS	-	expression tag	UNP P0AEX9
E	5	HIS	-	expression tag	UNP P0AEX9
E	6	HIS	-	expression tag	UNP P0AEX9
E	7	HIS	-	expression tag	UNP P0AEX9
E	8	HIS	-	expression tag	UNP P0AEX9
E	9	PRO	-	expression tag	UNP P0AEX9
E	10	MET	-	expression tag	UNP P0AEX9
E	92	ALA	ASP	engineered mutation	UNP P0AEX9
E	93	ALA	LYS	engineered mutation	UNP P0AEX9
E	249	ALA	LYS	engineered mutation	UNP P0AEX9
E	369	ALA	GLU	engineered mutation	UNP P0AEX9
E	372	ALA	LYS	engineered mutation	UNP P0AEX9
E	373	ALA	ASP	engineered mutation	UNP P0AEX9
E	377	ASN	ARG	engineered mutation	UNP P0AEX9
E	378	ALA	-	expression tag	UNP P0AEX9
E	379	ALA	-	expression tag	UNP P0AEX9
E	380	ALA	-	expression tag	UNP P0AEX9
E	381	ALA	-	expression tag	UNP P0AEX9
F	1	MET	-	initiating methionine	UNP P0AEX9
F	2	LYS	-	expression tag	UNP P0AEX9
F	3	HIS	-	expression tag	UNP P0AEX9
F	4	HIS	-	expression tag	UNP P0AEX9
F	5	HIS	-	expression tag	UNP P0AEX9
F	6	HIS	-	expression tag	UNP P0AEX9
F	7	HIS	-	expression tag	UNP P0AEX9
F	8	HIS	-	expression tag	UNP P0AEX9
F	9	PRO	-	expression tag	UNP P0AEX9
F	10	MET	-	expression tag	UNP P0AEX9
F	92	ALA	ASP	engineered mutation	UNP P0AEX9
F	93	ALA	LYS	engineered mutation	UNP P0AEX9
F	249	ALA	LYS	engineered mutation	UNP P0AEX9
F	369	ALA	GLU	engineered mutation	UNP P0AEX9
F	372	ALA	LYS	engineered mutation	UNP P0AEX9
F	373	ALA	ASP	engineered mutation	UNP P0AEX9
F	377	ASN	ARG	engineered mutation	UNP P0AEX9
F	378	ALA	-	expression tag	UNP P0AEX9
F	379	ALA	-	expression tag	UNP P0AEX9
F	380	ALA	-	expression tag	UNP P0AEX9
F	381	ALA	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP P0AEX9
G	2	LYS	-	expression tag	UNP P0AEX9
G	3	HIS	-	expression tag	UNP P0AEX9
G	4	HIS	-	expression tag	UNP P0AEX9
G	5	HIS	-	expression tag	UNP P0AEX9
G	6	HIS	-	expression tag	UNP P0AEX9
G	7	HIS	-	expression tag	UNP P0AEX9
G	8	HIS	-	expression tag	UNP P0AEX9
G	9	PRO	-	expression tag	UNP P0AEX9
G	10	MET	-	expression tag	UNP P0AEX9
G	92	ALA	ASP	engineered mutation	UNP P0AEX9
G	93	ALA	LYS	engineered mutation	UNP P0AEX9
G	249	ALA	LYS	engineered mutation	UNP P0AEX9
G	369	ALA	GLU	engineered mutation	UNP P0AEX9
G	372	ALA	LYS	engineered mutation	UNP P0AEX9
G	373	ALA	ASP	engineered mutation	UNP P0AEX9
G	377	ASN	ARG	engineered mutation	UNP P0AEX9
G	378	ALA	-	expression tag	UNP P0AEX9
G	379	ALA	-	expression tag	UNP P0AEX9
G	380	ALA	-	expression tag	UNP P0AEX9
G	381	ALA	-	expression tag	UNP P0AEX9
H	1	MET	-	initiating methionine	UNP P0AEX9
H	2	LYS	-	expression tag	UNP P0AEX9
H	3	HIS	-	expression tag	UNP P0AEX9
H	4	HIS	-	expression tag	UNP P0AEX9
H	5	HIS	-	expression tag	UNP P0AEX9
H	6	HIS	-	expression tag	UNP P0AEX9
H	7	HIS	-	expression tag	UNP P0AEX9
H	8	HIS	-	expression tag	UNP P0AEX9
H	9	PRO	-	expression tag	UNP P0AEX9
H	10	MET	-	expression tag	UNP P0AEX9
H	92	ALA	ASP	engineered mutation	UNP P0AEX9
H	93	ALA	LYS	engineered mutation	UNP P0AEX9
H	249	ALA	LYS	engineered mutation	UNP P0AEX9
H	369	ALA	GLU	engineered mutation	UNP P0AEX9
H	372	ALA	LYS	engineered mutation	UNP P0AEX9
H	373	ALA	ASP	engineered mutation	UNP P0AEX9
H	377	ASN	ARG	engineered mutation	UNP P0AEX9
H	378	ALA	-	expression tag	UNP P0AEX9
H	379	ALA	-	expression tag	UNP P0AEX9
H	380	ALA	-	expression tag	UNP P0AEX9
H	381	ALA	-	expression tag	UNP P0AEX9

- Molecule 3 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	11	Total	C	N	O	0	0	0
			91	58	14	19			
3	J	11	Total	C	N	O	0	0	0
			91	58	14	19			
3	K	12	Total	C	N	O	0	0	0
			100	63	16	21			
3	L	11	Total	C	N	O	0	0	0
			91	58	14	19			

There are 4 discrepancies between the modelled and reference sequences:

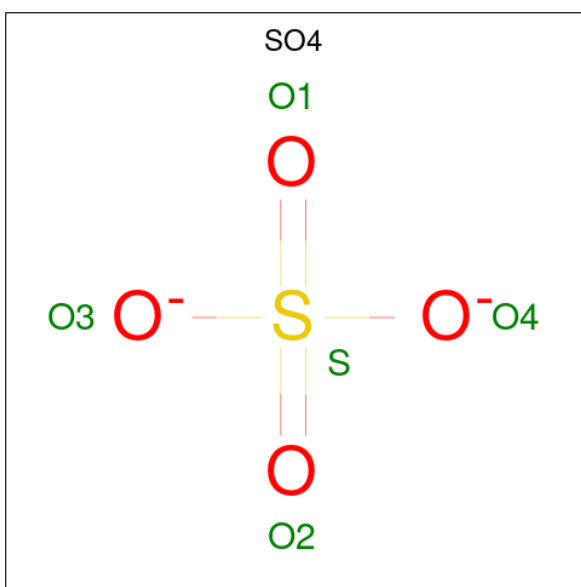
Chain	Residue	Modelled	Actual	Comment	Reference
I	80	MET	LEU	conflict	UNP P40078
J	80	MET	LEU	conflict	UNP P40078
K	80	MET	LEU	conflict	UNP P40078
L	80	MET	LEU	conflict	UNP P40078

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



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

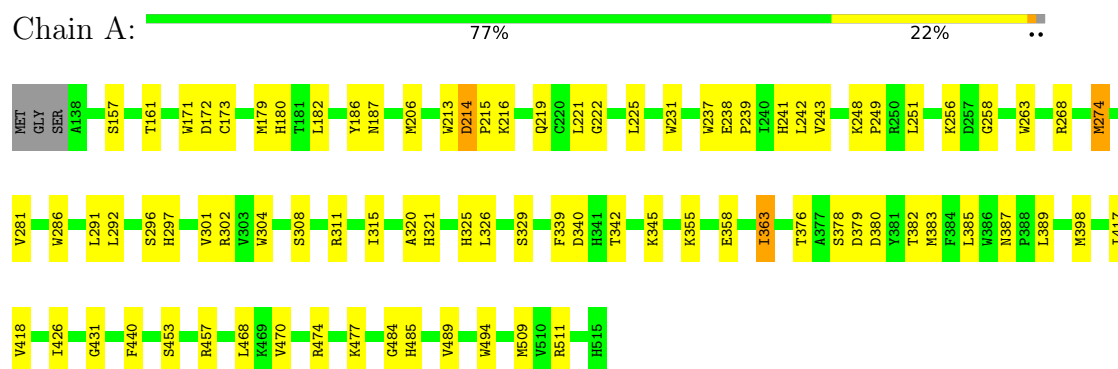


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total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

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.

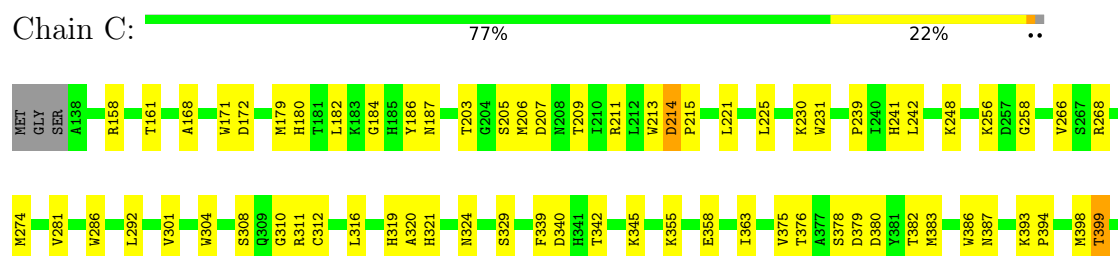
• Molecule 1: Ribosome assembly protein 4



