



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:56 PM GMT

PDB ID : 4GPB  
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.  
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

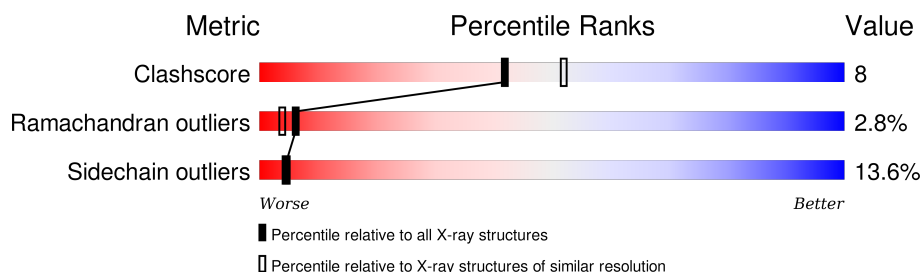
# 1 Overall quality at a glance ⓘ

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	 64% 25% 7% . .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7430 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.

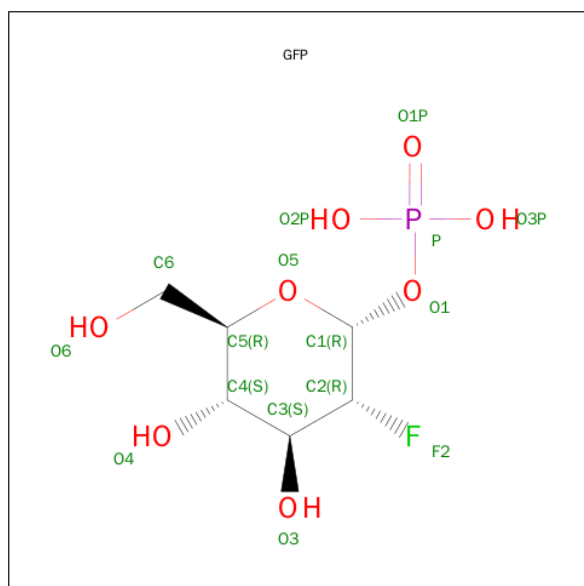
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	833	6779	4320	1197	1232	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

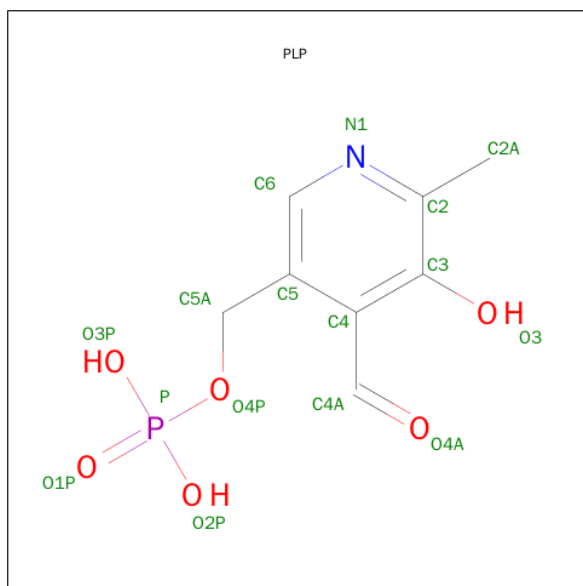
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489

- Molecule 2 is SUGAR (2-DEOXY-2-FLUORO-ALPHA-D-GLUCOSE-1-PHOSPHATE) (three-letter code: GFP) (formula:  $C_6H_{12}FO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	O	P		
2	A	1	16	6	1	8	1	0	0
2	A	1	16	6	1	8	1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



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.

