



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:40 PM GMT

PDB ID : 1GPY  
Title : CRYSTALLOGRAPHIC BINDING STUDIES ON THE ALLOSTERIC INHIBITOR GLUCOSE-6-PHOSPHATE TO T STATE GLYCOGEN PHOSPHORYLASE B  
Authors : Johnson, L.N.  
Deposited on : 1993-03-31  
Resolution : 2.40 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

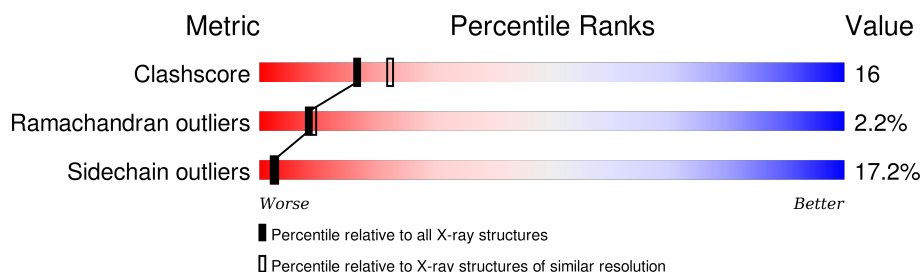
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	 50% 30% 14% . .

## 2 Entry composition [i](#)

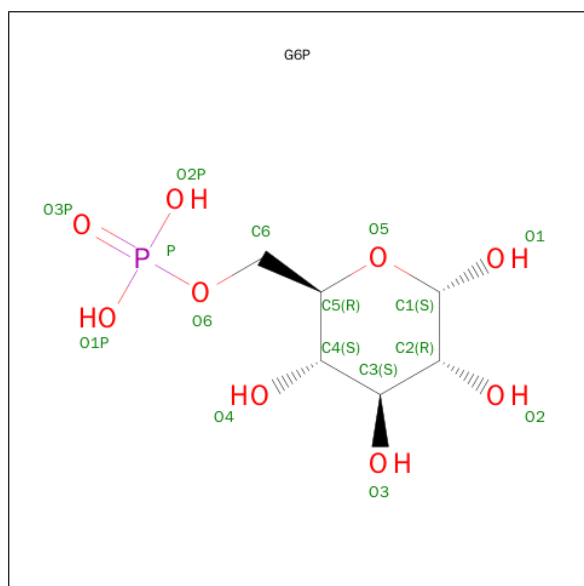
There are 4 unique types of molecules in this entry. The entry contains 7431 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	828	6727	4286	1186	1225	30	39	0	0

- Molecule 2 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	16	6	9	1	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	673	Total	O	0	0
			673	673		



## 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, $\alpha$ , $\beta$ , $\gamma$	128.50Å 128.50Å 116.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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: G6P, 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	1.20	17/6880 (0.2%)	2.12	274/9313 (2.9%)

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	10

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	ILE	C-N	19.12	1.78	1.34
1	A	309	ARG	C-N	17.14	1.73	1.34
1	A	20	GLY	C-N	9.09	1.54	1.34
1	A	16	ARG	NE-CZ	8.02	1.43	1.33
1	A	323	ARG	CZ-NH1	6.96	1.42	1.33
1	A	105	GLU	CD-OE1	-5.93	1.19	1.25
1	A	210	SER	CA-CB	5.78	1.61	1.52
1	A	14	SER	CA-C	5.73	1.67	1.52
1	A	16	ARG	CG-CD	5.66	1.66	1.51
1	A	828	GLU	CG-CD	5.51	1.60	1.51
1	A	17	GLY	C-N	5.28	1.46	1.34
1	A	509	GLU	CD-OE2	-5.27	1.19	1.25
1	A	433	GLU	CB-CG	5.22	1.62	1.52
1	A	67	TRP	CD1-NE1	-5.14	1.29	1.38
1	A	323	ARG	NE-CZ	5.12	1.39	1.33
1	A	716	GLU	CD-OE2	5.08	1.31	1.25
1	A	244	TRP	CD1-NE1	-5.08	1.29	1.38