• Molecule 1: Ribosome assembly protein 4

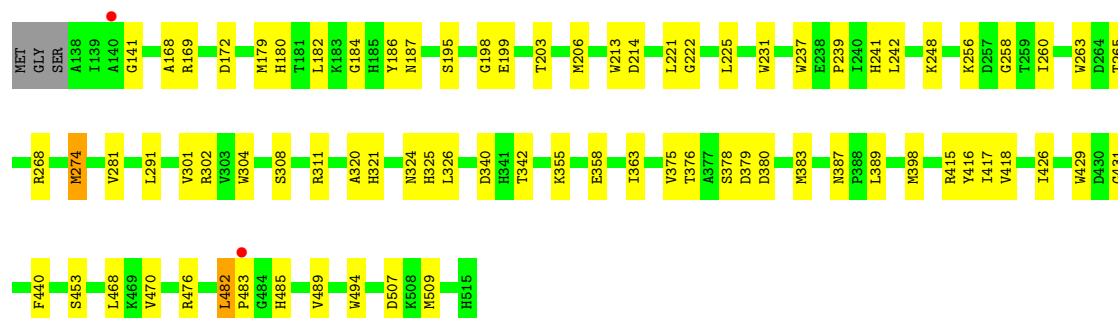
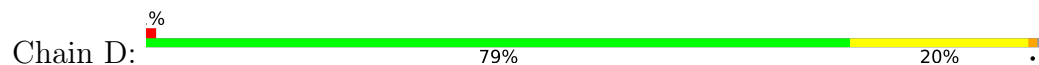


• Molecule 1: Ribosome assembly protein 4

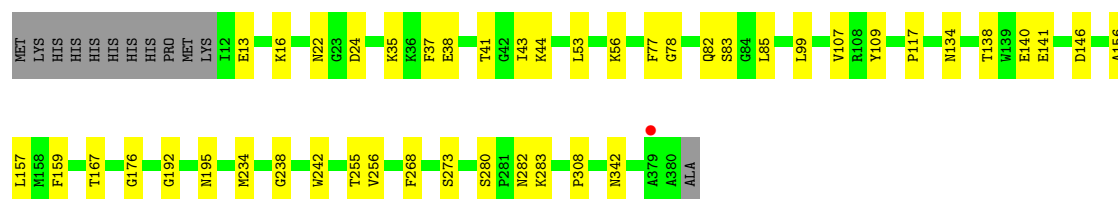
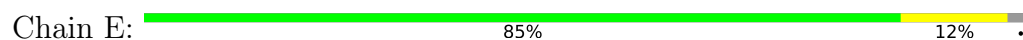




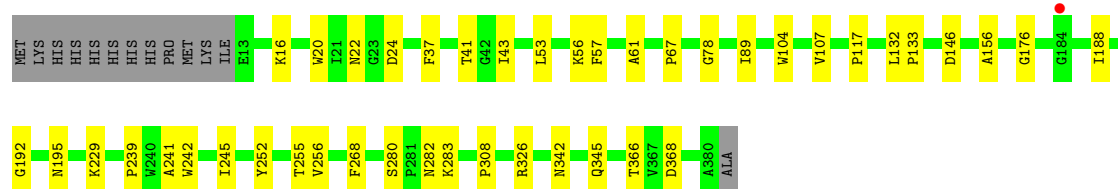
- Molecule 1: Ribosome assembly protein 4



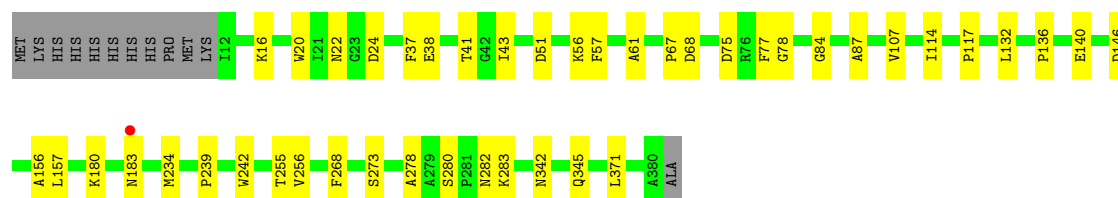
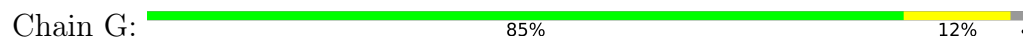
- Molecule 2: Maltose-binding periplasmic protein



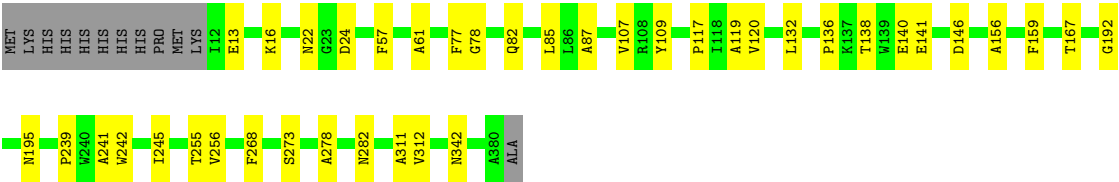
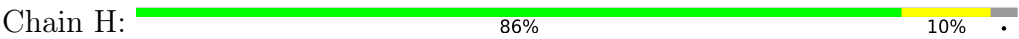
- Molecule 2: Maltose-binding periplasmic protein



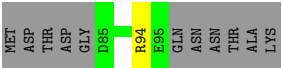
- Molecule 2: Maltose-binding periplasmic protein



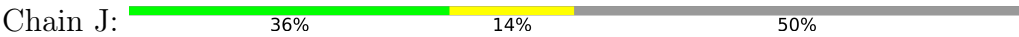
- Molecule 2: Maltose-binding periplasmic protein



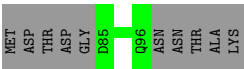
● Molecule 3: Ribosome biogenesis protein NSA2



● Molecule 3: Ribosome biogenesis protein NSA2



● Molecule 3: Ribosome biogenesis protein NSA2



● Molecule 3: Ribosome biogenesis protein NSA2



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



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

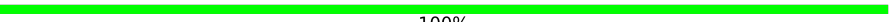


- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain O:  50% 50%

GLC1
GLC2

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

Chain P:  100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.58Å 96.49Å 196.44Å 90.00° 115.45° 90.00°	Depositor
Resolution (Å)	48.98 – 3.20 48.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.98-3.20) 96.5 (48.98-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.192 , 0.244 0.195 , 0.243	Depositor DCC
R_{free} test set	2823 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23675	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.28	0/3035	0.72	6/4116 (0.1%)
1	B	0.28	0/3035	0.72	4/4116 (0.1%)
1	C	0.28	0/3035	0.70	4/4116 (0.1%)
1	D	0.28	0/3035	0.71	4/4116 (0.1%)
2	E	0.33	0/2903	0.73	4/3948 (0.1%)
2	F	0.32	0/2895	0.72	0/3937
2	G	0.32	0/2903	0.73	0/3948
2	H	0.31	0/2903	0.72	0/3948
3	I	0.30	0/92	0.85	0/125
3	J	0.25	0/92	0.64	0/125
3	K	0.24	0/101	0.67	0/137
3	L	0.28	0/92	0.73	0/125
All	All	0.30	0/24121	0.72	22/32757 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	387	ASN	CA-C-N	6.92	126.44	119.24
1	D	387	ASN	C-N-CA	6.92	126.44	119.24
1	A	387	ASN	CA-C-N	6.85	126.36	119.24
1	A	387	ASN	C-N-CA	6.85	126.36	119.24
1	B	387	ASN	CA-C-N	6.75	126.26	119.24
1	B	387	ASN	C-N-CA	6.75	126.26	119.24
1	C	387	ASN	CA-C-N	6.69	126.20	119.24
1	C	387	ASN	C-N-CA	6.69	126.20	119.24
1	C	214	ASP	CA-C-N	6.62	126.31	119.56
1	C	214	ASP	C-N-CA	6.62	126.31	119.56
1	A	248	LYS	CA-C-N	6.17	125.93	119.76
1	A	248	LYS	C-N-CA	6.17	125.93	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ASP	CA-C-N	5.88	125.56	119.56
1	B	214	ASP	C-N-CA	5.88	125.56	119.56
1	A	214	ASP	CA-C-N	5.87	125.55	119.56
1	A	214	ASP	C-N-CA	5.87	125.55	119.56
1	D	214	ASP	CA-C-N	5.54	125.22	119.56
1	D	214	ASP	C-N-CA	5.54	125.22	119.56
2	E	134	ASN	CA-C-N	5.33	123.49	119.66
2	E	134	ASN	C-N-CA	5.33	123.49	119.66
2	E	238	GLY	CA-C-N	5.07	124.86	119.28
2	E	238	GLY	C-N-CA	5.07	124.86	119.28

