



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:35 AM GMT

PDB ID : 2AV6  
Title : X-Ray studies on maltodextrin phosphorylase complexes: recognition of substrates and catalytic mechanism of phosphorylase family  
Authors : Geremia, S.; Campagnolo, M.  
Deposited on : 2005-08-29  
Resolution : 2.01 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

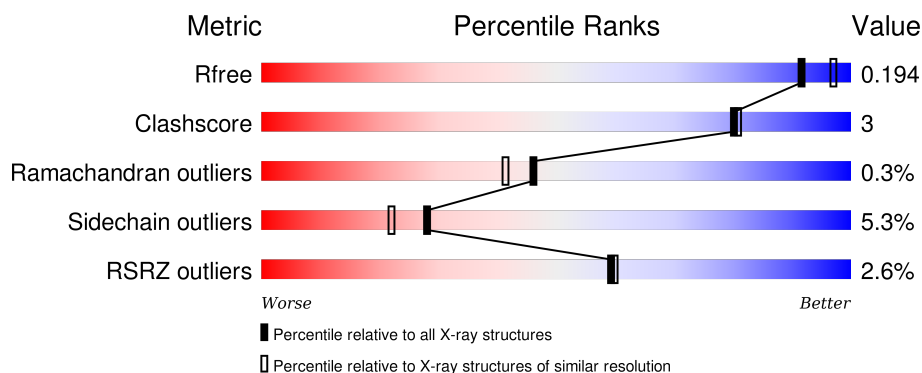
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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>87%</div> <div>12%</div> </div>
1	B	796	<div> <div>3%</div> <div>86%</div> <div>12%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	B	994	-	-	-	X
2	GLC	B	996	-	-	-	X
3	NO3	A	1999	-	X	-	-
3	NO3	B	2999	-	X	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14073 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			

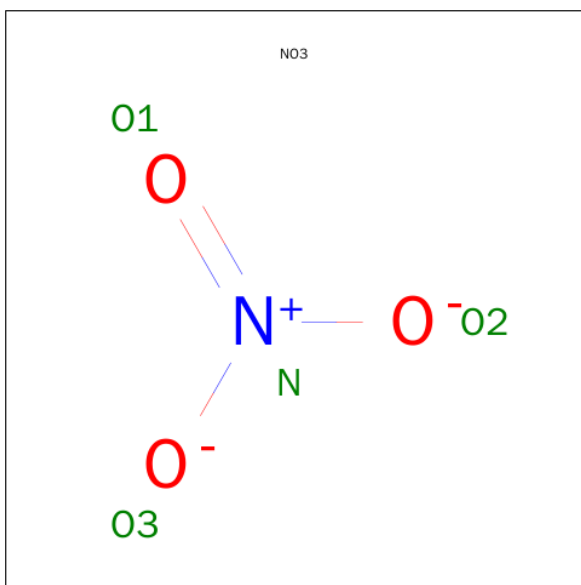
There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

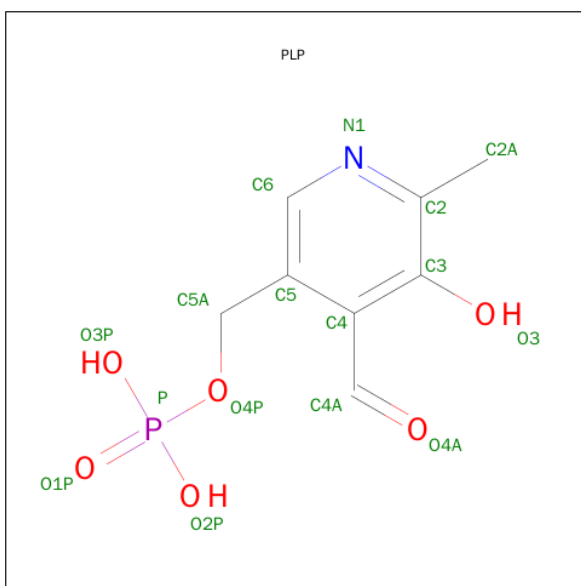
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	5	Total	C	O	0	0
			56	30	26		
2	B	5	Total	C	O	0	0
			56	30	26		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