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH2	-21.07	109.77	120.30
1	A	43	ARG	NE-CZ-NH1	19.05	129.83	120.30
1	A	457	ARG	NE-CZ-NH2	-18.56	111.02	120.30
1	A	601	ARG	NE-CZ-NH2	-17.51	111.54	120.30
1	A	242	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	A	457	ARG	NE-CZ-NH1	15.95	128.28	120.30
1	A	413	ARG	NE-CZ-NH2	-15.79	112.40	120.30
1	A	242	ARG	NE-CZ-NH2	-15.14	112.73	120.30
1	A	601	ARG	NE-CZ-NH1	13.73	127.17	120.30
1	A	323	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	A	649	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	A	424	ARG	NE-CZ-NH2	-11.35	114.63	120.30
1	A	795	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	A	160	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	A	269	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	A	381	PRO	O-C-N	-10.57	105.79	122.70
1	A	770	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	A	831	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	A	277	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	A	799	ARG	NE-CZ-NH2	-10.05	115.28	120.30
1	A	575	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	490	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	A	28	LYS	CA-CB-CG	9.79	134.95	113.40
1	A	424	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	815	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	A	551	ARG	NE-CZ-NH1	-9.50	115.55	120.30
1	A	724	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	753	LYS	CA-CB-CG	9.39	134.07	113.40
1	A	365	TRP	CD1-CG-CD2	9.25	113.70	106.30
1	A	413	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	A	815	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	A	244	TRP	CD1-CG-CD2	9.07	113.56	106.30
1	A	427	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	713	MET	CG-SD-CE	-8.90	85.96	100.20
1	A	277	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	A	551	ARG	NE-CZ-NH2	8.74	124.67	120.30
1	A	90	TYR	CB-CG-CD2	-8.68	115.79	121.00
1	A	799	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	387	TRP	CD1-CG-CD2	8.62	113.19	106.30
1	A	67	TRP	CD1-CG-CD2	8.49	113.09	106.30
1	A	215	TRP	CD1-CG-CD2	8.44	113.05	106.30
1	A	409	ARG	NE-CZ-NH2	-8.43	116.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	PRO	CA-N-CD	-8.41	99.72	111.50
1	A	398	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	754	GLN	CA-CB-CG	8.29	131.63	113.40
1	A	724	ARG	CA-CB-CG	8.28	131.61	113.40
1	A	224	MET	CG-SD-CE	8.18	113.29	100.20
1	A	613	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	A	323	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	A	318	CYS	CA-C-N	-8.11	99.36	117.20
1	A	365	TRP	CE2-CD2-CG	-8.07	100.84	107.30
1	A	321	PRO	O-C-N	8.06	135.59	122.70
1	A	182	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	A	387	TRP	CE2-CD2-CG	-8.02	100.88	107.30
1	A	215	TRP	CE2-CD2-CG	-8.02	100.89	107.30
1	A	174	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	A	205	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	238	VAL	CG1-CB-CG2	-7.91	98.25	110.90
1	A	244	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	A	754	GLN	N-CA-CB	-7.89	96.40	110.60
1	A	367	VAL	CG1-CB-CG2	-7.82	98.38	110.90
1	A	255	LYS	N-CA-CB	-7.81	96.54	110.60
1	A	67	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	A	136	LEU	CA-CB-CG	7.67	132.94	115.30
1	A	486	ILE	CA-CB-CG1	-7.66	96.44	111.00
1	A	255	LYS	N-CA-C	7.66	131.68	111.00
1	A	543	LEU	CA-CB-CG	7.61	132.81	115.30
