



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:02 AM EDT

PDB ID : 2AZD / pdb_00002azd
Title : X-Ray studies on Maltodextrin Phosphorylase (MalP) Complexes: recognition of substrates and CATALYTIC mechanism of phosphorylase family
Authors : Geremia, S.; Campagnolo, M.
Deposited on : 2005-09-10
Resolution : 2.16 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

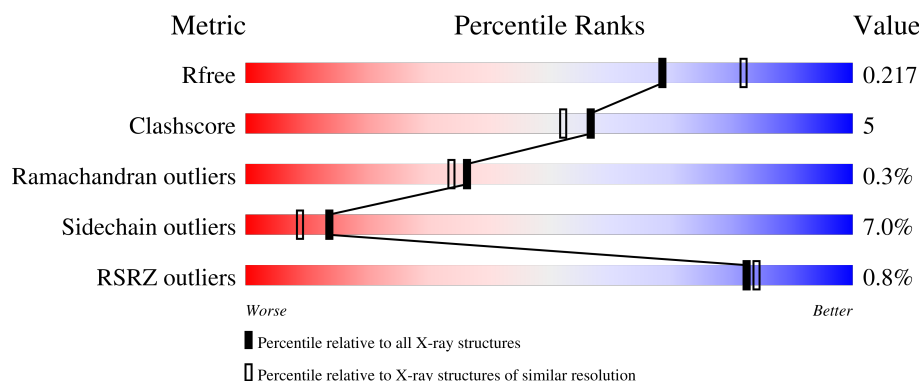
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	% 84% 14% .
1	B	796	% 81% 16% ..
2	C	4	75% 25%
2	D	4	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	VO4	A	999	-	-	X	-
3	VO4	B	1999	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13556 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
			6389	4079	1128	1162	20			
1	B	796	Total	C	N	O	S	0	0	0
			6389	4079	1128	1162	20			

There are 6 discrepancies between the modelled and reference sequences:

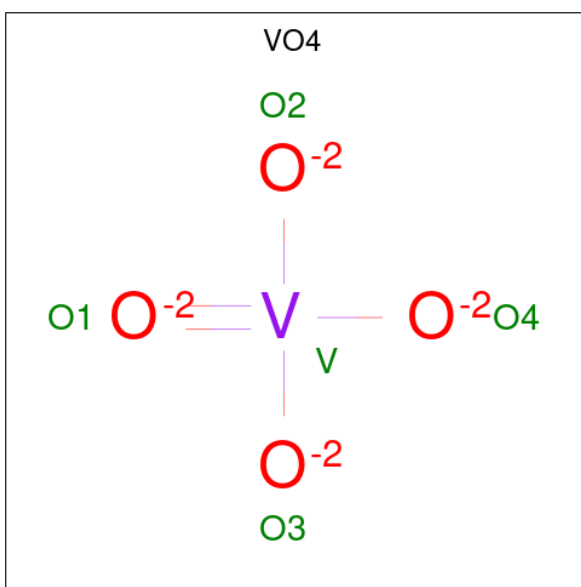
Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	HIS	engineered mutation	UNP P00490
A	262	PHE	THR	engineered mutation	UNP P00490
A	263	GLU	ALA	engineered mutation	UNP P00490
B	261	ALA	HIS	engineered mutation	UNP P00490
B	262	PHE	THR	engineered mutation	UNP P00490
B	263	GLU	ALA	engineered mutation	UNP P00490

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



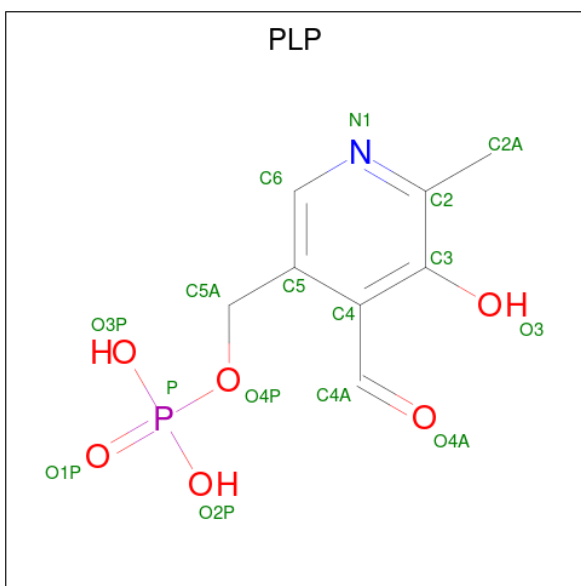
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	D	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is VANADATE ION (CCD ID: VO4) (formula: O₄V).



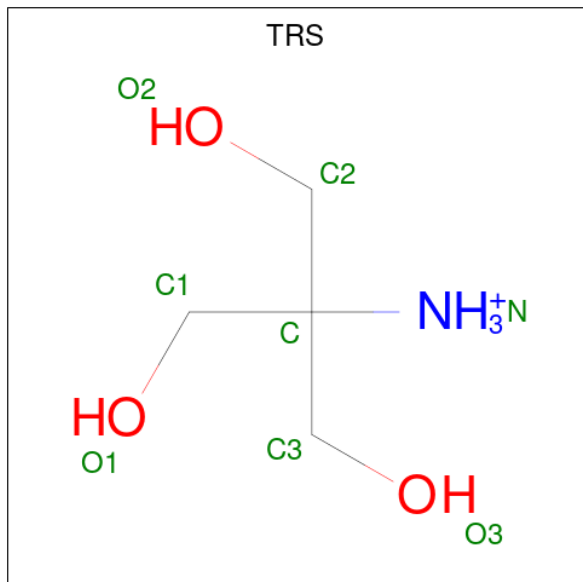
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	V		0	0
			5	4	1			
3	B	1	Total	O	V		0	0
			5	4	1			

- 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 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

