



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:20 AM GMT

PDB ID : 2GPB  
Title : COMPARISON OF THE BINDING OF GLUCOSE AND GLUCOSE-1-PHOSPHATE DERIVATIVES TO T-STATE GLYCOGEN PHOSPHORYLASE B  
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Deposited on : 1990-06-04  
Resolution : 2.30 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

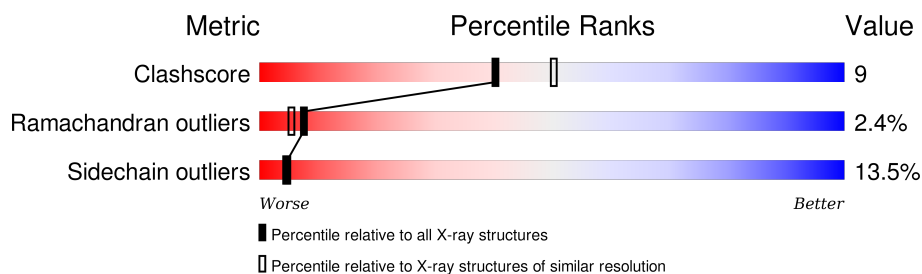
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	 65% 24% 7% . .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7361 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 GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	831	6759	4308	1191	1230	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489

- Molecule 2 is SUGAR (GLUCOSE) (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

- Molecule 4 is water.

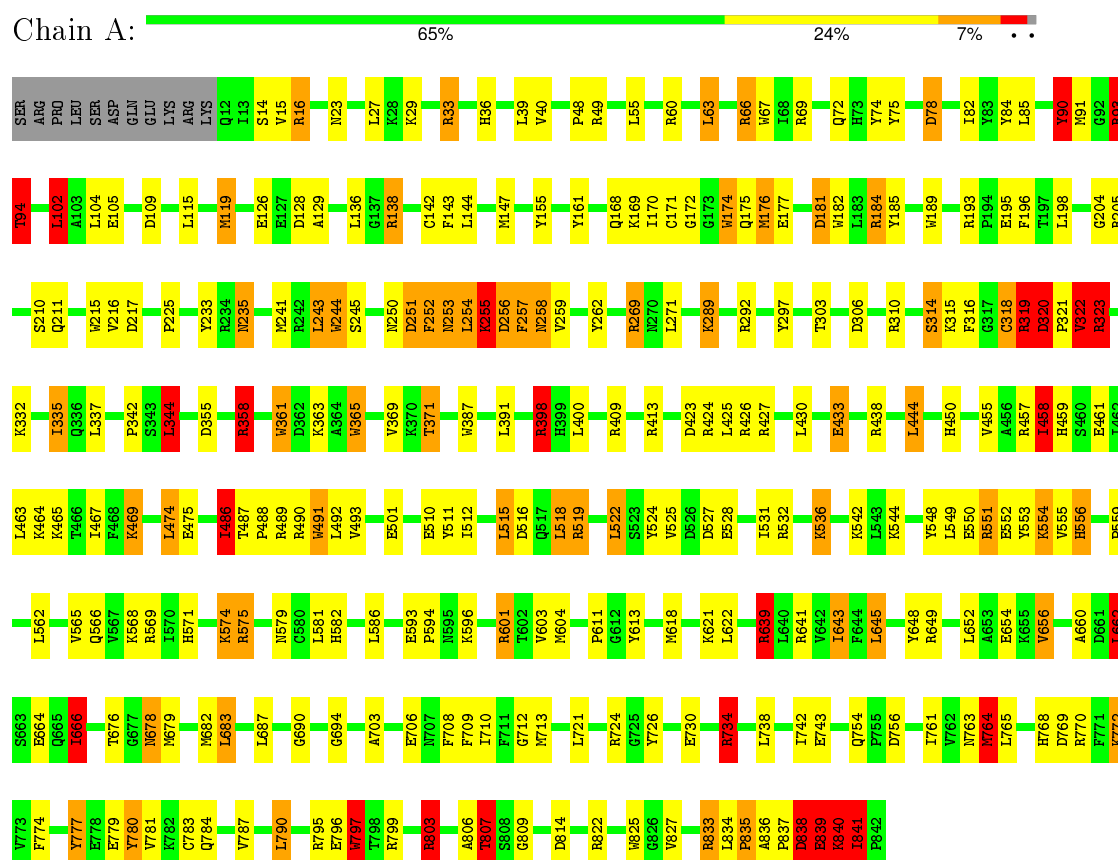
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	575	Total	O	0	0
			575	575		

### 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.

Note EDS was not executed.

