



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 PM UTC

PDB ID : 2GPB / pdb_00002gpb
Title : COMPARISON OF THE BINDING OF GLUCOSE AND GLUCOSE-1-PHOSPHATE DERIVATIVES TO T-STATE GLYCOGEN PHOSPHORYLASE B
Authors : Martin, J.L.; Johnson, L.N.
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.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

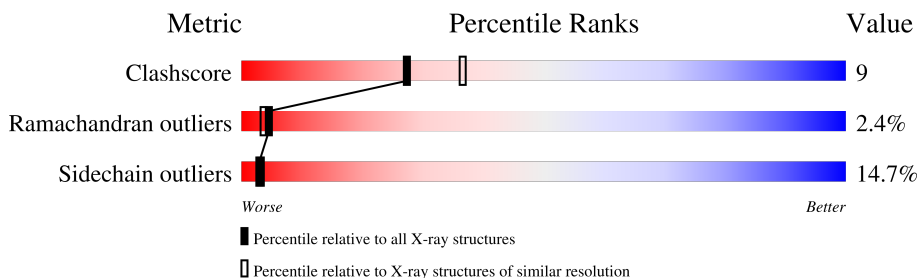
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	

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.

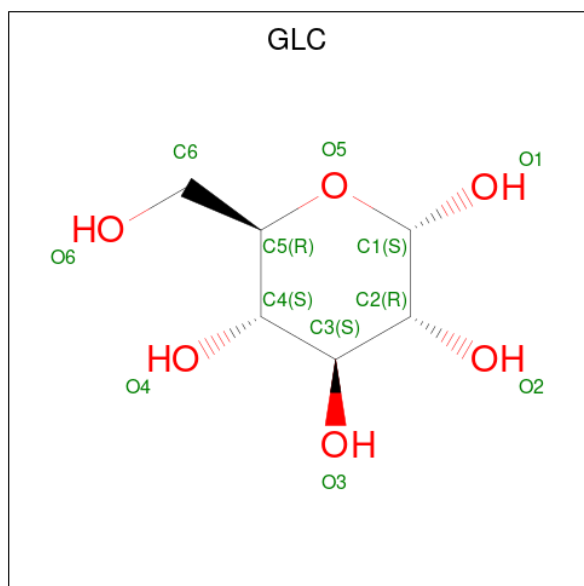
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

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:

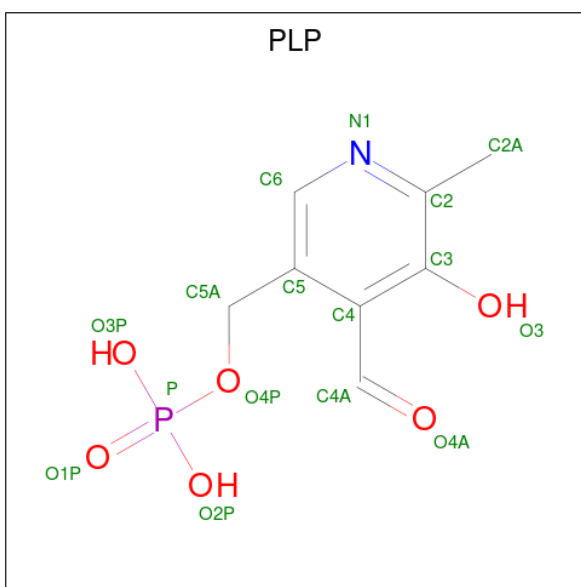
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.50Å 128.50Å 116.30Å 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 ²)	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	1.17	35/6913 (0.5%)	2.03	214/9356 (2.3%)