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

- 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		

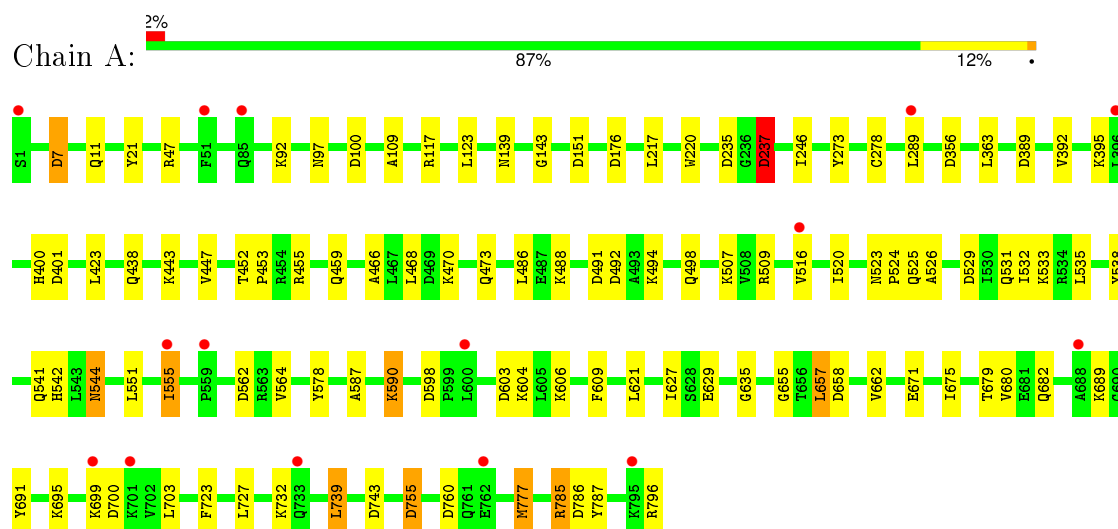
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	587	Total 587	O 587	0	0
5	B	558	Total 558	O 558	0	0

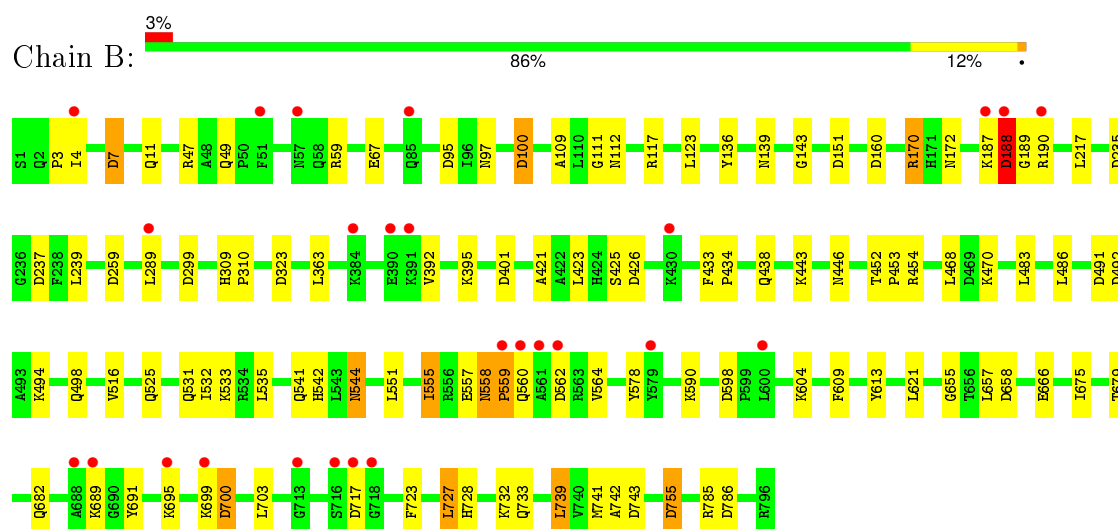
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.96Å 105.61Å 218.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.01 19.20 – 2.01	Depositor EDS
% Data completeness (in resolution range)	86.3 (15.00-2.01) 86.4 (19.20-2.01)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.190 , 0.244 0.200 , 0.194	Depositor DCC
$R_{free}$ test set	5033 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 100588 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GLC, BGC, NO3, 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	0.93	2/6539 (0.0%)	0.93	16/8865 (0.2%)
1	B	0.92	2/6539 (0.0%)	0.95	22/8865 (0.2%)
All	All	0.92	4/13078 (0.0%)	0.94	38/17730 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	TYR	CD1-CE1	5.91	1.48	1.39
1	A	273	TYR	CE2-CZ	-5.15	1.31	1.38
1	B	666	GLU	CD-OE2	5.04	1.31	1.25
1	A	777	MET	SD-CE	5.02	2.06	1.77