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	2958	0	2896	51	0
1	B	2958	0	2896	50	1
1	C	2958	0	2896	57	0
1	D	2958	0	2896	46	0
2	E	2834	0	2797	26	0
2	F	2826	0	2786	22	0
2	G	2834	0	2797	23	0
2	H	2834	0	2797	23	0
3	I	91	0	87	1	0
3	J	91	0	87	1	0
3	K	100	0	95	0	0
3	L	91	0	87	0	0
4	M	23	0	21	0	0
4	N	23	0	21	0	0
4	O	23	0	21	1	0
4	P	23	0	21	0	0
5	A	15	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	15	0	0	1	1
All	All	23675	0	23201	290	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:THR:HG22	1:C:399:THR:HG23	1.72	0.72
1:A:221:LEU:O	1:A:268:ARG:NH1	2.24	0.71
1:A:302:ARG:HG2	1:A:315:ILE:HG12	1.76	0.68
1:A:378:SER:OG	1:A:380:ASP:OD1	2.09	0.68
1:D:378:SER:OG	1:D:380:ASP:OD1	2.10	0.68
1:C:378:SER:OG	1:C:380:ASP:OD1	2.13	0.66
1:B:378:SER:OG	1:B:380:ASP:OD1	2.13	0.66
1:A:383:MET:HB2	1:A:398:MET:HG3	1.78	0.66
1:A:308:SER:HB3	1:A:311:ARG:HD2	1.79	0.65
1:B:383:MET:HB2	1:B:398:MET:HG3	1.78	0.65
1:D:324:ASN:ND2	1:D:379:ASP:OD1	2.26	0.64
1:B:221:LEU:O	1:B:268:ARG:NH1	2.31	0.64
1:D:308:SER:HB3	1:D:311:ARG:HD2	1.78	0.64
1:D:221:LEU:O	1:D:268:ARG:NH1	2.30	0.64
1:D:225:LEU:HD11	1:D:268:ARG:HE	1.62	0.64
1:D:320:ALA:O	1:D:321:HIS:ND1	2.32	0.63
2:G:280:SER:O	2:G:283:LYS:NZ	2.33	0.62
1:A:222:GLY:HA3	1:A:268:ARG:HH12	1.63	0.61
1:B:355:LYS:HA	1:B:358:GLU:HB3	1.83	0.61
1:B:320:ALA:O	1:B:321:HIS:ND1	2.34	0.61
1:C:383:MET:HB2	1:C:398:MET:HG3	1.82	0.61
1:D:383:MET:HB2	1:D:398:MET:HG3	1.83	0.60
1:C:355:LYS:HA	1:C:358:GLU:HB3	1.83	0.60
1:A:320:ALA:O	1:A:321:HIS:ND1	2.34	0.60
2:F:16:LYS:O	2:F:282:ASN:ND2	2.35	0.60
1:A:457:ARG:HH21	1:A:474:ARG:HD2	1.67	0.60
1:C:320:ALA:O	1:C:321:HIS:ND1	2.35	0.59
1:B:222:GLY:HA3	1:B:268:ARG:HH12	1.67	0.59
2:E:280:SER:O	2:E:283:LYS:NZ	2.36	0.59
1:D:187:ASN:HB3	1:D:206:MET:HB3	1.85	0.58
1:D:468:LEU:HD21	1:D:489:VAL:HG11	1.84	0.58
1:C:319:HIS:NE2	1:C:376:THR:OG1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:GLY:HA2	2:E:195:ASN:HD21	1.69	0.58
1:C:340:ASP:OD1	1:C:342:THR:OG1	2.23	0.57
1:C:301:VAL:HG21	1:C:376:THR:HG21	1.85	0.57
1:C:225:LEU:HD11	1:C:268:ARG:HE	1.69	0.56
1:A:186:TYR:HE1	1:C:186:TYR:HE1	1.53	0.56
1:A:355:LYS:HA	1:A:358:GLU:HB3	1.87	0.56
2:E:22:ASN:ND2	2:E:24:ASP:OD1	2.38	0.56
2:G:57:PHE:O	2:G:61:ALA:N	2.38	0.56
1:C:158:ARG:NH1	1:C:172:ASP:OD1	2.39	0.56
1:C:324:ASN:ND2	1:C:379:ASP:OD1	2.25	0.56
1:A:225:LEU:HD11	1:A:268:ARG:HE	1.70	0.55
1:B:187:ASN:HB3	1:B:206:MET:HB3	1.88	0.55
1:C:231:TRP:CZ2	1:C:256:LYS:HG3	2.42	0.55
1:B:324:ASN:ND2	1:B:379:ASP:OD1	2.28	0.55
2:E:16:LYS:O	2:E:282:ASN:ND2	2.39	0.54
1:B:340:ASP:OD1	1:B:342:THR:OG1	2.22	0.54
1:D:222:GLY:HA3	1:D:268:ARG:HH12	1.73	0.54
1:A:340:ASP:OD1	1:A:342:THR:OG1	2.22	0.53
2:G:16:LYS:O	2:G:282:ASN:ND2	2.41	0.53
2:F:22:ASN:ND2	2:F:24:ASP:OD1	2.42	0.53
1:B:426:ILE:HB	1:B:440:PHE:HB2	1.90	0.53
1:A:180:HIS:NE2	1:A:216:LYS:O	2.36	0.53
1:C:375:VAL:HG11	1:C:417:ILE:HD13	1.91	0.53
1:C:179:MET:O	1:C:180:HIS:ND1	2.41	0.53
2:E:82:GLN:OE1	2:E:109:TYR:OH	2.23	0.52
1:A:301:VAL:HG21	1:A:376:THR:HG21	1.91	0.52
2:E:107:VAL:HG21	2:E:117:PRO:HD3	1.91	0.52
2:E:192:GLY:O	2:E:195:ASN:ND2	2.42	0.52
1:B:308:SER:HB3	1:B:311:ARG:HD2	1.92	0.52
1:D:355:LYS:HA	1:D:358:GLU:HB3	1.91	0.52
2:E:159:PHE:HE1	2:E:167:THR:HG22	1.75	0.52
2:H:120:VAL:N	2:H:311:ALA:O	2.33	0.52
1:A:339:PHE:HE1	1:A:345:LYS:HG2	1.76	0.51
1:C:308:SER:HB3	1:C:311:ARG:HD2	1.93	0.51
2:H:61:ALA:HB3	2:H:85:LEU:HD13	1.92	0.51
1:C:203:THR:HG22	1:C:213:TRP:HE1	1.75	0.51
1:A:225:LEU:HD23	1:A:263:TRP:CD2	2.45	0.51
1:B:184:GLY:HA2	1:D:186:TYR:CZ	2.46	0.51
2:H:107:VAL:HG21	2:H:117:PRO:HD3	1.91	0.51
1:C:258:GLY:HA2	1:C:281:VAL:HG23	1.93	0.51
2:H:22:ASN:ND2	2:H:24:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ASP:OD1	1:D:342:THR:OG1	2.22	0.51
1:B:180:HIS:NE2	1:B:216:LYS:O	2.41	0.50
2:H:82:GLN:OE1	2:H:109:TYR:OH	2.28	0.50
2:F:107:VAL:HG21	2:F:117:PRO:HD3	1.92	0.50
1:D:172:ASP:HB2	1:D:179:MET:HE3	1.92	0.50
1:A:239:PRO:HB2	1:A:241:HIS:CE1	2.47	0.49
1:B:225:LEU:HD11	1:B:268:ARG:HE	1.76	0.49
2:G:239:PRO:HA	2:G:242:TRP:CE2	2.47	0.49
1:D:203:THR:HG22	1:D:213:TRP:HE1	1.78	0.49
2:F:252:TYR:OH	2:F:326:ARG:NH1	2.46	0.49
1:D:225:LEU:HD23	1:D:263:TRP:CD2	2.48	0.49
1:B:186:TYR:HE1	1:D:186:TYR:HE1	1.61	0.49
1:B:241:HIS:CE1	1:B:242:LEU:HG	2.48	0.49
1:B:179:MET:O	1:B:180:HIS:ND1	2.45	0.49
2:H:119:ALA:HA	2:H:312:VAL:HA	1.96	0.48
1:C:221:LEU:O	1:C:268:ARG:NH1	2.44	0.48
1:C:426:ILE:HB	1:C:440:PHE:HB2	1.95	0.48
1:A:417:ILE:HG13	1:A:431:GLY:HA2	1.94	0.48
1:D:241:HIS:CE1	1:D:242:LEU:HG	2.47	0.48
1:B:161:THR:HG22	1:B:171:TRP:HE1	1.78	0.48
2:H:16:LYS:O	2:H:282:ASN:ND2	2.47	0.48
1:D:301:VAL:HG21	1:D:376:THR:HG21	1.95	0.47
2:G:255:THR:OG1	2:G:256:VAL:N	2.46	0.47
1:B:203:THR:HG22	1:B:213:TRP:HE1	1.79	0.47
2:H:146:ASP:HA	2:H:156:ALA:HB2	1.96	0.47
2:H:239:PRO:HA	2:H:242:TRP:CE2	2.49	0.47
1:C:239:PRO:HB2	1:C:241:HIS:CE1	2.49	0.47
1:C:241:HIS:CE1	1:C:242:LEU:HG	2.50	0.47
2:F:57:PHE:O	2:F:61:ALA:N	2.46	0.47
1:A:241:HIS:CE1	1:A:242:LEU:HG	2.49	0.47
1:B:138:ALA:O	2:G:84:GLY:HA3	2.14	0.47
2:F:188:ILE:HG21	2:F:345:GLN:HG3	1.95	0.47
1:A:258:GLY:HA2	1:A:281:VAL:HG23	1.96	0.47
1:B:182:LEU:HD23	1:B:213:TRP:CD2	2.50	0.47
1:B:285:LYS:HE3	1:B:326:LEU:O	2.15	0.47
1:C:487:ASP:HB3	1:C:506:LYS:HB3	1.95	0.47
1:D:485:HIS:HB3	1:D:507:ASP:OD2	2.15	0.47
2:G:68:ASP:OD2	2:G:280:SER:OG	2.26	0.47
1:A:231:TRP:CZ2	1:A:256:LYS:HG3	2.50	0.47
1:A:426:ILE:HB	1:A:440:PHE:HB2	1.97	0.47
1:B:172:ASP:HB2	1:B:179:MET:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLY:HA2	1:B:281:VAL:HG23	1.97	0.47
2:F:53:LEU:HA	2:F:56:LYS:HB2	1.97	0.47
2:H:132:LEU:HD21	2:H:136:PRO:HD3	1.96	0.47
1:B:225:LEU:HD23	1:B:263:TRP:CD2	2.50	0.47
2:F:192:GLY:O	2:F:195:ASN:ND2	2.48	0.47
1:C:161:THR:CG2	1:C:171:TRP:HE1	2.29	0.46
1:B:239:PRO:HB2	1:B:241:HIS:CE1	2.51	0.46
2:H:138:THR:HG1	2:H:141:GLU:HG3	1.80	0.46
1:A:286:TRP:HA	1:A:292:LEU:HG	1.97	0.46
1:B:231:TRP:CZ2	1:B:256:LYS:HG3	2.50	0.46
1:D:476:ARG:NH2	5:D:602:SO4:O2	2.43	0.46
2:G:107:VAL:O	2:G:114:ILE:HG12	2.15	0.46
1:C:214:ASP:HB2	1:C:221:LEU:HD21	1.98	0.46
1:D:231:TRP:CZ2	1:D:256:LYS:HG3	2.50	0.46
1:D:482:LEU:H	1:D:482:LEU:HD23	1.80	0.46
2:E:78:GLY:HA3	2:E:342:ASN:O	2.15	0.46
2:G:20:TRP:CD2	2:G:67:PRO:HG3	2.50	0.46
1:D:179:MET:O	1:D:180:HIS:ND1	2.49	0.46
1:D:417:ILE:HG13	1:D:431:GLY:HA2	1.97	0.46
1:C:375:VAL:HG22	1:C:410:PHE:CE2	2.50	0.46
1:C:445:ALA:HB1	1:C:464:LYS:HB3	1.97	0.46
2:G:157:LEU:HB2	2:G:234:MET:HE3	1.97	0.46
2:E:13:GLU:HB3	2:E:16:LYS:HD3	1.97	0.46
2:G:77:PHE:HE2	2:G:273:SER:HB2	1.81	0.46
2:H:120:VAL:HB	2:H:311:ALA:HB3	1.97	0.46
1:D:260:ILE:HB	1:D:274:MET:HE2	1.98	0.45