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ILE	CA-CB	10.38	1.67	1.54
1	A	371	THR	CA-CB	9.17	1.68	1.53
1	A	94	THR	CA-CB	8.65	1.67	1.53
1	A	34	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	571	HIS	CD2-NE2	-6.88	1.30	1.37
1	A	450	HIS	CD2-NE2	-6.88	1.30	1.37
1	A	57	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	632	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	459	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	603	VAL	CA-CB	6.55	1.62	1.54
1	A	399	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	201	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	208	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	556	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	443	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	36	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	582	HIS	CD2-NE2	-5.98	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	477	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	390	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	787	VAL	CA-CB	5.79	1.62	1.54
1	A	582	HIS	CG-ND1	-5.73	1.31	1.38
1	A	34	HIS	CG-ND1	-5.70	1.31	1.38
1	A	632	HIS	CG-ND1	-5.68	1.32	1.38
1	A	165	ILE	CA-CB	5.67	1.60	1.54
1	A	767	HIS	CD2-NE2	-5.62	1.31	1.37
1	A	768	HIS	CD2-NE2	-5.59	1.31	1.37
1	A	436	VAL	CA-CB	5.50	1.62	1.54
1	A	263	ILE	CA-CB	5.43	1.60	1.54
1	A	450	HIS	CG-ND1	-5.32	1.32	1.38
1	A	571	HIS	CG-ND1	-5.19	1.32	1.38
1	A	341	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	629	VAL	CA-CB	5.10	1.59	1.54
1	A	565	VAL	CA-CB	5.05	1.62	1.54

