



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:43 PM UTC

PDB ID : 1L6I / pdb_00001l6i
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

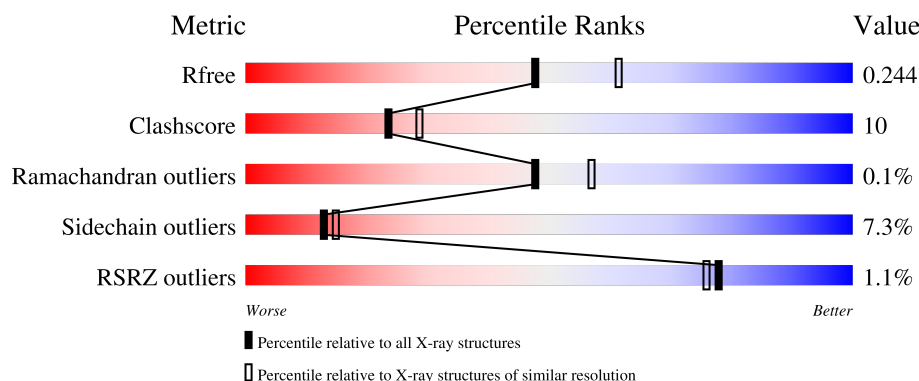
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	796	 71% 24% 5%
1	B	796	 2% 66% 29% 5%
2	C	5	 60% 40%
2	D	5	 80% 20%

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
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.



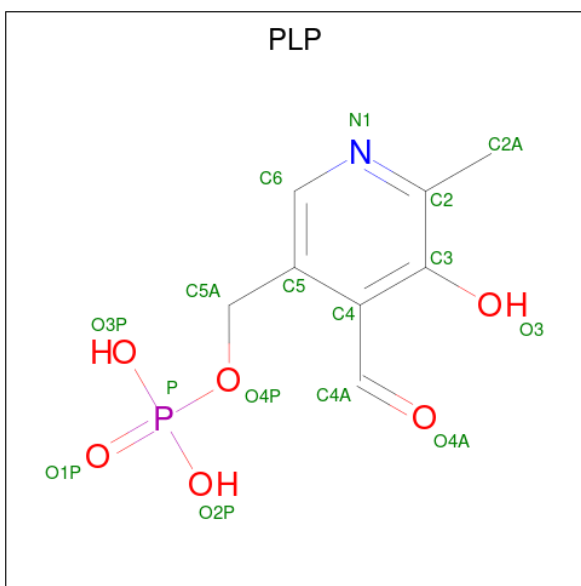
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total	C	O	0	0	0
			56	30	26			
2	D	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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 (CCD ID: 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		

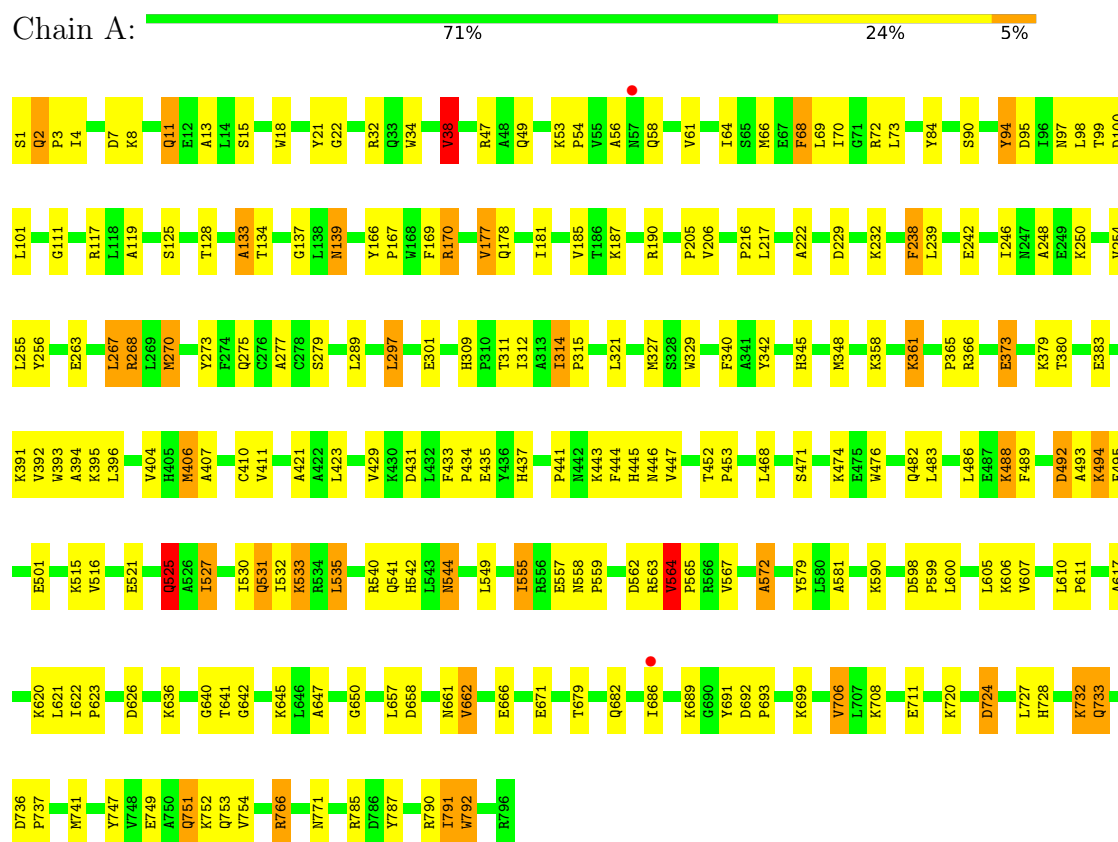
- Molecule 5 is water.