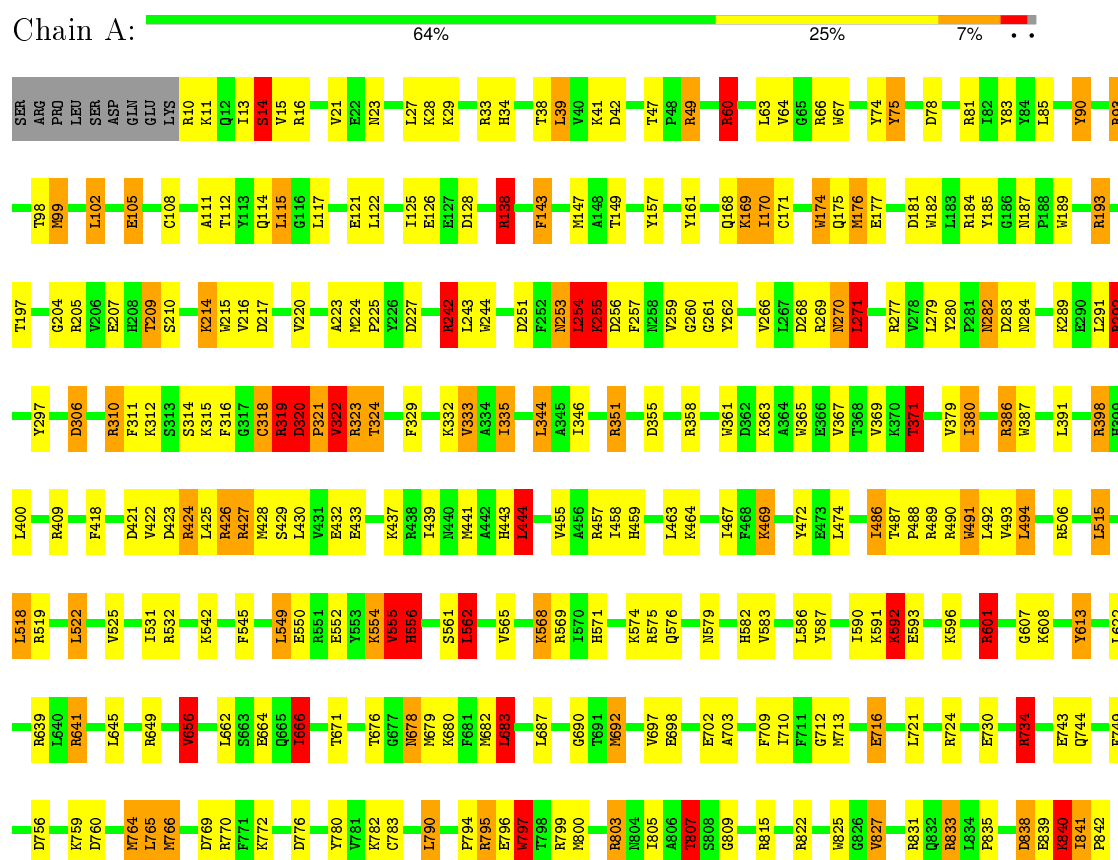
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	604	Total	O	0	0
			604	604		

### 3 Residue-property plots

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, $R_{free}$	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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: GFP, 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	0.94	2/6933 (0.0%)	1.81	173/9381 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	THR	CA-CB	5.82	1.68	1.53
1	A	177	GLU	CD-OE1	-5.65	1.19	1.25