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	LYS	N-CA-C	15.15	130.22	108.86
1	A	413	ARG	CB-CG-CD	-11.33	85.25	111.30
1	A	838	ASP	CA-CB-CG	-10.68	101.92	112.60
1	A	666	ILE	N-CA-CB	-9.90	94.89	111.23
1	A	458	ILE	CB-CA-C	-9.76	99.47	111.97
1	A	656	VAL	CB-CA-C	-9.70	98.84	112.22
1	A	556	HIS	N-CA-C	9.64	131.34	110.80
1	A	23	ASN	CA-CB-CG	-9.37	103.23	112.60
1	A	486	ILE	CA-CB-CG1	-9.24	94.69	110.40
1	A	807	THR	N-CA-CB	-9.19	96.49	110.73
1	A	490	ARG	CB-CA-C	-9.10	95.38	110.85
1	A	256	ASP	N-CA-C	-8.88	94.05	108.52
1	A	119	MET	CB-CA-C	-8.74	97.16	110.88
1	A	666	ILE	CA-CB-CG2	8.74	125.35	110.50
1	A	13	ILE	N-CA-C	-8.70	104.08	111.56
1	A	338	ASN	OD1-CG-ND2	-8.68	113.92	122.60
1	A	319	ARG	CA-CB-CG	8.61	131.33	114.10
1	A	97	ASN	CA-CB-CG	-8.52	104.08	112.60
1	A	763	ASN	CA-CB-CG	8.49	121.09	112.60
1	A	666	ILE	CA-CB-CG1	-8.43	96.07	110.40
1	A	405	GLU	CB-CG-CD	8.31	126.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ARG	N-CA-C	8.25	122.42	111.28
1	A	574	LYS	CA-CB-CG	8.25	130.60	114.10
1	A	678	ASN	CA-CB-CG	8.25	120.85	112.60
1	A	501	GLU	CB-CA-C	-8.20	97.95	110.90
1	A	486	ILE	CA-CB-CG2	8.06	124.20	110.50
1	A	490	ARG	N-CA-CB	7.89	121.83	110.16
1	A	318	CYS	N-CA-C	-7.78	94.24	110.80
1	A	251	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	576	GLN	OE1-CD-NE2	-7.73	114.87	122.60
1	A	838	ASP	O-C-N	7.68	132.81	122.59
1	A	62	HIS	CB-CG-CD2	-7.59	121.33	131.20
1	A	743	GLU	CB-CG-CD	7.56	125.45	112.60
1	A	15	VAL	CA-C-O	7.55	130.22	120.78
1	A	407	ASN	OD1-CG-ND2	-7.41	115.19	122.60
1	A	253	ASN	O-C-N	7.32	131.86	122.71
1	A	735	ILE	CA-C-N	7.32	126.85	119.24
1	A	735	ILE	C-N-CA	7.32	126.85	119.24
1	A	208	HIS	CA-CB-CG	-7.32	106.48	113.80
1	A	271	LEU	N-CA-C	-7.29	95.27	110.80
1	A	264	GLN	CA-C-O	-7.28	113.11	120.90
1	A	575	ARG	CB-CG-CD	-7.27	94.57	111.30
1	A	574	LYS	N-CA-C	-7.25	104.41	113.18
1	A	458	ILE	N-CA-CB	7.22	119.00	110.55
1	A	174	TRP	CG-CD2-CE3	7.17	141.07	133.90
1	A	175	GLN	OE1-CD-NE2	-7.16	115.44	122.60
1	A	253	ASN	CA-C-N	7.14	135.17	121.54
1	A	253	ASN	C-N-CA	7.14	135.17	121.54
1	A	119	MET	N-CA-CB	7.13	120.35	110.01
1	A	838	ASP	N-CA-C	7.13	125.98	110.80
1	A	93	ARG	CG-CD-NE	7.02	127.43	112.00
1	A	467	ILE	N-CA-CB	-7.01	101.71	110.47
1	A	807	THR	CB-CA-C	7.00	122.55	110.72
1	A	507	ILE	N-CA-C	6.97	119.73	112.83
1	A	62	HIS	CB-CG-ND1	6.92	133.08	122.70
1	A	724	ARG	CA-CB-CG	6.85	127.81	114.10
1	A	553	TYR	CA-CB-CG	6.83	126.20	113.90
1	A	784	GLN	OE1-CD-NE2	-6.79	115.81	122.60
1	A	797	TRP	CB-CG-CD1	-6.79	116.72	126.90
1	A	101	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	A	255	LYS	N-CA-C	6.68	125.03	110.80
1	A	768	HIS	CA-CB-CG	6.68	120.48	113.80
1	A	211	GLN	OE1-CD-NE2	-6.65	115.95	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	484	ASN	CA-CB-CG	6.60	119.20	112.60
1	A	797	TRP	CG-CD2-CE3	6.60	140.50	133.90
1	A	436	VAL	N-CA-C	-6.59	98.64	108.46
1	A	822	ARG	N-CA-C	6.58	118.53	111.36
1	A	477	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	A	105	GLU	N-CA-C	6.53	118.05	111.07
1	A	666	ILE	CB-CA-C	6.48	121.92	111.29
1	A	501	GLU	N-CA-CB	6.45	119.42	110.07
1	A	734	ARG	CB-CG-CD	6.43	126.10	111.30
1	A	323	ARG	N-CA-C	-6.42	97.12	110.80
1	A	413	ARG	N-CA-C	-6.39	103.82	111.69
1	A	744	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	A	661	ASP	N-CA-C	-6.34	105.19	113.12
1	A	57	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	A	195	GLU	CB-CA-C	-6.32	99.94	110.68
1	A	31	PHE	N-CA-C	-6.30	104.33	111.07
1	A	16	ARG	N-CA-C	-6.29	105.46	112.57
1	A	443	HIS	CA-CB-CG	6.29	120.09	113.80
1	A	576	GLN	N-CA-C	-6.26	104.55	111.82
1	A	106	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	571	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	A	678	ASN	OD1-CG-ND2	-6.25	116.36	122.60
1	A	469	LYS	CB-CG-CD	6.21	125.59	111.30
1	A	365	TRP	CG-CD2-CE3	6.18	140.08	133.90
1	A	365	TRP	CB-CG-CD1	-6.14	117.68	126.90
1	A	30	ASN	CA-CB-CG	-6.13	106.47	112.60
1	A	452	VAL	N-CA-C	-6.12	99.31	108.12
1	A	326	PHE	CA-CB-CG	-6.08	107.72	113.80
1	A	189	TRP	N-CA-C	-6.07	106.20	113.97
1	A	697	VAL	CA-C-O	-6.07	114.80	121.29
1	A	713	MET	CA-CB-CG	6.05	126.20	114.10
1	A	566	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	A	329	PHE	CA-C-N	6.02	125.70	119.56
1	A	329	PHE	C-N-CA	6.02	125.70	119.56
1	A	832	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	A	284	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	713	MET	N-CA-CB	-5.95	100.85	109.83
1	A	831	ARG	N-CA-C	-5.94	103.26	111.81
1	A	208	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	A	656	VAL	N-CA-CB	5.91	119.44	110.58
1	A	763	ASN	OD1-CG-ND2	-5.90	116.70	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	ARG	CA-C-O	-5.88	114.62	120.80
1	A	430	LEU	N-CA-C	-5.88	105.60	112.89