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

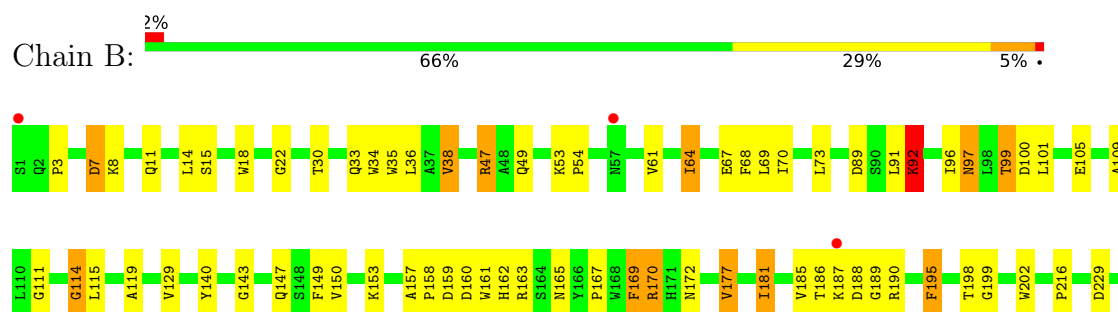
3 Residue-property plots

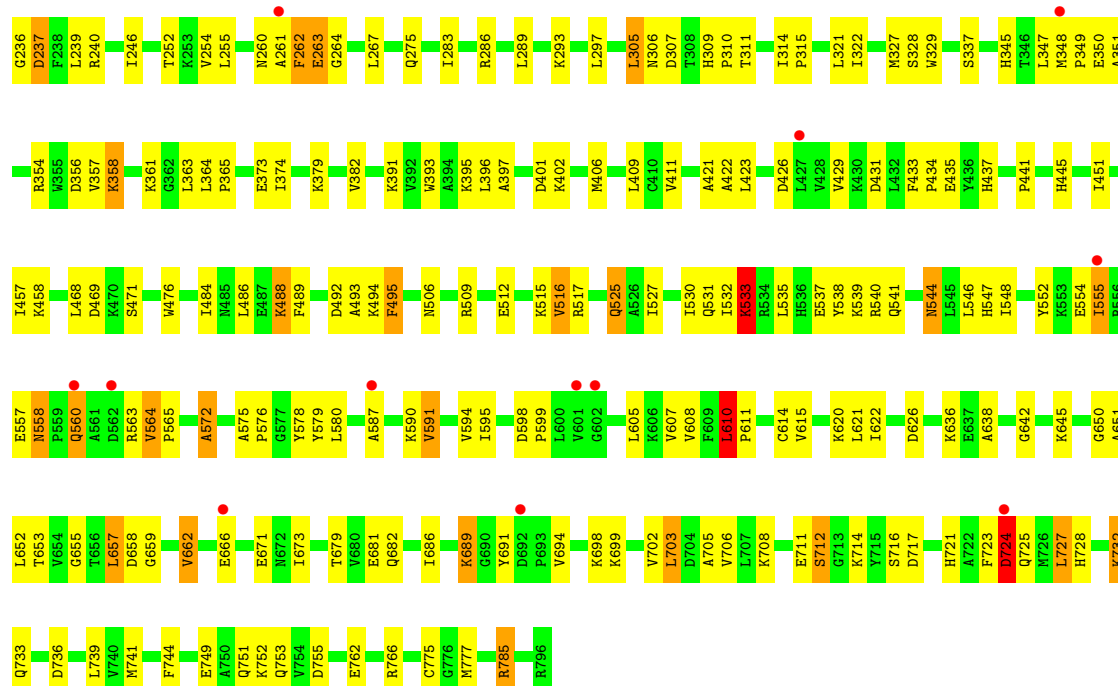
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	75.33Å 105.94Å 218.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-2.20) 90.9 (20.00-2.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	29.3	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

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: PLP, PO4, 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	1.49	45/6540 (0.7%)	1.45	44/8865 (0.5%)
1	B	1.51	36/6540 (0.6%)	1.46	61/8865 (0.7%)
All	All	1.50	81/13080 (0.6%)	1.46	105/17730 (0.6%)

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	THR	CA-CB	8.65	1.64	1.53
1	B	267	LEU	CA-C	8.58	1.64	1.52
1	B	622	ILE	CA-CB	8.30	1.58	1.54
1	A	256	TYR	C-O	7.89	1.27	1.23
1	B	306	ASN	CA-CB	-7.88	1.43	1.53
1	A	222	ALA	CA-CB	7.59	1.64	1.53
1	A	445	HIS	CA-C	-7.38	1.43	1.52
1	B	594	VAL	CA-CB	7.37	1.62	1.54
1	B	614	CYS	C-O	-7.32	1.15	1.23
1	A	11	GLN	C-O	-7.30	1.15	1.24
1	B	162	HIS	CA-C	-7.24	1.44	1.53
1	A	68	PHE	C-O	6.96	1.32	1.23
1	B	199	GLY	CA-C	-6.92	1.47	1.52
1	B	195	PHE	CA-C	6.89	1.61	1.52
1	B	160	ASP	C-O	-6.83	1.15	1.24
1	A	404	VAL	C-O	-6.80	1.16	1.24
1	A	205	PRO	CA-CB	-6.68	1.46	1.54
1	A	177	VAL	CA-CB	6.59	1.64	1.54
1	A	254	VAL	C-O	-6.35	1.17	1.24
1	B	307	ASP	CA-C	-6.22	1.44	1.52
1	B	638	ALA	CA-CB	-6.19	1.43	1.53
1	A	232	LYS	C-O	-6.18	1.16	1.24
1	A	72	ARG	CA-C	-6.18	1.45	1.52
1	B	527	ILE	CA-C	6.15	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	563	ARG	CA-C	-6.10	1.45	1.52
1	B	150	VAL	C-O	-6.09	1.17	1.24
1	A	277	ALA	CA-CB	6.05	1.62	1.53
1	A	279	SER	C-O	-6.04	1.17	1.24
1	B	147	GLN	CA-C	-6.00	1.45	1.52