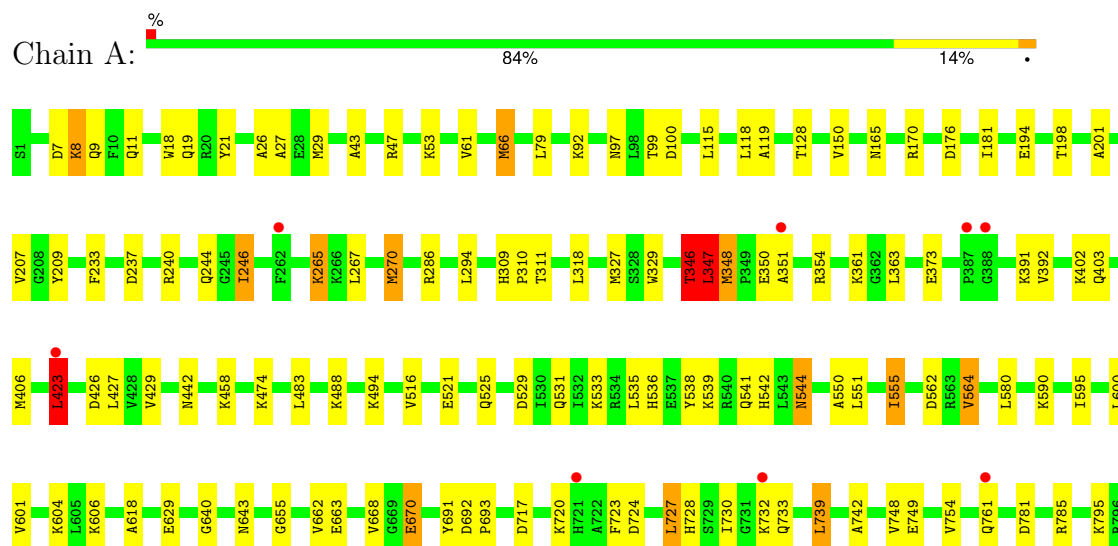
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	339	Total	O	0	0
			339	339		
6	B	293	Total	O	0	0
			293	293		