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ASP	CB-CG-OD2	10.21	127.49	118.30
1	B	786	ASP	CB-CG-OD2	8.66	126.09	118.30
1	B	491	ASP	CB-CG-OD2	8.52	125.97	118.30
1	B	492	ASP	CB-CG-OD2	8.41	125.87	118.30
1	B	95	ASP	CB-CG-OD2	8.23	125.70	118.30
1	A	492	ASP	CB-CG-OD2	8.12	125.61	118.30
1	A	658	ASP	CB-CG-OD2	7.47	125.02	118.30
1	B	562	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	760	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	743	ASP	CB-CG-OD2	6.62	124.25	118.30
1	A	7	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	755	ASP	CB-CG-OD2	6.53	124.18	118.30
1	B	59	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	176	ASP	CB-CG-OD2	6.35	124.02	118.30
1	B	598	ASP	CB-CG-OD2	6.35	124.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	717	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	491	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	743	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	598	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	426	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	151	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	658	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	389	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	603	ASP	CB-CG-OD2	5.61	123.34	118.30
1	B	299	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	7	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	235	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	235	ASP	CB-CG-OD2	5.38	123.15	118.30
1	B	100	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	151	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	237	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	170	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	356	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	160	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	786	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	755	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	700	ASP	CB-CG-OD2	5.05	122.84	118.30