1	A	51	TYR	CB-CG-CD1	-7.60	116.44	121.00
1	A	398	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	650	VAL	CG1-CB-CG2	-7.51	98.88	110.90
1	A	217	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	438	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	84	TYR	CB-CG-CD1	-7.47	116.52	121.00
1	A	20	GLY	CA-C-N	-7.44	100.83	117.20
1	A	387	TRP	CG-CD2-CE3	7.39	140.55	133.90
1	A	16	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	277	ARG	CA-CB-CG	-7.38	97.17	113.40
1	A	527	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	A	161	TYR	CB-CG-CD2	-7.34	116.59	121.00
1	A	404	TYR	CB-CG-CD2	-7.34	116.60	121.00
1	A	309	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	A	489	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	A	633	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	189	TRP	CD1-CG-CD2	7.17	112.04	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	LYS	CA-CB-CG	7.17	129.17	113.40
1	A	724	ARG	CD-NE-CZ	7.17	133.63	123.60
1	A	732	TYR	CB-CG-CD2	-7.16	116.71	121.00
1	A	710	ILE	CG1-CB-CG2	-7.15	95.67	111.40
1	A	575	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	174	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	A	825	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	A	255	LYS	CA-C-N	-7.04	101.71	117.20
1	A	797	TRP	NE1-CE2-CZ2	-7.03	122.67	130.40
1	A	825	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	A	138	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	20	GLY	O-C-N	-6.91	111.64	122.70
1	A	491	TRP	CG-CD2-CE3	6.87	140.08	133.90
1	A	825	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	A	760	ASP	N-CA-CB	-6.79	98.38	110.60
1	A	109	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	319	ARG	N-CA-C	-6.75	92.78	111.00
1	A	182	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	836	ALA	N-CA-CB	-6.71	100.70	110.10
1	A	314	SER	CA-C-N	-6.71	102.44	117.20
1	A	50	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	121	GLU	CA-CB-CG	6.66	128.05	113.40
1	A	193	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	280	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	A	233	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	A	734	ARG	O-C-N	-6.57	112.18	122.70
1	A	321	PRO	CA-C-N	-6.57	102.74	117.20
1	A	322	VAL	CA-CB-CG2	-6.57	101.05	110.90
1	A	361	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	A	831	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	641	ARG	CA-CB-CG	6.55	127.81	113.40
1	A	256	ASP	CB-CG-OD1	-6.54	112.41	118.30
1	A	648	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	A	491	TRP	CE2-CD2-CG	-6.44	102.14	107.30
1	A	189	TRP	CE2-CD2-CG	-6.44	102.15	107.30
1	A	639	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	381	PRO	CA-C-N	6.43	131.34	117.20
1	A	224	MET	CA-CB-CG	-6.38	102.46	113.30
1	A	314	SER	O-C-N	6.28	132.75	122.70
1	A	244	TRP	CG-CD1-NE1	-6.27	103.83	110.10
1	A	337	LEU	CA-CB-CG	6.27	129.71	115.30
1	A	527	ASP	CB-CG-OD1	6.24	123.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	ILE	CA-CB-CG2	6.22	123.34	110.90
1	A	85	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	359	LEU	CB-CG-CD2	-6.12	100.60	111.00
1	A	795	ARG	CB-CG-CD	6.07	127.39	111.60
1	A	472	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	322	VAL	N-CA-C	-6.07	94.62	111.00
1	A	355	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	764	MET	CG-SD-CE	-6.05	90.53	100.20
1	A	491	TRP	CD1-CG-CD2	6.04	111.13	106.30
1	A	340	THR	N-CA-CB	-5.99	98.91	110.30