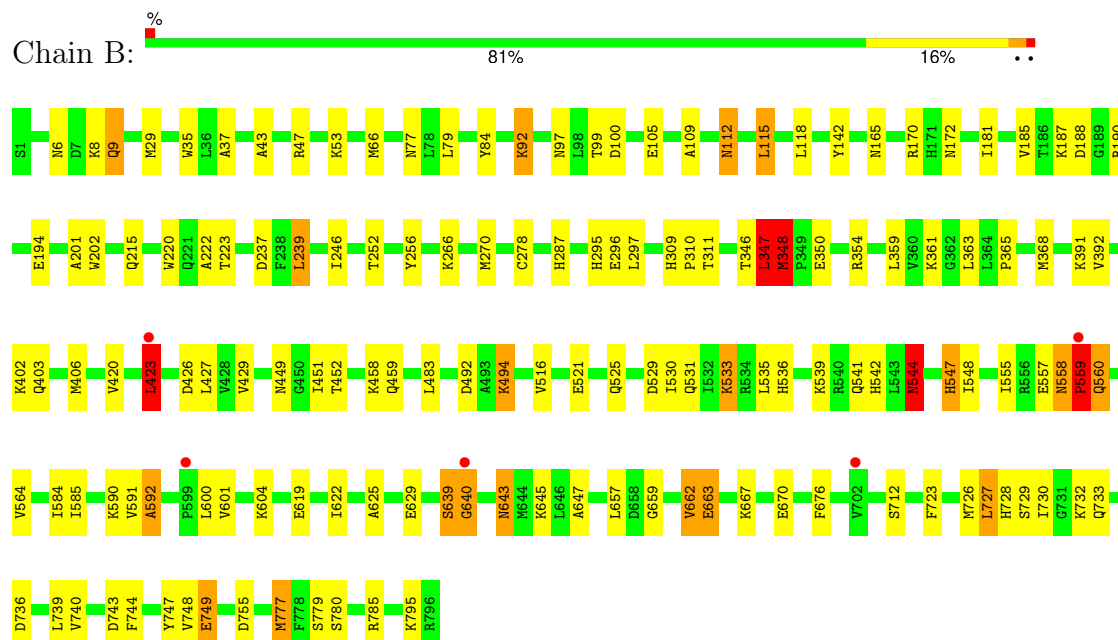
3 Residue-property plots

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)-beta-D-glucopyranose

Chain C:  75% 25%

BGC1
GLC2
GLC3
GLC4

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

Chain D:  50% 50%

BGC1
GLC2
GLC3
GLC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.78Å 105.89Å 220.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.83 – 2.16 6.83 – 2.16	Depositor EDS
% Data completeness (in resolution range)	91.5 (6.83-2.16) 88.3 (6.83-2.16)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.250 0.215 , 0.217	Depositor DCC
R_{free} test set	4477 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13556	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: TRS, BGC, VO4, 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	1.45	33/6539 (0.5%)	1.20	9/8865 (0.1%)
1	B	1.50	37/6539 (0.6%)	1.26	21/8865 (0.2%)
All	All	1.48	70/13078 (0.5%)	1.23	30/17730 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	662	VAL	CA-CB	10.02	1.68	1.54
1	B	222	ALA	CA-CB	-9.35	1.40	1.53
1	B	348	MET	SD-CE	9.27	2.02	1.79
1	B	736	ASP	C-O	-8.98	1.19	1.23
1	B	109	ALA	CA-CB	-8.89	1.41	1.52
1	B	736	ASP	N-CA	8.68	1.52	1.46
1	B	201	ALA	CA-CB	-7.46	1.42	1.53
1	A	595	ILE	CA-CB	-7.30	1.46	1.54
1	A	618	ALA	CA-CB	-7.26	1.42	1.53
1	A	233	PHE	C-O	-7.00	1.16	1.24
1	A	748	VAL	CA-CB	6.99	1.63	1.54
1	A	761	GLN	CG-CD	6.93	1.69	1.52
1	A	201	ALA	CA-CB	-6.91	1.44	1.53
1	A	781	ASP	C-O	-6.68	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ARG	C-O	-6.65	1.15	1.24
1	A	27	ALA	CA-CB	6.52	1.64	1.53
1	B	494	LYS	CA-C	6.42	1.60	1.52
1	B	740	VAL	CA-CB	-6.38	1.46	1.54
1	B	643	ASN	CG-OD1	6.35	1.35	1.23
1	A	742	ALA	CA-CB	-6.28	1.42	1.53
1	A	327	MET	SD-CE	-6.27	1.63	1.79
1	B	29	MET	SD-CE	6.27	1.95	1.79
1	B	622	ILE	CA-CB	6.17	1.57	1.54
1	A	754	VAL	C-O	-6.10	1.17	1.24
1	B	744	PHE	CA-CB	-6.08	1.44	1.53
1	A	580	LEU	C-O	-6.05	1.17	1.24
1	B	112	ASN	N-CA	-5.94	1.40	1.46
1	B	584	ILE	CA-C	5.92	1.60	1.52
1	A	198	THR	C-O	-5.84	1.17	1.24
1	B	647	ALA	CA-CB	-5.82	1.44	1.53
1	A	176	ASP	CA-C	5.82	1.59	1.52
1	A	209	TYR	C-O	-5.80	1.17	1.24
1	A	318	LEU	C-O	-5.79	1.17	1.24
1	B	726	MET	CG-SD	5.77	1.95	1.80
1	B	559	PRO	CA-C	5.76	1.60	1.52
1	A	286	ARG	CA-C	5.75	1.60	1.52
1	A	8	LYS	C-O	-5.75	1.17	1.24
1	B	9	GLN	CA-C	5.64	1.60	1.52
1	A	550	ALA	CA-CB	-5.62	1.44	1.53
1	B	118	LEU	N-CA	-5.61	1.39	1.46
1	B	368	MET	SD-CE	-5.59	1.65	1.79
1	A	351	ALA	CA-C	5.57	1.60	1.52
1	B	619	GLU	C-O	-5.54	1.17	1.24
1	A	119	ALA	CA-CB	-5.53	1.44	1.53
1	A	150	VAL	CA-CB	-5.49	1.47	1.54
1	A	423	LEU	CG-CD1	5.44	1.70	1.52
1	B	622	ILE	CA-C	5.39	1.57	1.52
1	B	256	TYR	C-O	-5.36	1.21	1.23
1	A	19	GLN	C-O	-5.34	1.17	1.24
1	B	142	TYR	C-O	-5.34	1.16	1.24
1	B	223	THR	C-O	-5.34	1.17	1.23
1	A	270	MET	CG-SD	5.31	1.94	1.80
1	B	592	ALA	N-CA	-5.30	1.40	1.46
1	B	202	TRP	C-O	5.27	1.30	1.24
1	B	423	LEU	CG-CD1	5.26	1.70	1.52
1	B	92	LYS	CA-C	-5.23	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	GLN	CA-C	5.22	1.59	1.52
1	B	777	MET	SD-CE	5.21	1.92	1.79
1	B	215	GLN	C-O	-5.20	1.18	1.24
1	B	780	SER	C-O	5.20	1.30	1.24
1	B	77	ASN	CA-C	5.19	1.59	1.52
1	B	37	ALA	C-O	-5.18	1.18	1.24
1	A	668	VAL	CA-CB	5.17	1.60	1.54
1	B	779	SER	C-O	-5.17	1.17	1.23
1	A	474	LYS	CD-CE	5.09	1.67	1.52
1	A	43	ALA	C-O	-5.09	1.18	1.24
1	A	207	VAL	C-O	-5.06	1.18	1.24
1	A	742	ALA	C-O	5.03	1.30	1.24
1	B	585	ILE	C-O	5.02	1.30	1.24
1	A	61	VAL	CA-CB	5.01	1.60	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	LEU	N-CA-C	-6.50	99.33	109.72
1	A	118	LEU	N-CA-C	-6.45	104.17	111.14
1	B	420	VAL	N-CA-C	6.33	118.25	112.43
1	B	748	VAL	O-C-N	6.18	127.86	121.87
1	B	647	ALA	N-CA-C	-6.15	104.27	110.97
1	A	564	VAL	N-CA-CB	6.06	117.79	110.33
1	B	544	ASN	N-CA-C	-5.99	104.75	111.28
1	B	622	ILE	N-CA-C	5.96	119.50	112.35
1	A	265	LYS	N-CA-C	-5.92	104.18	111.40
1	B	452	THR	CA-C-N	5.84	125.52	119.56
1	B	452	THR	C-N-CA	5.84	125.52	119.56
1	B	743	ASP	N-CA-C	-5.82	105.51	113.30
1	B	239	LEU	N-CA-C	5.76	117.36	111.14
1	B	749	GLU	N-CA-C	-5.73	104.73	110.97
1	B	640	GLY	N-CA-C	-5.58	99.96	113.18
1	A	442	ASN	N-CA-C	5.56	119.81	113.19
1	B	347	LEU	N-CA-C	-5.56	100.34	109.40
1	B	663	GLU	N-CA-C	-5.51	105.35	111.36
1	B	748	VAL	CA-C-N	5.47	127.87	120.65
1	B	748	VAL	C-N-CA	5.47	127.87	120.65
1	A	18	TRP	N-CA-C	-5.46	105.49	111.82
1	B	547	HIS	CA-C-N	-5.42	112.21	121.97
1	B	547	HIS	C-N-CA	-5.42	112.21	121.97
1	B	252	THR	OG1-CB-CG2	-5.33	98.64	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	THR	N-CA-C	5.29	118.18	109.72
1	A	655	GLY	N-CA-C	5.24	118.93	110.87
1	A	640	GLY	N-CA-C	-5.22	100.82	113.18
1	B	730	ILE	CB-CA-C	-5.20	104.75	111.20
1	B	115	LEU	CA-C-N	5.09	125.60	120.00
1	B	115	LEU	C-N-CA	5.09	125.60	120.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	562	ASP	Peptide
1	B	559	PRO	Peptide

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	6389	0	6332	44	0
1	B	6389	0	6333	60	0
2	C	45	0	39	3	0
2	D	45	0	39	4	0
3	A	5	0	0	7	0
3	B	5	0	0	8	0
4	A	15	0	6	0	0
4	B	15	0	7	1	0
5	A	8	0	12	1	0
5	B	8	0	12	1	0
6	A	339	0	0	8	0
6	B	293	0	0	6	0
All	All	13556	0	12780	117	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 5.