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ARG	NE-CZ-NH2	-13.93	113.33	120.30
1	A	575	ARG	NE-CZ-NH2	-13.44	113.58	120.30
1	A	138	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	138	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	A	519	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	A	60	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	A	424	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	601	ARG	NE-CZ-NH2	-9.47	115.57	120.30
1	A	333	VAL	CG1-CB-CG2	-9.43	95.81	110.90
1	A	575	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	A	489	ARG	NE-CZ-NH1	9.21	124.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	TRP	CD1-CG-CD2	9.14	113.61	106.30
1	A	822	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	387	TRP	CD1-CG-CD2	8.90	113.42	106.30
1	A	457	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	A	766	MET	CG-SD-CE	8.66	114.05	100.20
1	A	666	ILE	CA-CB-CG1	-8.61	94.65	111.00
1	A	803	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	A	409	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	682	MET	CG-SD-CE	8.50	113.80	100.20
1	A	490	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	90	TYR	CB-CG-CD2	-8.31	116.01	121.00
1	A	182	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	A	613	TYR	CB-CG-CD2	-8.30	116.02	121.00
1	A	797	TRP	CE2-CD2-CG	-8.29	100.67	107.30
1	A	365	TRP	CE2-CD2-CG	-8.27	100.69	107.30
1	A	67	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	649	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	361	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	A	666	ILE	N-CA-CB	-8.08	92.23	110.80
1	A	797	TRP	CB-CG-CD1	-8.06	116.52	127.00
1	A	215	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	A	494	LEU	CA-CB-CG	7.93	133.53	115.30
1	A	797	TRP	CG-CD2-CE3	7.91	141.02	133.90
1	A	365	TRP	CG-CD2-CE3	7.75	140.87	133.90
1	A	562	LEU	CA-CB-CG	7.73	133.09	115.30
1	A	361	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	A	67	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	182	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	A	161	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	A	838	ASP	CA-C-N	-7.42	100.88	117.20
1	A	555	VAL	N-CA-C	7.41	131.01	111.00
1	A	807	THR	N-CA-CB	-7.41	96.22	110.30
1	A	244	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	A	292	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	519	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	797	TRP	NE1-CE2-CZ2	-7.31	122.35	130.40
1	A	825	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	666	ILE	CA-CB-CG2	7.27	125.44	110.90
1	A	387	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	A	174	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	A	60	ARG	CA-CB-CG	7.21	129.27	113.40
1	A	74	TYR	CB-CG-CD2	-7.19	116.68	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	601	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	185	TYR	CB-CG-CD1	-7.17	116.70	121.00
1	A	489	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	75	TYR	CB-CG-CD2	-7.14	116.71	121.00
1	A	215	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	A	205	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	713	MET	CA-CB-CG	7.10	125.37	113.30
1	A	277	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	838	ASP	N-CA-C	7.05	130.04	111.00
1	A	174	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	A	365	TRP	CB-CG-CD1	-7.00	117.89	127.00
1	A	351	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	297	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	A	683	LEU	CB-CA-C	-6.98	96.94	110.20
1	A	491	TRP	CG-CD2-CE3	6.95	140.16	133.90
1	A	827	VAL	CG1-CB-CG2	-6.95	99.78	110.90
1	A	253	ASN	CA-C-N	-6.94	101.92	117.20
1	A	427	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	825	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	A	269	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	66	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	60	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	244	TRP	CE2-CD2-CG	-6.67	101.97	107.30
1	A	189	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	A	312	LYS	CA-CB-CG	-6.56	98.96	113.40
1	A	428	MET	CA-CB-CG	-6.56	102.14	113.30
1	A	255	LYS	CA-C-N	-6.56	102.77	117.20
1	A	189	TRP	CD1-CG-CD2	6.47	111.48	106.30
1	A	490	ARG	CB-CA-C	-6.45	97.49	110.40
1	A	656	VAL	CB-CA-C	-6.45	99.14	111.40
1	A	464	LYS	CB-CG-CD	-6.43	94.89	111.60
1	A	310	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	256	ASP	N-CA-C	-6.34	93.87	111.00