1	A	94	TYR	CA-C	-5.99	1.44	1.52
1	A	267	LEU	CA-C	5.96	1.60	1.52
1	A	572	ALA	C-O	-5.94	1.16	1.24
1	A	139	ASN	C-O	5.78	1.31	1.23
1	B	165	ASN	CA-C	-5.76	1.45	1.52
1	B	14	LEU	N-CA	-5.72	1.39	1.46
1	B	354	ARG	N-CA	-5.71	1.38	1.46
1	A	206	VAL	C-O	-5.65	1.17	1.24
1	A	238	PHE	N-CA	-5.64	1.39	1.46
1	A	791	ILE	C-O	-5.61	1.17	1.24
1	A	312	ILE	CA-CB	5.60	1.62	1.54
1	B	129	VAL	C-O	-5.59	1.15	1.23
1	B	457	ILE	C-O	-5.59	1.17	1.24
1	A	531	GLN	C-O	-5.57	1.17	1.24
1	B	379	LYS	C-O	-5.54	1.17	1.24
1	B	61	VAL	C-O	-5.52	1.17	1.24
1	A	345	HIS	CA-C	-5.45	1.45	1.52
1	A	406	MET	SD-CE	-5.43	1.66	1.79
1	B	275	GLN	C-O	5.38	1.30	1.24
1	A	117	ARG	CA-C	5.38	1.60	1.52
1	A	273	TYR	CA-CB	5.38	1.61	1.53
1	B	229	ASP	CA-C	5.36	1.59	1.53
1	A	13	ALA	CA-CB	-5.35	1.44	1.53
1	A	327	MET	CA-C	-5.34	1.46	1.52
1	A	38	VAL	CA-CB	5.29	1.61	1.54
1	B	322	ILE	C-O	5.27	1.30	1.24
1	A	771	ASN	C-O	-5.26	1.17	1.24
1	B	328	SER	C-O	-5.24	1.16	1.23
1	A	229	ASP	C-O	-5.23	1.18	1.24
1	B	724	ASP	N-CA	5.23	1.52	1.46
1	A	410	CYS	CA-C	-5.19	1.46	1.52
1	B	47	ARG	NE-CZ	5.19	1.38	1.33
1	B	70	ILE	C-O	-5.18	1.18	1.24
1	A	70	ILE	C-O	-5.17	1.17	1.24
1	B	33	GLN	C-O	-5.16	1.18	1.24
1	B	254	VAL	C-O	-5.16	1.18	1.24
1	A	617	ALA	CA-C	5.15	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	777	MET	SD-CE	5.14	1.92	1.79
1	A	567	VAL	C-O	-5.14	1.18	1.24
1	B	261	ALA	CA-CB	5.11	1.61	1.53
1	B	572	ALA	C-O	-5.11	1.17	1.23
1	A	270	MET	SD-CE	-5.10	1.66	1.79
1	A	133	ALA	C-O	-5.09	1.17	1.23
1	A	407	ALA	C-O	5.09	1.30	1.24
1	B	785	ARG	C-O	-5.09	1.18	1.24
1	A	47	ARG	CA-C	5.08	1.59	1.52
1	A	248	ALA	CA-CB	-5.06	1.45	1.53
1	A	527	ILE	C-O	-5.04	1.19	1.24
1	A	134	THR	C-O	-5.04	1.18	1.24
1	A	314	ILE	CA-CB	5.04	1.60	1.54
1	B	305	LEU	CA-C	-5.02	1.46	1.52
1	A	206	VAL	N-CA	5.02	1.52	1.46