2:G:140:GLU:OE1	2:G:140:GLU:N	2.46	0.45
2:F:41:THR:HG23	2:F:43:ILE:H	1.82	0.45
2:G:107:VAL:HG21	2:G:117:PRO:HD3	1.97	0.45
2:H:77:PHE:HE2	2:H:273:SER:HB2	1.82	0.45
1:C:187:ASN:HB3	1:C:206:MET:HB3	1.99	0.45
1:D:239:PRO:HB2	1:D:241:HIS:CE1	2.52	0.45
2:G:22:ASN:ND2	2:G:24:ASP:OD1	2.50	0.45
1:A:237:TRP:CE2	1:A:251:LEU:HD13	2.52	0.45
1:A:385:LEU:HB2	1:A:398:MET:HE3	1.99	0.45
1:A:243:VAL:HG21	1:A:249:PRO:HB3	1.99	0.45
1:B:487:ASP:HB3	1:B:506:LYS:HB3	1.99	0.45
1:B:186:TYR:OH	1:D:184:GLY:HA2	2.17	0.44
2:E:146:ASP:HA	2:E:156:ALA:HB2	1.98	0.44
2:F:78:GLY:HA3	2:F:342:ASN:O	2.17	0.44
1:A:157:SER:HA	1:A:173:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:242:TRP:HB2	2:F:308:PRO:HG2	1.99	0.44
1:C:286:TRP:HA	1:C:292:LEU:HG	2.00	0.44
2:H:78:GLY:HA3	2:H:342:ASN:O	2.18	0.44
1:D:482:LEU:HB2	1:D:483:PRO:HD2	1.99	0.44
1:A:485:HIS:CD2	1:A:511:ARG:HD2	2.51	0.44
1:B:445:ALA:HB1	1:B:464:LYS:HB3	1.99	0.44
2:H:255:THR:OG1	2:H:256:VAL:N	2.50	0.44
2:E:157:LEU:HB2	2:E:234:MET:HE3	2.00	0.44
1:C:203:THR:CG2	1:C:213:TRP:HE1	2.31	0.44
1:C:301:VAL:HB	1:C:316:LEU:HB2	1.99	0.44
1:D:375:VAL:HG11	1:D:417:ILE:HD13	2.00	0.44
2:G:87:ALA:HB2	2:G:278:ALA:HA	2.00	0.44
2:G:78:GLY:HA3	2:G:342:ASN:O	2.18	0.44
1:B:248:LYS:HD2	1:B:266:VAL:HG22	2.00	0.43
1:B:329:SER:HA	1:B:410:PHE:CG	2.53	0.43
1:C:172:ASP:HB2	1:C:179:MET:HE3	2.00	0.43
2:F:89:ILE:HD11	2:F:104:TRP:HZ3	1.83	0.43
1:B:286:TRP:HA	1:B:292:LEU:HG	2.01	0.43
1:B:386:TRP:CH2	1:B:394:PRO:HG3	2.53	0.43
1:D:415:ARG:HD3	1:D:416:TYR:CZ	2.53	0.43
2:E:255:THR:OG1	2:E:256:VAL:N	2.52	0.43
1:D:199:GLU:OE1	1:D:248:LYS:NZ	2.35	0.43
1:D:258:GLY:HA2	1:D:281:VAL:HG23	2.01	0.43
1:A:161:THR:HG22	1:A:171:TRP:HE1	1.84	0.43
1:A:219:GLN:HG2	2:E:44:LYS:HG2	1.99	0.43
1:C:274:MET:HE2	1:C:310:GLY:HA2	2.00	0.43
1:D:426:ILE:HB	1:D:440:PHE:HB2	2.01	0.43
1:B:453:SER:HB2	1:B:494:TRP:CE2	2.53	0.43
2:E:99:LEU:HD22	2:E:117:PRO:HG2	1.99	0.43
2:F:239:PRO:HA	2:F:242:TRP:CE2	2.54	0.43
1:B:286:TRP:CE2	1:B:292:LEU:HD11	2.53	0.43
2:F:20:TRP:CD2	2:F:67:PRO:HG3	2.54	0.43
1:C:182:LEU:HD23	1:C:213:TRP:CD2	2.54	0.43
1:C:379:ASP:OD2	3:I:94:ARG:NH1	2.46	0.43
2:E:37:PHE:O	2:E:41:THR:HG22	2.19	0.43
2:G:51:ASP:O	2:G:56:LYS:HE2	2.19	0.43
1:A:325:HIS:CG	1:A:326:LEU:H	2.37	0.42
1:B:485:HIS:HB3	1:B:507:ASP:OD2	2.18	0.42
1:C:179:MET:HE3	1:C:179:MET:HB2	1.94	0.42
1:D:141:GLY:O	1:D:169:ARG:NE	2.52	0.42
2:E:41:THR:HG23	2:E:43:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:146:ASP:HA	2:G:156:ALA:HB2	2.01	0.42
1:A:182:LEU:HD23	1:A:213:TRP:CG	2.54	0.42
1:A:219:GLN:NE2	2:E:44:LYS:HG2	2.34	0.42
2:F:37:PHE:O	2:F:41:THR:HG22	2.19	0.42
2:F:176:GLY:HA2	2:F:195:ASN:HD21	1.84	0.42
1:A:468:LEU:HD21	1:A:489:VAL:HG11	2.00	0.42
1:C:485:HIS:N	1:C:485:HIS:CD2	2.88	0.42
1:D:453:SER:HB2	1:D:494:TRP:CE2	2.55	0.42
2:G:41:THR:HG23	2:G:43:ILE:H	1.85	0.42
3:J:88:PRO:HD2	3:J:91:LEU:HD12	2.00	0.42
1:B:214:ASP:HA	1:B:215:PRO:HD2	1.86	0.42
1:D:398:MET:H	1:D:398:MET:HG2	1.70	0.42
2:G:75:ASP:OD2	4:O:2:GLC:O3	2.27	0.42
2:H:192:GLY:O	2:H:195:ASN:ND2	2.51	0.42
1:A:238:GLU:HA	1:A:239:PRO:HD3	1.86	0.42
1:C:468:LEU:HB2	1:C:482:LEU:HB2	2.01	0.42
2:E:242:TRP:HB2	2:E:308:PRO:HG2	2.02	0.42
1:D:179:MET:HE3	1:D:179:MET:HB2	1.98	0.42
1:A:182:LEU:HD23	1:A:213:TRP:CD2	2.54	0.42
1:B:186:TYR:HE1	1:D:186:TYR:CE1	2.38	0.42
1:B:468:LEU:HD21	1:B:489:VAL:HG11	2.02	0.42
1:C:161:THR:HG22	1:C:171:TRP:HE1	1.84	0.42
1:C:386:TRP:CH2	1:C:394:PRO:HG3	2.55	0.42
2:E:83:SER:HB2	2:E:85:LEU:HG	2.02	0.42
1:A:214:ASP:HA	1:A:215:PRO:HD2	1.86	0.42
1:A:380:ASP:O	1:A:382:THR:HG23	2.19	0.42
1:A:477:LYS:HE2	1:A:477:LYS:HB3	1.81	0.42
1:B:154:HIS:CD2	1:B:155:THR:HG22	2.54	0.42
2:H:140:GLU:OE1	2:H:140:GLU:N	2.48	0.42
1:C:214:ASP:HA	1:C:215:PRO:HD2	1.85	0.42
1:D:325:HIS:CG	1:D:326:LEU:H	2.37	0.42
1:A:187:ASN:HB3	1:A:206:MET:HB3	2.01	0.42
1:B:319:HIS:NE2	1:B:376:THR:OG1	2.42	0.42
1:C:184:GLY:O	1:C:211:ARG:NE	2.53	0.42
1:C:339:PHE:HE1	1:C:345:LYS:HG2	1.85	0.42
2:G:37:PHE:O	2:G:41:THR:HG22	2.20	0.42
2:H:57:PHE:O	2:H:61:ALA:N	2.52	0.42
1:A:329:SER:O	1:A:363:ILE:HD11	2.21	0.41
1:B:238:GLU:HA	1:B:239:PRO:HD3	1.92	0.41
1:C:230:LYS:HB3	1:C:256:LYS:HB3	2.02	0.41
1:C:468:LEU:HD21	1:C:489:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ALA:HB3	1:C:182:LEU:HB2	2.02	0.41
1:C:329:SER:HA	1:C:410:PHE:CG	2.55	0.41
2:F:241:ALA:O	2:F:245:ILE:HG13	2.21	0.41
2:F:255:THR:OG1	2:F:256:VAL:N	2.52	0.41
2:H:138:THR:OG1	2:H:141:GLU:HG3	2.18	0.41
1:B:161:THR:CG2	1:B:171:TRP:HE1	2.31	0.41
1:B:380:ASP:O	1:B:382:THR:HG23	2.21	0.41
1:C:462:CYS:HB2	1:C:489:VAL:HB	2.02	0.41
2:H:13:GLU:HB3	2:H:16:LYS:HD3	2.01	0.41
2:E:140:GLU:OE1	2:E:140:GLU:N	2.52	0.41
1:A:180:HIS:CE1	2:E:35:LYS:HE3	2.56	0.41
1:A:214:ASP:HB2	1:A:221:LEU:HD21	2.03	0.41
1:C:477:LYS:HE2	1:C:477:LYS:HB3	1.81	0.41
1:C:485:HIS:CD2	1:C:511:ARG:HD2	2.56	0.41
1:D:291:LEU:HD11	1:D:389:LEU:HD12	2.03	0.41
1:C:304:TRP:CZ3	1:C:312:CYS:HB2	2.55	0.41
1:D:195:SER:O	1:D:198:GLY:N	2.52	0.41
2:H:241:ALA:O	2:H:245:ILE:HG13	2.21	0.41
1:A:291:LEU:HD11	1:A:389:LEU:HD12	2.02	0.41
1:B:304:TRP:CZ3	1:B:312:CYS:HB2	2.55	0.41
1:B:375:VAL:HG11	1:B:417:ILE:HD13	2.01	0.41
1:C:207:ASP:OD1	1:C:209:THR:OG1	2.39	0.41
1:D:398:MET:HB2	1:D:429:TRP:CZ3	2.56	0.41
1:A:172:ASP:HB2	1:A:179:MET:HE3	2.03	0.41
1:A:274:MET:HE1	1:A:292:LEU:HD22	2.03	0.41
1:B:286:TRP:CZ2	1:B:306:ILE:HG12	2.55	0.41
1:C:248:LYS:HD3	1:C:266:VAL:HG22	2.02	0.41
1:C:393:LYS:HA	1:C:394:PRO:HD3	1.94	0.41
1:D:168:ALA:HB3	1:D:182:LEU:HB2	2.02	0.41
1:D:237:TRP:CZ3	1:D:265:THR:HG21	2.56	0.41
1:D:302:ARG:HD3	1:D:304:TRP:CZ2	2.56	0.41
2:H:159:PHE:HE1	2:H:167:THR:HG22	1.85	0.41
1:A:179:MET:O	1:A:180:HIS:ND1	2.54	0.41
1:B:462:CYS:HB2	1:B:489:VAL:HB	2.03	0.41
2:E:53:LEU:HA	2:E:56:LYS:HB2	2.03	0.41
2:E:77:PHE:CE2	2:E:273:SER:HB2	2.56	0.41
2:H:87:ALA:HB2	2:H:278:ALA:HA	2.03	0.41
1:A:296:SER:OG	1:A:297:HIS:N	2.54	0.40
1:C:398:MET:HB2	1:C:429:TRP:CZ3	2.56	0.40
2:G:132:LEU:HD21	2:G:136:PRO:HD3	2.01	0.40
1:A:453:SER:HB2	1:A:494:TRP:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:SER:OG	1:C:206:MET:N	2.54	0.40
2:E:77:PHE:HE2	2:E:273:SER:HB2	1.86	0.40
2:F:366:THR:HG22	2:F:368:ASP:H	1.86	0.40
1:A:321:HIS:HB3	1:A:379:ASP:HB2	2.02	0.40
1:C:380:ASP:O	1:C:382:THR:HG23	2.21	0.40
2:G:371:LEU:HD23	2:G:371:LEU:HA	1.92	0.40
1:A:302:ARG:HD3	1:A:304:TRP:CZ2	2.57	0.40
2:E:138:THR:OG1	2:E:141:GLU:HG3	2.22	0.40
2:F:146:ASP:HA	2:F:156:ALA:HB2	2.04	0.40
1:B:296:SER:OG	1:B:297:HIS:N	2.54	0.40
2:F:132:LEU:HA	2:F:133:PRO:HD2	1.96	0.40
2:F:280:SER:O	2:F:283:LYS:NZ	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:TYR:OH	5:D:602:SO4:O3[1_565]	2.17	0.03

