



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:47 PM BST

PDB ID : 1L6I  
Title : Crystal Structure of the Maltodextrin Phosphorylase complexed with the products of the enzymatic reaction between glucose-1-phosphate and maltopentaose  
Authors : Geremia, S.; Campagnolo, M.; Schinzel, R.; Johnson, L.N.  
Deposited on : 2002-03-11  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

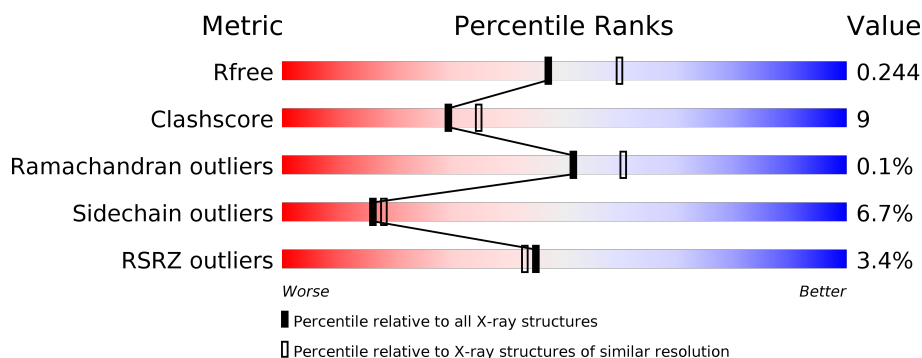
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	796	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	796	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>.</div> </div> </div>
2	C	5	<div> <div></div> <div> <div>60%</div> <div>40%</div> </div> </div>
2	D	5	<div> <div></div> <div> <div>80%</div> <div>20%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	999	-	-	X	-
3	PO4	B	999	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14135 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	S	0	0	0
			6390	4079	1128	1163	20			
1	B	796	Total	C	N	O	S	0	0	0
			6390	4079	1128	1163	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	HIS	SEE REMARK 999	GB 606352
A	262	PHE	THR	SEE REMARK 999	GB 606352
A	263	GLU	ALA	SEE REMARK 999	GB 606352
B	261	ALA	HIS	SEE REMARK 999	GB 606352
B	262	PHE	THR	SEE REMARK 999	GB 606352
B	263	GLU	ALA	SEE REMARK 999	GB 606352

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



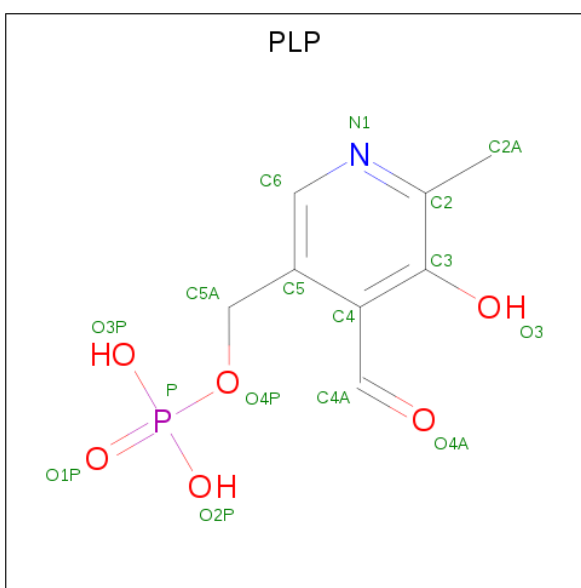
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total	C	O	0	0	0
			56	30	26			
2	D	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	P		0	0
			5	4	1			
3	B	1	Total	O	P		0	0
			5	4	1			

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

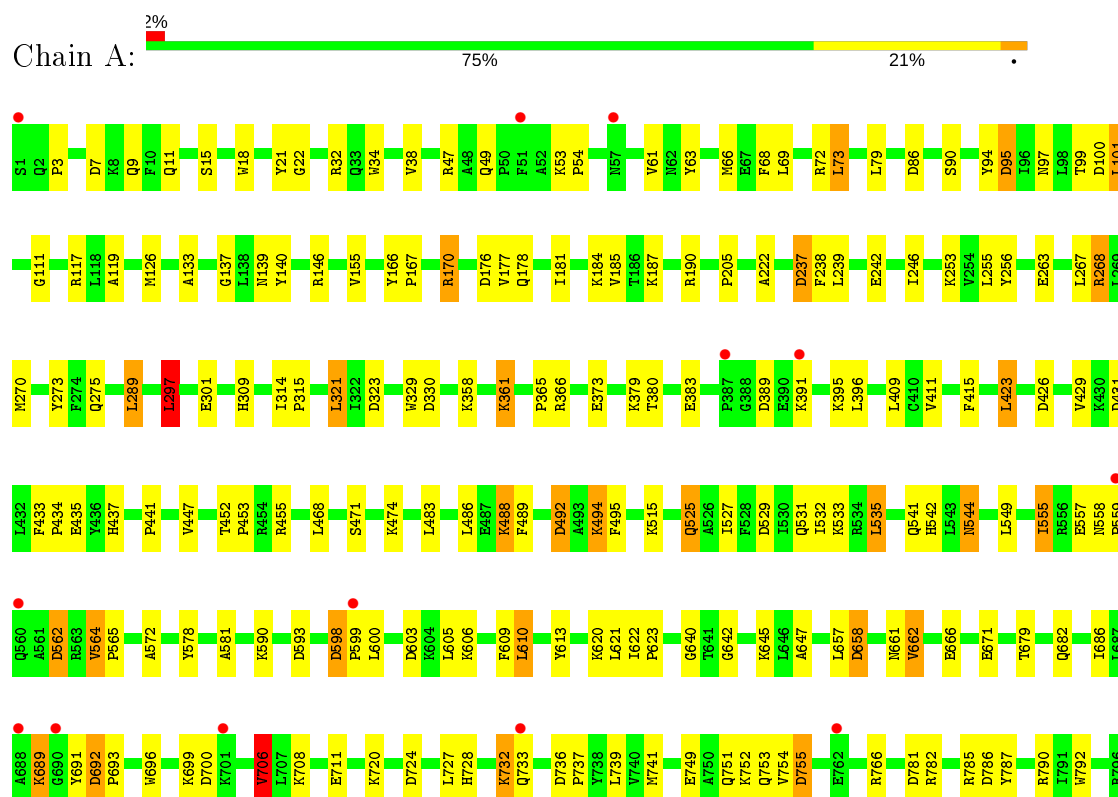
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	606	Total 606	O 606	0	0
5	B	597	Total 597	O 597	0	0