1	A	727	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	A	224	MET	CA-C-N	5.86	125.77	119.85
1	A	224	MET	C-N-CA	5.86	125.77	119.85
1	A	174	TRP	CB-CG-CD1	-5.85	118.12	126.90
1	A	413	ARG	CA-CB-CG	5.84	125.78	114.10
1	A	554	LYS	CA-C-N	5.80	132.42	121.97
1	A	554	LYS	C-N-CA	5.80	132.42	121.97
1	A	128	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	763	ASN	CB-CG-ND2	5.80	125.10	116.40
1	A	529	ALA	N-CA-C	-5.79	104.89	111.14
1	A	464	LYS	CB-CG-CD	-5.72	98.14	111.30
1	A	785	GLU	CB-CG-CD	5.71	122.31	112.60
1	A	756	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	312	LYS	CA-CB-CG	-5.67	102.75	114.10
1	A	216	VAL	N-CA-CB	-5.67	102.95	112.47
1	A	13	ILE	O-C-N	5.65	127.01	121.98
1	A	578	LEU	N-CA-C	-5.64	105.21	111.36
1	A	643	ILE	N-CA-CB	-5.64	103.63	111.41
1	A	707	ASN	CA-CB-CG	-5.62	106.98	112.60
1	A	841	ILE	N-CA-C	-5.61	96.76	108.88
1	A	29	LYS	CA-CB-CG	5.61	125.31	114.10
1	A	797	TRP	CB-CA-C	-5.60	102.08	110.88
1	A	554	LYS	O-C-N	5.60	130.23	122.78
1	A	201	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	A	458	ILE	CB-CG1-CD1	-5.58	102.08	113.80
1	A	322	VAL	CA-C-N	5.57	132.18	121.54
1	A	322	VAL	C-N-CA	5.57	132.18	121.54
1	A	549	LEU	CA-C-O	-5.56	115.17	121.00
1	A	713	MET	CG-SD-CE	-5.55	88.69	100.90
1	A	754	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	A	457	ARG	NE-CZ-NH2	-5.54	114.22	119.20
1	A	322	VAL	CA-C-O	5.53	127.70	120.78
1	A	280	TYR	CA-C-N	5.53	126.75	119.84
1	A	280	TYR	C-N-CA	5.53	126.75	119.84
1	A	553	TYR	O-C-N	-5.52	115.32	121.84
1	A	174	TRP	CE2-CD2-CG	-5.52	100.58	107.20
1	A	507	ILE	O-C-N	-5.51	116.80	122.14
1	A	767	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	A	358	ARG	N-CA-C	5.49	119.15	111.74
1	A	19	ALA	N-CA-C	-5.47	102.00	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	A	664	GLU	CA-C-O	-5.45	114.75	120.58
1	A	399	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	A	446	ILE	N-CA-C	-5.45	105.06	111.00
1	A	811	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	692	MET	N-CA-CB	-5.42	102.77	110.58
1	A	477	HIS	CB-CG-ND1	5.42	130.83	122.70
1	A	370	LYS	CG-CD-CE	5.41	123.73	111.30
1	A	509	GLU	O-C-N	-5.40	115.59	122.34
1	A	590	ILE	CA-CB-CG2	-5.39	101.34	110.50
1	A	734	ARG	CA-CB-CG	5.39	124.88	114.10
1	A	715	VAL	CA-C-O	-5.37	115.48	121.17
1	A	712	GLY	O-C-N	5.35	129.26	122.68
1	A	729	GLN	CA-C-O	-5.35	114.75	120.42
1	A	527	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	499	LEU	N-CA-C	-5.33	105.38	111.14
1	A	772	LYS	CA-CB-CG	5.33	124.75	114.10
1	A	380	ILE	CA-C-N	5.32	124.95	119.05
1	A	380	ILE	C-N-CA	5.32	124.95	119.05
1	A	481	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	840	LYS	N-CA-C	5.31	122.10	110.80
1	A	73	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	A	764	MET	CG-SD-CE	-5.28	89.30	100.90
1	A	797	TRP	NE1-CE2-CZ2	-5.27	122.19	130.10
1	A	626	ILE	N-CA-C	-5.25	105.38	110.42
1	A	341	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	A	469	LYS	CA-CB-CG	5.24	124.59	114.10
1	A	78	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	632	HIS	CA-CB-CG	-5.23	108.57	113.80
1	A	678	ASN	CB-CG-ND2	5.22	124.23	116.40
1	A	682	MET	CA-C-O	-5.22	114.89	120.42
1	A	235	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	839	GLU	CA-C-N	5.21	131.48	121.54
1	A	839	GLU	C-N-CA	5.21	131.48	121.54
1	A	215	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	A	469	LYS	O-C-N	-5.19	116.70	122.09
1	A	176	MET	N-CA-C	-5.18	100.46	108.90
1	A	729	GLN	N-CA-C	-5.18	105.72	111.36
1	A	797	TRP	N-CA-CB	5.18	117.52	110.01
1	A	161	TYR	CA-C-N	-5.17	112.45	122.06
1	A	161	TYR	C-N-CA	-5.17	112.45	122.06
1	A	167	ASN	OD1-CG-ND2	-5.17	117.43	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	A	602	THR	N-CA-C	-5.14	100.15	108.52
1	A	532	ARG	CA-CB-CG	5.12	124.33	114.10
1	A	467	ILE	N-CA-C	5.11	116.44	110.62
1	A	387	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	A	239	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	42	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	187	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	689	ILE	O-C-N	-5.07	117.40	123.03
1	A	806	ALA	CA-C-O	5.07	125.61	119.38
1	A	287	GLU	CB-CG-CD	-5.06	104.00	112.60
1	A	564	ASP	CA-CB-CG	5.05	117.66	112.60
1	A	70	THR	N-CA-C	-5.05	105.69	111.14
1	A	840	LYS	O-C-N	5.05	129.31	122.59
1	A	398	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	272	ALA	O-C-N	-5.04	116.32	122.22
1	A	579	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	213	ALA	N-CA-C	-5.04	103.02	110.48
1	A	496	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	677	GLY	N-CA-C	-5.04	106.69	112.73
1	A	461	GLU	N-CA-C	5.03	116.84	111.36
1	A	94	THR	O-C-N	-5.02	116.27	122.20
1	A	743	GLU	N-CA-CB	-5.01	102.07	110.39
1	A	29	LYS	CB-CA-C	-5.01	102.47	110.79
1	A	170	ILE	O-C-N	-5.00	116.37	122.97