#### • Molecule 1: GLYCOGEN PHOSPHORYLASE B



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.50 Å   128.50 Å   116.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.91	3/6913 (0.0%)	1.75	168/9356 (1.8%)

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	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	THR	CA-CB	5.74	1.68	1.53
1	A	335	ILE	CA-CB	5.39	1.67	1.54
1	A	94	THR	CA-CB	5.25	1.67	1.53

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	A	138	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	A	424	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	A	649	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	413	ARG	CB-CG-CD	-10.13	85.25	111.60
1	A	490	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	613	TYR	CB-CG-CD2	-9.87	115.08	121.00
1	A	409	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	A	215	TRP	CD1-CG-CD2	9.43	113.85	106.30
1	A	575	ARG	NE-CZ-NH2	-9.37	115.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	A	387	TRP	CD1-CG-CD2	8.90	113.42	106.30
1	A	601	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	A	639	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	365	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	A	486	ILE	CA-CB-CG1	-8.59	94.69	111.00
1	A	174	TRP	CE2-CD2-CG	-8.40	100.58	107.30
1	A	90	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	A	822	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	A	174	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	A	16	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	319	ARG	CA-CB-CG	8.15	131.33	113.40
1	A	174	TRP	CG-CD2-CE3	7.96	141.07	133.90
1	A	189	TRP	CD1-CG-CD2	7.93	112.65	106.30
1	A	457	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	185	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	A	215	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	A	797	TRP	CB-CG-CD1	-7.91	116.72	127.00
1	A	666	ILE	CA-CB-CG1	-7.86	96.07	111.00
1	A	574	LYS	CA-CB-CG	7.82	130.60	113.40
1	A	387	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	A	413	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	797	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	A	713	MET	CA-CB-CG	7.59	126.20	113.30
1	A	556	HIS	N-CA-C	7.53	131.34	111.00
1	A	182	TRP	CD1-CG-CD2	7.53	112.32	106.30
1	A	490	ARG	CB-CA-C	-7.51	95.38	110.40
1	A	797	TRP	NE1-CE2-CZ2	-7.46	122.19	130.40
1	A	93	ARG	CG-CD-NE	7.45	127.43	111.80
1	A	361	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	A	244	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	A	797	TRP	CG-CD2-CE3	7.33	140.50	133.90
1	A	365	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	A	67	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	807	THR	N-CA-CB	-7.27	96.49	110.30
1	A	63	LEU	CA-CB-CG	7.26	131.99	115.30
1	A	838	ASP	CA-C-N	-7.24	101.27	117.20
1	A	803	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	A	666	ILE	CA-CB-CG2	7.23	125.35	110.90
1	A	489	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	713	MET	CG-SD-CE	-7.20	88.69	100.20
1	A	365	TRP	CB-CG-CD1	-7.17	117.68	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	825	TRP	CE2-CD2-CG	-7.16	101.58	107.30
1	A	554	LYS	N-CA-C	7.12	130.22	111.00
1	A	639	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	780	TYR	CB-CG-CD2	-7.01	116.79	121.00
1	A	189	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	182	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	A	666	ILE	N-CA-CB	-6.92	94.89	110.80
1	A	413	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	398	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	365	TRP	CG-CD2-CE3	6.86	140.08	133.90
1	A	770	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	601	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	174	TRP	CB-CG-CD1	-6.83	118.12	127.00
1	A	244	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	A	764	MET	CG-SD-CE	-6.82	89.30	100.20
1	A	553	TYR	CA-CB-CG	6.74	126.20	113.40
1	A	358	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	825	TRP	CD1-CG-CD2	6.66	111.63	106.30
1	A	486	ILE	CA-CB-CG2	6.65	124.20	110.90
1	A	554	LYS	CA-C-N	-6.63	102.62	117.20
1	A	119	MET	CB-CA-C	-6.62	97.16	110.40
1	A	361	TRP	CE2-CD2-CG	-6.62	102.01	107.30
1	A	656	VAL	CB-CA-C	-6.61	98.84	111.40
1	A	491	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	A	575	ARG	CB-CG-CD	-6.55	94.57	111.60
1	A	724	ARG	CA-CB-CG	6.55	127.81	113.40
1	A	78	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	777	TYR	CB-CG-CD2	-6.54	117.08	121.00