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	ILE	N-CA-C	9.90	122.44	107.99
1	A	640	GLY	N-CA-C	-8.97	100.15	112.18
1	A	641	THR	N-CA-C	-8.58	104.84	114.62
1	A	626	ASP	N-CA-C	-8.40	102.97	113.55
1	B	530	ILE	N-CA-C	8.38	119.98	107.75
1	B	723	PHE	N-CA-C	8.01	121.62	112.57
1	A	268	ARG	NE-CZ-NH2	-7.80	112.18	119.20
1	B	744	PHE	N-CA-C	7.64	119.61	111.28
1	A	792	TRP	N-CA-C	7.53	119.49	111.28
1	A	268	ARG	CD-NE-CZ	7.46	134.85	124.40
1	B	169	PHE	N-CA-C	7.36	120.88	110.50
1	A	238	PHE	N-CA-C	7.31	119.25	111.28
1	A	564	VAL	CB-CA-C	7.29	118.15	111.00
1	B	114	GLY	N-CA-C	7.22	121.64	112.83
1	B	626	ASP	N-CA-C	-7.22	104.45	113.55
1	A	444	PHE	N-CA-C	7.20	121.57	109.76
1	B	283	ILE	N-CA-C	-7.17	103.47	110.72
1	A	268	ARG	NE-CZ-NH1	7.11	128.61	121.50
1	B	579	TYR	N-CA-C	7.01	119.77	111.71
1	B	724	ASP	N-CA-CB	6.86	120.02	110.07
1	B	712	SER	N-CA-C	6.69	121.28	113.18
1	B	622	ILE	CA-C-O	6.67	123.16	118.69
1	A	579	TYR	N-CA-C	6.40	118.25	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	615	VAL	N-CA-C	6.36	117.03	110.36
1	A	72	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	A	56	ALA	N-CA-C	6.28	119.03	110.55
1	B	471	SER	N-CA-C	6.26	119.09	111.82
1	A	38	VAL	N-CA-CB	6.23	119.93	110.58
1	B	177	VAL	N-CA-C	6.20	117.62	108.45
1	B	263	GLU	N-CA-C	-6.16	104.86	112.38
1	B	610	LEU	CB-CA-C	-6.15	99.66	109.51
1	B	458	LYS	N-CA-C	6.06	118.66	111.33
1	B	607	VAL	CA-C-N	-6.01	115.11	123.10
1	B	607	VAL	C-N-CA	-6.01	115.11	123.10
1	A	4	ILE	N-CA-C	6.00	116.56	108.17
1	B	469	ASP	N-CA-C	-6.00	104.74	111.28
1	B	140	TYR	N-CA-C	5.99	119.03	110.10
1	A	724	ASP	N-CA-C	5.97	118.75	111.82
1	B	495	PHE	N-CA-C	-5.97	104.85	111.36
1	B	540	ARG	N-CA-C	5.87	119.74	112.58
1	B	650	GLY	N-CA-C	5.74	123.81	115.32
1	A	342	TYR	N-CA-C	5.74	118.31	109.07
1	B	345	HIS	CB-CA-C	-5.71	100.52	110.17
1	A	540	ARG	N-CA-C	5.71	119.44	111.74
1	B	714	LYS	N-CA-C	5.64	118.16	111.33
1	A	751	GLN	N-CA-C	-5.63	105.67	112.54
1	A	125	SER	N-CA-C	5.62	117.08	111.07
1	A	431	ASP	CB-CA-C	-5.61	99.94	109.03
1	A	747	TYR	N-CA-C	-5.60	105.08	111.07
1	A	98	LEU	N-CA-C	5.59	117.82	111.11
1	B	563	ARG	CA-C-N	-5.57	111.82	122.13
1	B	563	ARG	C-N-CA	-5.57	111.82	122.13
1	A	38	VAL	N-CA-C	5.57	116.34	110.72
1	A	340	PHE	N-CA-C	5.55	118.67	109.46
1	B	652	LEU	CA-C-N	-5.53	114.39	122.19
1	B	652	LEU	C-N-CA	-5.53	114.39	122.19
1	B	703	LEU	N-CA-C	-5.48	104.53	111.11
1	B	364	LEU	CA-C-N	5.47	124.93	119.24
1	B	364	LEU	C-N-CA	5.47	124.93	119.24
1	B	198	THR	OG1-CB-CG2	-5.46	98.37	109.30
1	A	254	VAL	N-CA-C	5.45	116.59	108.46
1	B	337	SER	CA-C-N	-5.45	114.09	122.60
1	B	337	SER	C-N-CA	-5.45	114.09	122.60
1	A	640	GLY	CA-C-O	-5.44	117.63	121.88
1	A	611	PRO	CB-CA-C	-5.43	103.98	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	493	ALA	N-CA-C	5.42	117.89	111.33
1	A	84	TYR	N-CA-C	5.42	117.63	111.02
1	B	431	ASP	CB-CA-C	-5.40	100.28	109.03
1	A	169	PHE	N-CA-C	5.38	117.63	110.53
1	A	766	ARG	N-CA-C	-5.38	105.42	111.28
1	B	374	ILE	N-CA-C	-5.38	105.29	110.72
1	A	493	ALA	N-CA-C	5.37	117.89	111.71
1	B	262	PHE	N-CA-C	5.35	117.11	111.28
1	B	216	PRO	N-CA-C	5.34	121.84	112.01
1	B	8	LYS	N-CA-C	-5.33	105.55	111.36
1	A	650	GLY	N-CA-C	5.32	123.41	115.64
1	B	591	VAL	N-CA-C	-5.29	104.44	111.05
1	B	775	CYS	N-CA-C	5.29	118.75	112.72
1	B	160	ASP	N-CA-CB	-5.28	101.27	109.87
1	A	525	GLN	N-CA-C	-5.27	106.89	113.38
1	A	268	ARG	CB-CG-CD	5.27	123.41	111.30
1	A	607	VAL	CB-CA-C	-5.24	104.18	110.99
1	A	8	LYS	N-CA-C	-5.23	105.75	111.82
1	A	205	PRO	N-CD-CG	-5.22	95.37	103.20
1	B	655	GLY	N-CA-C	5.22	120.99	110.97
1	A	482	GLN	N-CA-C	-5.21	106.02	112.38
1	B	651	ALA	CA-C-N	-5.21	114.89	122.65
1	B	651	ALA	C-N-CA	-5.21	114.89	122.65
1	A	117	ARG	N-CA-C	5.19	117.84	111.82
1	A	217	LEU	N-CA-C	-5.17	98.84	107.99
1	B	327	MET	N-CA-C	5.16	117.77	110.50
1	B	364	LEU	N-CA-C	5.14	117.99	108.94
1	B	724	ASP	N-CA-C	5.14	116.69	111.14
1	B	189	GLY	N-CA-C	5.13	121.83	114.64
1	B	92	LYS	N-CA-C	-5.08	105.75	111.28
1	B	30	THR	CA-C-N	5.07	124.52	119.24
1	B	30	THR	C-N-CA	5.07	124.52	119.24
1	B	260	ASN	N-CA-C	-5.05	105.96	111.82
1	B	426	ASP	N-CA-C	-5.04	105.48	111.69
1	A	216	PRO	N-CA-C	5.03	120.08	111.68
1	B	306	ASN	N-CA-C	5.03	116.80	108.20
1	B	64	ILE	N-CA-C	5.02	115.32	107.99
1	B	7	ASP	N-CA-C	5.01	116.74	111.28
1	B	546	LEU	N-CA-C	-5.01	105.90	111.36
1	A	492	ASP	CB-CG-OD2	5.00	129.91	118.40