All (117) 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:B:348:MET:SD	1:B:348:MET:CE	2.02	1.47
1:B:557:GLU:O	1:B:558:ASN:HB2	1.76	0.86
1:B:347:LEU:O	1:B:348:MET:HB2	1.74	0.85
1:A:347:LEU:O	1:A:348:MET:HB2	1.82	0.77
1:B:295:HIS:CD2	1:B:296:GLU:HG3	2.22	0.74
3:A:999:VO4:O3	2:C:4:GLC:H62	1.87	0.73
1:B:97:ASN:HD21	1:B:99:THR:HB	1.54	0.72
1:B:547:HIS:O	1:B:548:ILE:C	2.31	0.72
1:B:729:SER:HB2	6:B:2164:HOH:O	1.89	0.71
3:B:1999:VO4:V	3:B:1999:VO4:O1	1.49	0.69
3:B:1999:VO4:V	3:B:1999:VO4:O2	1.51	0.67
3:A:999:VO4:O4	3:A:999:VO4:V	1.51	0.67
3:A:999:VO4:V	3:A:999:VO4:O1	1.50	0.67
3:B:1999:VO4:V	3:B:1999:VO4:O3	1.50	0.67
3:A:999:VO4:O3	3:A:999:VO4:V	1.50	0.67
3:B:1999:VO4:O3	2:D:4:GLC:H62	1.95	0.67
1:A:97:ASN:HD21	1:A:99:THR:HB	1.61	0.64
3:A:999:VO4:V	3:A:999:VO4:O2	1.53	0.64
3:B:1999:VO4:V	3:B:1999:VO4:O4	1.54	0.64
1:B:97:ASN:HD22	1:B:100:ASP:H	1.46	0.63
1:A:531:GLN:HE22	1:A:541:GLN:HA	1.64	0.63
1:A:97:ASN:HD22	1:A:100:ASP:H	1.47	0.62
1:B:79:LEU:HD11	1:B:458:LYS:HG2	1.82	0.61
1:A:79:LEU:HD11	1:A:458:LYS:HG2	1.85	0.59
1:B:459:GLN:NE2	6:B:2274:HOH:O	2.36	0.58
1:A:606:LYS:HG3	6:A:1122:HOH:O	2.04	0.58
1:A:270:MET:HG2	1:A:363:LEU:HD21	1.86	0.57
3:B:1999:VO4:O1	5:B:1990:TRS:H31	2.05	0.57
1:A:66:MET:HG3	1:A:309:HIS:CB	2.35	0.56
1:B:533:LYS:HB2	6:B:2223:HOH:O	2.05	0.56
1:A:311:THR:HB	1:A:406:MET:HE3	1.86	0.56
1:A:423:LEU:HD13	6:A:1264:HOH:O	2.05	0.56
1:B:530:ILE:HD12	1:B:625:ALA:HB2	1.87	0.56
1:B:97:ASN:ND2	1:B:99:THR:HB	2.20	0.55
1:B:66:MET:HG3	1:B:309:HIS:HB3	1.89	0.55
1:B:423:LEU:HD13	6:B:2257:HOH:O	2.05	0.55
1:A:97:ASN:ND2	1:A:99:THR:HB	2.21	0.54
1:A:728:HIS:HB3	1:A:733:GLN:HB2	1.89	0.54
1:B:66:MET:HG3	1:B:309:HIS:CB	2.38	0.54
1:A:246:ILE:HD13	1:B:239:LEU:HD12	1.89	0.53
1:B:270:MET:HG2	1:B:363:LEU:HD21	1.90	0.53
1:B:531:GLN:HE22	1:B:541:GLN:HA	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:PHE:HB2	1:A:727:LEU:HD22	1.91	0.53
1:B:115:LEU:H	2:D:4:GLC:H61	1.74	0.53
1:B:311:THR:HB	1:B:406:MET:HE3	1.90	0.53
1:B:112:ASN:HD22	2:D:3:GLC:H61	1.74	0.52
1:B:558:ASN:H	1:B:559:PRO:HD3	1.75	0.52
1:B:639:SER:OG	1:B:640:GLY:N	2.40	0.52
1:B:492:ASP:OD1	1:B:492:ASP:C	2.54	0.51
1:A:9:GLN:HG3	6:A:1239:HOH:O	2.10	0.51
1:A:670:GLU:HB3	6:A:1321:HOH:O	2.10	0.51
1:A:115:LEU:H	2:C:4:GLC:H61	1.75	0.50
1:A:309:HIS:N	1:A:310:PRO:CD	2.74	0.50
1:A:724:ASP:HB2	6:A:1290:HOH:O	2.11	0.50
1:B:728:HIS:HB3	1:B:733:GLN:HB2	1.93	0.50
1:A:21:TYR:O	1:B:172:ASN:HB2	2.10	0.50
1:A:246:ILE:HD13	1:B:239:LEU:CD1	2.41	0.50
1:B:115:LEU:HB2	2:D:4:GLC:H4	1.93	0.49
1:A:329:TRP:CZ3	1:A:373:GLU:HG2	2.47	0.49
1:B:723:PHE:HB2	1:B:727:LEU:HD22	1.93	0.49
1:A:691:TYR:CE2	1:A:739:LEU:HD22	2.47	0.49
1:B:560:GLN:HB3	6:B:2283:HOH:O	2.12	0.49
1:B:97:ASN:ND2	1:B:100:ASP:H	2.10	0.49
1:B:667:LYS:HE2	1:B:777:MET:SD	2.53	0.48
1:B:591:VAL:O	1:B:592:ALA:C	2.55	0.48
1:B:35:TRP:CZ2	1:B:105:GLU:HG3	2.49	0.48
1:B:220:TRP:CD2	1:B:278:CYS:HB3	2.49	0.48
1:A:267:LEU:HA	1:A:270:MET:HE3	1.95	0.48
1:B:43:ALA:O	1:B:47:ARG:HG3	2.14	0.48
1:B:659:GLY:O	6:B:2130:HOH:O	2.20	0.47
1:A:544:ASN:C	1:A:544:ASN:HD22	2.22	0.47
1:B:529:ASP:OD1	1:B:629:GLU:OE2	2.32	0.47
1:B:676:PHE:CE2	1:B:747:TYR:HB2	2.49	0.47
1:A:47:ARG:HD2	1:A:170:ARG:HD3	1.97	0.47
1:A:346:THR:HG23	6:A:1313:HOH:O	2.14	0.47
1:A:488:LYS:HG2	6:A:1270:HOH:O	2.15	0.47
1:B:185:VAL:HG23	1:B:365:PRO:HB2	1.97	0.46
1:B:354:ARG:HD2	1:B:403:GLN:NE2	2.30	0.46
3:A:999:VO4:O4	3:A:999:VO4:O2	2.33	0.46
1:A:66:MET:HG3	1:A:309:HIS:HB3	1.99	0.45
1:B:266:LYS:HG3	1:B:359:LEU:HD11	1.97	0.45
1:B:84:TYR:C	1:B:84:TYR:CD1	2.94	0.45
1:B:47:ARG:HD2	1:B:170:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:LYS:NZ	4:B:900:PLP:O3	2.49	0.44
1:A:7:ASP:O	1:A:11:GLN:HG2	2.17	0.44
1:A:97:ASN:ND2	1:A:100:ASP:H	2.14	0.44
1:A:601:VAL:O	1:A:604:LYS:HB2	2.18	0.44
3:B:1999:VO4:O2	3:B:1999:VO4:O4	2.36	0.44
1:A:536:HIS:HB3	1:A:539:LYS:HG2	1.98	0.43
1:B:309:HIS:N	1:B:310:PRO:CD	2.80	0.43
1:A:53:LYS:HB3	1:A:53:LYS:HE3	1.87	0.43
1:A:354:ARG:HD2	1:A:403:GLN:NE2	2.34	0.43
1:B:557:GLU:O	1:B:558:ASN:CB	2.54	0.43
1:A:529:ASP:OD1	1:A:629:GLU:OE2	2.36	0.43
5:A:990:TRS:H32	6:A:1108:HOH:O	2.18	0.43
1:B:270:MET:CG	1:B:363:LEU:HD21	2.48	0.43
1:B:295:HIS:CD2	1:B:296:GLU:CG	3.00	0.42
1:B:451:ILE:HG21	1:B:645:LYS:HG3	2.00	0.42
1:B:601:VAL:O	1:B:604:LYS:HB2	2.19	0.42
3:A:999:VO4:O3	3:A:999:VO4:O4	2.37	0.42
3:B:1999:VO4:O3	3:B:1999:VO4:O4	2.37	0.42
1:A:26:ALA:HA	1:A:29:MET:HE2	2.02	0.42
1:B:536:HIS:HB3	1:B:539:LYS:HG2	2.02	0.42
1:A:536:HIS:HD1	1:A:538:TYR:H	1.68	0.41
1:B:53:LYS:HB3	1:B:53:LYS:HE3	1.83	0.41
1:A:717:ASP:O	1:A:717:ASP:CG	2.63	0.41
1:B:6:ASN:HB3	1:B:9:GLN:HE21	1.85	0.41
1:B:287:HIS:CE1	1:B:297:LEU:HA	2.56	0.41
1:A:692:ASP:HA	1:A:693:PRO:HD2	1.92	0.41
1:A:270:MET:CG	1:A:363:LEU:HD21	2.51	0.41
1:B:309:HIS:HB2	1:B:310:PRO:HD3	2.03	0.41
1:A:590:LYS:HA	1:A:590:LYS:HD2	1.97	0.41
1:A:115:LEU:HB2	2:C:4:GLC:H4	2.03	0.40
1:B:544:ASN:HD22	1:B:544:ASN:C	2.30	0.40
1:B:590:LYS:HD2	1:B:590:LYS:HA	1.84	0.40
1:A:551:LEU:O	1:A:555:ILE:HG23	2.22	0.40
1:B:266:LYS:O	1:B:270:MET:HG3	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%)	772 (97%)	21 (3%)	1 (0%)	48	50
1	B	794/796 (100%)	758 (96%)	32 (4%)	4 (0%)	24	20
All	All	1588/1592 (100%)	1530 (96%)	53 (3%)	5 (0%)	36	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	449	ASN
1	B	558	ASN
1	B	348	MET
1	A	348	MET
1	B	639	SER