1	A	81	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	683	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	469	LYS	CA-CB-CG	6.30	127.26	113.40
1	A	822	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	491	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	A	592	LYS	CB-CG-CD	6.25	127.86	111.60
1	A	253	ASN	O-C-N	6.25	132.69	122.70
1	A	99	MET	CG-SD-CE	-6.23	90.23	100.20
1	A	255	LYS	N-CA-C	6.18	127.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	TRP	CG-CD1-NE1	-6.18	103.92	110.10
1	A	838	ASP	O-C-N	6.17	132.57	122.70
1	A	575	ARG	CB-CG-CD	-6.14	95.64	111.60
1	A	712	GLY	CA-C-N	-6.14	103.69	117.20
1	A	800	MET	CG-SD-CE	-6.11	90.43	100.20
1	A	64	VAL	CG1-CB-CG2	-6.08	101.18	110.90
1	A	244	TRP	CB-CG-CD1	-6.05	119.13	127.00
1	A	10	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	770	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	324	THR	CA-C-N	-5.99	104.02	117.20
1	A	270	ASN	CA-C-N	-5.98	104.05	117.20
1	A	835	PRO	CA-C-N	-5.95	104.12	117.20
1	A	320	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	797	TRP	CD1-CG-CD2	5.92	111.03	106.30
1	A	361	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	A	369	VAL	CG1-CB-CG2	-5.91	101.45	110.90
1	A	583	VAL	CG1-CB-CG2	-5.89	101.48	110.90
1	A	63	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	486	ILE	CA-CB-CG1	-5.84	99.91	111.00
1	A	93	ARG	CB-CG-CD	-5.82	96.48	111.60
1	A	491	TRP	CD1-CG-CD2	5.80	110.94	106.30
1	A	121	GLU	CA-CB-CG	5.79	126.15	113.40
1	A	556	HIS	CA-C-N	-5.79	104.47	117.20
1	A	90	TYR	CB-CG-CD1	5.78	124.47	121.00
1	A	641	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	115	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	66	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	592	LYS	CG-CD-CE	5.72	129.07	111.90
1	A	776	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	666	ILE	CB-CA-C	5.66	122.93	111.60
1	A	472	TYR	CB-CG-CD1	-5.66	117.61	121.00
1	A	83	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	A	209	THR	CA-C-N	-5.64	104.80	117.20
1	A	282	ASN	N-CA-CB	-5.63	100.47	110.60
1	A	387	TRP	CG-CD1-NE1	-5.61	104.50	110.10
1	A	177	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	A	444	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	765	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	220	VAL	CG1-CB-CG2	-5.52	102.07	110.90
1	A	387	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	A	522	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	A	833	ARG	CA-CB-CG	5.47	125.44	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	639	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	262	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	A	60	ARG	CG-CD-NE	5.43	123.21	111.80
1	A	207	GLU	N-CA-CB	5.41	120.33	110.60
1	A	323	ARG	N-CA-C	-5.39	96.43	111.00
1	A	840	LYS	CA-CB-CG	5.35	125.18	113.40
1	A	344	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	209	THR	O-C-N	5.35	131.26	122.70
1	A	532	ARG	CA-CB-CG	5.35	125.16	113.40
1	A	322	VAL	CA-CB-CG2	-5.30	102.94	110.90
1	A	67	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	A	143	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	207	GLU	CB-CA-C	-5.30	99.80	110.40
1	A	346	ILE	CA-C-N	5.30	131.93	117.10
1	A	214	LYS	CB-CG-CD	-5.29	97.83	111.60
1	A	613	TYR	CB-CG-CD1	5.29	124.17	121.00
1	A	306	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	49	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	422	VAL	CA-C-N	5.22	128.69	117.20
1	A	426	ARG	CG-CD-NE	5.21	122.75	111.80
1	A	380	ILE	CG1-CB-CG2	-5.21	99.95	111.40
1	A	386	ARG	CB-CG-CD	-5.21	98.07	111.60
1	A	15	VAL	CA-C-O	5.20	131.02	120.10
1	A	493	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	A	361	TRP	CB-CG-CD1	-5.20	120.25	127.00
1	A	587	TYR	CB-CG-CD1	-5.19	117.88	121.00
1	A	683	LEU	N-CA-CB	5.14	120.68	110.40
1	A	358	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	769	ASP	CB-CG-OD1	5.13	122.91	118.30
1	A	174	TRP	CG-CD2-CE3	5.12	138.50	133.90
1	A	128	ASP	CB-CG-OD1	5.11	122.89	118.30
1	A	506	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	734	ARG	CB-CG-CD	5.06	124.75	111.60
1	A	242	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	601	ARG	CA-CB-CG	5.04	124.50	113.40
1	A	671	THR	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ASP	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	6779	0	6729	114	0
2	A	32	0	20	0	0
3	A	15	0	7	0	0
4	A	604	0	0	18	0
All	All	7430	0	6756	114	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 8.