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	116	0
1	B	6390	0	6333	154	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	262	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (262) 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:OE1	1:A:733:GLN:N	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:733:GLN:H	1:A:733:GLN:CD	1.96	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:733:GLN:H	1:B:733:GLN:CD	2.00	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:544:ASN:HD22	1:B:544:ASN:C	2.02	0.67
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:B:658:ASP:O	1:B:659:GLY:C	2.38	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:97:ASN:ND2	1:B:100:ASP:H	1.97	0.62
1:B:476:TRP:CD1	1:B:476:TRP:H	2.15	0.62
1:B:492:ASP:OD1	1:B:492:ASP:C	2.41	0.62
3:A:999:PO4:O4	2:C:4:GLC:H61	2.00	0.62
1:A:69:LEU:HD13	1:A:111:GLY:C	2.25	0.61
1:B:557:GLU:O	1:B:558:ASN:HB2	2.00	0.61
1:B:590:LYS:NZ	5:B:1312:HOH:O	2.27	0.61
1:B:115:LEU:H	2:D:4:GLC:H61	1.65	0.60
1:A:598:ASP:OD1	1:A:598:ASP:C	2.45	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: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
1:A:185:VAL:HG23	1:A:365:PRO:HB2	1.86	0.57
1:A:348:MET:HE1	1:A:636:LYS:HD2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:717:ASP:CG	1:B:717:ASP:O	2.51	0.54
1:A:658:ASP:O	1:A:661:ASN:HB2	2.08	0.54
1:A:492:ASP:C	1:A:492:ASP:OD1	2.50	0.53
1:A:263:GLU:OE2	1:B:236:GLY:O	2.26	0.53
1:B:15:SER:HA	1:B:18:TRP:NE1	2.24	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:671:GLU:CD	1:A:671:GLU:H	2.17	0.53
1:A:544:ASN:C	1:A:544:ASN:HD22	2.18	0.52
5:A:1517:HOH:O	2:C:1:GLC:H1	2.09	0.52
1:B:489:PHE:HB3	1:B:495:PHE:CG	2.44	0.52
1:B:560:GLN:HA	1:B:560:GLN:NE2	2.24	0.52
1:A:476:TRP:H	1:A:476:TRP:CD1	2.27	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:HE21	1:A:525:GLN:HA	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:311:THR:HB	1:A:406:MET:HE3	1.93	0.51
1:B:724:ASP:O	1:B:725:GLN:C	2.52	0.51
1:A:7:ASP:O	1:A:11:GLN:HG2	2.11	0.50
1:A:751:GLN:O	1:A:754:VAL:HB	2.11	0.50
1:B:69:LEU:HD13	1:B:111:GLY:C	2.36	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:99:THR:HB	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:ND2	1:A:100:ASP:H	2.06	0.50
1:B:699:LYS:HA	1:B:699:LYS:HE2	1.94	0.50
1:A:3:PRO:HB3	1:A:49:GLN:CD	2.37	0.50
1:B:558:ASN:OD1	1:B:558:ASN:C	2.54	0.50
1:B:544:ASN:O	1:B:548:ILE:HG13	2.12	0.49
1:A:250:LYS:HE3	1:A:270:MET:HE1	1.94	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:B:329:TRP:CZ3	1:B:373:GLU:HG2	2.47	0.49
1:B:358:LYS:O	1:B:358:LYS:HG2	2.10	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:554:GLU:HA	5:B:1474:HOH:O	2.13	0.49
1:A:535:LEU:HD12	1:A:581:ALA:HB1	1.94	0.49
1:A:7:ASP:OD1	1:A:90:SER:OG	2.26	0.48
1:B:598:ASP:C	1:B:598:ASP:OD1	2.56	0.48
1:A:238:PHE:HE2	1:B:263:GLU:CG	2.27	0.48
1:B:356:ASP:O	1:B:357:VAL:C	2.55	0.48
1:A:61:VAL:O	1:A:133:ALA:HA	2.14	0.48
1:A:94:TYR:O	1:A:95:ASP:HB2	2.12	0.48
1:A:622:ILE:N	1:A:623:PRO:CD	2.77	0.48
1:A:379:LYS:O	1:A:380:THR:C	2.56	0.48
1:B:149:PHE:HA	1:B:153:LYS:O	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLU:HB2	1:B:111:GLY:HA2	1.98	0.46
1:B:188:ASP:OD1	1:B:188:ASP:C	2.58	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:A:720:LYS:HD2	5:A:1465:HOH:O	2.16	0.46
1:B:349:PRO:O	1:B:350:GLU:C	2.58	0.46
1:B:421:ALA:O	1:B:422:ALA:C	2.59	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:238:PHE:CE2	1:B:263:GLU:HG3	2.50	0.45
1:A:489:PHE:HB3	1:A:495:PHE:CD1	2.51	0.45
1:B:653:THR:HB	1:B:673:ILE:HG13	1.98	0.45
1:B:68:PHE:CE1	1:B:119:ALA:HB1	2.52	0.45
1:B:186:THR:O	1:B:187:LYS:C	2.59	0.45
1:B:657:LEU:HD22	1:B:662:VAL:HB	1.98	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: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:B:681:GLU:H	1:B:681:GLU:CD	2.25	0.45
1:B:311:THR:HB	1:B:406:MET:HE3	1.97	0.45
1:A:393:TRP:O	1:A:394:ALA:C	2.60	0.44
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:HD2	1:B:590:LYS:HA	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:671:GLU:CD	1:B:671:GLU:H	2.25	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
1:A:32:ARG:NH2	5:A:1585:HOH:O	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:VAL:HG21	1:A:792:TRP:CE3	2.52	0.44
1:A:452:THR:HA	1:A:453:PRO:HD3	1.86	0.44
1:B:531:GLN:HE22	1:B:541:GLN:HA	1.83	0.44
1:B:555:ILE:HG23	1:B:555:ILE:HD13	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:101:LEU:HD12	1:B:101:LEU:HA	1.62	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:702:VAL:O	1:B:703:LEU:C	2.60	0.43
1:B:727:LEU:HA	1:B:727:LEU:HD12	1.53	0.43
1:A:239:LEU:HG	1:B:239:LEU:HD21	2.01	0.43
1:B:97:ASN:ND2	1:B:97:ASN:C	2.75	0.43
1:B:506:ASN:OD1	1:B:509:ARG:NH2	2.51	0.43
1:B:753:GLN:H	1:B:753:GLN:HG3	1.56	0.43
1:B:262:PHE:C	1:B:264:GLY:N	2.76	0.43
1:B:608:VAL:HG12	1:B:610:LEU:HD22	2.01	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:B:451:ILE:C	1:B:451:ILE:HD12	2.44	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:A:66:MET:HG3	1:A:309:HIS:CB	2.49	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
1:A:790:ARG:C	1:A:791:ILE:HG13	2.44	0.42
1:B:484:ILE:HD12	1:B:484:ILE:HA	1.90	0.42
1:A:170:ARG:HD2	1:B:22:GLY:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:CD1	1:A:167:PRO:HD2	2.55	0.42
1:A:238:PHE:CE2	1:B:263:GLU:CG	3.02	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: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:396:LEU:HD21	1:B:435:GLU:HB2	2.01	0.41
1:B:401:ASP:O	1:B:402:LYS:HB2	2.20	0.41
1:A:101:LEU:HD12	1:A:101:LEU:HA	1.50	0.41
1:A:657:LEU:HD23	1:A:657:LEU:HA	1.93	0.41
1:B:348:MET:HE1	1:B:636:LYS:HD2	2.02	0.41
1:B:558:ASN:OD1	1:B:558:ASN:O	2.38	0.41
1:B:532:ILE:HG21	1:B:621:LEU:HD13	2.02	0.41
1:B:476:TRP:CD1	1:B:476:TRP:N	2.86	0.41
1:A:421:ALA:C	1:A:446:ASN:HD21	2.28	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: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:A:1:SER:O	1:A:2:GLN:C	2.63	0.41
1:B:564:VAL:HA	1:B:565:PRO:HD3	1.84	0.41
1:B:564:VAL:HG13	1:B:755:ASP:CG	2.46	0.41
1:A:736:ASP:N	1:A:737:PRO:HD3	2.36	0.40
1:A:267:LEU:HA	1:A:270:MET:HE2	2.03	0.40
1:A:692:ASP:HA	1:A:693:PRO:HD2	1.88	0.40
1:B:558:ASN:C	1:B:560:GLN:N	2.79	0.40
1:B:689:LYS:O	1:B:689:LYS:HG2	2.20	0.40
1:B:716:SER:O	1:B:717:ASP:C	2.64	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:537:GLU:HB2	1:B:578:TYR:OH	2.22	0.40
1:B:575:ALA:HA	1:B:576:PRO:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:LYS:NZ	5:B:1524:HOH:O	2.31	0.40
1:B:733:GLN:N	1:B:733:GLN:CD	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	794/796 (100%)	766 (96%)	28 (4%)	0	100	100
1	B	794/796 (100%)	759 (96%)	33 (4%)	2 (0%)	36	42
All	All	1588/1592 (100%)	1525 (96%)	61 (4%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	533	LYS
1	B	558	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	667/667 (100%)	616 (92%)	51 (8%)	12	14
1	B	667/667 (100%)	621 (93%)	46 (7%)	14	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1334/1334 (100%)	1237 (93%)	97 (7%)	13	15