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	6389	0	6333	47	0
1	B	6389	0	6333	43	0
2	A	56	0	48	0	0
2	B	56	0	48	1	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	15	0	7	0	0
4	B	15	0	6	1	0
5	A	587	0	0	10	0
5	B	558	0	0	2	0
All	All	14073	0	12775	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (87) 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:777:MET:CE	1:A:777:MET:SD	2.06	1.43
1:A:123:LEU:HD11	1:A:217:LEU:HD13	1.55	0.87
1:B:97:ASN:HD22	1:B:100:ASP:H	1.24	0.84
1:A:785:ARG:HG2	5:A:2546:HOH:O	1.76	0.83
1:B:188:ASP:OD1	1:B:188:ASP:C	2.22	0.76
1:A:470:LYS:NZ	1:A:498:GLN:HE22	1.85	0.74
1:B:470:LYS:NZ	1:B:498:GLN:HE22	1.86	0.73
1:B:551:LEU:O	1:B:555:ILE:HG23	1.88	0.72
1:A:97:ASN:HD22	1:A:100:ASP:H	1.36	0.72
1:B:470:LYS:HZ3	1:B:498:GLN:HE22	1.36	0.72
1:B:739:LEU:HB3	1:B:742:ALA:HB3	1.76	0.66
1:A:520:ILE:HD11	5:A:2551:HOH:O	1.96	0.64
1:A:551:LEU:O	1:A:555:ILE:HG23	1.98	0.62
1:A:488:LYS:HE3	5:A:2498:HOH:O	2.02	0.59
1:A:466:ALA:HB2	5:A:2481:HOH:O	2.02	0.58
1:A:47:ARG:HD3	5:A:2512:HOH:O	2.07	0.55
1:A:470:LYS:HZ2	1:A:498:GLN:HE22	1.53	0.55
1:A:470:LYS:HZ3	1:A:498:GLN:HE22	1.51	0.55
1:A:470:LYS:NZ	1:A:498:GLN:NE2	2.55	0.54
1:A:21:TYR:O	1:B:172:ASN:HB2	2.07	0.54
1:B:728:HIS:ND1	1:B:733:GLN:HG2	2.23	0.54
1:A:679:THR:OG1	1:A:682:GLN:HG3	2.08	0.53
1:B:109:ALA:HB1	1:B:143:GLY:HA3	1.91	0.52
1:A:555:ILE:HD13	1:A:604:LYS:HD3	1.92	0.52
1:B:123:LEU:HD11	1:B:217:LEU:HD13	1.92	0.51
1:B:7:ASP:O	1:B:11:GLN:HG2	2.11	0.51
1:B:679:THR:OG1	1:B:682:GLN:HG3	2.12	0.50
1:B:557:GLU:O	1:B:558:ASN:HB2	2.12	0.49
1:B:97:ASN:ND2	1:B:100:ASP:H	2.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:CD1	1:A:217:LEU:HD13	2.35	0.49
1:A:700:ASP:HB3	1:A:703:LEU:HB3	1.94	0.49
1:A:507:LYS:NZ	1:A:526:ALA:O	2.38	0.49
1:B:425:SER:OG	1:B:446:ASN:ND2	2.36	0.49
1:B:470:LYS:NZ	1:B:498:GLN:NE2	2.60	0.48
1:B:67:GLU:HB2	1:B:111:GLY:HA2	1.95	0.48
1:A:109:ALA:HB1	1:A:143:GLY:HA3	1.96	0.47
1:B:188:ASP:OD1	1:B:189:GLY:N	2.47	0.47
1:B:544:ASN:HD22	1:B:544:ASN:C	2.18	0.47
1:B:655:GLY:O	1:B:675:ILE:HA	2.15	0.47
1:A:468:LEU:CD2	1:A:486:LEU:HD11	2.44	0.47
1:A:246:ILE:HD13	1:B:239:LEU:HD12	1.97	0.47
1:A:587:ALA:HA	1:A:723:PHE:CE1	2.49	0.47
1:B:700:ASP:HB3	1:B:703:LEU:HB3	1.96	0.47
1:B:723:PHE:O	1:B:727:LEU:HD22	2.15	0.46
1:B:532:ILE:HG21	1:B:621:LEU:HD13	1.98	0.46
1:B:703:LEU:HD11	1:B:741:MET:CE	2.45	0.45
1:A:544:ASN:ND2	5:A:2049:HOH:O	2.48	0.45
1:A:590:LYS:HD2	1:A:590:LYS:HA	1.82	0.45
1:A:237:ASP:OD1	5:A:2565:HOH:O	2.21	0.45
1:B:590:LYS:HA	1:B:590:LYS:HD2	1.78	0.45
1:B:483:LEU:O	1:B:486:LEU:HB2	2.17	0.45
1:A:529:ASP:OD1	1:A:629:GLU:OE2	2.34	0.44
1:B:3:PRO:HB3	1:B:49:GLN:OE1	2.17	0.44
1:A:635:GLY:N	1:A:680:VAL:HG22	2.32	0.44
1:A:220:TRP:CE2	1:A:278:CYS:HB3	2.53	0.44
1:A:220:TRP:CD2	1:A:278:CYS:HB3	2.53	0.44
1:B:112:ASN:HD22	2:B:996:GLC:H61	1.82	0.44
1:A:7:ASP:O	1:A:11:GLN:HG2	2.18	0.44
1:B:421:ALA:C	1:B:446:ASN:HD21	2.21	0.43
1:A:531:GLN:HE22	1:A:541:GLN:HA	1.82	0.43
1:B:613:TYR:CE2	4:B:900:PLP:H2A2	2.53	0.43
1:A:657:LEU:HD22	1:A:662:VAL:HB	2.00	0.43
1:A:671:GLU:H	1:A:671:GLU:CD	2.22	0.43
1:A:246:ILE:CD1	1:B:239:LEU:HD12	2.49	0.43
1:B:555:ILE:HD13	1:B:604:LYS:HD3	2.00	0.43
1:B:170:ARG:NH2	5:B:3092:HOH:O	2.51	0.43
1:B:691:TYR:CE2	1:B:739:LEU:HD22	2.54	0.42
1:A:544:ASN:HD22	1:A:544:ASN:C	2.23	0.42
1:B:187:LYS:O	1:B:188:ASP:HB3	2.19	0.42
1:B:309:HIS:N	1:B:310:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ILE:HG21	1:A:621:LEU:HD13	2.02	0.41
1:A:455:ARG:HA	1:A:459:GLN:HE21	1.84	0.41
1:B:47:ARG:HD3	5:B:3203:HOH:O	2.20	0.41
1:A:509:ARG:HD3	5:A:2548:HOH:O	2.20	0.41
1:B:559:PRO:HB2	1:B:560:GLN:NE2	2.35	0.41
1:B:531:GLN:HE22	1:B:541:GLN:HA	1.85	0.41
1:A:691:TYR:CE2	1:A:739:LEU:HD22	2.55	0.41
1:A:606:LYS:HG3	5:A:2091:HOH:O	2.20	0.41
1:A:523:ASN:HA	1:A:524:PRO:HD3	1.98	0.41
1:B:452:THR:HA	1:B:453:PRO:HD3	1.91	0.41
1:A:655:GLY:O	1:A:675:ILE:HA	2.21	0.41
1:A:447:VAL:HG11	1:A:787:TYR:CD2	2.57	0.40
1:B:433:PHE:N	1:B:434:PRO:CD	2.84	0.40
1:B:468:LEU:CD2	1:B:486:LEU:HD11	2.52	0.40
1:A:529:ASP:HA	1:A:627:ILE:HB	2.02	0.40
1:A:452:THR:HA	1:A:453:PRO:HD3	1.86	0.40
1:A:400:HIS:HD2	5:A:2241:HOH:O	2.05	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%)	770 (97%)	23 (3%)	1 (0%)	56	53
1	B	794/796 (100%)	765 (96%)	26 (3%)	3 (0%)	39	33
All	All	1588/1592 (100%)	1535 (97%)	49 (3%)	4 (0%)	46	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	ASP