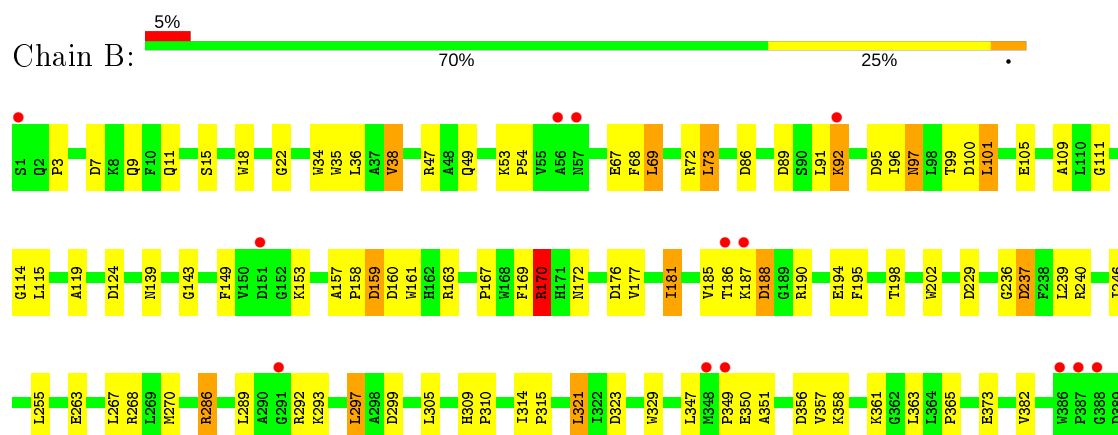
### 3 Residue-property plots

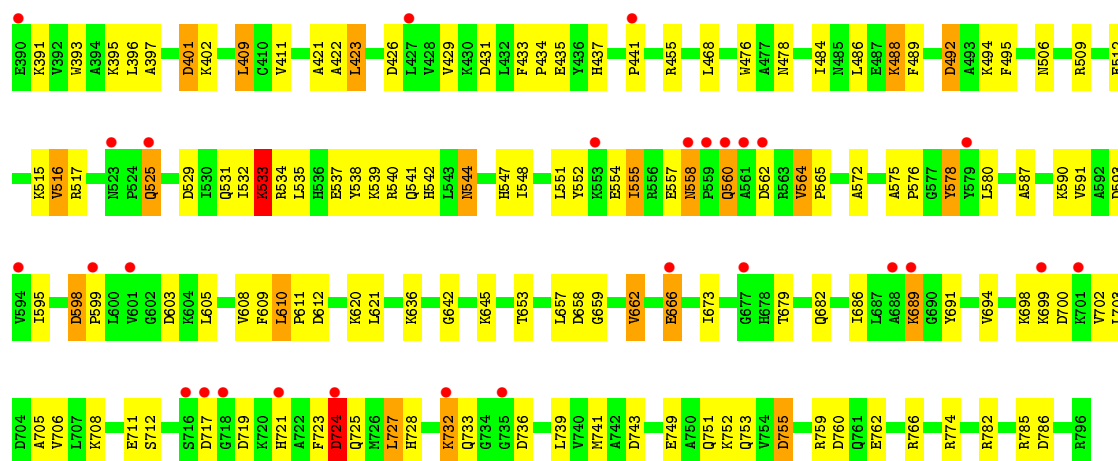
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: MALTODEXTRIN PHOSPHORYLASE



#### • Molecule 1: MALTODEXTRIN PHOSPHORYLASE





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

Chain C: 60% 40%



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

Chain D: 80% 20%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.33Å 105.94Å 218.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 18.54 – 2.18	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-2.20) 90.4 (18.54-2.18)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.197 , 0.243 0.198 , 0.244	Depositor DCC
$R_{free}$ test set	4091 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, GLC, PLP

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	1.18	10/6540 (0.2%)	1.23	52/8865 (0.6%)
1	B	1.18	5/6540 (0.1%)	1.20	50/8865 (0.6%)
All	All	1.18	15/13080 (0.1%)	1.22	102/17730 (0.6%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	723	PHE	CE2-CZ	6.05	1.48	1.37
1	A	696	TRP	CB-CG	-5.96	1.39	1.50
1	A	140	TYR	CE2-CZ	-5.67	1.31	1.38
1	B	194	GLU	CD-OE1	5.63	1.31	1.25
1	A	222	ALA	CA-CB	5.61	1.64	1.52
1	A	613	TYR	CD2-CE2	-5.50	1.31	1.39
1	A	415	PHE	CE2-CZ	5.31	1.47	1.37
1	A	63	TYR	CE1-CZ	-5.28	1.31	1.38
1	A	155	VAL	CB-CG1	5.24	1.63	1.52
1	A	256	TYR	CD1-CE1	5.20	1.47	1.39
1	B	170	ARG	CG-CD	5.13	1.64	1.51
1	B	759	ARG	CZ-NH1	5.11	1.39	1.33
1	A	662	VAL	CB-CG2	-5.11	1.42	1.52
1	B	666	GLU	CD-OE2	5.03	1.31	1.25
1	A	706	VAL	CB-CG1	-5.01	1.42	1.52

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ARG	NE-CZ-NH1	16.63	128.61	120.30
1	A	268	ARG	NE-CZ-NH2	-16.25	112.18	120.30
1	A	492	ASP	CB-CG-OD2	12.90	129.91	118.30
1	A	72	ARG	NE-CZ-NH1	-10.21	115.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ASP	CB-CG-OD2	9.97	127.27	118.30
1	B	323	ASP	CB-CG-OD2	9.81	127.13	118.30
1	A	117	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	B	286	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	529	ASP	CB-CG-OD2	8.69	126.12	118.30
1	B	286	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	B	786	ASP	CB-CG-OD2	8.38	125.84	118.30
1	A	95	ASP	CB-CG-OD2	8.07	125.57	118.30
1	A	268	ARG	CD-NE-CZ	8.03	134.85	123.60
1	A	755	ASP	CB-CG-OD2	8.01	125.51	118.30
1	B	529	ASP	CB-CG-OD2	7.93	125.44	118.30
1	B	229	ASP	CB-CG-OD1	7.93	125.43	118.30
1	B	124	ASP	CB-CG-OD2	7.74	125.26	118.30
1	B	86	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	658	ASP	CB-CG-OD2	7.52	125.06	118.30
1	B	101	LEU	CB-CG-CD1	-7.42	98.39	111.00
1	B	759	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	786	ASP	CB-CG-OD2	7.18	124.76	118.30
1	A	562	ASP	CB-CG-OD2	7.17	124.76	118.30
1	B	492	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	781	ASP	CB-CG-OD2	6.99	124.59	118.30
1	B	724	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	389	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	159	ASP	CB-CG-OD2	6.86	124.48	118.30
1	A	700	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	47	ARG	NE-CZ-NH1	-6.71	116.95	120.30
1	A	790	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	101	LEU	CB-CG-CD1	-6.64	99.72	111.00
1	A	237	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	593	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	289	LEU	CB-CG-CD1	-6.50	99.95	111.00
1	A	297	LEU	CB-CG-CD2	6.50	122.04	111.00
1	B	124	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	B	760	ASP	CB-CG-OD2	6.31	123.97	118.30
1	B	426	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	409	LEU	CA-CB-CG	6.29	129.77	115.30
1	B	297	LEU	CA-CB-CG	6.28	129.75	115.30
1	B	95	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	268	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	86	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	426	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	598	ASP	CB-CG-OD2	6.06	123.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	593	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	176	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	692	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	755	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	321	LEU	CA-CB-CG	5.80	128.65	115.30
1	B	540	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	658	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	A	790	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	409	LEU	CA-CB-CG	5.73	128.49	115.30
1	B	401	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	321	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	455	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	B	423	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	782	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	126	MET	CG-SD-CE	5.63	109.21	100.20
1	B	724	ASP	CB-CG-OD1	-5.58	113.27	118.30
1	B	610	LEU	CB-CA-C	-5.55	99.66	110.20
1	A	177	VAL	CG1-CB-CG2	5.51	119.72	110.90
1	B	719	ASP	CB-CG-OD2	5.47	123.23	118.30
1	B	455	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	B	743	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	72	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	610	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	A	330	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	774	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	146	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	603	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	612	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	297	LEU	CA-CB-CG	5.29	127.48	115.30
1	A	492	ASP	OD1-CG-OD2	-5.28	113.26	123.30
1	A	72	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	176	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	79	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	724	ASP	N-CA-CB	5.24	120.02	110.60
1	A	431	ASP	CB-CA-C	-5.23	99.94	110.40
1	A	253	LYS	CD-CE-NZ	-5.22	99.68	111.70
1	A	205	PRO	N-CD-CG	-5.22	95.37	103.20
1	A	273	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	B	739	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	423	LEU	CA-CB-CG	5.21	127.27	115.30
1	B	69	LEU	CB-CG-CD1	5.18	119.81	111.00
1	B	160	ASP	N-CA-CB	-5.18	101.27	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	GLY	N-CA-C	-5.18	100.15	113.10
1	B	292	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	534	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	739	LEU	CA-CB-CG	5.15	127.14	115.30
1	B	700	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	782	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	598	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	603	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	73	LEU	CA-CB-CG	5.06	126.95	115.30
1	B	431	ASP	CB-CA-C	-5.06	100.28	110.40
1	B	198	THR	OG1-CB-CG2	-5.05	98.37	110.00
1	B	73	LEU	CB-CG-CD1	5.05	119.58	111.00
1	B	299	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	289	LEU	CB-CG-CD1	-5.03	102.45	111.00