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	38	VAL
1	A	58	GLN
1	A	64	ILE
1	A	73	LEU
1	A	128	THR
1	A	139	ASN
1	A	170	ARG
1	A	177	VAL
1	A	181	ILE
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	373	GLU
1	A	391	LYS
1	A	392	VAL
1	A	411	VAL
1	A	423	LEU
1	A	429	VAL
1	A	443	LYS
1	A	471	SER
1	A	483	LEU
1	A	488	LYS
1	A	494	LYS
1	A	501	GLU
1	A	515	LYS
1	A	516	VAL
1	A	521	GLU
1	A	525	GLN
1	A	533	LYS
1	A	535	LEU
1	A	542	HIS
1	A	544	ASN

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Mol	Chain	Res	Type
1	A	555	ILE
1	A	562	ASP
1	A	564	VAL
1	A	605	LEU
1	A	610	LEU
1	A	662	VAL
1	A	666	GLU
1	A	689	LYS
1	A	706	VAL
1	A	727	LEU
1	A	732	LYS
1	A	733	GLN
1	A	766	ARG
1	A	785	ARG
1	B	38	VAL
1	B	64	ILE
1	B	73	LEU
1	B	92	LYS
1	B	97	ASN
1	B	99	THR
1	B	170	ARG
1	B	177	VAL
1	B	181	ILE
1	B	237	ASP
1	B	255	LEU
1	B	289	LEU
1	B	297	LEU
1	B	321	LEU
1	B	358	LYS
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	445	HIS
1	B	488	LYS
1	B	494	LYS
1	B	515	LYS
1	B	516	VAL
1	B	525	GLN

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Mol	Chain	Res	Type
1	B	533	LYS
1	B	535	LEU
1	B	544	ASN
1	B	555	ILE
1	B	560	GLN
1	B	564	VAL
1	B	605	LEU
1	B	610	LEU
1	B	657	LEU
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	739	LEU
1	B	785	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	88	GLN
1	A	97	ASN
1	A	139	ASN
1	A	178	GLN
1	A	260	ASN
1	A	275	GLN
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	A	672	ASN
1	B	2	GLN
1	B	57	ASN
1	B	88	GLN
1	B	97	ASN
1	B	112	ASN
1	B	244	GLN

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Mol	Chain	Res	Type
1	B	260	ASN
1	B	326	GLN
1	B	405	HIS
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
1	B	672	ASN
1	B	753	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	0.82	0	17,17,17	1.59	5 (29%)
2	GLC	C	2	2	11,11,12	1.15	1 (9%)	15,15,17	1.19	0
2	GLC	C	3	2	11,11,12	1.07	1 (9%)	15,15,17	1.47	3 (20%)
2	GLC	C	4	2	11,11,12	1.14	2 (18%)	15,15,17	1.50	4 (26%)
2	GLC	C	5	2	11,11,12	1.14	1 (9%)	15,15,17	3.28	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.99	1 (9%)	15,15,17	1.10	1 (6%)
2	GLC	D	3	2	11,11,12	0.73	0	15,15,17	1.32	2 (13%)
2	GLC	D	4	2	11,11,12	0.66	0	15,15,17	1.37	3 (20%)
2	GLC	D	5	2	11,11,12	0.77	0	15,15,17	2.29	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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	GLC	O5-C1	-2.60	1.39	1.43
2	C	2	GLC	O5-C5	-2.51	1.38	1.43
2	C	3	GLC	O5-C1	-2.33	1.39	1.43
2	D	2	GLC	C2-C3	2.24	1.55	1.52
2	C	5	GLC	C2-C3	2.06	1.55	1.52
2	C	4	GLC	C2-C3	2.03	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	GLC	C1-O5-C5	10.80	126.66	112.19
2	D	5	GLC	C1-O5-C5	5.89	120.08	112.19
2	D	5	GLC	C1-C2-C3	4.57	116.30	109.64
2	C	5	GLC	C1-C2-C3	4.10	115.62	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	C1-C2-C3	3.60	117.69	110.36
2	C	4	GLC	C1-O5-C5	3.26	116.56	112.19
2	D	4	GLC	C1-O5-C5	3.25	116.54	112.19
2	D	1	GLC	O5-C5-C4	3.10	115.28	109.70
2	C	4	GLC	O4-C4-C3	3.03	117.53	110.38
2	D	4	GLC	O3-C3-C2	-3.03	103.87	110.05
2	D	5	GLC	O2-C2-C1	2.96	116.00	109.22
2	C	5	GLC	O3-C3-C4	-2.79	103.79	110.38
2	D	1	GLC	O2-C2-C3	-2.73	103.94	110.38
2	C	1	GLC	O5-C5-C4	2.72	114.59	109.70
2	C	3	GLC	C6-C5-C4	-2.71	106.35	113.02
2	D	2	GLC	O5-C5-C6	2.46	112.45	107.66
2	D	1	GLC	O6-C6-C5	-2.45	102.98	111.33
2	D	3	GLC	O6-C6-C5	-2.45	102.98	111.33
2	C	3	GLC	C1-C2-C3	2.43	113.19	109.64
2	C	4	GLC	C1-C2-C3	2.41	113.15	109.64
2	C	3	GLC	O3-C3-C2	2.33	114.82	110.05
2	C	5	GLC	C3-C4-C5	-2.30	106.05	110.23
2	D	3	GLC	O5-C5-C4	2.18	116.13	110.83
2	C	1	GLC	O2-C2-C3	-2.17	105.26	110.38
2	D	4	GLC	O4-C4-C3	2.15	115.45	110.38
2	C	1	GLC	O3-C3-C4	2.15	115.44	110.38
2	C	5	GLC	O3-C3-C2	2.12	114.38	110.05
2	C	1	GLC	O1-C1-O5	-2.10	104.17	110.41
2	C	1	GLC	C1-O5-C5	2.10	117.71	113.65
2	C	4	GLC	C6-C5-C4	-2.06	107.97	113.02
2	D	5	GLC	C6-C5-C4	-2.05	107.98	113.02
2	D	5	GLC	C3-C4-C5	-2.05	106.51	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