1	A	67	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	A	553	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	A	491	TRP	CD1-CG-CD2	6.46	111.47	106.30
1	A	138	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	490	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	838	ASP	O-C-N	6.32	132.81	122.70
1	A	215	TRP	CG-CD1-NE1	-6.31	103.79	110.10
1	A	256	ASP	N-CA-C	-6.28	94.05	111.00
1	A	524	TYR	CB-CG-CD1	-6.26	117.25	121.00
1	A	490	ARG	N-CA-CB	6.24	121.83	110.60
1	A	501	GLU	CB-CA-C	-6.23	97.95	110.40
1	A	318	CYS	N-CA-C	-6.21	94.24	111.00
1	A	613	TYR	CB-CG-CD1	6.19	124.71	121.00
1	A	161	TYR	CB-CG-CD2	-6.13	117.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	TYR	CB-CG-CD2	-6.11	117.34	121.00
1	A	253	ASN	CA-C-N	-6.08	103.82	117.20
1	A	458	ILE	CB-CA-C	-6.06	99.47	111.60
1	A	205	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	84	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	A	426	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	181	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	814	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	310	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	797	TRP	CD1-CG-CD2	5.90	111.02	106.30
1	A	489	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	271	LEU	N-CA-C	-5.83	95.27	111.00
1	A	93	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	682	MET	CG-SD-CE	5.78	109.44	100.20
1	A	365	TRP	CG-CD1-NE1	-5.77	104.33	110.10
1	A	253	ASN	O-C-N	5.73	131.86	122.70
1	A	322	VAL	CA-CB-CG2	-5.71	102.33	110.90
1	A	438	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	575	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	527	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	413	ARG	CA-CB-CG	5.63	125.78	113.40
1	A	803	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	734	ARG	CB-CG-CD	5.58	126.10	111.60
1	A	93	ARG	CD-NE-CZ	5.57	131.40	123.60
1	A	838	ASP	N-CA-C	5.55	125.98	111.00
1	A	712	GLY	CA-C-N	-5.47	105.16	117.20
1	A	825	TRP	CG-CD2-CE3	5.46	138.82	133.90
1	A	216	VAL	CG1-CB-CG2	-5.44	102.19	110.90
1	A	654	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	A	840	LYS	CA-C-N	-5.43	105.26	117.20
1	A	433	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	A	713	MET	N-CA-CB	-5.42	100.85	110.60
1	A	119	MET	N-CA-CB	5.42	120.35	110.60
1	A	29	LYS	CA-CB-CG	5.41	125.31	113.40
1	A	553	TYR	CA-C-N	5.41	129.10	117.20
1	A	155	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	A	253	ASN	C-N-CA	5.39	135.17	121.70
1	A	66	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	469	LYS	CB-CG-CD	5.38	125.59	111.60
1	A	262	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	444	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	184	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	TRP	CG-CD2-CE3	5.33	138.70	133.90
1	A	205	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	387	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	A	67	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	A	841	ILE	N-CA-C	-5.28	96.76	111.00
1	A	195	GLU	CB-CA-C	-5.23	99.94	110.40
1	A	734	ARG	CA-CB-CG	5.22	124.88	113.40
1	A	838	ASP	CA-CB-CG	-5.22	101.92	113.40
1	A	734	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	74	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	255	LYS	N-CA-C	5.20	125.03	111.00
1	A	491	TRP	CG-CD2-CE3	5.20	138.58	133.90
1	A	734	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	49	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	136	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	464	LYS	CB-CG-CD	-5.18	98.14	111.60
1	A	102	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	662	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	666	ILE	CB-CA-C	5.16	121.92	111.60
1	A	772	LYS	CA-CB-CG	5.16	124.75	113.40
1	A	738	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	323	ARG	N-CA-C	-5.14	97.12	111.00
1	A	233	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	469	LYS	CA-CB-CG	5.09	124.59	113.40
1	A	344	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	297	TYR	CB-CG-CD1	5.08	124.05	121.00
1	A	269	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	322	VAL	CA-CB-CG1	5.04	118.47	110.90
1	A	660	ALA	CB-CA-C	-5.04	102.53	110.10
1	A	430	LEU	CB-CG-CD1	-5.03	102.46	111.00
1	A	262	TYR	CB-CG-CD1	5.01	124.00	121.00
1	A	322	VAL	CA-C-N	-5.00	106.20	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	519	ARG	Sidechain
1	A	841	ILE	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	6759	0	6703	117	0
2	A	12	0	12	0	0
3	A	15	0	7	0	0
4	A	575	0	0	11	0
All	All	7361	0	6722	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 9.