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%)	621 (93%)	46 (7%)	14	9
1	B	667/667 (100%)	620 (93%)	47 (7%)	14	9
All	All	1334/1334 (100%)	1241 (93%)	93 (7%)	14	9

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS

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Mol	Chain	Res	Type
1	A	66	MET
1	A	92	LYS
1	A	128	THR
1	A	165	ASN
1	A	181	ILE
1	A	194	GLU
1	A	237	ASP
1	A	246	ILE
1	A	265	LYS
1	A	294	LEU
1	A	346	THR
1	A	347	LEU
1	A	350	GLU
1	A	361	LYS
1	A	391	LYS
1	A	392	VAL
1	A	402	LYS
1	A	423	LEU
1	A	426	ASP
1	A	427	LEU
1	A	429	VAL
1	A	483	LEU
1	A	494	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
1	A	555	ILE
1	A	564	VAL
1	A	600	LEU
1	A	643	ASN
1	A	662	VAL
1	A	663	GLU
1	A	670	GLU
1	A	720	LYS
1	A	727	LEU
1	A	730	ILE
1	A	732	LYS
1	A	739	LEU

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Mol	Chain	Res	Type
1	A	749	GLU
1	A	785	ARG
1	A	795	LYS
1	B	8	LYS
1	B	92	LYS
1	B	165	ASN
1	B	181	ILE
1	B	187	LYS
1	B	188	ASP
1	B	190	ARG
1	B	194	GLU
1	B	237	ASP
1	B	246	ILE
1	B	346	THR
1	B	347	LEU
1	B	350	GLU
1	B	361	LYS
1	B	391	LYS
1	B	392	VAL
1	B	402	LYS
1	B	423	LEU
1	B	426	ASP
1	B	427	LEU
1	B	429	VAL
1	B	483	LEU
1	B	494	LYS
1	B	516	VAL
1	B	521	GLU
1	B	525	GLN
1	B	533	LYS
1	B	535	LEU
1	B	542	HIS
1	B	544	ASN
1	B	555	ILE
1	B	560	GLN
1	B	564	VAL
1	B	600	LEU
1	B	643	ASN
1	B	657	LEU
1	B	662	VAL
1	B	663	GLU
1	B	670	GLU

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Mol	Chain	Res	Type
1	B	712	SER
1	B	727	LEU
1	B	732	LYS
1	B	739	LEU
1	B	749	GLU
1	B	755	ASP
1	B	785	ARG
1	B	795	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	9	GLN
1	A	97	ASN
1	A	112	ASN
1	A	260	ASN
1	A	400	HIS
1	A	403	GLN
1	A	446	ASN
1	A	498	GLN
1	A	504	GLN
1	A	531	GLN
1	A	544	ASN
1	A	678	HIS
1	B	9	GLN
1	B	97	ASN
1	B	112	ASN
1	B	178	GLN
1	B	244	GLN
1	B	260	ASN
1	B	295	HIS
1	B	400	HIS
1	B	403	GLN
1	B	446	ASN
1	B	498	GLN
1	B	531	GLN
1	B	544	ASN
1	B	558	ASN
1	B	672	ASN
1	B	678	HIS