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	123	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	123	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 (123) 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:713:MET:HE1	1:A:775:ALA:HB1	1.80	0.64
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:95:LEU:HG	1:A:99:MET:HE3	1.84	0.58
1:A:322:VAL:O	1:A:323:ARG:HD3	2.04	0.58
1:A:455:VAL:H	1:A:459:HIS:HD2	1.50	0.57
1:A:795:ARG:O	1:A:799:ARG:HG3	2.04	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:699:MET:HE2	1:A:708:PHE:HZ	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ARG:HG3	1:A:639:ARG:HH11	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:604:MET:HB3	1:A:645:LEU:HD22	1.90	0.54
1:A:690:GLY:O	1:A:710:ILE:HA	2.08	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:343:SER:OG	1:A:441:MET:HE3	2.13	0.49
1:A:15:VAL:HG13	1:A:15:VAL:O	2.13	0.48
1:A:562:LEU:HD21	1:A:662:LEU:HB2	1.95	0.48
1:A:790:LEU:HD13	1:A:797:TRP:CD1	2.48	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:319:ARG:HH21	1:A:320:ASP:CG	2.22	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:251:ASP:CG	1:A:252:PHE:H	2.21	0.47
1:A:90:TYR:HE1	4:A:1211:HOH:O	1.96	0.47
1:A:790:LEU:HB3	1:A:797:TRP:CD1	2.49	0.47
1:A:289:LYS:NZ	4:A:1427:HOH:O	2.47	0.47
1:A:344:LEU:HB2	4:A:1411:HOH:O	2.14	0.47
1:A:764:MET:HE2	1:A:769:ASP:HA	1.97	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:252:PHE:HD1	1:A:256:ASP:HB2	1.80	0.46
1:A:519:ARG:NH2	4:A:1060:HOH:O	2.47	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:33:ARG:HH11	1:A:33:ARG:HG3	1.80	0.46
1:A:109:ASP:HA	1:A:119:MET:HG3	1.97	0.46
1:A:839:GLU:O	1:A:840:LYS:NZ	2.48	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: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:257:PHE:O	1:A:258:ASN:HB2	2.14	0.45
1:A:618:MET:HB3	1:A:761:ILE:HD11	1.99	0.45
1:A:809:GLY:HA3	4:A:1059:HOH:O	2.15	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:457:ARG:HH22	1:A:701:GLU:CD	2.24	0.44
1:A:144:LEU:HD12	1:A:147:MET:HE1	1.98	0.44
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: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:251:ASP:CG	1:A:252:PHE:N	2.77	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ARG:HH22	1:A:473:GLU:CD	2.29	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:93:ARG:NH1	1:A:126:GLU:O	2.54	0.40
1:A:511:TYR:CE1	1:A:512:ILE:HD13	2.56	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 [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	829/842 (98%)	768 (93%)	41 (5%)	20 (2%)	4 4