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:A:571:HIS:HB2	1:A:574:LYS:HG2	1.55	0.86
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.69	0.75
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.70	0.72
1:A:703:ALA:HA	1:A:807:THR:HG21	1.71	0.70
1:A:730:GLU:O	1:A:734:ARG:HG2	1.91	0.69
1:A:193:ARG:HB3	1:A:196:PHE:HD2	1.57	0.68
1:A:177:GLU:HG2	1:A:611:PRO:HG3	1.76	0.67
1:A:550:GLU:HA	1:A:554:LYS:HB2	1.77	0.66
1:A:474:LEU:HD13	1:A:475:GLU:HG3	1.78	0.65
1:A:14:SER:HB3	1:A:16:ARG:HG3	1.78	0.65
1:A:181:ASP:HB3	1:A:184:ARG:HH11	1.62	0.65
1:A:458:ILE:HD11	1:A:694:GLY:N	2.12	0.64
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.80	0.62
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.65	0.62
1:A:764:MET:CE	1:A:769:ASP:HA	2.31	0.61
1:A:703:ALA:CA	1:A:807:THR:HG21	2.31	0.60
1:A:519:ARG:O	1:A:522:LEU:HB2	2.02	0.60
1:A:463:LEU:HA	1:A:467:ILE:HG22	1.85	0.59
1:A:144:LEU:HD12	1:A:147:MET:CE	2.33	0.58
1:A:516:ASP:HA	4:A:1059:HOH:O	2.04	0.58
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.86	0.58
1:A:322:VAL:O	1:A:323:ARG:HD3	2.04	0.58
1:A:795:ARG:O	1:A:799:ARG:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:H	1:A:459:HIS:HD2	1.50	0.57
1:A:60:ARG:HA	1:A:63:LEU:HD23	1.87	0.57
1:A:423:ASP:O	1:A:427:ARG:HB2	2.05	0.57
1:A:169:LYS:HB2	1:A:176:MET:HB2	1.86	0.57
1:A:639:ARG:HH11	1:A:639:ARG:HG3	1.70	0.56
1:A:320:ASP:HB3	1:A:321:PRO:CD	2.36	0.56
1:A:515:LEU:HD13	1:A:809:GLY:HA2	1.88	0.55
1:A:548:TYR:HA	1:A:551:ARG:HD3	1.87	0.54
1:A:690:GLY:O	1:A:710:ILE:HA	2.08	0.54
1:A:604:MET:HB3	1:A:645:LEU:HD22	1.90	0.54
1:A:171:CYS:SG	1:A:176:MET:HG2	2.49	0.53
1:A:181:ASP:O	1:A:184:ARG:NH1	2.42	0.53
1:A:172:GLY:O	1:A:621:LYS:NZ	2.42	0.53
1:A:193:ARG:HB3	1:A:196:PHE:CD2	2.42	0.52
1:A:319:ARG:NE	1:A:320:ASP:H	2.06	0.52
1:A:542:LYS:HE2	1:A:559:PRO:O	2.10	0.52
1:A:225:PRO:HG3	1:A:244:TRP:CZ3	2.44	0.52
1:A:803:ARG:O	1:A:807:THR:HB	2.10	0.51
1:A:486:ILE:CD1	1:A:676:THR:HB	2.40	0.51
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.94	0.50
1:A:365:TRP:O	1:A:369:VAL:HG12	2.11	0.49
1:A:142:CYS:SG	1:A:487:THR:HG22	2.52	0.49
1:A:790:LEU:HD13	1:A:797:TRP:CD1	2.48	0.48
1:A:562:LEU:HD21	1:A:662:LEU:HB2	1.95	0.48
1:A:15:VAL:HG13	1:A:15:VAL:O	2.13	0.48
1:A:257:PHE:H	1:A:257:PHE:HD1	1.61	0.48
1:A:554:LYS:HD3	1:A:555:VAL:H	1.78	0.48
1:A:14:SER:HB3	1:A:16:ARG:CG	2.42	0.48
1:A:72:GLN:O	1:A:75:TYR:HB3	2.14	0.48
1:A:85:LEU:HD11	1:A:303:THR:HG21	1.95	0.48
1:A:487:THR:O	1:A:491:TRP:HB2	2.13	0.48
1:A:678:ASN:HD22	1:A:679:MET:H	1.61	0.48
1:A:790:LEU:HB3	1:A:797:TRP:CD1	2.49	0.47
1:A:90:TYR:HE1	4:A:1211:HOH:O	1.96	0.47
1:A:257:PHE:O	1:A:258:ASN:HB2	2.14	0.47
1:A:344:LEU:HB2	4:A:1411:HOH:O	2.14	0.47