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	376/381 (99%)	357 (95%)	18 (5%)	1 (0%)	36	68
1	B	376/381 (99%)	358 (95%)	18 (5%)	0	100	100
1	C	376/381 (99%)	358 (95%)	18 (5%)	0	100	100
1	D	376/381 (99%)	358 (95%)	18 (5%)	0	100	100
2	E	367/381 (96%)	356 (97%)	11 (3%)	0	100	100
2	F	366/381 (96%)	354 (97%)	12 (3%)	0	100	100
2	G	367/381 (96%)	355 (97%)	11 (3%)	1 (0%)	36	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	367/381 (96%)	355 (97%)	12 (3%)	0	100	100
3	I	9/22 (41%)	8 (89%)	1 (11%)	0	100	100
3	J	9/22 (41%)	8 (89%)	1 (11%)	0	100	100
3	K	10/22 (46%)	9 (90%)	1 (10%)	0	100	100
3	L	9/22 (41%)	8 (89%)	1 (11%)	0	100	100
All	All	3008/3136 (96%)	2884 (96%)	122 (4%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	GLY
2	G	183	ASN

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	328/330 (99%)	323 (98%)	5 (2%)	57	76
1	B	328/330 (99%)	324 (99%)	4 (1%)	63	79
1	C	328/330 (99%)	324 (99%)	4 (1%)	63	79
1	D	328/330 (99%)	322 (98%)	6 (2%)	51	74
2	E	287/298 (96%)	285 (99%)	2 (1%)	76	83
2	F	286/298 (96%)	284 (99%)	2 (1%)	76	83
2	G	287/298 (96%)	283 (99%)	4 (1%)	59	77
2	H	287/298 (96%)	286 (100%)	1 (0%)	86	88
3	I	10/19 (53%)	10 (100%)	0	100	100
3	J	10/19 (53%)	9 (90%)	1 (10%)	7	30
3	K	11/19 (58%)	11 (100%)	0	100	100
3	L	10/19 (53%)	9 (90%)	1 (10%)	7	30
All	All	2500/2588 (97%)	2470 (99%)	30 (1%)	63	79

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	MET
1	A	363	ILE
1	A	418	VAL
1	A	470	VAL
1	A	509	MET
1	B	247	SER
1	B	363	ILE
1	B	418	VAL
1	B	470	VAL
1	C	363	ILE
1	C	399	THR
1	C	418	VAL
1	C	470	VAL
1	D	274	MET
1	D	363	ILE
1	D	418	VAL
1	D	470	VAL
1	D	482	LEU
1	D	509	MET
2	E	38	GLU
2	E	268	PHE
2	F	229	LYS
2	F	268	PHE
2	G	38	GLU
2	G	180	LYS
2	G	268	PHE
2	G	345	GLN
2	H	268	PHE
3	J	93	ASP
3	L	95	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	219	GLN
1	D	353	GLN
2	E	195	ASN
2	E	377	ASN
2	F	359	ASN
2	F	365	GLN
2	F	377	ASN

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Mol	Chain	Res	Type
2	H	377	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GLC	M	1	4	12,12,12	0.57	0	17,17,17	0.55	0
4	GLC	M	2	4	11,11,12	0.60	0	15,15,17	0.63	0
4	GLC	N	1	4	12,12,12	0.54	0	17,17,17	0.50	0
4	GLC	N	2	4	11,11,12	0.61	0	15,15,17	0.70	0
4	GLC	O	1	4	12,12,12	0.55	0	17,17,17	0.51	0
4	GLC	O	2	4	11,11,12	0.63	0	15,15,17	0.68	0
4	GLC	P	1	4	12,12,12	0.53	0	17,17,17	0.49	0
4	GLC	P	2	4	11,11,12	0.66	0	15,15,17	0.61	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	GLC	M	1	4	-	0/2/22/22	0/1/1/1
4	GLC	M	2	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	N	1	4	-	0/2/22/22	0/1/1/1
4	GLC	N	2	4	-	0/2/19/22	0/1/1/1
4	GLC	O	1	4	-	0/2/22/22	0/1/1/1
4	GLC	O	2	4	-	0/2/19/22	0/1/1/1
4	GLC	P	1	4	-	1/2/22/22	0/1/1/1
4	GLC	P	2	4	-	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:

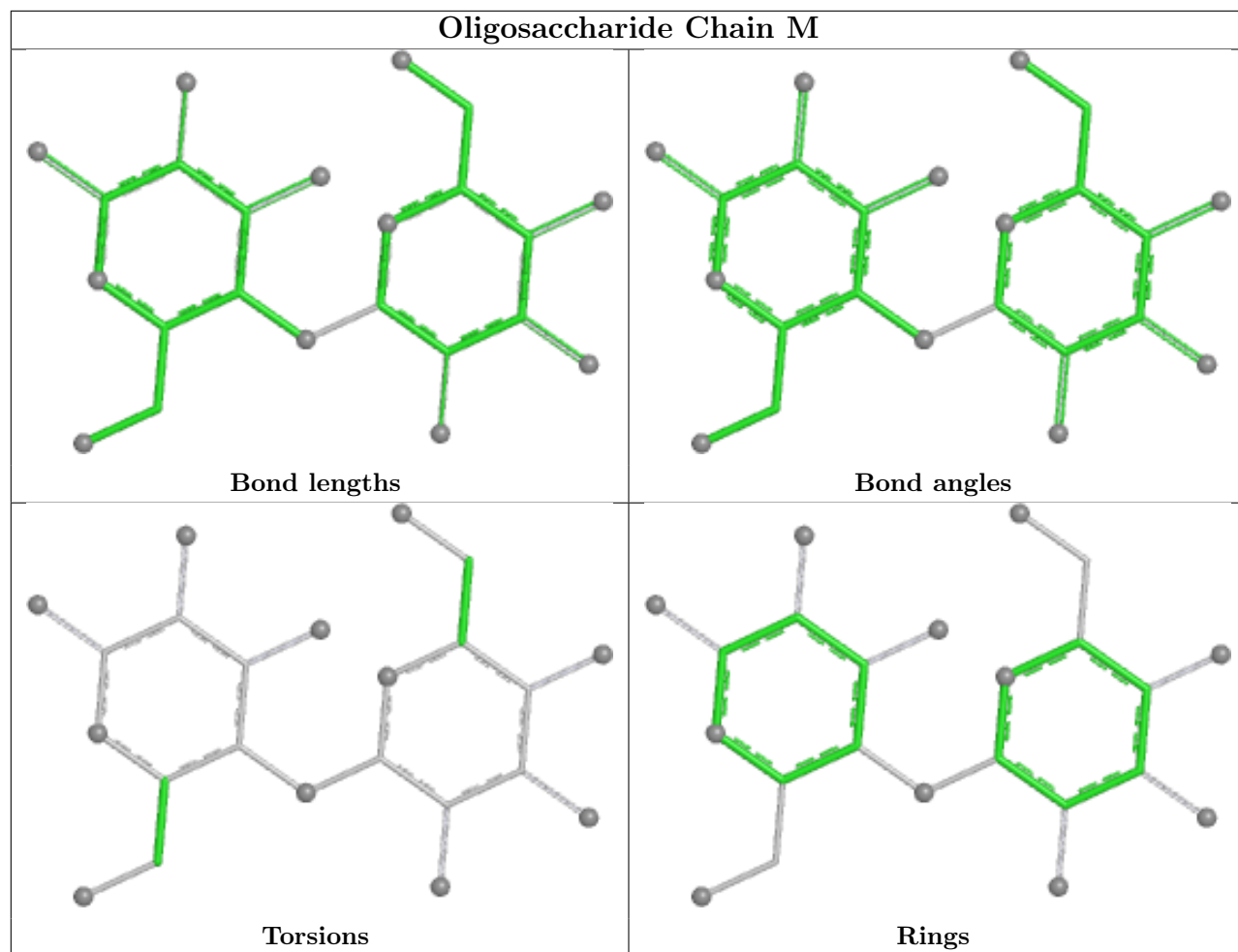
Mol	Chain	Res	Type	Atoms
4	P	1	GLC	C4-C5-C6-O6

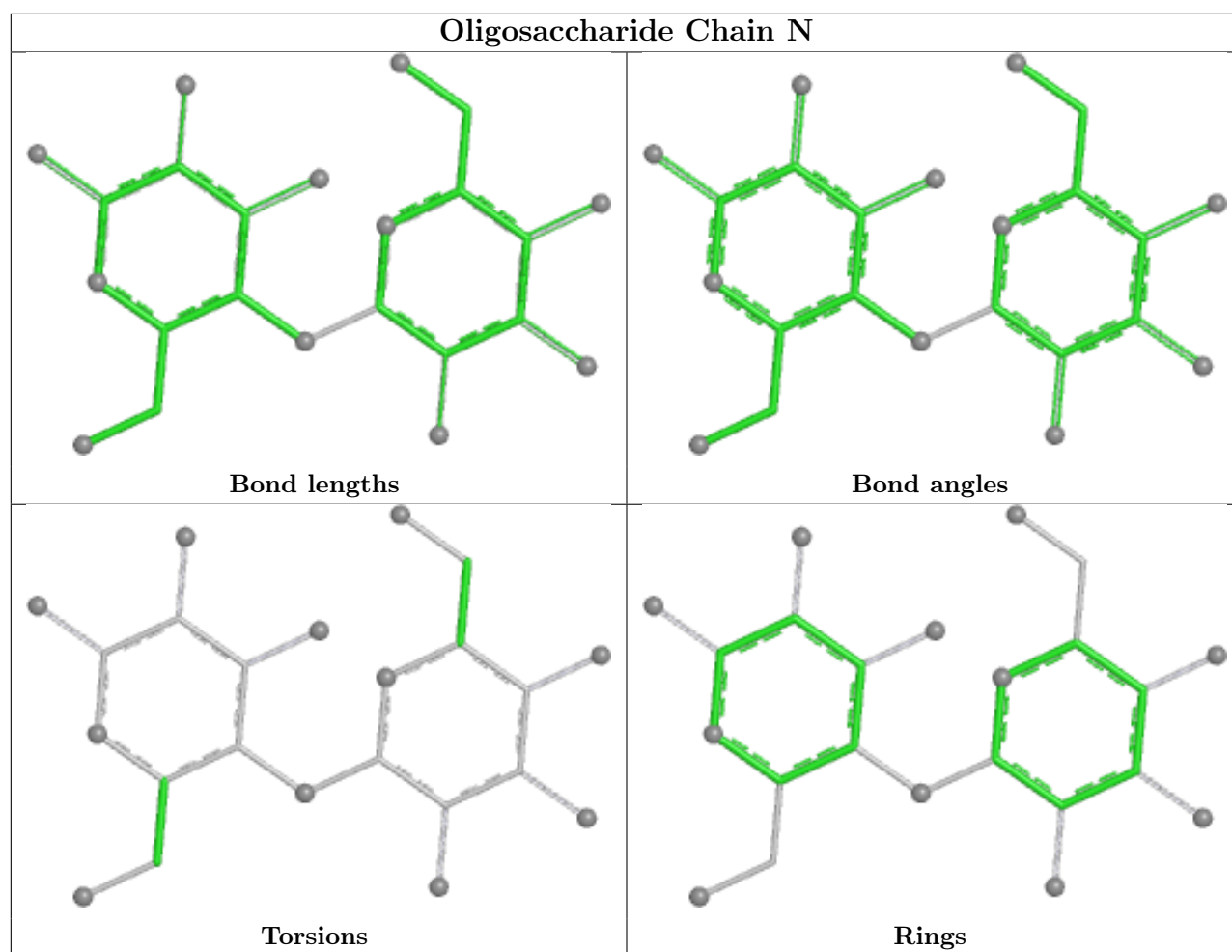
There are no ring outliers.

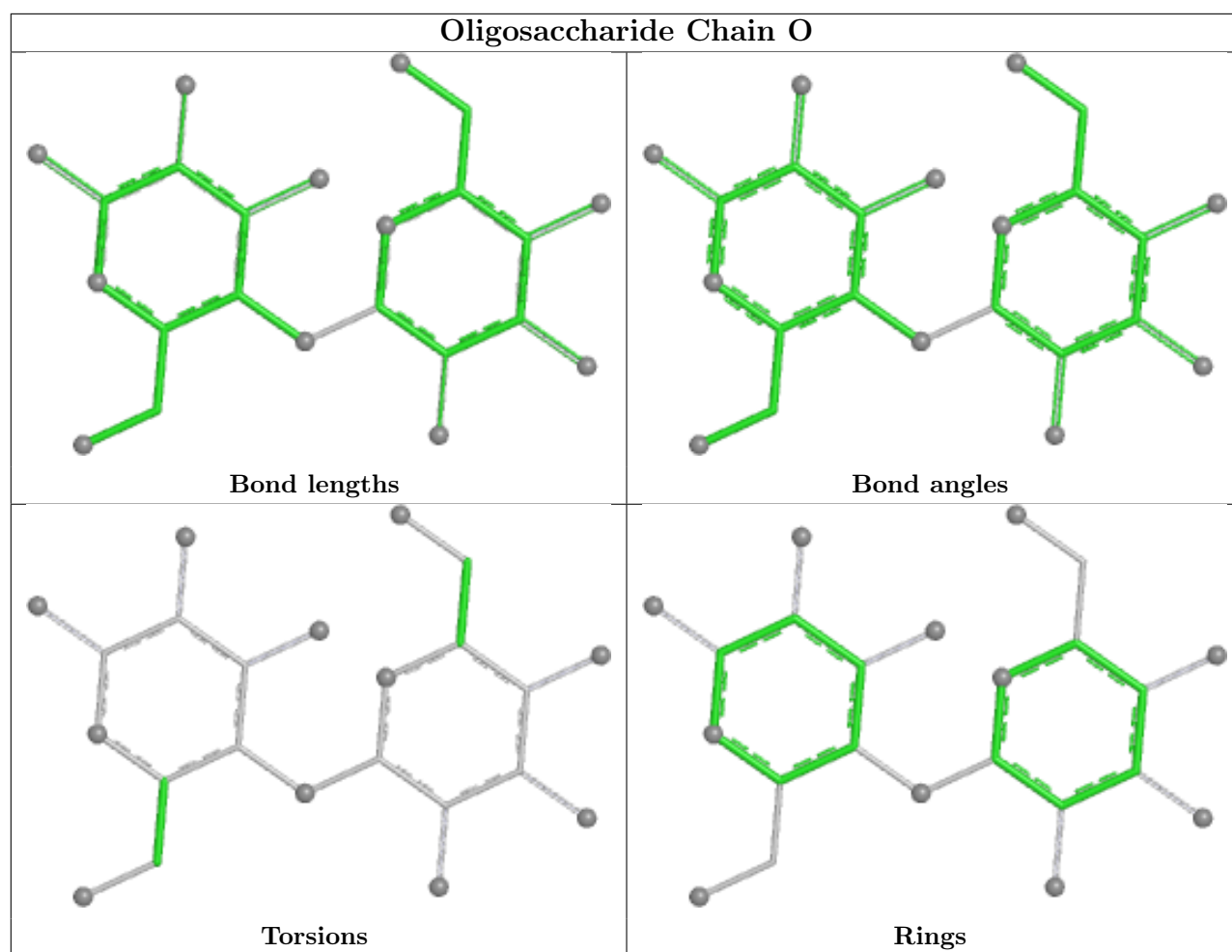
1 monomer is involved in 1 short contact:

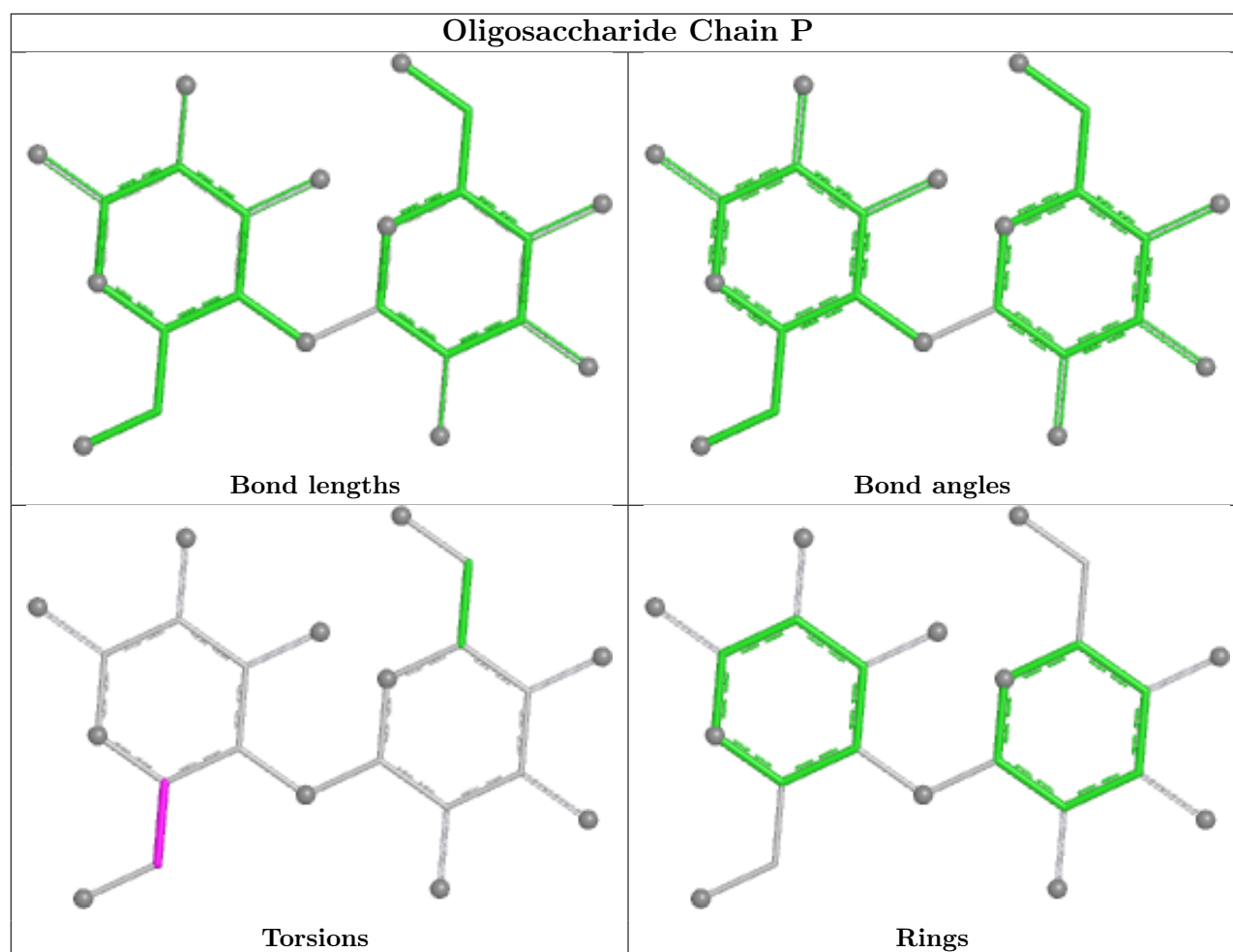
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	2	GLC	1	0

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









5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
5	SO4	A	601	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	D	602	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	C	602	-	4,4,4	0.23	0	6,6,6	0.14	0
5	SO4	D	601	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	B	602	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	D	603	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	B	601	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	A	602	-	4,4,4	0.23	0	6,6,6	0.17	0
5	SO4	C	601	-	4,4,4	0.23	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	602	SO4	1	1

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/381 (99%)	-0.16	0 100 100	45, 83, 146, 187	0
1	B	378/381 (99%)	-0.31	0 100 100	39, 57, 113, 168	0
1	C	378/381 (99%)	-0.18	1 (0%) 90 81	41, 69, 133, 168	0
1	D	378/381 (99%)	-0.26	2 (0%) 87 76	38, 61, 123, 190	0
2	E	369/381 (96%)	-0.54	1 (0%) 90 81	34, 51, 80, 113	0
2	F	368/381 (96%)	-0.43	1 (0%) 90 81	36, 59, 106, 147	0
2	G	369/381 (96%)	-0.49	1 (0%) 90 81	29, 56, 110, 145	0
2	H	369/381 (96%)	-0.27	0 100 100	37, 74, 132, 156	0
3	I	11/22 (50%)	0.02	0 100 100	58, 64, 110, 112	0
3	J	11/22 (50%)	-0.19	0 100 100	51, 60, 119, 126	0
3	K	12/22 (54%)	0.10	0 100 100	61, 64, 126, 142	0
3	L	11/22 (50%)	0.03	0 100 100	50, 53, 84, 112	0
All	All	3032/3136 (96%)	-0.32	6 (0%) 91 85	29, 62, 124, 190	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	184	GLY	2.2
1	D	140	ALA	2.2
1	C	483	PRO	2.2
2	E	379	ALA	2.2
2	G	183	ASN	2.1
1	D	483	PRO	2.1

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

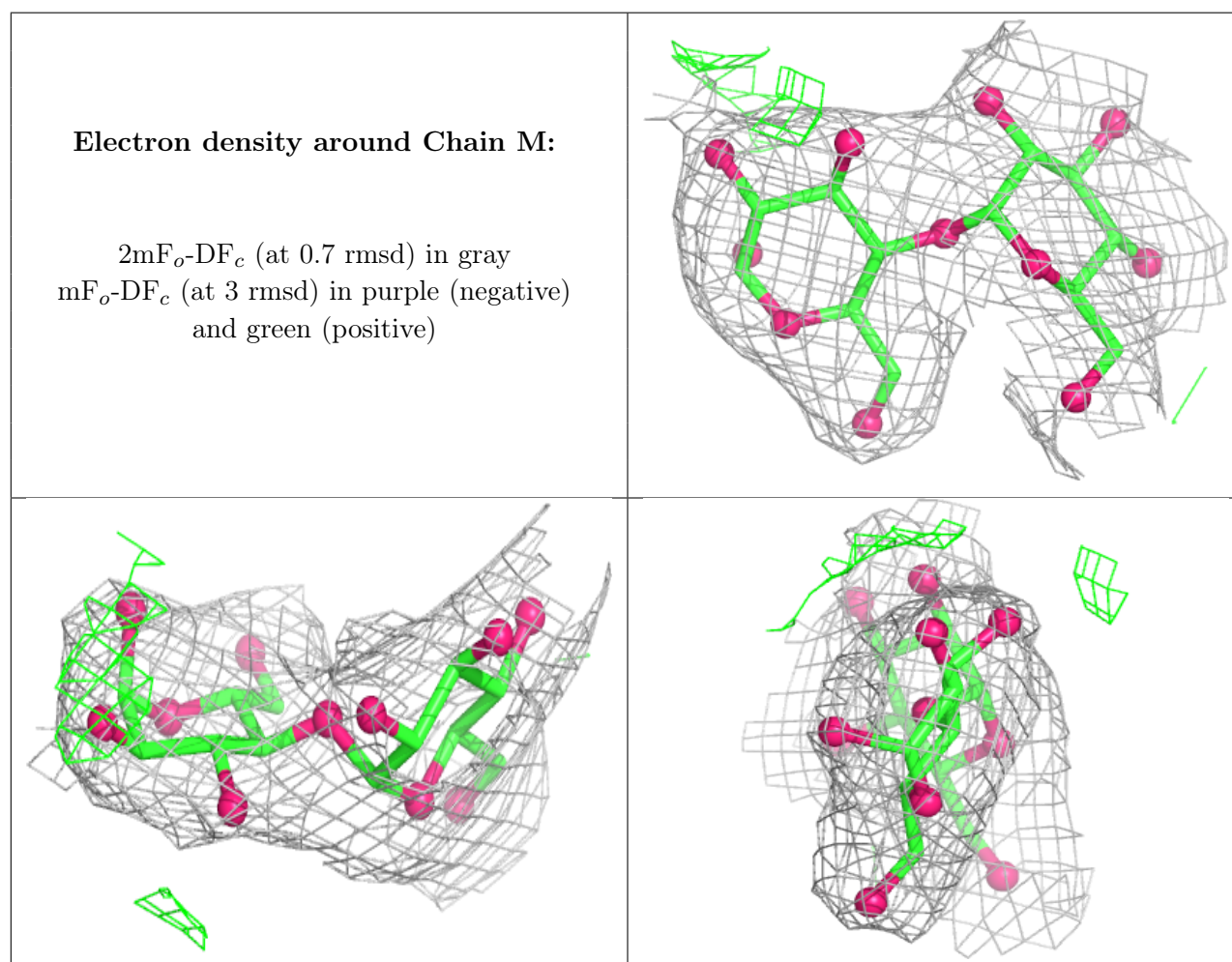
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