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
2	BGC	C	1	2	12,12,12	0.68	0	17,17,17	1.40	3 (17%)
2	GLC	C	2	2	11,11,12	0.85	0	15,15,17	1.72	3 (20%)
2	GLC	C	3	2	11,11,12	0.74	0	15,15,17	1.03	1 (6%)
2	GLC	C	4	2	11,11,12	0.94	1 (9%)	15,15,17	2.24	2 (13%)
2	BGC	D	1	2	12,12,12	0.64	0	17,17,17	1.69	7 (41%)
2	GLC	D	2	2	11,11,12	1.12	1 (9%)	15,15,17	1.72	3 (20%)
2	GLC	D	3	2	11,11,12	0.75	0	15,15,17	1.31	2 (13%)
2	GLC	D	4	2	11,11,12	0.90	0	15,15,17	2.18	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	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	BGC	D	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	2	2	-	2/2/19/22	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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	GLC	C2-C3	2.50	1.56	1.52
2	D	2	GLC	C4-C5	2.31	1.58	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	GLC	C1-O5-C5	6.87	121.40	112.19
2	C	4	GLC	C1-O5-C5	6.67	121.12	112.19
2	C	2	GLC	C1-O5-C5	4.92	118.78	112.19
2	D	2	GLC	C1-O5-C5	4.84	118.67	112.19
2	C	4	GLC	O2-C2-C3	3.83	118.07	110.15
2	D	1	BGC	C3-C4-C5	3.18	116.00	110.23
2	D	3	GLC	O2-C2-C3	2.78	115.91	110.15
2	D	1	BGC	O2-C2-C1	2.76	115.61	109.25
2	C	1	BGC	C3-C4-C5	2.74	115.20	110.23
2	D	2	GLC	O3-C3-C2	2.61	115.37	110.05
2	C	1	BGC	C1-O5-C5	-2.40	109.00	113.65
2	D	1	BGC	O5-C1-C2	-2.32	106.22	110.30
2	C	3	GLC	C1-C2-C3	2.32	113.02	109.64
2	D	1	BGC	O2-C2-C3	-2.29	104.98	110.38
2	D	4	GLC	O2-C2-C3	2.25	114.82	110.15
2	D	4	GLC	O6-C6-C5	2.22	118.89	111.33
2	D	1	BGC	O5-C5-C4	2.20	113.66	109.70
2	D	3	GLC	O2-C2-C1	-2.17	104.24	109.22
2	C	1	BGC	O2-C2-C3	-2.17	105.26	110.38
2	C	2	GLC	O2-C2-C3	2.17	114.64	110.15
2	D	2	GLC	C2-C3-C4	-2.13	107.11	110.86
2	D	1	BGC	C1-O5-C5	-2.11	109.58	113.65
2	C	2	GLC	C2-C3-C4	-2.05	107.26	110.86
2	D	1	BGC	O1-C1-C2	2.01	114.81	108.98

There are no chirality outliers.

All (8) torsion outliers are listed below:

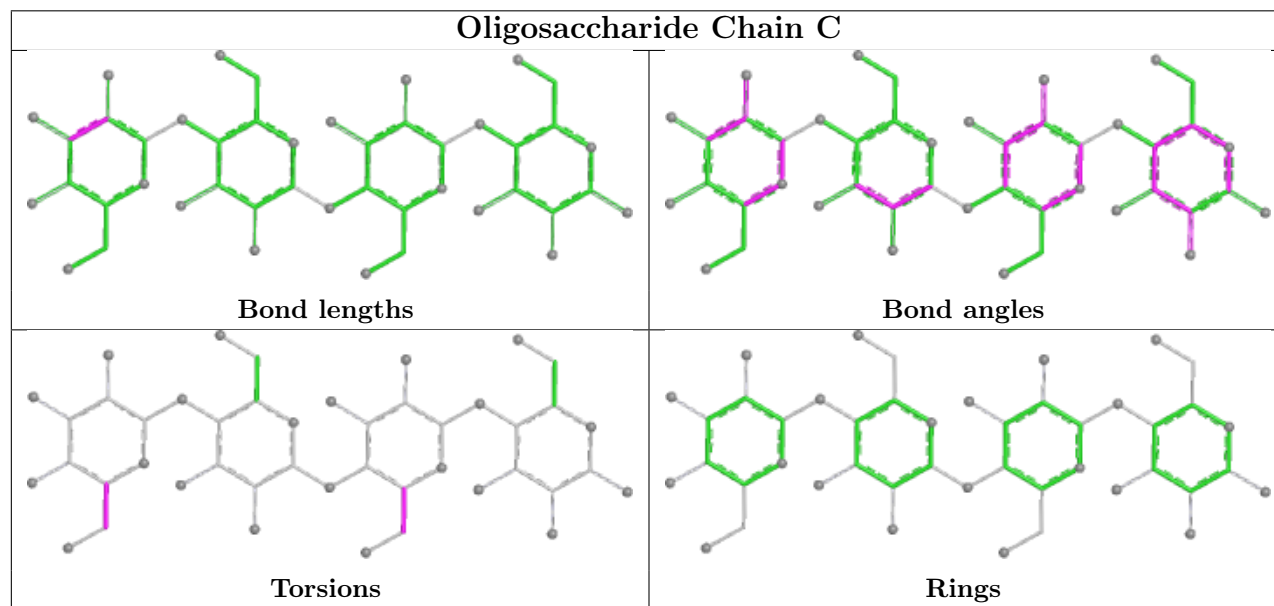
Mol	Chain	Res	Type	Atoms
2	D	4	GLC	O5-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6