1	A	213	ALA	N-CA-C	-5.98	94.85	111.00
1	A	524	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	A	638	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	321	PRO	N-CA-C	5.95	127.57	112.10
1	A	351	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	69	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	769	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	362	ASP	CB-CG-OD2	5.89	123.61	118.30
1	A	536	LYS	CB-CG-CD	-5.88	96.30	111.60
1	A	365	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	A	491	TRP	CB-CG-CD1	-5.88	119.36	127.00
1	A	387	TRP	CB-CG-CD1	-5.87	119.37	127.00
1	A	361	TRP	CD1-CG-CD2	5.86	110.99	106.30
1	A	649	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	734	ARG	CA-CB-CG	5.84	126.25	113.40
1	A	365	TRP	CB-CG-CD1	-5.84	119.41	127.00
1	A	29	LYS	CA-CB-CG	5.84	126.24	113.40
1	A	759	LYS	CA-CB-CG	-5.83	100.57	113.40
1	A	47	THR	N-CA-CB	-5.82	99.25	110.30
1	A	840	LYS	CA-C-N	-5.82	104.40	117.20
1	A	629	VAL	CG1-CB-CG2	-5.82	101.60	110.90
1	A	39	LEU	CA-CB-CG	-5.80	101.96	115.30
1	A	332	LYS	CG-CD-CE	5.80	129.29	111.90
1	A	797	TRP	CE2-CD2-CG	-5.80	102.66	107.30
1	A	29	LYS	N-CA-CB	-5.79	100.18	110.60
1	A	825	TRP	CG-CD1-NE1	-5.77	104.33	110.10
1	A	67	TRP	CG-CD1-NE1	-5.76	104.33	110.10
1	A	78	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	325	ASN	N-CA-C	5.76	126.55	111.00
1	A	244	TRP	CG-CD2-CE3	5.76	139.08	133.90
1	A	408	GLN	N-CA-CB	-5.74	100.27	110.60
1	A	699	MET	CG-SD-CE	5.74	109.38	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	639	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	33	ARG	CA-CB-CG	5.73	126.00	113.40
1	A	770	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	210	SER	N-CA-C	5.72	126.46	111.00
1	A	354	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	A	93	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	365	TRP	CG-CD2-CE3	5.69	139.02	133.90
1	A	117	LEU	N-CA-C	5.68	126.33	111.00
1	A	102	LEU	CB-CG-CD2	-5.68	101.35	111.00
1	A	763	ASN	CA-CB-CG	-5.68	100.91	113.40
1	A	100	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	A	436	VAL	N-CA-C	-5.66	95.73	111.00
1	A	763	ASN	N-CA-CB	-5.63	100.47	110.60
1	A	569	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	152	LEU	CB-CG-CD2	-5.61	101.47	111.00
1	A	734	ARG	CG-CD-NE	5.60	123.56	111.80
1	A	315	LYS	CG-CD-CE	5.60	128.69	111.90
1	A	435	ALA	CB-CA-C	-5.59	101.71	110.10
1	A	455	VAL	CG1-CB-CG2	-5.56	102.01	110.90
1	A	215	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	A	49	ARG	CA-CB-CG	5.55	125.62	113.40
1	A	325	ASN	CA-C-N	-5.55	104.99	117.20
1	A	182	TRP	CG-CD1-NE1	-5.55	104.55	110.10
1	A	601	ARG	CA-CB-CG	5.53	125.56	113.40
1	A	325	ASN	O-C-N	5.52	131.53	122.70
1	A	313	SER	CA-C-N	-5.52	105.06	117.20
1	A	430	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	63	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	807	THR	N-CA-CB	-5.51	99.83	110.30
1	A	178	GLU	CA-CB-CG	-5.50	101.29	113.40
1	A	407	ASN	CA-C-N	-5.49	105.13	117.20
1	A	641	ARG	N-CA-C	-5.49	96.19	111.00
1	A	551	ARG	CA-CB-CG	5.48	125.46	113.40
1	A	323	ARG	N-CA-C	-5.48	96.20	111.00
1	A	138	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	641	ARG	N-CA-CB	-5.46	100.78	110.60
1	A	370	LYS	CA-CB-CG	5.43	125.35	113.40
1	A	662	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	387	TRP	CG-CD1-NE1	-5.42	104.67	110.10
1	A	244	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	A	584	ILE	CG1-CB-CG2	-5.40	99.52	111.40