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	6390	0	6333	109	0
1	B	6390	0	6333	143	0
2	C	56	0	48	3	0
2	D	56	0	48	3	0
3	A	5	0	0	2	0
3	B	5	0	0	3	0
4	A	15	0	7	0	0
4	B	15	0	7	0	0
5	A	606	0	0	11	0
5	B	597	0	0	16	0
All	All	14135	0	12776	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:GLN:N	1:A:733:GLN:OE1	2.05	0.88
1:A:22:GLY:CA	1:B:170:ARG:HD2	2.11	0.79
1:B:733:GLN:OE1	1:B:733:GLN:N	2.14	0.79
1:A:22:GLY:HA3	1:B:170:ARG:HD2	1.65	0.79
1:A:437:HIS:CD2	1:A:441:PRO:HA	2.17	0.78
1:B:97:ASN:HD21	1:B:99:THR:HB	1.47	0.78
1:B:762:GLU:O	1:B:766:ARG:HG3	1.85	0.76
1:B:97:ASN:HD22	1:B:100:ASP:H	1.31	0.76
1:A:699:LYS:HB2	5:A:1321:HOH:O	1.86	0.74
1:B:702:VAL:HA	5:B:1510:HOH:O	1.86	0.74
1:A:97:ASN:HD22	1:A:100:ASP:H	1.34	0.74
1:A:3:PRO:HB3	1:A:49:GLN:OE1	1.91	0.71
1:A:97:ASN:HD21	1:A:99:THR:HB	1.54	0.70
1:A:492:ASP:OD2	1:A:494:LYS:HE3	1.92	0.70
1:B:47:ARG:HD3	5:B:1594:HOH:O	1.92	0.70
1:B:89:ASP:O	1:B:92:LYS:HG2	1.93	0.69
1:A:749:GLU:O	1:A:752:LYS:HB2	1.91	0.69
1:B:599:PRO:HA	5:B:1549:HOH:O	1.95	0.67
1:A:361:LYS:HE3	5:A:1046:HOH:O	1.95	0.66
1:A:642:GLY:HA2	1:A:645:LYS:HD2	1.77	0.66
1:A:468:LEU:HD23	1:A:486:LEU:HD11	1.77	0.66
1:B:437:HIS:CD2	1:B:441:PRO:HA	2.30	0.66
1:B:537:GLU:OE1	1:B:580:LEU:HD23	1.95	0.65
1:B:636:LYS:NZ	5:B:1524:HOH:O	2.31	0.63
1:B:544:ASN:HD22	1:B:544:ASN:C	2.02	0.63
1:B:97:ASN:ND2	1:B:100:ASP:H	1.97	0.62
1:B:733:GLN:H	1:B:733:GLN:CD	2.00	0.62
3:A:999:PO4:O4	2:C:4:GLC:H61	2.00	0.62
1:B:557:GLU:O	1:B:558:ASN:HB2	2.00	0.61
1:B:658:ASP:O	1:B:659:GLY:C	2.38	0.61
1:B:115:LEU:H	2:D:4:GLC:H61	1.65	0.60
1:A:238:PHE:HE2	1:B:263:GLU:HG3	1.67	0.60
1:B:488:LYS:HG3	5:B:1468:HOH:O	2.02	0.60
1:A:733:GLN:H	1:A:733:GLN:CD	1.96	0.60
1:A:15:SER:HA	1:A:18:TRP:NE1	2.16	0.59
1:B:558:ASN:OD1	1:B:560:GLN:HB2	2.02	0.59
3:B:999:PO4:O4	2:D:4:GLC:H61	2.01	0.59
1:A:728:HIS:ND1	1:A:733:GLN:HG2	2.18	0.58
1:B:7:ASP:O	1:B:11:GLN:HG2	2.03	0.58
1:B:532:ILE:O	1:B:533:LYS:HB3	2.02	0.58
1:B:3:PRO:HB3	1:B:49:GLN:OE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:VAL:HG23	1:A:365:PRO:HB2	1.86	0.57
1:B:492:ASP:C	1:B:492:ASP:OD1	2.41	0.57
1:A:69:LEU:HD13	1:A:111:GLY:C	2.25	0.57
1:A:395:LYS:NZ	1:A:435:GLU:OE1	2.38	0.57
1:B:286:ARG:NE	5:B:1505:HOH:O	2.22	0.57
1:B:686:ILE:HG22	1:B:691:TYR:HB2	1.86	0.56
1:B:724:ASP:OD1	1:B:724:ASP:N	2.38	0.56
1:A:489:PHE:HB3	1:A:495:PHE:CG	2.40	0.56
1:B:35:TRP:CE2	1:B:105:GLU:HB2	2.40	0.56
1:B:305:LEU:HD22	1:B:310:PRO:HB2	1.88	0.56
1:A:396:LEU:HD21	1:A:435:GLU:HB2	1.88	0.56
1:A:598:ASP:OD1	1:A:598:ASP:C	2.45	0.55
1:B:395:LYS:NZ	1:B:435:GLU:OE1	2.39	0.55
1:A:329:TRP:CZ3	1:A:373:GLU:HG2	2.40	0.55
1:B:590:LYS:NZ	5:B:1312:HOH:O	2.27	0.55
1:A:468:LEU:CD2	1:A:486:LEU:HD11	2.36	0.55
1:A:329:TRP:CH2	1:A:373:GLU:HG2	2.41	0.55
1:B:525:GLN:HE21	1:B:525:GLN:HA	1.71	0.55
1:A:21:TYR:O	1:B:172:ASN:HB2	2.06	0.55
1:A:686:ILE:HG22	1:A:691:TYR:HB2	1.88	0.55
1:B:620:LYS:NZ	5:B:1334:HOH:O	2.40	0.55
1:B:749:GLU:O	1:B:752:LYS:HB2	2.07	0.54
1:B:181:ILE:HG22	1:B:195:PHE:HB3	1.88	0.54
1:A:658:ASP:O	1:A:661:ASN:HB2	2.08	0.54
1:B:15:SER:HA	1:B:18:TRP:NE1	2.24	0.53
1:A:263:GLU:OE2	1:B:236:GLY:O	2.26	0.53
1:B:538:TYR:CZ	1:B:539:LYS:HE2	2.43	0.53
1:A:474:LYS:HD2	5:A:1367:HOH:O	2.08	0.53
1:A:728:HIS:ND1	1:A:733:GLN:NE2	2.56	0.53
1:B:433:PHE:N	1:B:434:PRO:CD	2.72	0.53
1:A:7:ASP:OD1	1:A:90:SER:OG	2.26	0.52
1:B:489:PHE:HB3	1:B:495:PHE:CG	2.44	0.52
1:B:560:GLN:NE2	1:B:560:GLN:HA	2.24	0.52
5:A:1517:HOH:O	2:C:1:GLC:H1	2.09	0.52
1:B:109:ALA:HB1	1:B:143:GLY:HA3	1.91	0.52
3:B:999:PO4:O4	2:D:4:GLC:O4	2.26	0.52
3:A:999:PO4:O4	2:C:4:GLC:O4	2.27	0.52
1:A:525:GLN:HA	1:A:525:GLN:HE21	1.75	0.51
1:A:178:GLN:NE2	5:A:1443:HOH:O	2.43	0.51
1:B:721:HIS:O	1:B:724:ASP:OD1	2.28	0.51