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Mol	Chain	Res	Type
1	B	559	PRO
1	B	558	ASN
1	A	533	LYS

### 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%)	631 (95%)	36 (5%)	27	21
1	B	667/667 (100%)	632 (95%)	35 (5%)	29	23
All	All	1334/1334 (100%)	1263 (95%)	71 (5%)	28	22

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
1	A	117	ARG
1	A	139	ASN
1	A	237	ASP
1	A	289	LEU
1	A	363	LEU
1	A	392	VAL
1	A	395	LYS
1	A	401	ASP
1	A	423	LEU
1	A	438	GLN
1	A	443	LYS
1	A	473	GLN
1	A	494	LYS
1	A	516	VAL
1	A	525	GLN
1	A	535	LEU
1	A	538	TYR
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	578	TYR
1	A	590	LYS
1	A	609	PHE
1	A	657	LEU
1	A	689	LYS
1	A	695	LYS
1	A	699	LYS
1	A	727	LEU
1	A	732	LYS
1	A	739	LEU
1	A	755	ASP
1	A	785	ARG
1	A	796	ARG
1	B	4	ILE
1	B	117	ARG
1	B	139	ASN
1	B	188	ASP
1	B	190	ARG
1	B	237	ASP
1	B	289	LEU
1	B	363	LEU
1	B	392	VAL
1	B	395	LYS
1	B	401	ASP
1	B	423	LEU
1	B	438	GLN
1	B	443	LYS
1	B	454	ARG
1	B	494	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	555	ILE
1	B	564	VAL
1	B	578	TYR
1	B	609	PHE

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Mol	Chain	Res	Type
1	B	657	LEU
1	B	689	LYS
1	B	695	LYS
1	B	699	LYS
1	B	727	LEU
1	B	732	LYS
1	B	739	LEU
1	B	755	ASP
1	B	785	ARG