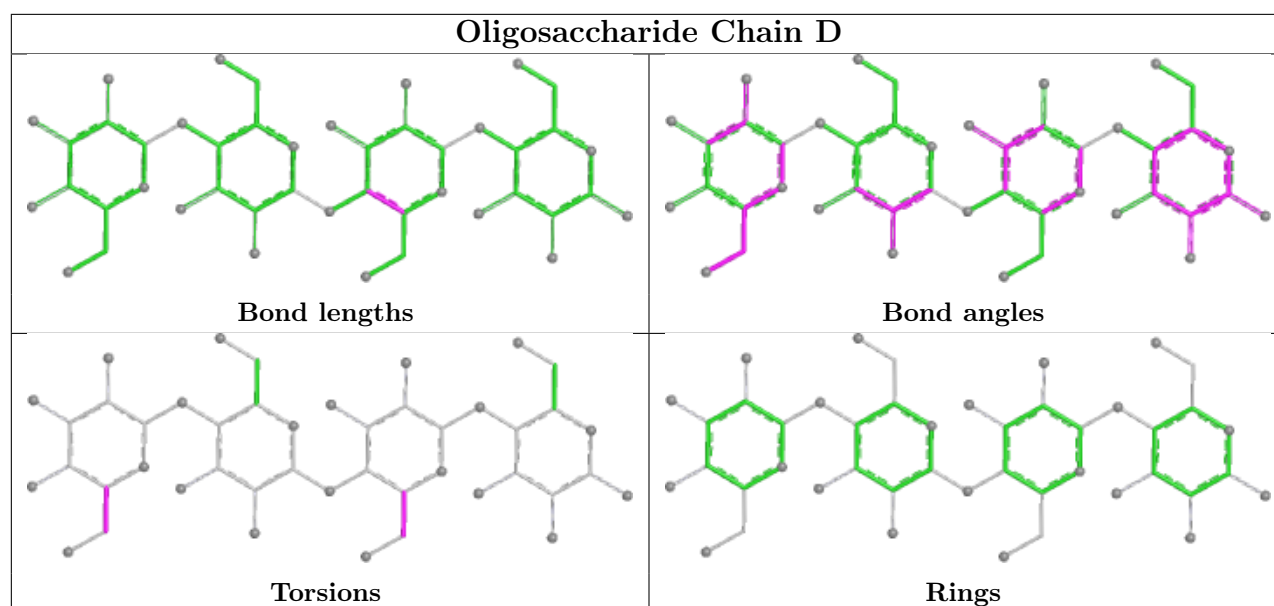
There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

6 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	VO4	A	999	-	0,4,4	-	-	-	-	-
4	PLP	A	900	1	15,15,16	1.34	3 (20%)	21,22,23	1.56	5 (23%)
3	VO4	B	1999	-	0,4,4	-	-	-	-	-
4	PLP	B	900	1	15,15,16	1.31	1 (6%)	21,22,23	1.19	2 (9%)
5	TRS	B	1990	-	7,7,7	0.49	0	9,9,9	1.72	2 (22%)
5	TRS	A	990	-	7,7,7	0.76	0	9,9,9	1.56	2 (22%)

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
5	TRS	A	990	-	-	2/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	B	900	1	-	0/6/6/8	0/1/1/1
5	TRS	B	1990	-	-	2/9/9/9	-
4	PLP	A	900	1	-	1/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	PLP	C2-N1	2.93	1.39	1.33
4	B	900	PLP	C2-N1	2.78	1.38	1.33
4	A	900	PLP	C6-N1	2.65	1.39	1.34
4	A	900	PLP	O3-C3	-2.18	1.31	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1990	TRS	O3-C3-C	-3.48	101.18	110.88
4	B	900	PLP	C3-C4-C5	3.00	122.19	118.59
4	A	900	PLP	C4A-C4-C3	-2.91	115.67	120.52
4	A	900	PLP	C2A-C2-N1	2.82	122.95	117.64
4	A	900	PLP	C4A-C4-C5	2.80	123.83	120.94
5	A	990	TRS	O3-C3-C	-2.73	103.26	110.88
5	B	1990	TRS	C1-C-N	2.70	115.04	108.17
4	B	900	PLP	C4A-C4-C3	-2.56	116.25	120.52
4	A	900	PLP	C5A-C5-C6	-2.24	115.70	119.36
5	A	990	TRS	C1-C-N	2.14	113.63	108.17
4	A	900	PLP	C3-C2-N1	-2.14	118.26	120.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	990	TRS	N-C-C1-O1
5	B	1990	TRS	N-C-C1-O1
5	B	1990	TRS	C3-C-C1-O1
4	A	900	PLP	C6-C5-C5A-O4P
5	A	990	TRS	C3-C-C1-O1

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	VO4	7	0
3	B	1999	VO4	8	0
4	B	900	PLP	1	0
5	B	1990	TRS	1	0
5	A	990	TRS	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.36	8 (1%) 79 82	22, 37, 59, 74	0
1	B	796/796 (100%)	-0.28	5 (0%) 85 87	22, 37, 60, 76	0
All	All	1592/1592 (100%)	-0.32	13 (0%) 82 84	22, 37, 60, 76	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	PHE	3.8
1	B	599	PRO	3.3
1	A	423	LEU	3.3
1	A	351	ALA	3.2
1	B	702	VAL	3.0
1	A	761	GLN	2.7
1	A	388	GLY	2.3
1	B	423	LEU	2.3
1	A	387	PRO	2.3
1	B	559	PRO	2.2
1	B	640	GLY	2.2
1	A	721	HIS	2.2
1	A	732	LYS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