1	A	734	ARG	CA-C-N	5.39	129.06	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	CYS	N-CA-C	-5.38	96.48	111.00
1	A	310	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	468	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	A	377	HIS	CA-C-N	5.35	128.98	117.20
1	A	663	SER	N-CA-CB	-5.35	102.48	110.50
1	A	720	ARG	CB-CG-CD	-5.34	97.70	111.60
1	A	708	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	A	525	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	A	386	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	797	TRP	NE1-CE2-CD2	5.34	112.64	107.30
1	A	613	TYR	CB-CG-CD1	5.32	124.19	121.00
1	A	60	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	259	VAL	CA-CB-CG2	-5.30	102.94	110.90
1	A	367	VAL	CA-CB-CG2	5.30	118.85	110.90
1	A	730	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	A	226	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	A	102	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	91	MET	CG-SD-CE	5.28	108.65	100.20
1	A	94	THR	CA-C-N	5.26	128.78	117.20
1	A	392	LEU	CA-CB-CG	-5.26	103.19	115.30
1	A	724	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	473	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	A	367	VAL	CA-C-N	5.24	128.73	117.20
1	A	532	ARG	CA-CB-CG	5.24	124.93	113.40
1	A	108	CYS	CA-CB-SG	-5.22	104.60	114.00
1	A	84	TYR	CG-CD2-CE2	-5.22	117.13	121.30
1	A	253	ASN	CA-C-N	-5.22	105.72	117.20
1	A	489	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	355	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	506	ARG	CG-CD-NE	5.19	122.71	111.80
1	A	90	TYR	CA-CB-CG	5.19	123.27	113.40
1	A	519	ARG	CA-CB-CG	-5.19	101.98	113.40
1	A	334	ALA	N-CA-CB	5.19	117.36	110.10
1	A	318	CYS	CB-CA-C	5.18	120.77	110.40
1	A	754	GLN	N-CA-C	-5.18	97.02	111.00
1	A	756	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	123	GLU	CA-CB-CG	-5.17	102.03	113.40
1	A	441	MET	CA-CB-CG	5.17	122.08	113.30
1	A	691	THR	O-C-N	-5.17	114.44	122.70
1	A	318	CYS	O-C-N	5.16	130.95	122.70
1	A	294	LYS	CG-CD-CE	-5.15	96.46	111.90
1	A	472	TYR	CD1-CG-CD2	5.14	123.56	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	786	ARG	CG-CD-NE	5.14	122.60	111.80
1	A	770	ARG	CG-CD-NE	5.14	122.59	111.80
1	A	181	ASP	N-CA-CB	-5.13	101.36	110.60
1	A	732	TYR	CD1-CG-CD2	5.13	123.55	117.90
1	A	107	ALA	CA-C-N	5.13	128.48	117.20
1	A	554	LYS	CB-CG-CD	-5.12	98.28	111.60
1	A	16	ARG	O-C-N	-5.12	114.50	123.20
1	A	435	ALA	O-C-N	5.11	130.88	122.70
1	A	319	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	615	MET	CG-SD-CE	5.10	108.36	100.20
1	A	275	ILE	CB-CA-C	-5.09	101.42	111.60
1	A	198	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	836	ALA	CB-CA-C	5.06	117.69	110.10
1	A	825	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	A	357	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	A	25	THR	N-CA-CB	-5.04	100.72	110.30
1	A	720	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	55	LEU	CA-CB-CG	5.03	126.87	115.30
1	A	257	PHE	CA-C-O	5.03	130.66	120.10
1	A	49	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	189	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	A	244	TRP	CH2-CZ2-CE2	5.02	122.42	117.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ARG	Mainchain
1	A	185	TYR	Sidechain
1	A	20	GLY	Mainchain
1	A	318	CYS	Mainchain
1	A	381	PRO	Mainchain
1	A	472	TYR	Sidechain
1	A	51	TYR	Sidechain
1	A	777	TYR	Sidechain
1	A	831	ARG	Sidechain
1	A	840	LYS	Mainchain