1:A:314:SER:O	1:A:315:LYS:HD2	2.14	0.47
1:A:94:THR:HG22	4:A:1423:HOH:O	2.15	0.47
1:A:492:LEU:HB2	1:A:683:LEU:HD22	1.96	0.47
1:A:519:ARG:NH2	4:A:1060:HOH:O	2.47	0.46
1:A:252:PHE:HD1	1:A:256:ASP:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:VAL:O	1:A:531:ILE:HD11	2.16	0.46
1:A:109:ASP:HA	1:A:119:MET:HG3	1.97	0.46
1:A:33:ARG:HH11	1:A:33:ARG:HG3	1.80	0.46
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.97	0.46
1:A:316:PHE:HA	1:A:320:ASP:HB2	1.98	0.46
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.51	0.46
1:A:834:LEU:HG	1:A:835:PRO:HD2	1.98	0.46
1:A:78:ASP:OD2	1:A:332:LYS:NZ	2.49	0.46
1:A:16:ARG:HB3	1:A:105:GLU:HB3	1.98	0.45
1:A:601:ARG:NH2	1:A:784:GLN:OE1	2.48	0.45
1:A:618:MET:HB3	1:A:761:ILE:HD11	1.99	0.45
1:A:289:LYS:NZ	4:A:1427:HOH:O	2.47	0.45
1:A:809:GLY:HA3	4:A:1059:HOH:O	2.15	0.45
1:A:839:GLU:O	1:A:840:LYS:NZ	2.48	0.45
1:A:355:ASP:OD1	1:A:398:ARG:NH1	2.50	0.45
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.98	0.45
1:A:754:GLN:HB3	4:A:1174:HOH:O	2.16	0.45
1:A:204:GLY:HA2	1:A:217:ASP:O	2.17	0.45
1:A:170:ILE:HA	1:A:174:TRP:O	2.17	0.45
1:A:461:GLU:OE1	1:A:465:LYS:NZ	2.51	0.44
1:A:66:ARG:HG3	1:A:837:PRO:HB3	2.00	0.44
1:A:241:MET:HG2	1:A:243:LEU:HD13	1.99	0.44
1:A:144:LEU:HD12	1:A:147:MET:HE1	2.00	0.44
1:A:320:ASP:HB3	1:A:321:PRO:HD3	1.99	0.43
1:A:450:HIS:HE1	4:A:1568:HOH:O	2.00	0.43
1:A:102:LEU:HD23	1:A:104:LEU:HD22	1.99	0.43
1:A:604:MET:HB3	1:A:645:LEU:CD2	2.48	0.43
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.59	0.43
1:A:319:ARG:HH21	1:A:320:ASP:CG	2.22	0.43
1:A:251:ASP:CG	1:A:252:PHE:H	2.21	0.43
1:A:129:ALA:HB2	4:A:1423:HOH:O	2.18	0.43
1:A:721:LEU:HD23	1:A:772:LYS:HD3	2.01	0.42
1:A:777:TYR:O	1:A:781:VAL:HG13	2.20	0.42
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.19	0.42
1:A:69:ARG:HD3	1:A:837:PRO:HA	2.01	0.42
1:A:522:LEU:HD13	1:A:806:ALA:HB3	2.01	0.42
1:A:594:PRO:O	1:A:639:ARG:NH2	2.50	0.42
1:A:764:MET:HE2	1:A:769:ASP:HA	2.01	0.42
1:A:522:LEU:HD13	1:A:806:ALA:CB	2.50	0.41
1:A:532:ARG:O	1:A:536:LYS:HB2	2.21	0.41
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:THR:HA	1:A:488:PRO:HD2	1.83	0.41
1:A:493:VAL:HG22	1:A:512:ILE:HD12	2.02	0.41
1:A:355:ASP:O	1:A:358:ARG:NH1	2.53	0.41
1:A:772:LYS:HE3	4:A:1124:HOH:O	2.21	0.41
1:A:314:SER:OG	1:A:332:LYS:NZ	2.53	0.41
1:A:36:HIS:O	1:A:40:VAL:HA	2.20	0.41
1:A:554:LYS:HE3	1:A:643:ILE:HD13	2.03	0.40
1:A:575:ARG:HD2	1:A:666:ILE:O	2.21	0.40
1:A:69:ARG:NH1	1:A:838:ASP:O	2.54	0.40
1:A:511:TYR:CE1	1:A:512:ILE:HD13	2.56	0.40
1:A:93:ARG:NH1	1:A:126:GLU:O	2.54	0.40
1:A:143:PHE:O	1:A:147:MET:HG3	2.21	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	829/842 (98%)	768 (93%)	41 (5%)	20 (2%)	7 5