Some 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	139	ASN
1	A	178	GLN
1	A	221	GLN
1	A	260	ASN
1	A	400	HIS
1	A	446	ASN
1	A	459	GLN
1	A	498	GLN
1	A	525	GLN
1	A	531	GLN
1	A	544	ASN
1	B	2	GLN
1	B	9	GLN
1	B	97	ASN
1	B	112	ASN
1	B	139	ASN
1	B	178	GLN
1	B	260	ASN
1	B	446	ASN
1	B	459	GLN
1	B	498	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 carbohydrates 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	A	994	2	12,12,12	0.86	0	17,17,17	0.90	0
2	GLC	A	995	2	11,11,12	1.17	1 (9%)	14,15,17	1.03	1 (7%)
2	GLC	A	996	2	11,11,12	1.42	1 (9%)	14,15,17	1.00	1 (7%)
2	GLC	A	997	2	11,11,12	0.91	1 (9%)	14,15,17	1.87	3 (21%)
2	GLC	A	998	2	11,11,12	0.90	1 (9%)	14,15,17	2.71	2 (14%)
2	BGC	B	994	2	12,12,12	0.80	0	17,17,17	0.73	0
2	GLC	B	995	2	11,11,12	0.66	0	14,15,17	1.21	1 (7%)
2	GLC	B	996	2	11,11,12	0.72	0	14,15,17	0.74	0
2	GLC	B	997	2	11,11,12	0.88	0	14,15,17	2.18	3 (21%)
2	GLC	B	998	2	11,11,12	0.80	0	14,15,17	2.39	2 (14%)

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	A	994	2	-	0/2/22/22	0/1/1/1
2	GLC	A	995	2	-	0/2/19/22	0/1/1/1
2	GLC	A	996	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	997	2	-	0/2/19/22	0/1/1/1
2	GLC	A	998	2	-	0/2/19/22	0/1/1/1
2	BGC	B	994	2	-	0/2/22/22	0/1/1/1
2	GLC	B	995	2	-	0/2/19/22	0/1/1/1
2	GLC	B	996	2	-	0/2/19/22	0/1/1/1
2	GLC	B	997	2	-	0/2/19/22	0/1/1/1
2	GLC	B	998	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	996	GLC	O5-C1	-2.98	1.38	1.43
2	A	997	GLC	C2-C3	2.25	1.55	1.52
2	A	998	GLC	C2-C3	2.35	1.55	1.52
2	A	995	GLC	C2-C3	3.15	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	996	GLC	O2-C2-C1	2.17	113.56	109.21
2	A	997	GLC	O2-C2-C3	2.20	114.54	110.12
2	A	997	GLC	O4-C4-C3	2.34	115.61	110.34
2	A	995	GLC	C1-C2-C3	2.55	112.55	109.54
2	B	995	GLC	C1-C2-C3	2.70	112.73	109.54
2	B	997	GLC	O2-C2-C3	3.13	116.42	110.12
2	B	997	GLC	O4-C4-C3	3.39	117.96	110.34
2	B	998	GLC	C1-O5-C5	4.71	118.23	112.25
2	A	997	GLC	C1-O5-C5	5.49	119.22	112.25
2	B	997	GLC	C1-O5-C5	6.42	120.40	112.25
2	A	998	GLC	C1-C2-C3	6.51	117.24	109.54
2	B	998	GLC	C1-C2-C3	6.63	117.38	109.54
2	A	998	GLC	C1-O5-C5	6.88	120.98	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	996	GLC	1	0

## 5.6 Ligand geometry

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	NO3	A	1999	-	3,3,3	3.41	3 (100%)	3,3,3	0.21	0
4	PLP	A	900	1	15,15,16	1.99	2 (13%)	21,22,23	1.98	9 (42%)
3	NO3	B	2999	-	3,3,3	3.79	3 (100%)	3,3,3	0.37	0
4	PLP	B	900	1	15,15,16	1.28	3 (20%)	21,22,23	1.69	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
3	NO3	A	1999	-	-	0/0/0/0	0/0/0/0
4	PLP	A	900	1	-	0/6/6/8	0/1/1/1
3	NO3	B	2999	-	-	0/0/0/0	0/0/0/0
4	PLP	B	900	1	-	0/6/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	PLP	C3-C2	-5.94	1.36	1.40
4	A	900	PLP	C4A-C4	-3.06	1.45	1.51
4	B	900	PLP	C5-C4	-2.39	1.37	1.40
4	B	900	PLP	C3-C2	-2.22	1.39	1.40
4	B	900	PLP	C4A-C4	-2.05	1.47	1.51
3	A	1999	NO3	O2-N	2.91	1.40	1.25
3	B	2999	NO3	O2-N	2.97	1.40	1.25
3	A	1999	NO3	O3-N	3.15	1.41	1.25
3	B	2999	NO3	O3-N	3.58	1.43	1.25
3	A	1999	NO3	O1-N	4.06	1.41	1.24
3	B	2999	NO3	O1-N	4.64	1.43	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	PLP	C4A-C4-C3	-3.00	114.92	120.36
4	A	900	PLP	C6-C5-C4	-2.99	115.61	118.15
4	B	900	PLP	C6-C5-C4	-2.99	115.61	118.15
4	B	900	PLP	C3-C2-N1	-2.94	116.54	120.61
4	A	900	PLP	O3P-P-O1P	-2.24	103.38	110.58
4	A	900	PLP	C3-C2-N1	-2.21	117.56	120.61
4	A	900	PLP	C5-C6-N1	-2.15	120.12	123.86
4	A	900	PLP	O2P-P-O1P	2.02	117.07	110.58
4	B	900	PLP	C6-N1-C2	2.09	123.55	119.28
4	A	900	PLP	C6-N1-C2	2.21	123.78	119.28
4	A	900	PLP	O4P-P-O1P	2.34	113.11	107.14
4	B	900	PLP	O2P-P-O1P	2.49	118.60	110.58
4	B	900	PLP	C2A-C2-C3	2.68	124.27	121.04
4	B	900	PLP	C3-C4-C5	3.42	122.51	118.78
4	A	900	PLP	C3-C4-C5	4.80	124.02	118.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	900	PLP	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 ⓘ