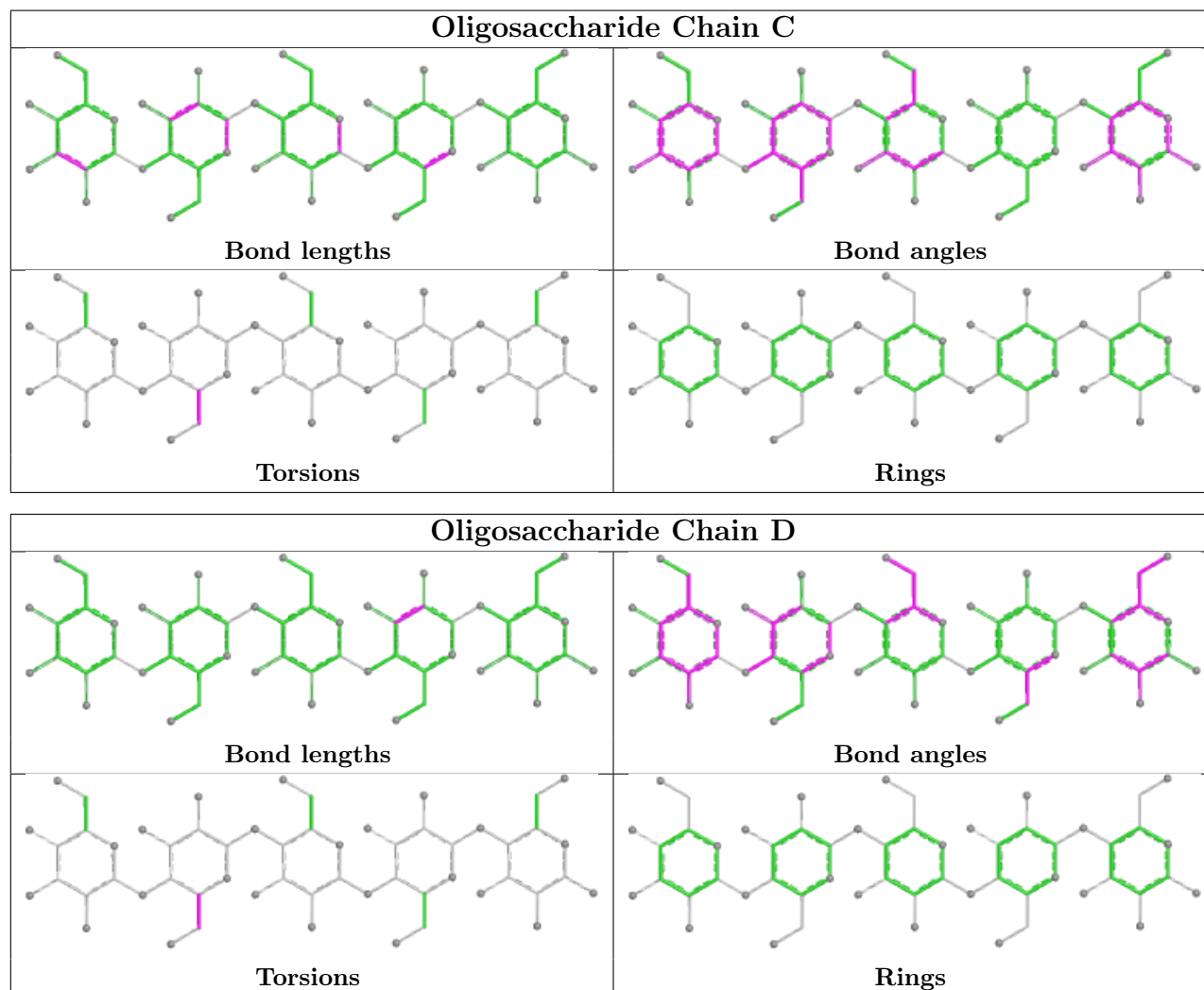
Mol	Chain	Res	Type	Atoms
2	D	4	GLC	O5-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	1	0
2	D	4	GLC	3	0
2	C	4	GLC	2	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	$\# Z > 2$
3	PO4	A	999	-	4,4,4	0.88	0	6,6,6	1.03	0
4	PLP	B	900	1	15,15,16	2.35	3 (20%)	21,22,23	3.07	9 (42%)
3	PO4	B	999	-	4,4,4	0.77	0	6,6,6	0.89	0
4	PLP	A	900	1	15,15,16	1.63	1 (6%)	21,22,23	2.06	6 (28%)

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	-6.54	1.34	1.41
4	A	900	PLP	C3-C2	-4.95	1.35	1.41
4	B	900	PLP	C5-C4	-3.96	1.36	1.40
4	B	900	PLP	C4A-C4	-2.66	1.46	1.51

All (15) 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	-5.45	113.62	118.10
4	B	900	PLP	C3-C2-N1	-5.29	114.29	120.96
4	B	900	PLP	C3-C4-C5	5.18	124.80	118.59
4	B	900	PLP	C5A-C5-C6	4.44	126.60	119.36
4	A	900	PLP	O4P-P-O1P	3.56	116.07	106.44
4	A	900	PLP	C4A-C4-C5	-3.56	117.27	120.94
4	B	900	PLP	C6-N1-C2	3.36	125.28	119.20
4	A	900	PLP	O3P-P-O4P	3.33	115.34	106.67
4	A	900	PLP	O4P-C5A-C5	-3.23	103.30	109.36
4	A	900	PLP	C3-C4-C5	3.12	122.34	118.59
4	B	900	PLP	C2A-C2-N1	3.01	123.31	117.64
4	B	900	PLP	C5A-C5-C4	-2.53	117.64	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	PLP	O4P-C5A-C5	-2.28	105.08	109.36
4	A	900	PLP	O3P-P-O2P	-2.27	99.29	107.80

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	A	900	PLP	C4-C5-C5A-O4P
4	B	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 [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	796/796 (100%)	-0.05	2 (0%) 90 88	18, 32, 51, 65	0
1	B	796/796 (100%)	0.06	15 (1%) 66 63	18, 33, 52, 73	0
All	All	1592/1592 (100%)	0.00	17 (1%) 78 76	18, 32, 52, 73	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	ASN	3.1
1	B	261	ALA	3.0
1	A	57	ASN	2.9
1	B	560	GLN	2.9
1	B	562	ASP	2.9
1	B	187	LYS	2.8
1	B	555	ILE	2.4
1	B	587	ALA	2.3
1	B	348	MET	2.3
1	B	724	ASP	2.2
1	B	1	SER	2.2
1	B	692	ASP	2.1
1	B	427	LEU	2.1
1	B	602	GLY	2.1
1	B	666	GLU	2.0
1	A	686	ILE	2.0
1	B	601	VAL	2.0