1:A:751:GLN:O	1:A:754:VAL:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASP:O	1:A:11:GLN:HG2	2.11	0.50
1:A:68:PHE:CE1	1:A:119:ALA:HB1	2.45	0.50
1:B:309:HIS:HB2	1:B:310:PRO:HD3	1.93	0.50
1:A:531:GLN:HE22	1:A:541:GLN:HA	1.75	0.50
1:B:237:ASP:OD2	1:B:240:ARG:NH1	2.45	0.50
1:A:97:ASN:ND2	1:A:100:ASP:H	2.06	0.50
1:A:97:ASN:ND2	1:A:99:THR:HB	2.24	0.50
1:B:699:LYS:HE2	1:B:699:LYS:HA	1.94	0.50
1:B:544:ASN:O	1:B:548:ILE:HG13	2.12	0.49
1:B:34:TRP:O	1:B:38:VAL:HG13	2.12	0.49
1:B:682:GLN:HB3	5:B:1469:HOH:O	2.10	0.49
1:B:694:VAL:O	1:B:698:LYS:HG2	2.11	0.49
1:B:185:VAL:HG23	1:B:365:PRO:HB2	1.93	0.49
1:A:94:TYR:O	1:A:95:ASP:HB2	2.12	0.49
1:B:358:LYS:HG2	1:B:358:LYS:O	2.10	0.49
1:B:329:TRP:CZ3	1:B:373:GLU:HG2	2.47	0.49
1:B:433:PHE:N	1:B:434:PRO:HD3	2.27	0.49
1:A:606:LYS:HE3	5:A:1509:HOH:O	2.12	0.49
1:B:157:ALA:HB1	1:B:158:PRO:CD	2.43	0.49
1:B:185:VAL:CG2	1:B:365:PRO:HB2	2.43	0.49
1:B:512:GLU:O	1:B:516:VAL:HG13	2.13	0.49
1:B:717:ASP:O	1:B:717:ASP:CG	2.51	0.49
1:B:554:GLU:HA	5:B:1474:HOH:O	2.13	0.49
1:A:492:ASP:C	1:A:492:ASP:OD1	2.50	0.49
1:A:535:LEU:HD12	1:A:581:ALA:HB1	1.94	0.49
1:A:267:LEU:HA	1:A:270:MET:HE2	1.95	0.48
1:B:267:LEU:HA	1:B:270:MET:HE2	1.95	0.48
1:A:238:PHE:HE2	1:B:263:GLU:CG	2.27	0.48
1:A:61:VAL:O	1:A:133:ALA:HA	2.14	0.48
1:A:622:ILE:N	1:A:623:PRO:CD	2.77	0.48
1:A:671:GLU:CD	1:A:671:GLU:H	2.17	0.48
1:B:149:PHE:HA	1:B:153:LYS:O	2.14	0.48
1:A:544:ASN:C	1:A:544:ASN:HD22	2.18	0.48
1:A:69:LEU:HD13	1:A:111:GLY:CA	2.44	0.48
1:B:314:ILE:HB	1:B:315:PRO:HD3	1.96	0.47
1:B:727:LEU:HD13	1:B:727:LEU:N	2.29	0.47
1:B:53:LYS:HA	1:B:54:PRO:HD3	1.63	0.47
1:A:185:VAL:HA	1:A:190:ARG:O	2.15	0.47
1:B:159:ASP:OD2	5:B:1093:HOH:O	2.20	0.47
1:B:703:LEU:HD11	1:B:741:MET:SD	2.54	0.47
1:A:297:LEU:HD22	1:A:301:GLU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:LYS:HA	1:B:711:GLU:OE1	2.14	0.47
1:B:468:LEU:HD23	1:B:486:LEU:HD11	1.97	0.47
1:A:170:ARG:HD2	1:B:22:GLY:HA3	1.96	0.47
1:B:35:TRP:CZ2	1:B:105:GLU:HB2	2.49	0.47
1:B:185:VAL:HA	1:B:190:ARG:O	2.15	0.46
1:B:67:GLU:HB2	1:B:111:GLY:HA2	1.98	0.46
1:B:724:ASP:O	1:B:725:GLN:C	2.52	0.46
1:B:468:LEU:CD2	1:B:486:LEU:HD11	2.45	0.46
1:B:564:VAL:HG23	1:B:565:PRO:HD2	1.98	0.46
1:B:587:ALA:O	1:B:591:VAL:HG23	2.16	0.46
1:B:679:THR:OG1	1:B:682:GLN:HG3	2.16	0.46
1:B:69:LEU:HD13	1:B:111:GLY:C	2.36	0.46
1:A:720:LYS:HD2	5:A:1465:HOH:O	2.16	0.46
1:B:114:GLY:H	3:B:999:PO4:P	2.39	0.45
1:B:708:LYS:O	1:B:712:SER:HB3	2.16	0.45
1:A:598:ASP:HA	1:A:599:PRO:HD2	1.81	0.45
1:A:489:PHE:HB3	1:A:495:PHE:CD1	2.51	0.45
1:A:238:PHE:CE2	1:B:263:GLU:HG3	2.50	0.45
1:B:653:THR:HB	1:B:673:ILE:HG13	1.98	0.45
1:B:657:LEU:HD22	1:B:662:VAL:HB	1.98	0.45
1:B:68:PHE:CE1	1:B:119:ALA:HB1	2.52	0.45
1:A:3:PRO:HB3	1:A:49:GLN:CD	2.37	0.45
1:A:549:LEU:HB3	1:A:706:VAL:HG22	1.98	0.45
1:B:547:HIS:CE1	1:B:751:GLN:HG3	2.51	0.45
1:B:558:ASN:OD1	1:B:558:ASN:C	2.54	0.45
1:B:699:LYS:HB2	5:B:1347:HOH:O	2.15	0.45
1:A:474:LYS:CD	5:A:1367:HOH:O	2.64	0.45
1:A:246:ILE:CD1	1:B:239:LEU:HD12	2.47	0.45
1:B:517:ARG:NH2	1:B:611:PRO:O	2.50	0.45
1:A:732:LYS:HD3	1:A:732:LYS:HA	1.79	0.45
1:A:724:ASP:N	1:A:724:ASP:OD1	2.49	0.44
1:B:161:TRP:CE2	1:B:163:ARG:HB2	2.51	0.44
1:B:329:TRP:CH2	1:B:373:GLU:HG2	2.52	0.44
1:B:552:TYR:O	1:B:555:ILE:HG12	2.17	0.44
1:B:590:LYS:HA	1:B:590:LYS:HD2	1.77	0.44
1:A:53:LYS:HA	1:A:54:PRO:HD3	1.78	0.44
1:A:527:ILE:HD12	1:A:564:VAL:HG22	2.00	0.44
1:B:36:LEU:HD23	1:B:167:PRO:HG3	1.98	0.44
1:B:728:HIS:ND1	1:B:733:GLN:HG2	2.32	0.44
1:B:642:GLY:HA2	1:B:645:LYS:HD2	1.99	0.44
1:A:590:LYS:HD2	1:A:590:LYS:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:NH2	5:A:1585:HOH:O	2.41	0.44
1:A:452:THR:HA	1:A:453:PRO:HD3	1.86	0.44
1:A:61:VAL:HG21	1:A:792:TRP:CE3	2.52	0.44
1:B:531:GLN:HE22	1:B:541:GLN:HA	1.83	0.44