All (114) 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:225:PRO:HB2	1:A:242:ARG:HD2	1.60	0.82
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.65	0.77
1:A:367:VAL:O	1:A:371:THR:HG22	1.85	0.76
1:A:593:GLU:HB2	1:A:596:LYS:HD2	1.73	0.70
1:A:730:GLU:O	1:A:734:ARG:HG2	1.91	0.70
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.74	0.69
1:A:716:GLU:HB2	4:A:1115:HOH:O	1.93	0.66
1:A:463:LEU:HA	1:A:467:ILE:HG23	1.79	0.64
1:A:756:ASP:HB2	1:A:759:LYS:HD3	1.82	0.62
1:A:78:ASP:HB3	1:A:315:LYS:NZ	2.15	0.61
1:A:329:PHE:O	1:A:333:VAL:HG12	2.01	0.61
1:A:703:ALA:HA	1:A:807:THR:HG21	1.85	0.57
1:A:430:LEU:HD22	1:A:443:HIS:HB3	1.85	0.57
1:A:315:LYS:O	1:A:318:CYS:HB2	2.04	0.57
1:A:841:ILE:HD13	1:A:842:PRO:HD2	1.84	0.57
1:A:28:LYS:HG2	1:A:115:LEU:HD22	1.87	0.57
1:A:143:PHE:O	1:A:147:MET:HG3	2.05	0.56
1:A:455:VAL:H	1:A:459:HIS:HD2	1.53	0.56
1:A:794:PRO:HA	4:A:1072:HOH:O	2.06	0.56
1:A:764:MET:HE1	4:A:1339:HOH:O	2.04	0.55
1:A:169:LYS:HG3	1:A:176:MET:HB3	1.88	0.55
1:A:698:GLU:O	1:A:702:GLU:HB2	2.08	0.54
1:A:157:TYR:OH	1:A:310:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HA	1:A:125:ILE:HD12	1.90	0.53
1:A:545:PHE:CZ	1:A:656:VAL:HG13	2.44	0.53
1:A:678:ASN:HD22	1:A:679:MET:H	1.57	0.53
1:A:292:ARG:NH2	4:A:1421:HOH:O	2.41	0.53
1:A:379:VAL:HG22	4:A:1443:HOH:O	2.08	0.53
1:A:486:ILE:CD1	1:A:676:THR:HB	2.38	0.53
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.91	0.53
1:A:28:LYS:HG3	1:A:111:ALA:HB1	1.92	0.52
1:A:441:MET:HE3	1:A:444:LEU:HD12	1.91	0.52
1:A:525:VAL:O	1:A:531:ILE:HD11	2.09	0.52
1:A:664:GLU:OE1	1:A:666:ILE:HD13	2.10	0.52
1:A:463:LEU:HA	1:A:467:ILE:CG2	2.40	0.52
1:A:561:SER:HB2	1:A:601:ARG:HA	1.92	0.52
1:A:795:ARG:O	1:A:799:ARG:HG3	2.10	0.51
1:A:75:TYR:HB2	4:A:1009:HOH:O	2.10	0.50
1:A:815:ARG:HB2	4:A:1485:HOH:O	2.11	0.50
1:A:99:MET:HE1	1:A:108:CYS:HB2	1.94	0.49
1:A:251:ASP:O	1:A:255:LYS:N	2.45	0.49
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.94	0.49
1:A:486:ILE:HG12	1:A:680:LYS:CG	2.43	0.48
1:A:592:LYS:HE2	4:A:1140:HOH:O	2.13	0.48
1:A:78:ASP:HB3	1:A:315:LYS:HZ1	1.77	0.48
1:A:486:ILE:HG12	1:A:680:LYS:HG2	1.95	0.48
1:A:790:LEU:HD13	1:A:797:TRP:CD1	2.49	0.48
1:A:759:LYS:HE2	4:A:1539:HOH:O	2.14	0.47
1:A:85:LEU:HD13	1:A:335:ILE:HD12	1.97	0.47
1:A:321:PRO:O	1:A:322:VAL:HB	2.15	0.47
1:A:197:THR:HA	1:A:223:ALA:O	2.15	0.47
1:A:187:ASN:ND2	4:A:1036:HOH:O	2.48	0.47
1:A:105:GLU:HB2	4:A:1019:HOH:O	2.14	0.46
1:A:98:THR:O	1:A:102:LEU:HB2	2.15	0.46
1:A:311:PHE:HE1	1:A:332:LYS:HG3	1.81	0.46
1:A:171:CYS:HB2	1:A:176:MET:SD	2.56	0.45
1:A:562:LEU:HB3	1:A:601:ARG:HB3	1.98	0.45
1:A:423:ASP:O	1:A:427:ARG:HG3	2.15	0.45