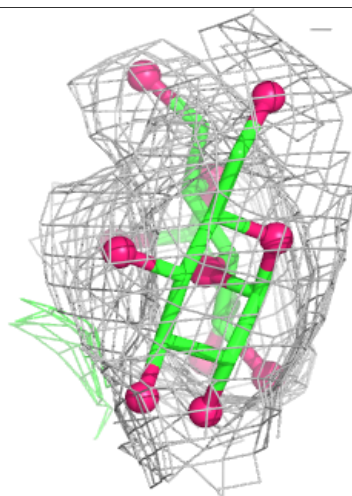
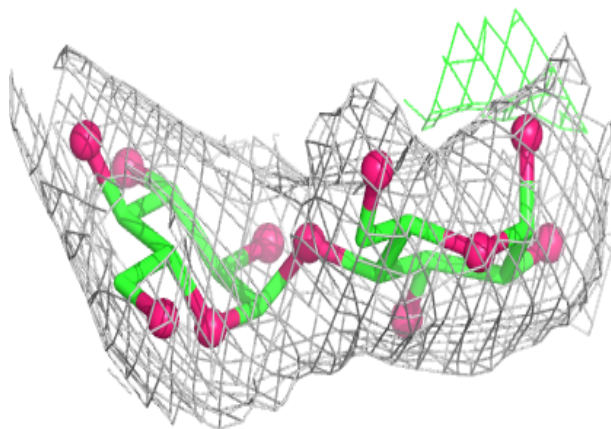
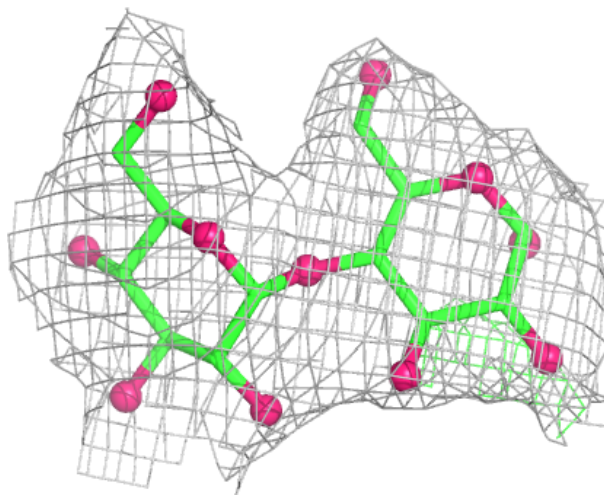
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GLC	N	1	12/12	0.94	0.06	41,49,52,52	0
4	GLC	P	1	12/12	0.94	0.08	47,55,69,73	0
4	GLC	P	2	11/12	0.94	0.07	41,46,53,57	0
4	GLC	N	2	11/12	0.95	0.05	40,47,52,60	0
4	GLC	M	2	11/12	0.95	0.06	20,31,39,44	0
4	GLC	M	1	12/12	0.95	0.06	33,44,48,50	0
4	GLC	O	1	12/12	0.96	0.06	29,36,49,68	0
4	GLC	O	2	11/12	0.96	0.05	22,26,36,40	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.



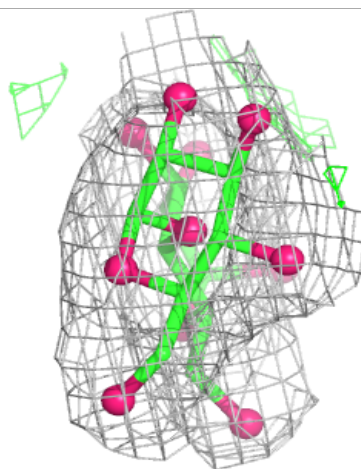
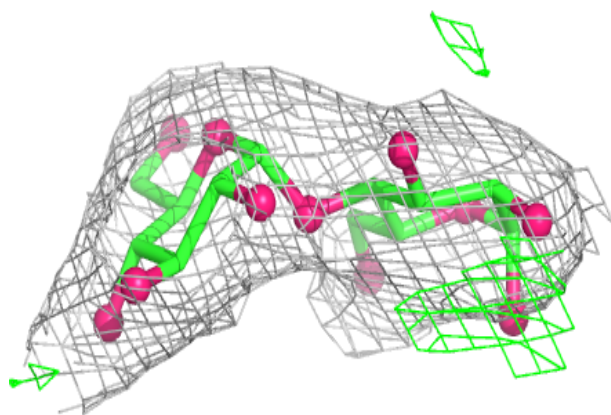
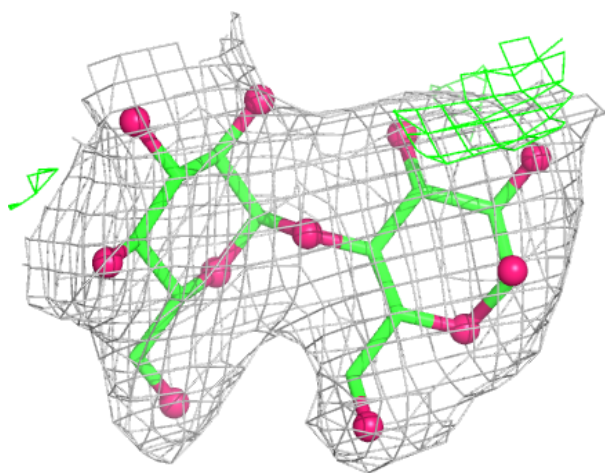
Electron density around Chain N:

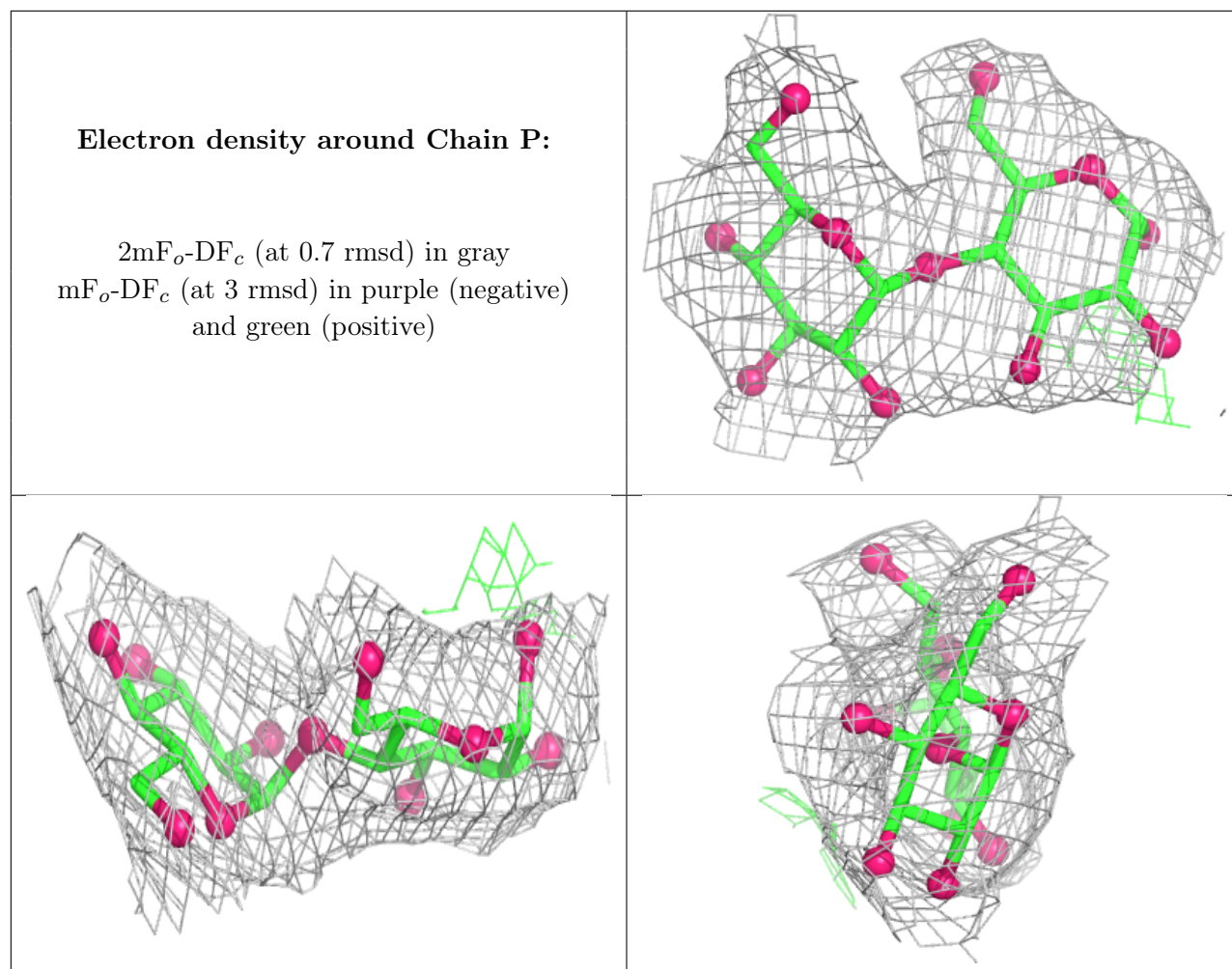
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain O:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	A	602	5/5	0.70	0.15	69,78,85,92	0
5	SO4	A	603	5/5	0.86	0.08	105,106,107,115	0
5	SO4	C	601	5/5	0.87	0.07	83,84,87,92	0
5	SO4	B	602	5/5	0.88	0.09	77,79,80,84	0
5	SO4	A	601	5/5	0.91	0.06	80,80,83,85	0
5	SO4	B	601	5/5	0.92	0.07	70,70,74,77	0
5	SO4	C	602	5/5	0.93	0.06	64,65,69,70	0
5	SO4	D	601	5/5	0.93	0.06	65,68,69,73	0
5	SO4	D	603	5/5	0.95	0.05	62,63,66,70	0
5	SO4	D	602	5/5	0.97	0.05	42,43,45,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.