1:B:555:ILE:HD13	1:B:555:ILE:HG23	1.77	0.44
1:A:657:LEU:HD22	1:A:662:VAL:HB	2.00	0.44
1:B:393:TRP:CE2	1:B:397:ALA:HB2	2.53	0.44
1:B:590:LYS:CE	5:B:1312:HOH:O	2.66	0.44
1:A:532:ILE:HG21	1:A:621:LEU:HD13	1.99	0.43
1:B:598:ASP:C	1:B:598:ASP:OD1	2.56	0.43
1:B:101:LEU:HA	1:B:101:LEU:HD12	1.62	0.43
1:B:356:ASP:O	1:B:357:VAL:C	2.55	0.43
1:B:382:VAL:HG11	1:B:393:TRP:HE3	1.83	0.43
1:A:379:LYS:O	1:A:383:GLU:HB2	2.17	0.43
1:A:620:LYS:NZ	5:A:1308:HOH:O	2.50	0.43
1:B:512:GLU:HG3	5:B:1169:HOH:O	2.16	0.43
1:B:727:LEU:HD12	1:B:727:LEU:HA	1.53	0.43
1:A:239:LEU:HG	1:B:239:LEU:HD21	2.01	0.43
1:B:506:ASN:OD1	1:B:509:ARG:NH2	2.51	0.43
1:B:753:GLN:HG3	1:B:753:GLN:H	1.56	0.43
1:B:608:VAL:HG12	1:B:610:LEU:HD22	2.01	0.43
1:A:379:LYS:O	1:A:380:THR:C	2.56	0.43
1:A:689:LYS:O	1:A:689:LYS:HG2	2.17	0.43
1:A:753:GLN:H	1:A:753:GLN:HG3	1.55	0.43
1:B:533:LYS:O	1:B:572:ALA:HB2	2.18	0.43
1:A:564:VAL:HA	1:A:565:PRO:HD3	1.85	0.43
1:A:598:ASP:OD1	1:A:600:LEU:N	2.46	0.42
1:A:433:PHE:N	1:A:434:PRO:CD	2.82	0.42
1:A:555:ILE:HD12	1:A:555:ILE:HG21	1.80	0.42
1:A:557:GLU:O	1:A:558:ASN:HB2	2.19	0.42
1:A:647:ALA:HA	5:A:1103:HOH:O	2.19	0.42
1:B:349:PRO:O	1:B:351:ALA:N	2.53	0.42
1:B:478:ASN:N	1:B:478:ASN:OD1	2.53	0.42
1:A:66:MET:HG3	1:A:309:HIS:CB	2.49	0.42
1:B:349:PRO:O	1:B:350:GLU:C	2.58	0.42
1:B:169:PHE:CE1	1:B:202:TRP:HB3	2.54	0.42
1:A:137:GLY:HA2	1:A:275:GLN:NE2	2.34	0.42
1:A:242:GLU:HG3	1:B:246:ILE:HD13	2.01	0.42
1:B:91:LEU:HB3	1:B:96:ILE:HB	2.01	0.42
1:A:187:LYS:HD3	1:A:187:LYS:HA	1.49	0.42
1:A:533:LYS:O	1:A:572:ALA:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ILE:HA	1:B:484:ILE:HD12	1.90	0.42
1:A:170:ARG:HD2	1:B:22:GLY:CA	2.49	0.42
1:A:166:TYR:CD1	1:A:167:PRO:HD2	2.55	0.42
1:A:532:ILE:O	1:A:532:ILE:HG13	2.19	0.42
1:A:679:THR:OG1	1:A:682:GLN:HG3	2.20	0.42
1:A:238:PHE:CE2	1:B:263:GLU:CG	3.02	0.42
1:B:309:HIS:N	1:B:310:PRO:CD	2.83	0.42
1:B:347:LEU:HA	1:B:347:LEU:HD23	1.79	0.42
1:B:732:LYS:HA	1:B:732:LYS:HD3	1.72	0.42
1:B:401:ASP:O	1:B:402:LYS:HB2	2.20	0.41
1:B:396:LEU:HD21	1:B:435:GLU:HB2	2.01	0.41
1:A:101:LEU:HD12	1:A:101:LEU:HA	1.50	0.41
1:A:657:LEU:HA	1:A:657:LEU:HD23	1.93	0.41
1:B:558:ASN:O	1:B:558:ASN:OD1	2.38	0.41
1:B:188:ASP:OD1	1:B:188:ASP:C	2.58	0.41
1:B:532:ILE:HG21	1:B:621:LEU:HD13	2.02	0.41
1:B:476:TRP:N	1:B:476:TRP:CD1	2.86	0.41
1:A:366:ARG:HH11	1:A:366:ARG:HD2	1.71	0.41
1:B:293:LYS:HA	1:B:293:LYS:HD3	1.86	0.41
1:B:421:ALA:O	1:B:422:ALA:C	2.59	0.41
1:B:705:ALA:HB1	5:B:1284:HOH:O	2.19	0.41
1:A:34:TRP:O	1:A:38:VAL:HG13	2.21	0.41
1:A:691:TYR:OH	1:A:741:MET:HB2	2.20	0.41
1:B:736:ASP:OD1	5:B:1283:HOH:O	2.22	0.41
1:B:186:THR:O	1:B:187:LYS:C	2.59	0.41
1:B:564:VAL:HA	1:B:565:PRO:HD3	1.84	0.41
1:A:736:ASP:N	1:A:737:PRO:HD3	2.36	0.40
1:A:692:ASP:HA	1:A:693:PRO:HD2	1.88	0.40
1:B:689:LYS:O	1:B:689:LYS:HG2	2.20	0.40
1:A:314:ILE:HB	1:A:315:PRO:HD3	2.03	0.40
1:A:447:VAL:HG11	1:A:787:TYR:CD2	2.56	0.40
1:A:558:ASN:HA	1:A:559:PRO:HD2	1.89	0.40
1:A:708:LYS:HA	1:A:711:GLU:OE1	2.21	0.40
1:B:591:VAL:HG12	1:B:595:ILE:HD12	2.04	0.40
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.81	0.40
1:A:447:VAL:HG11	1:A:787:TYR:CE2	2.56	0.40
1:A:488:LYS:H	1:A:488:LYS:HG3	1.75	0.40
1:B:575:ALA:HA	1:B:576:PRO:HD3	1.88	0.40
1:B:537:GLU:HB2	1:B:578:TYR:OH	2.22	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	794/796 (100%)	766 (96%)	28 (4%)	0	100	100
1	B	794/796 (100%)	759 (96%)	33 (4%)	2 (0%)	41	46
All	All	1588/1592 (100%)	1525 (96%)	61 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	533	LYS
1	B	558	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	667/667 (100%)	625 (94%)	42 (6%)	18	20
1	B	667/667 (100%)	620 (93%)	47 (7%)	15	16
All	All	1334/1334 (100%)	1245 (93%)	89 (7%)	16	18