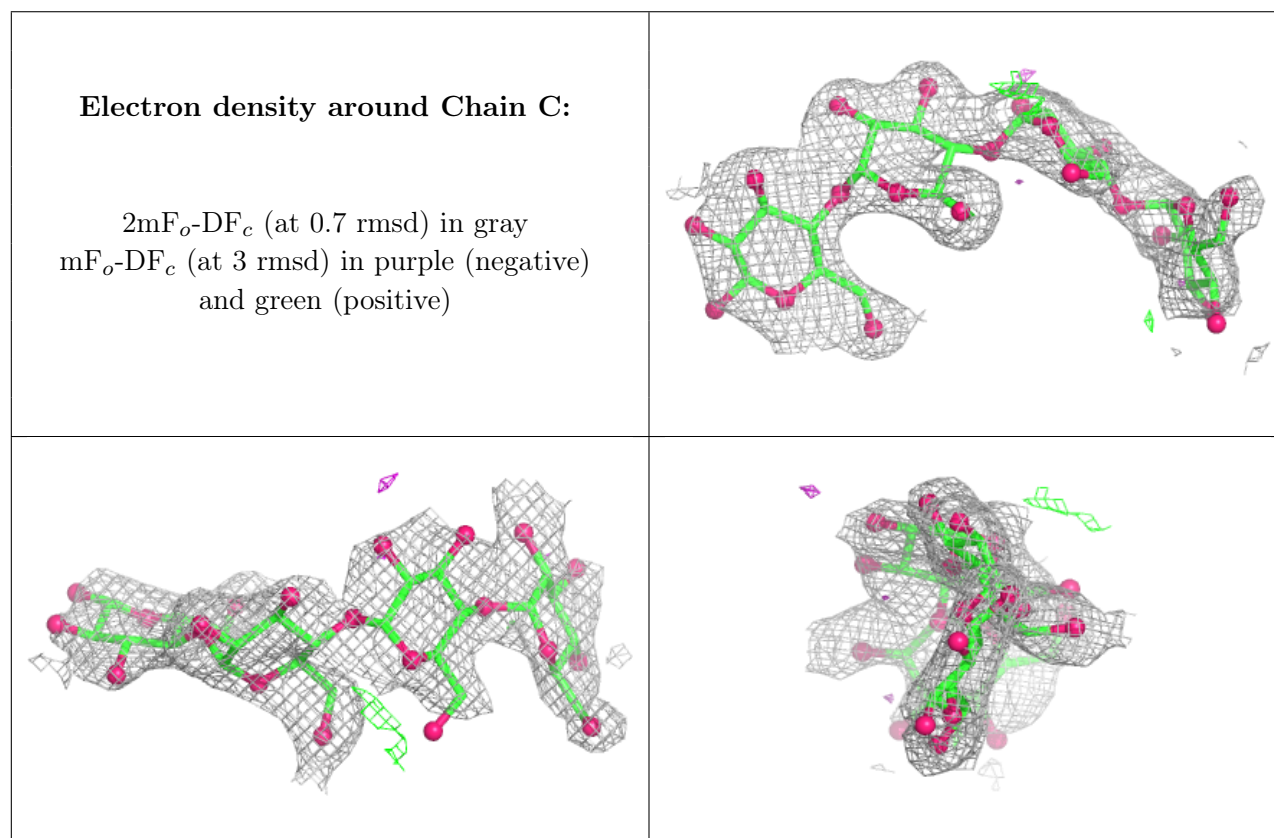
6.3 Carbohydrates [i](#)

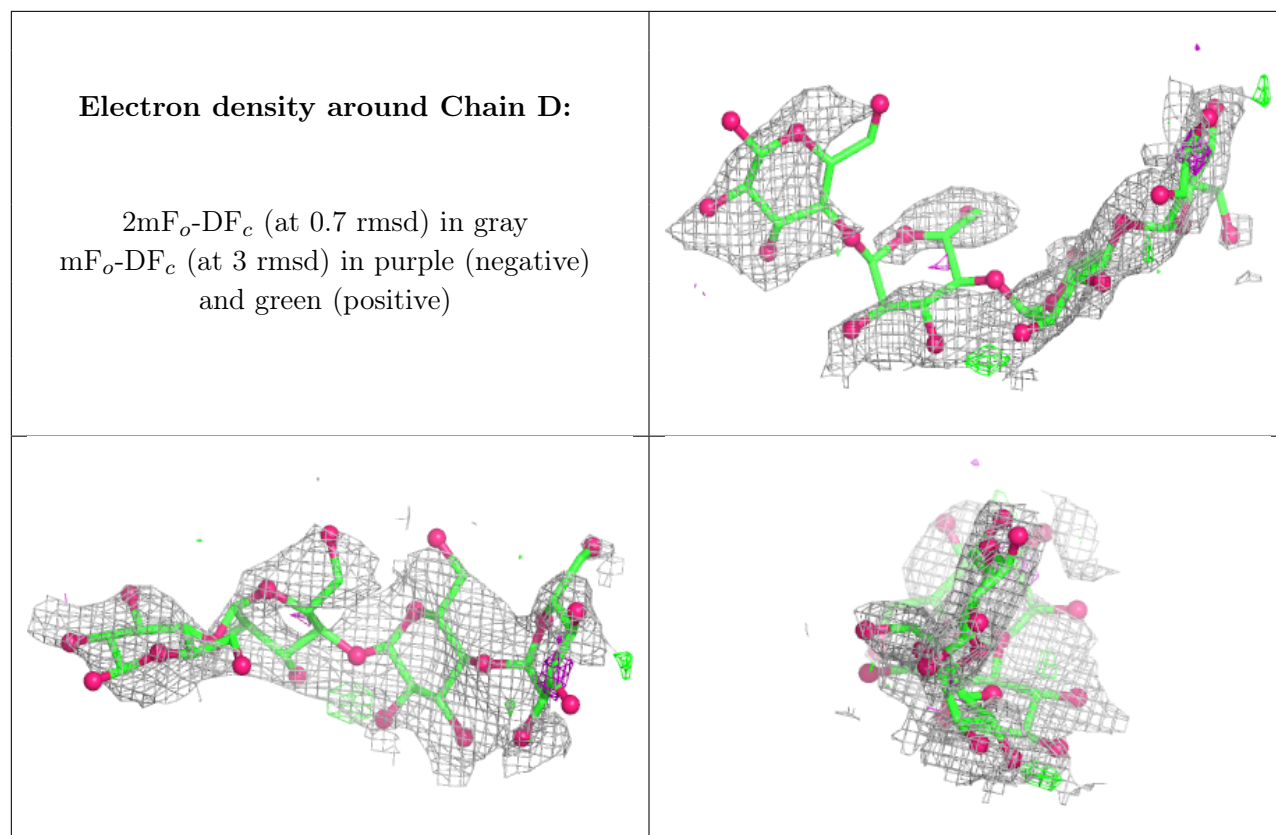
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
2	GLC	D	2	11/12	0.49	0.12	74,76,77,77	0
2	GLC	D	4	11/12	0.56	0.15	73,77,79,79	0
2	GLC	C	4	11/12	0.65	0.13	73,77,78,78	0
2	GLC	D	3	11/12	0.68	0.12	71,73,75,77	0
2	GLC	C	2	11/12	0.68	0.12	73,76,77,77	0
2	BGC	D	1	12/12	0.71	0.11	77,79,80,81	0
2	GLC	C	3	11/12	0.84	0.11	70,73,75,77	0
2	BGC	C	1	12/12	0.85	0.10	77,79,79,81	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	VO4	A	999	5/5	0.83	0.16	75,75,77,82	0
5	TRS	A	990	8/8	0.84	0.09	47,49,50,55	0
5	TRS	B	1990	8/8	0.86	0.08	48,49,50,53	0
3	VO4	B	1999	5/5	0.89	0.15	75,76,77,83	0
4	PLP	B	900	15/16	0.95	0.06	25,29,40,42	0
4	PLP	A	900	15/16	0.98	0.04	20,26,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.