### 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%)	-0.04	15 (1%) 70 70	14, 25, 44, 59	0
1	B	796/796 (100%)	-0.00	26 (3%) 50 51	14, 25, 46, 59	0
All	All	1592/1592 (100%)	-0.02	41 (2%) 59 60	14, 25, 45, 59	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	562	ASP	5.4
1	B	560	GLN	5.1
1	B	57	ASN	4.7
1	A	51	PHE	3.9
1	B	559	PRO	3.8
1	B	187	LYS	3.7
1	B	561	ALA	3.4
1	B	718	GLY	3.3
1	B	579	TYR	3.2
1	A	289	LEU	2.8
1	B	688	ALA	2.8
1	A	699	LYS	2.7
1	B	188	ASP	2.7
1	B	716	SER	2.7
1	A	701	LYS	2.7
1	B	4	ILE	2.7
1	A	85	GLN	2.6
1	A	1	SER	2.6
1	B	717	ASP	2.6
1	B	391	LYS	2.5
1	B	689	LYS	2.5
1	B	390	GLU	2.4
1	A	688	ALA	2.4
1	A	555	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	762	GLU	2.4
1	B	190	ARG	2.3
1	A	795	LYS	2.3
1	B	600	LEU	2.3
1	B	51	PHE	2.3
1	A	516	VAL	2.2
1	B	713	GLY	2.2
1	A	396	LEU	2.2
1	B	695	LYS	2.2
1	A	733	GLN	2.2
1	A	600	LEU	2.1
1	B	384	LYS	2.1
1	B	85	GLN	2.1
1	B	289	LEU	2.1
1	B	699	LYS	2.1
1	B	430	LYS	2.0
1	A	559	PRO	2.0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BGC	B	994	12/12	0.93	0.20	2.67	32,34,37,42	0
2	GLC	B	996	11/12	0.95	0.13	2.07	20,23,24,24	0
2	BGC	A	994	12/12	0.94	0.12	1.83	33,34,37,42	0
2	GLC	B	997	11/12	0.94	0.10	0.98	24,27,30,31	0
2	GLC	B	998	11/12	0.94	0.13	0.91	32,35,36,37	0
2	GLC	A	998	11/12	0.91	0.15	0.61	31,35,37,37	0
2	GLC	B	995	11/12	0.92	0.12	0.51	20,24,28,28	0
2	GLC	A	997	11/12	0.96	0.08	-0.29	24,27,29,31	0
2	GLC	A	996	11/12	0.97	0.08	-0.89	19,23,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	A	995	11/12	0.95	0.09	-0.96	22,23,27,28	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NO3	B	2999	4/4	0.83	0.23	5.57	42,45,46,46	0
3	NO3	A	1999	4/4	0.94	0.15	0.88	42,45,45,46	0
4	PLP	A	900	15/16	0.98	0.09	-0.44	15,20,32,36	0
4	PLP	B	900	15/16	0.97	0.08	-0.71	14,19,32,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.