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	73	LEU
1	A	139	ASN
1	A	170	ARG

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Mol	Chain	Res	Type
1	A	181	ILE
1	A	184	LYS
1	A	237	ASP
1	A	255	LEU
1	A	268	ARG
1	A	289	LEU
1	A	297	LEU
1	A	321	LEU
1	A	358	LYS
1	A	361	LYS
1	A	391	LYS
1	A	411	VAL
1	A	423	LEU
1	A	429	VAL
1	A	471	SER
1	A	483	LEU
1	A	488	LYS
1	A	494	LYS
1	A	515	LYS
1	A	525	GLN
1	A	535	LEU
1	A	542	HIS
1	A	544	ASN
1	A	555	ILE
1	A	562	ASP
1	A	564	VAL
1	A	578	TYR
1	A	605	LEU
1	A	609	PHE
1	A	610	LEU
1	A	666	GLU
1	A	689	LYS
1	A	706	VAL
1	A	727	LEU
1	A	732	LYS
1	A	755	ASP
1	A	766	ARG
1	A	785	ARG
1	B	9	GLN
1	B	38	VAL
1	B	73	LEU
1	B	92	LYS

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Mol	Chain	Res	Type
1	B	97	ASN
1	B	139	ASN
1	B	170	ARG
1	B	177	VAL
1	B	181	ILE
1	B	188	ASP
1	B	237	ASP
1	B	255	LEU
1	B	297	LEU
1	B	321	LEU
1	B	361	LYS
1	B	363	LEU
1	B	391	LYS
1	B	409	LEU
1	B	411	VAL
1	B	423	LEU
1	B	429	VAL
1	B	488	LYS
1	B	494	LYS
1	B	515	LYS
1	B	516	VAL
1	B	525	GLN
1	B	533	LYS
1	B	535	LEU
1	B	542	HIS
1	B	544	ASN
1	B	551	LEU
1	B	555	ILE
1	B	560	GLN
1	B	562	ASP
1	B	564	VAL
1	B	578	TYR
1	B	605	LEU
1	B	609	PHE
1	B	662	VAL
1	B	666	GLU
1	B	689	LYS
1	B	706	VAL
1	B	724	ASP
1	B	727	LEU
1	B	732	LYS
1	B	755	ASP

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Mol	Chain	Res	Type
1	B	785	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	112	ASN
1	A	139	ASN
1	A	171	HIS
1	A	178	GLN
1	A	260	ASN
1	A	437	HIS
1	A	446	ASN
1	A	459	GLN
1	A	525	GLN
1	A	531	GLN
1	A	544	ASN
1	B	57	ASN
1	B	97	ASN
1	B	112	ASN
1	B	178	GLN
1	B	260	ASN
1	B	437	HIS
1	B	446	ASN
1	B	459	GLN
1	B	525	GLN
1	B	531	GLN
1	B	544	ASN
1	B	560	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

10 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	GLC	C	1	2	12,12,12	0.84	0	17,17,17	1.60	5 (29%)
2	GLC	C	2	2	11,11,12	1.15	1 (9%)	15,15,17	1.33	2 (13%)
2	GLC	C	3	2	11,11,12	1.11	1 (9%)	15,15,17	1.63	4 (26%)
2	GLC	C	4	2	11,11,12	1.18	2 (18%)	15,15,17	1.56	4 (26%)
2	GLC	C	5	2	11,11,12	1.18	1 (9%)	15,15,17	3.41	7 (46%)
2	GLC	D	1	2	12,12,12	0.69	0	17,17,17	1.67	4 (23%)
2	GLC	D	2	2	11,11,12	1.02	1 (9%)	15,15,17	1.32	1 (6%)
2	GLC	D	3	2	11,11,12	0.76	0	15,15,17	1.37	2 (13%)
2	GLC	D	4	2	11,11,12	0.68	0	15,15,17	1.40	3 (20%)
2	GLC	D	5	2	11,11,12	0.80	1 (9%)	15,15,17	2.47	5 (33%)

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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	2/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	GLC	O5-C1	-2.74	1.39	1.43
2	C	3	GLC	O5-C1	-2.47	1.39	1.43
2	C	2	GLC	O5-C5	-2.42	1.38	1.43
2	D	2	GLC	C2-C3	2.32	1.55	1.52
2	C	5	GLC	C2-C3	2.12	1.55	1.52
2	C	4	GLC	C2-C3	2.10	1.55	1.52
2	D	5	GLC	C1-C2	2.09	1.57	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	GLC	C1-O5-C5	10.68	126.66	112.19
2	D	5	GLC	C1-O5-C5	5.82	120.08	112.19
2	D	5	GLC	C1-C2-C3	5.40	116.30	109.67
2	C	5	GLC	C1-C2-C3	4.84	115.62	109.67
2	D	1	GLC	C1-C2-C3	3.55	117.69	110.31
2	D	5	GLC	O2-C2-C1	3.35	116.00	109.15
2	D	2	GLC	O5-C5-C6	3.35	112.45	107.20
2	C	4	GLC	C1-O5-C5	3.22	116.56	112.19
2	D	4	GLC	C1-O5-C5	3.21	116.54	112.19
2	D	4	GLC	O3-C3-C2	-3.20	103.87	109.99
2	C	4	GLC	O4-C4-C3	3.10	117.53	110.35
2	D	1	GLC	O5-C5-C4	3.08	115.28	109.69
2	C	3	GLC	C1-C2-C3	2.87	113.19	109.67
2	C	3	GLC	C6-C5-C4	-2.84	106.35	113.00
2	C	5	GLC	O3-C3-C4	-2.84	103.79	110.35
2	C	4	GLC	C1-C2-C3	2.83	113.15	109.67
2	D	1	GLC	O2-C2-C3	-2.77	103.94	110.35
2	C	5	GLC	O5-C5-C6	2.75	111.51	107.20
2	C	1	GLC	O5-C5-C4	2.70	114.59	109.69
2	C	5	GLC	O5-C1-C2	-2.58	106.79	110.77
2	C	3	GLC	O3-C3-C2	2.52	114.82	109.99
2	D	1	GLC	O6-C6-C5	-2.42	102.98	111.29
2	D	3	GLC	O6-C6-C5	-2.42	102.98	111.29
2	C	5	GLC	C3-C4-C5	-2.35	106.05	110.24
2	C	2	GLC	O5-C1-C2	-2.34	107.16	110.77
2	C	3	GLC	O5-C5-C6	2.30	110.81	107.20
2	C	5	GLC	O3-C3-C2	2.29	114.38	109.99
2	D	4	GLC	O4-C4-C3	2.21	115.45	110.35
2	C	1	GLC	O2-C2-C3	-2.20	105.26	110.35
2	C	1	GLC	O3-C3-C4	2.20	115.44	110.35
2	D	3	GLC	O5-C5-C4	2.18	116.13	110.83
2	C	4	GLC	C6-C5-C4	-2.15	107.97	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	C1-O5-C5	2.15	117.71	113.66
2	D	5	GLC	C6-C5-C4	-2.15	107.98	113.00
2	D	5	GLC	C3-C4-C5	-2.09	106.51	110.24
2	C	1	GLC	O1-C1-O5	-2.07	104.17	110.38
2	C	2	GLC	O3-C3-C2	2.04	113.90	109.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

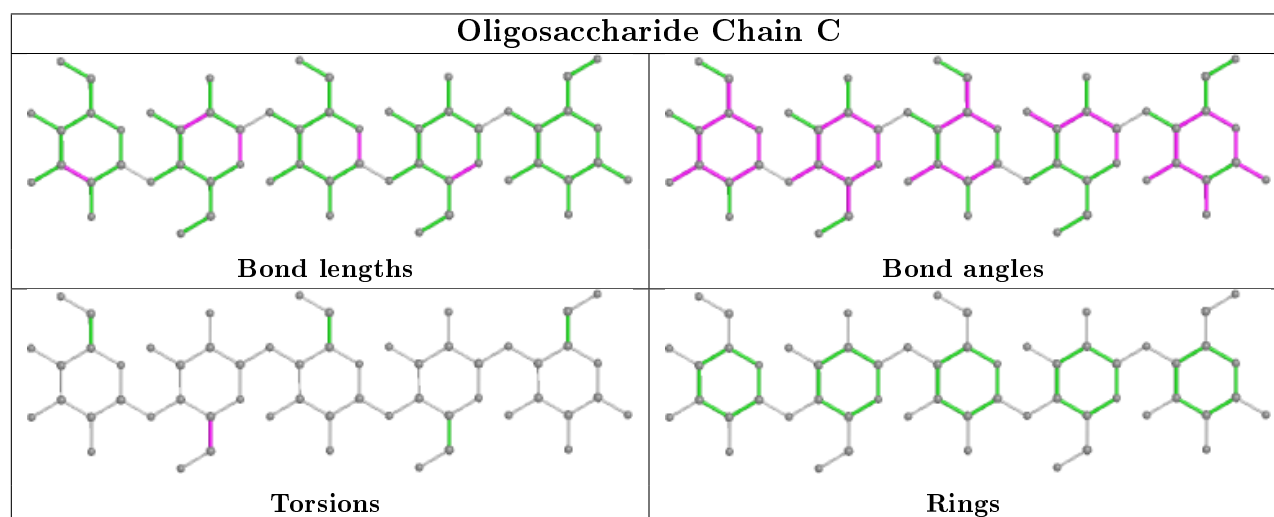
Mol	Chain	Res	Type	Atoms
2	D	4	GLC	O5-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6