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	SER
1	A	252	PHE
1	A	254	LEU
1	A	320	ASP
1	A	556	HIS
1	A	839	GLU
1	A	840	LYS
1	A	258	ASN
1	A	259	VAL

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Mol	Chain	Res	Type
1	A	318	CYS
1	A	323	ARG
1	A	551	ARG
1	A	251	ASP
1	A	255	LYS
1	A	836	ALA
1	A	838	ASP
1	A	319	ARG
1	A	835	PRO
1	A	322	VAL
1	A	342	PRO

### 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	720/731 (98%)	623 (86%)	97 (14%)	<b>5</b> <b>4</b>

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

Mol	Chain	Res	Type
1	A	23	ASN
1	A	27	LEU
1	A	33	ARG
1	A	39	LEU
1	A	48	PRO
1	A	55	LEU
1	A	90	TYR
1	A	93	ARG
1	A	94	THR
1	A	102	LEU
1	A	115	LEU
1	A	128	ASP
1	A	138	ARG
1	A	176	MET
1	A	198	LEU

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Mol	Chain	Res	Type
1	A	211	GLN
1	A	235	ASN
1	A	243	LEU
1	A	245	SER
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	257	PHE
1	A	289	LYS
1	A	292	ARG
1	A	306	ASP
1	A	314	SER
1	A	319	ARG
1	A	320	ASP
1	A	323	ARG
1	A	335	ILE
1	A	337	LEU
1	A	344	LEU
1	A	358	ARG
1	A	361	TRP
1	A	363	LYS
1	A	371	THR
1	A	391	LEU
1	A	398	ARG
1	A	400	LEU
1	A	425	LEU
1	A	433	GLU
1	A	444	LEU
1	A	458	ILE
1	A	469	LYS
1	A	474	LEU
1	A	486	ILE
1	A	510	GLU
1	A	515	LEU
1	A	518	LEU
1	A	522	LEU
1	A	528	GLU
1	A	536	LYS
1	A	544	LYS
1	A	549	LEU
1	A	552	GLU
1	A	565	VAL

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Mol	Chain	Res	Type
1	A	568	LYS
1	A	569	ARG
1	A	579	ASN
1	A	581	LEU
1	A	586	LEU
1	A	593	GLU
1	A	596	LYS
1	A	603	VAL
1	A	622	LEU
1	A	639	ARG
1	A	641	ARG
1	A	643	ILE
1	A	645	LEU
1	A	656	VAL
1	A	662	LEU
1	A	666	ILE
1	A	678	ASN
1	A	683	LEU
1	A	687	LEU
1	A	706	GLU
1	A	708	PHE
1	A	734	ARG
1	A	743	GLU
1	A	756	ASP
1	A	763	ASN
1	A	764	MET
1	A	765	LEU
1	A	768	HIS
1	A	779	GLU
1	A	787	VAL
1	A	790	LEU
1	A	796	GLU
1	A	797	TRP
1	A	803	ARG
1	A	807	THR
1	A	833	ARG
1	A	838	ASP
1	A	839	GLU
1	A	840	LYS
1	A	841	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	62	HIS
1	A	97	ASN
1	A	235	ASN
1	A	390	HIS
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	566	GLN
1	A	579	ASN
1	A	614	HIS
1	A	678	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
2	GLC	A	910	-	12,12,12	1.06	1 (8%)	17,17,17	0.85	1 (5%)
3	PLP	A	999	1	15,15,16	2.07	2 (13%)	21,22,23	1.26	3 (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	GLC	A	910	-	-	0/2/22/22	0/1/1/1
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C3-C2	-6.56	1.36	1.40
3	A	999	PLP	P-O2P	-2.05	1.47	1.54
2	A	910	GLC	C4-C5	2.47	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	PLP	C5-C6-N1	-2.26	119.93	123.86
3	A	999	PLP	O4P-C5A-C5	2.36	112.90	108.99
2	A	910	GLC	O5-C1-C2	2.77	114.21	109.80
3	A	999	PLP	O2P-P-O1P	3.19	120.85	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.