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

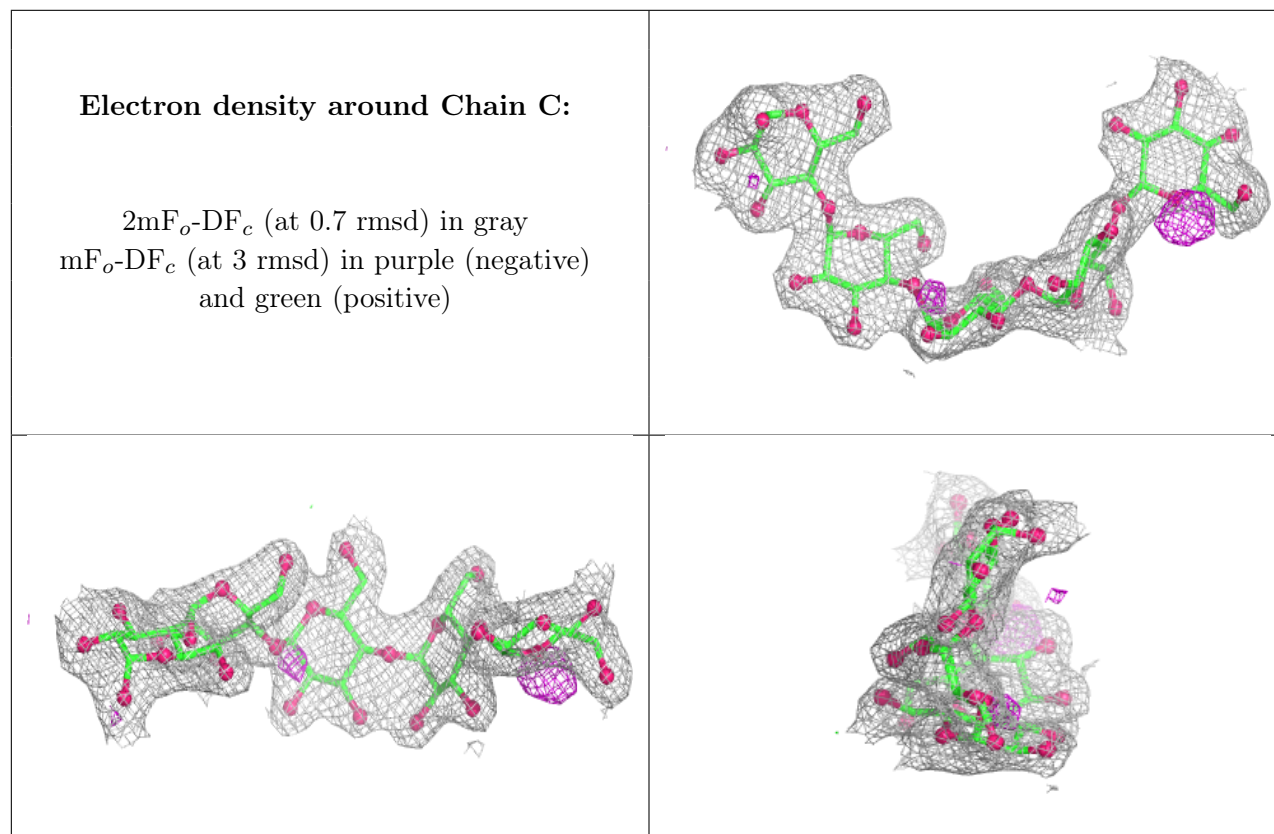
There are no non-standard protein/DNA/RNA residues in this entry.

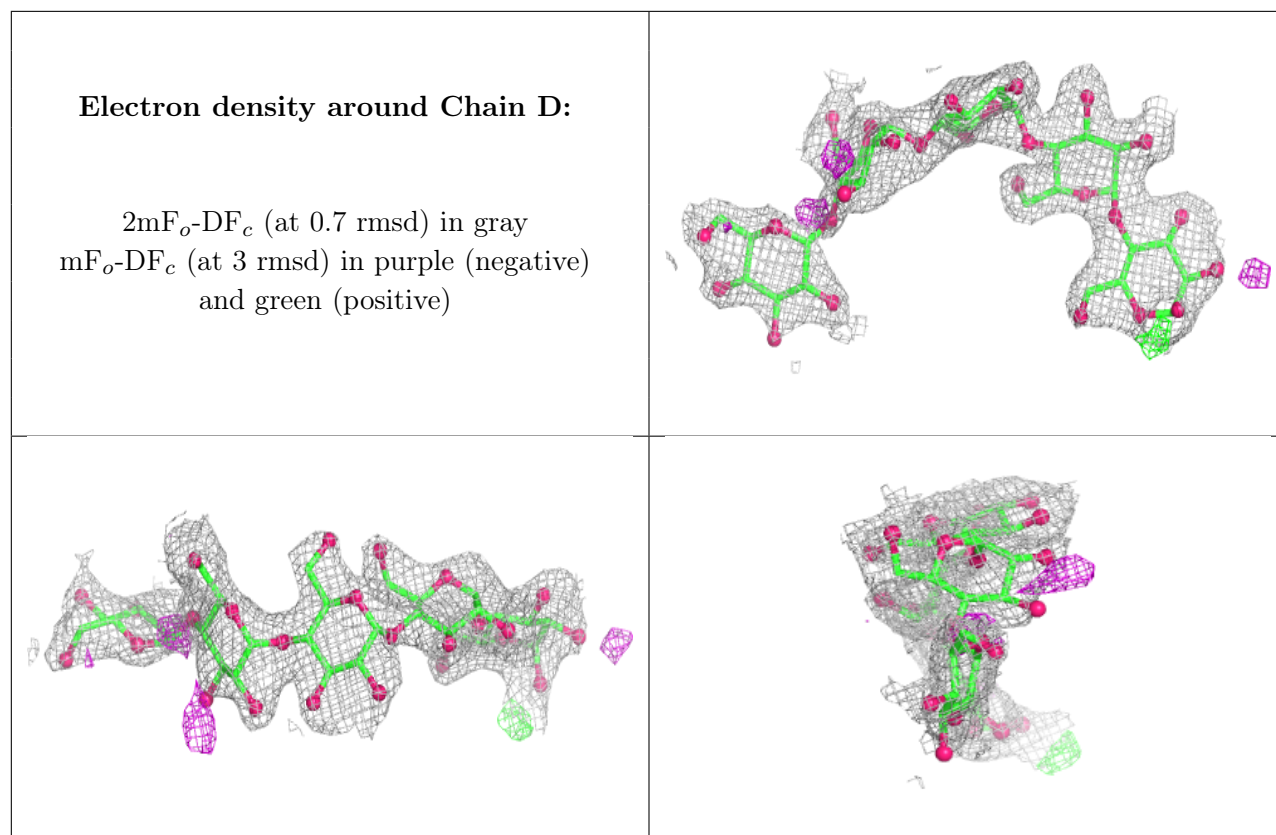
6.3 Carbohydrates ⓘ

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
2	GLC	D	2	11/12	0.78	0.12	39,45,46,46	0
2	GLC	D	4	11/12	0.78	0.13	43,45,46,48	0
2	GLC	D	1	12/12	0.83	0.09	43,45,48,54	0
2	GLC	C	5	11/12	0.85	0.10	38,43,46,47	0
2	GLC	D	5	11/12	0.85	0.11	40,44,46,48	0
2	GLC	C	2	11/12	0.88	0.10	39,45,46,46	0
2	GLC	C	4	11/12	0.91	0.10	42,45,47,47	0
2	GLC	C	3	11/12	0.91	0.10	38,40,43,45	0
2	GLC	D	3	11/12	0.92	0.07	39,41,43,46	0
2	GLC	C	1	12/12	0.94	0.07	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, 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	PO4	B	999	5/5	0.89	0.20	58,61,62,62	0
3	PO4	A	999	5/5	0.91	0.16	59,60,61,62	0
4	PLP	B	900	15/16	0.95	0.07	18,26,34,34	0
4	PLP	A	900	15/16	0.96	0.07	18,24,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.