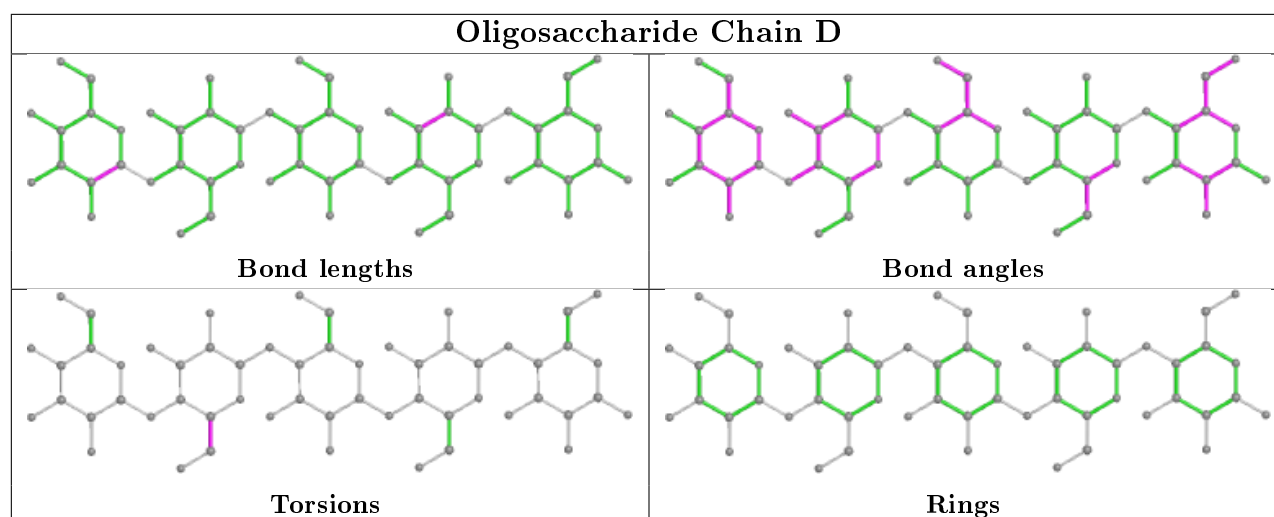
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	GLC	2	0
2	C	1	GLC	1	0
2	D	4	GLC	3	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PLP	B	900	1	15,15,16	2.36	3 (20%)	20,22,23	3.12	8 (40%)
4	PLP	A	900	1	15,15,16	1.64	1 (6%)	20,22,23	2.07	6 (30%)
3	PO4	A	999	-	4,4,4	0.85	0	6,6,6	1.00	0
3	PO4	B	999	-	4,4,4	0.72	0	6,6,6	0.85	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	PLP	B	900	1	-	3/6/6/8	0/1/1/1
4	PLP	A	900	1	-	2/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	PLP	C3-C2	-6.72	1.34	1.40
4	A	900	PLP	C3-C2	-5.07	1.35	1.40
4	B	900	PLP	C5-C4	-4.00	1.36	1.40
4	B	900	PLP	C4A-C4	-2.57	1.46	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	PLP	C4A-C4-C5	-6.72	114.01	120.94
4	B	900	PLP	C6-C5-C4	-5.76	113.62	118.16
4	B	900	PLP	C3-C4-C5	5.61	124.80	118.74
4	B	900	PLP	C3-C2-N1	-5.02	114.29	120.77
4	B	900	PLP	C5A-C5-C6	4.39	126.60	119.37
4	A	900	PLP	C4A-C4-C5	-3.55	117.27	120.94
4	A	900	PLP	O4P-P-O1P	3.42	116.07	106.47
4	A	900	PLP	C3-C4-C5	3.33	122.34	118.74
4	B	900	PLP	C6-N1-C2	3.30	125.28	119.17
4	A	900	PLP	O3P-P-O4P	3.24	115.34	106.73
4	A	900	PLP	O4P-C5A-C5	-3.17	103.30	109.35
4	B	900	PLP	C2A-C2-N1	2.89	123.31	117.67
4	B	900	PLP	O4P-C5A-C5	-2.24	105.08	109.35
4	A	900	PLP	O3P-P-O2P	-2.18	99.29	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	900	PLP	C5A-O4P-P-O1P
4	B	900	PLP	C5A-O4P-P-O3P
4	B	900	PLP	C4-C5-C5A-O4P
4	A	900	PLP	C4-C5-C5A-O4P
4	A	900	PLP	C5A-O4P-P-O1P

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	PO4	2	0
3	B	999	PO4	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	796/796 (100%)	-0.13	13 (1%) 72 70	18, 32, 51, 65	0
1	B	796/796 (100%)	0.03	41 (5%) 27 26	18, 33, 52, 73	0
All	All	1592/1592 (100%)	-0.05	54 (3%) 45 43	18, 32, 52, 73	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	560	GLN	6.4
1	B	562	ASP	5.8
1	B	57	ASN	5.6
1	B	689	LYS	4.4
1	B	688	ALA	4.3
1	B	187	LYS	4.1
1	B	559	PRO	4.0
1	B	721	HIS	3.6
1	A	560	GLN	3.6
1	B	92	LYS	3.5
1	A	688	ALA	3.4
1	B	579	TYR	3.4
1	A	559	PRO	3.4
1	A	51	PHE	3.3
1	A	1	SER	3.3
1	B	387	PRO	3.1
1	A	701	LYS	3.1
1	B	427	LEU	3.1
1	A	599	PRO	2.9
1	A	57	ASN	2.9
1	A	387	PRO	2.9
1	B	677	GLY	2.8
1	B	348	MET	2.8
1	B	599	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	151	ASP	2.7
1	B	386	TRP	2.7
1	A	762	GLU	2.6
1	B	349	PRO	2.6
1	B	717	ASP	2.6
1	B	724	ASP	2.6
1	B	291	GLY	2.6
1	B	1	SER	2.5
1	B	388	GLY	2.5
1	B	558	ASN	2.5
1	A	733	GLN	2.5
1	B	718	GLY	2.4
1	B	553	LYS	2.3
1	B	561	ALA	2.3
1	B	735	GLY	2.3
1	B	441	PRO	2.3
1	B	56	ALA	2.3
1	B	732	LYS	2.2
1	B	390	GLU	2.2
1	B	601	VAL	2.2
1	B	666	GLU	2.2
1	B	525	GLN	2.2
1	B	699	LYS	2.1
1	B	716	SER	2.1
1	A	391	LYS	2.0
1	B	523	ASN	2.0
1	B	594	VAL	2.0
1	A	690	GLY	2.0
1	B	701	LYS	2.0
1	B	186	THR	2.0