1:A:138:ARG:HB3	4:A:1520:HOH:O	2.16	0.45
1:A:204:GLY:HA2	1:A:217:ASP:O	2.16	0.45
1:A:99:MET:HE1	1:A:108:CYS:CB	2.46	0.45
1:A:550:GLU:O	1:A:554:LYS:HA	2.16	0.45
1:A:703:ALA:CA	1:A:807:THR:HG21	2.46	0.45
1:A:487:THR:HA	1:A:488:PRO:HD2	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:O	1:A:271:LEU:HB2	2.17	0.44
1:A:181:ASP:O	1:A:184:ARG:HG3	2.17	0.44
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.57	0.44
1:A:316:PHE:HA	1:A:319:ARG:O	2.17	0.44
1:A:112:THR:HG23	1:A:117:LEU:HB2	2.00	0.43
1:A:488:PRO:O	1:A:492:LEU:HB3	2.18	0.43
1:A:721:LEU:HD23	1:A:772:LYS:HD3	1.99	0.43
1:A:441:MET:CE	1:A:444:LEU:HD12	2.48	0.43
1:A:170:ILE:HA	1:A:174:TRP:O	2.19	0.43
1:A:796:GLU:OE1	1:A:799:ARG:NH1	2.52	0.43
1:A:386:ARG:HA	1:A:439:ILE:O	2.19	0.43
1:A:181:ASP:O	1:A:184:ARG:NH1	2.52	0.43
1:A:433:GLU:OE2	1:A:437:LYS:NZ	2.51	0.43
1:A:335:ILE:HG13	1:A:335:ILE:O	2.15	0.43
1:A:554:LYS:HE2	4:A:1332:HOH:O	2.19	0.43
1:A:569:ARG:HD2	1:A:608:LYS:O	2.19	0.42
1:A:254:LEU:HD21	1:A:266:VAL:HG22	2.01	0.42
1:A:790:LEU:HB3	1:A:797:TRP:CD1	2.54	0.42
1:A:492:LEU:HB2	1:A:683:LEU:HD22	2.00	0.42
1:A:355:ASP:OD1	1:A:398:ARG:NH1	2.53	0.42
1:A:690:GLY:O	1:A:710:ILE:HA	2.19	0.42
1:A:351:ARG:O	1:A:355:ASP:HB2	2.19	0.42
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.54	0.42
1:A:280:TYR:OH	1:A:291:LEU:HB3	2.20	0.42
1:A:34:HIS:O	1:A:38:THR:HB	2.20	0.42
1:A:749:PHE:HB2	4:A:1537:HOH:O	2.20	0.42
1:A:744:GLN:HA	4:A:1537:HOH:O	2.20	0.42
1:A:93:ARG:NH1	1:A:126:GLU:O	2.53	0.42
1:A:568:LYS:O	1:A:607:GLY:HA3	2.20	0.41
1:A:724:ARG:NH2	4:A:1533:HOH:O	2.53	0.41
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.20	0.41
1:A:803:ARG:NH2	4:A:1315:HOH:O	2.46	0.41
1:A:571:HIS:HB3	1:A:574:LYS:HG3	2.01	0.41
1:A:257:PHE:CD1	1:A:257:PHE:N	2.88	0.41
1:A:678:ASN:ND2	1:A:679:MET:H	2.17	0.41
1:A:14:SER:HB3	1:A:16:ARG:CG	2.50	0.41
1:A:542:LYS:NZ	4:A:1517:HOH:O	2.52	0.41
1:A:549:LEU:HG	1:A:555:VAL:HG21	2.03	0.41
1:A:60:ARG:HH11	1:A:60:ARG:HG2	1.85	0.41
1:A:418:PHE:CD2	1:A:424:ARG:HD3	2.56	0.41
1:A:29:LYS:HE2	1:A:29:LYS:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:O	1:A:831:ARG:HD2	2.21	0.40
1:A:319:ARG:NH1	1:A:320:ASP:OD1	2.54	0.40
1:A:549:LEU:HD12	1:A:549:LEU:HA	1.83	0.40
1:A:421:ASP:O	1:A:425:LEU:HD23	2.21	0.40
1:A:49:ARG:HA	1:A:125:ILE:HG21	2.04	0.40
1:A:487:THR:O	1:A:491:TRP:HB2	2.21	0.40
1:A:805:ILE:HD13	1:A:805:ILE:HG21	1.91	0.40
1:A:39:LEU:HD12	1:A:39:LEU:HA	1.92	0.40
1:A:193:ARG:HH11	1:A:193:ARG:HD2	1.69	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	831/842 (99%)	753 (91%)	55 (7%)	23 (3%)	<b>6</b> <b>4</b>