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
1	A	318	CYS

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Mol	Chain	Res	Type
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 [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	720/731 (98%)	614 (85%)	106 (15%)	3 3

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
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	93	ARG
1	A	94	THR
1	A	102	LEU
1	A	104	LEU
1	A	115	LEU
1	A	119	MET
1	A	122	LEU
1	A	138	ARG
1	A	176	MET

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Mol	Chain	Res	Type
1	A	198	LEU
1	A	211	GLN
1	A	234	ARG
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	258	ASN
1	A	292	ARG
1	A	304	LEU
1	A	306	ASP
1	A	308	ILE
1	A	314	SER
1	A	319	ARG
1	A	320	ASP
1	A	322	VAL
1	A	323	ARG
1	A	335	ILE
1	A	337	LEU
1	A	344	LEU
1	A	356	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	437	LYS
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	513	SER
1	A	515	LEU
1	A	518	LEU

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Mol	Chain	Res	Type
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
1	A	568	LYS
1	A	569	ARG
1	A	581	LEU
1	A	586	LEU
1	A	590	ILE
1	A	593	GLU
1	A	596	LYS
1	A	603	VAL
1	A	622	LEU
1	A	639	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	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	716	GLU
1	A	730	GLU
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	781	VAL
1	A	787	VAL
1	A	790	LEU
1	A	796	GLU

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Mol	Chain	Res	Type
1	A	797	TRP
1	A	807	THR
1	A	833	ARG
1	A	838	ASP
1	A	840	LYS
1	A	841	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	62	HIS
1	A	235	ASN
1	A	270	ASN
1	A	305	GLN
1	A	390	HIS
1	A	412	ASN
1	A	450	HIS
1	A	453	ASN
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	614	HIS
1	A	678	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	1.05	1 (8%)	17,17,17	0.73	1 (5%)
3	PLP	A	999	1	15,15,16	1.74	3 (20%)	21,22,23	1.20	2 (9%)

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	-	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)
3	A	999	PLP	C3-C2	-4.57	1.36	1.41
2	A	910	GLC	C4-C5	2.49	1.58	1.53
3	A	999	PLP	C2-N1	2.15	1.37	1.33
3	A	999	PLP	P-O2P	-2.01	1.47	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	PLP	O2P-P-O1P	2.57	120.85	110.83
3	A	999	PLP	C5-C6-N1	-2.40	119.93	123.83
2	A	910	GLC	O5-C1-C2	2.22	114.21	110.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PLP	C4-C5-C5A-O4P

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.