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

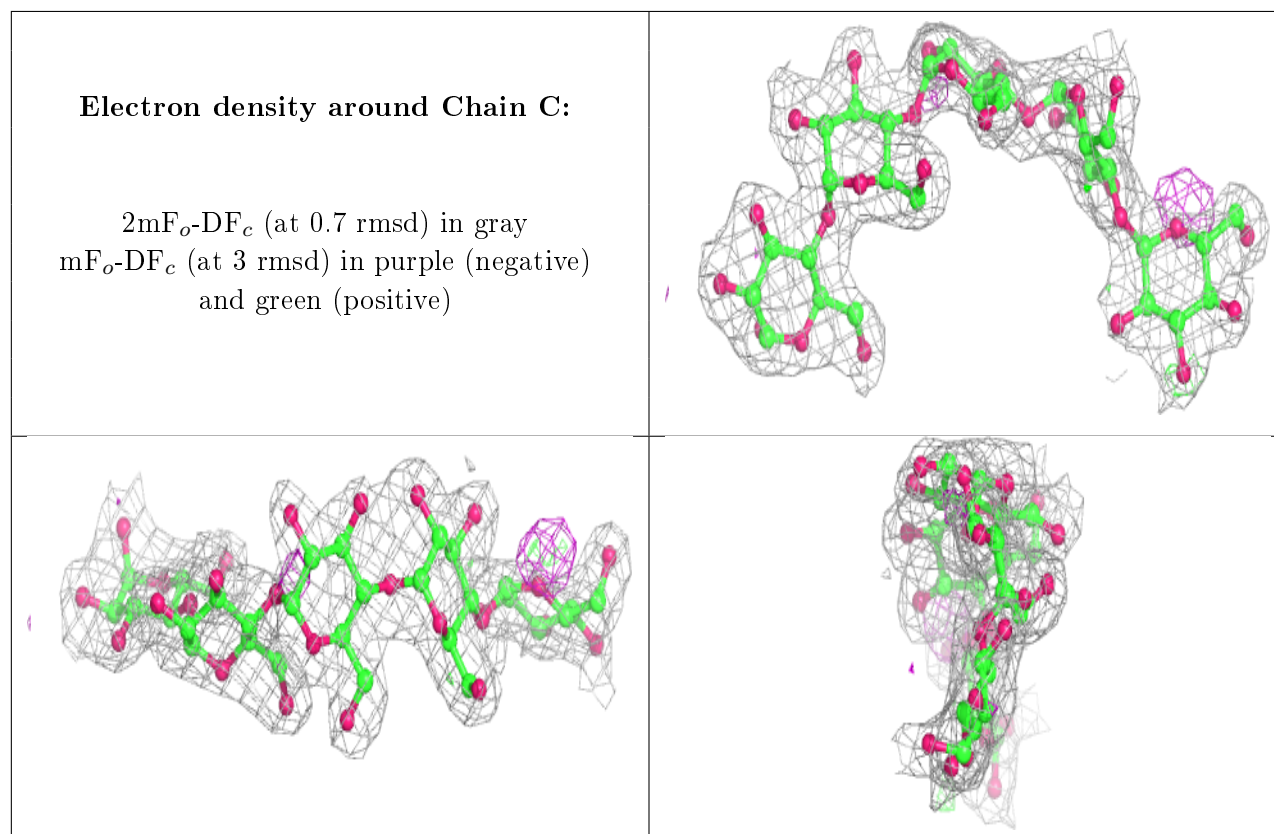
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

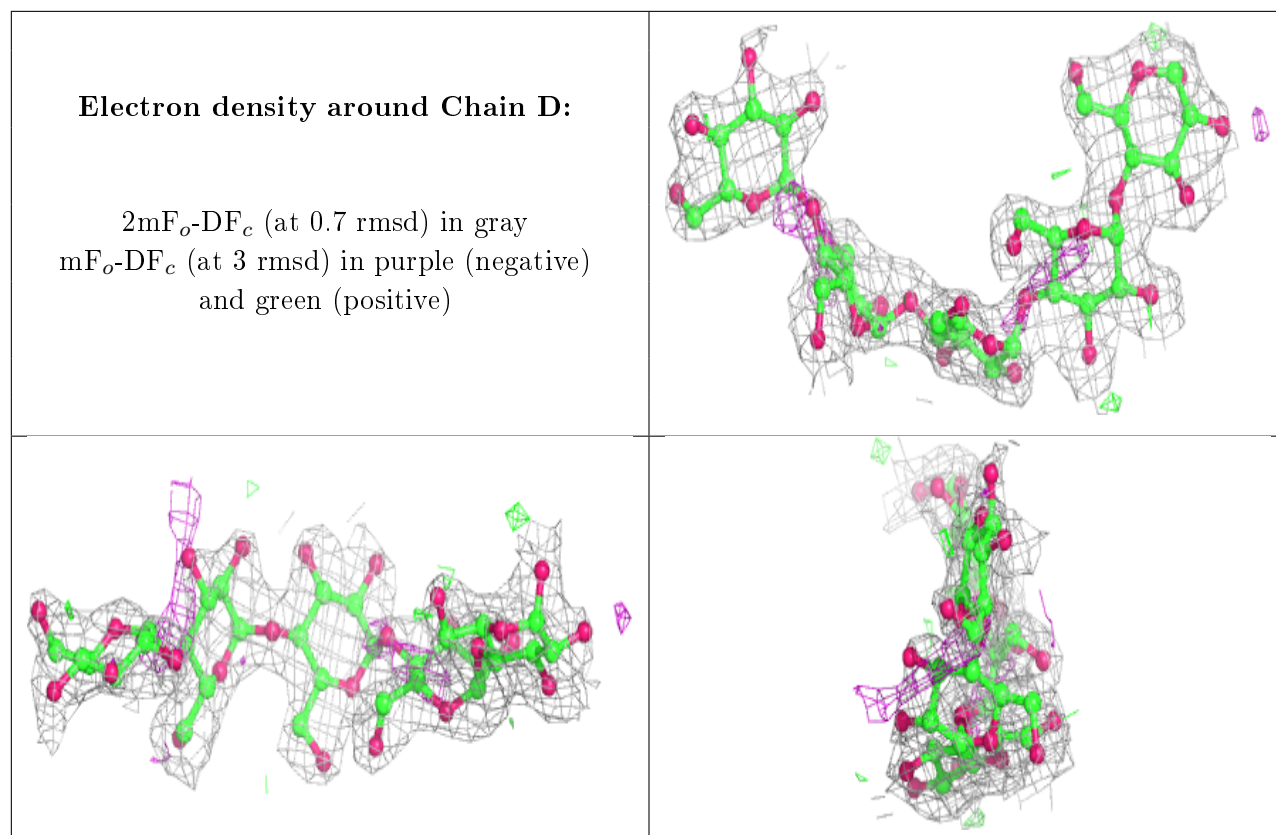
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	GLC	D	4	11/12	0.78	0.23	43,45,46,48	0
2	GLC	D	2	11/12	0.78	0.21	39,45,46,46	0
2	GLC	C	2	11/12	0.81	0.14	39,45,46,46	0
2	GLC	C	5	11/12	0.81	0.19	38,43,46,47	0
2	GLC	D	5	11/12	0.83	0.20	40,44,46,48	0
2	GLC	D	1	12/12	0.85	0.21	43,45,48,54	0
2	GLC	C	4	11/12	0.89	0.13	42,45,47,47	0
2	GLC	C	3	11/12	0.90	0.15	38,40,43,45	0
2	GLC	D	3	11/12	0.93	0.14	39,41,43,46	0
2	GLC	C	1	12/12	0.94	0.10	42,45,48,53	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PO4	B	999	5/5	0.92	0.31	58,61,62,62	0
4	PLP	B	900	15/16	0.95	0.09	18,26,34,34	0
4	PLP	A	900	15/16	0.96	0.10	18,24,34,35	0
3	PO4	A	999	5/5	0.97	0.15	59,60,61,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.