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	114	GLN
1	A	254	LEU
1	A	259	VAL
1	A	318	CYS
1	A	320	ASP
1	A	321	PRO
1	A	322	VAL
1	A	323	ARG
1	A	324	THR
1	A	555	VAL
1	A	556	HIS

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Mol	Chain	Res	Type
1	A	839	GLU
1	A	210	SER
1	A	261	GLY
1	A	314	SER
1	A	840	LYS
1	A	14	SER
1	A	271	LEU
1	A	319	ARG
1	A	554	LYS
1	A	284	ASN
1	A	260	GLY

### 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	722/731 (99%)	624 (86%)	98 (14%)	<b>5</b> <b>4</b>

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	13	ILE
1	A	14	SER
1	A	23	ASN
1	A	27	LEU
1	A	33	ARG
1	A	39	LEU
1	A	41	LYS
1	A	42	ASP
1	A	47	THR
1	A	60	ARG
1	A	90	TYR
1	A	102	LEU
1	A	105	GLU
1	A	138	ARG

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Mol	Chain	Res	Type
1	A	169	LYS
1	A	170	ILE
1	A	176	MET
1	A	193	ARG
1	A	209	THR
1	A	214	LYS
1	A	216	VAL
1	A	224	MET
1	A	242	ARG
1	A	243	LEU
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	270	ASN
1	A	271	LEU
1	A	279	LEU
1	A	282	ASN
1	A	283	ASP
1	A	289	LYS
1	A	292	ARG
1	A	306	ASP
1	A	319	ARG
1	A	320	ASP
1	A	335	ILE
1	A	344	LEU
1	A	363	LYS
1	A	371	THR
1	A	380	ILE
1	A	391	LEU
1	A	398	ARG
1	A	400	LEU
1	A	426	ARG
1	A	429	SER
1	A	432	GLU
1	A	444	LEU
1	A	458	ILE
1	A	469	LYS
1	A	474	LEU
1	A	494	LEU
1	A	515	LEU
1	A	518	LEU
1	A	522	LEU

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Mol	Chain	Res	Type
1	A	549	LEU
1	A	552	GLU
1	A	556	HIS
1	A	562	LEU
1	A	565	VAL
1	A	568	LYS
1	A	576	GLN
1	A	579	ASN
1	A	586	LEU
1	A	590	ILE
1	A	591	LYS
1	A	592	LYS
1	A	601	ARG
1	A	613	TYR
1	A	622	LEU
1	A	641	ARG
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	692	MET
1	A	716	GLU
1	A	734	ARG
1	A	743	GLU
1	A	760	ASP
1	A	764	MET
1	A	765	LEU
1	A	766	MET
1	A	782	LYS
1	A	790	LEU
1	A	795	ARG
1	A	797	TRP
1	A	807	THR
1	A	827	VAL
1	A	833	ARG
1	A	838	ASP
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	12	GLN
1	A	34	HIS
1	A	57	HIS
1	A	62	HIS
1	A	253	ASN
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	576	GLN
1	A	678	ASN
1	A	763	ASN
1	A	767	HIS
1	A	768	HIS

### 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](#)

3 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	GFP	A	900	-	14,16,16	0.83	1 (7%)	19,24,24	2.11	3 (15%)
2	GFP	A	901	-	14,16,16	1.56	3 (21%)	19,24,24	1.57	4 (21%)
3	PLP	A	999	1	15,15,16	2.20	1 (6%)	21,22,23	1.31	4 (19%)

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	GFP	A	900	-	-	0/6/27/27	0/1/1/1
2	GFP	A	901	-	-	0/6/27/27	0/1/1/1
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C3-C2	-7.48	1.35	1.40
2	A	900	GFP	O5-C1	2.13	1.47	1.41
2	A	901	GFP	C4-C5	2.52	1.58	1.53
2	A	901	GFP	O5-C1	2.72	1.48	1.41
2	A	901	GFP	C2-C3	2.79	1.54	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	GFP	C1-C2-C3	-4.39	104.76	111.52
2	A	900	GFP	O3-C3-C4	-3.26	102.99	110.34
2	A	901	GFP	C1-C2-C3	-3.00	106.90	111.52
3	A	999	PLP	C5-C6-N1	-2.27	119.93	123.86
3	A	999	PLP	C6-C5-C4	2.02	119.86	118.15
3	A	999	PLP	O4P-C5A-C5	2.06	112.41	108.99
2	A	901	GFP	O1-C1-C2	2.10	112.32	108.39
2	A	901	GFP	O3-C3-C2	2.23	113.04	109.05
3	A	999	PLP	O2P-P-O1P	2.95	120.06	110.58
2	A	901	GFP	F2-C2-C3	4.56	111.76	108.52
2	A	900	GFP	F2-C2-C3	6.18	112.91	108.52

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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