## 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	6727	0	6655	220	2
2	A	16	0	11	2	0
3	A	15	0	6	0	0
4	A	673	0	0	33	2
All	All	7431	0	6672	220	2

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 16.

All (220) 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:309:ARG:C	1:A:310:ARG:N	1.73	1.42
1:A:308:ILE:C	1:A:309:ARG:N	1.78	1.37
1:A:841:ILE:CB	4:A:1672:HOH:O	1.77	1.29
1:A:67:TRP:HE1	1:A:240:THR:HG22	1.35	0.91
1:A:730:GLU:O	1:A:734:ARG:HB2	1.78	0.83
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.65	0.79
1:A:756:ASP:HA	1:A:759:LYS:HD3	1.65	0.79
1:A:528:GLU:HG3	1:A:532:ARG:HH12	1.48	0.78
1:A:833:ARG:HD2	1:A:833:ARG:N	1.99	0.78
1:A:309:ARG:NH2	1:A:310:ARG:HG3	2.00	0.77
1:A:437:LYS:HE2	4:A:1540:HOH:O	1.86	0.76
1:A:528:GLU:HG3	1:A:532:ARG:NH1	2.01	0.75
1:A:309:ARG:HH21	1:A:310:ARG:HG3	1.50	0.75
1:A:794:PRO:HG3	4:A:1640:HOH:O	1.86	0.75
1:A:593:GLU:HG2	1:A:596:LYS:HE3	1.68	0.75
1:A:703:ALA:HA	1:A:807:THR:HG21	1.70	0.72
1:A:316:PHE:HA	1:A:319:ARG:HE	1.54	0.71
1:A:304:LEU:HD23	1:A:307:ILE:HD12	1.73	0.70
1:A:322:VAL:HG13	1:A:323:ARG:H	1.57	0.69
1:A:30:ASN:HB2	1:A:58:THR:HG23	1.76	0.68
1:A:47:THR:HG21	4:A:1564:HOH:O	1.95	0.66
1:A:833:ARG:H	1:A:833:ARG:HD2	1.60	0.65
1:A:340:THR:HG22	1:A:385:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.79	0.65
1:A:314:SER:O	1:A:316:PHE:HB2	1.99	0.63
1:A:405:GLU:HA	1:A:408:GLN:HE21	1.64	0.63
1:A:548:TYR:CE2	1:A:552:GLU:HG3	2.33	0.62
1:A:138:ARG:HB3	4:A:1507:HOH:O	1.99	0.62
1:A:651:SER:O	1:A:655:LYS:HD2	2.00	0.62
1:A:252:PHE:CE1	1:A:256:ASP:HB2	2.34	0.62
1:A:196:PHE:CE1	1:A:309:ARG:NH1	2.67	0.62
1:A:392:LEU:HB3	1:A:400:LEU:HG	1.81	0.61
1:A:506:ARG:HG3	1:A:506:ARG:HH11	1.65	0.60
1:A:75:TYR:CZ	1:A:315:LYS:HE3	2.37	0.60
1:A:304:LEU:HD12	1:A:348:GLU:HG3	1.82	0.60
1:A:322:VAL:HG13	1:A:323:ARG:N	2.17	0.60
1:A:251:ASP:HB2	1:A:255:LYS:NZ	2.17	0.59
1:A:255:LYS:HB3	1:A:255:LYS:NZ	2.18	0.59
1:A:404:TYR:O	1:A:408:GLN:HB2	2.03	0.59
1:A:335:ILE:HD11	1:A:337:LEU:HD13	1.84	0.59
1:A:404:TYR:HB3	4:A:1261:HOH:O	2.03	0.59
1:A:252:PHE:CZ	1:A:256:ASP:HB2	2.38	0.59
1:A:405:GLU:O	1:A:408:GLN:HB3	2.03	0.59
1:A:466:THR:O	1:A:469:LYS:HD2	2.00	0.59
1:A:204:GLY:HA3	1:A:218:THR:HG22	1.85	0.59
1:A:256:ASP:HB3	1:A:258:ASN:ND2	2.18	0.58
1:A:256:ASP:HB3	1:A:258:ASN:OD1	2.04	0.58
1:A:703:ALA:CA	1:A:807:THR:HG21	2.33	0.57
1:A:641:ARG:HG3	1:A:643:ILE:HD11	1.86	0.57
1:A:256:ASP:HB3	1:A:258:ASN:CG	2.25	0.57
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.69	0.57
1:A:77:LYS:HD3	4:A:1567:HOH:O	2.04	0.57
1:A:322:VAL:HG11	1:A:325:ASN:HB2	1.86	0.57
1:A:710:ILE:HD12	1:A:710:ILE:H	1.69	0.57
1:A:309:ARG:C	1:A:310:ARG:CA	2.70	0.56
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.69	0.56
1:A:319:ARG:NH2	1:A:320:ASP:HA	2.19	0.56
1:A:423:ASP:O	1:A:426:ARG:HG3	2.05	0.56
1:A:335:ILE:HD11	1:A:337:LEU:CD1	2.36	0.56
1:A:309:ARG:CA	1:A:310:ARG:N	2.65	0.56
1:A:514:ASP:HB2	1:A:831:ARG:NH2	2.20	0.56
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.05	0.56
1:A:207:GLU:HG2	1:A:214:LYS:HB3	1.87	0.55
1:A:321:PRO:O	1:A:322:VAL:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLY:O	1:A:69:ARG:HB2	2.06	0.55
1:A:548:TYR:HA	1:A:551:ARG:HG3	1.88	0.55
1:A:548:TYR:HA	1:A:551:ARG:CG	2.37	0.55
1:A:424:ARG:HH22	1:A:473:GLU:CD	2.10	0.55
1:A:303:THR:O	1:A:307:ILE:HG13	2.07	0.54
1:A:502:ILE:HA	1:A:505:GLU:HG3	1.88	0.54
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.42	0.54
1:A:831:ARG:O	1:A:833:ARG:NH1	2.40	0.54
1:A:225:PRO:CB	1:A:242:ARG:HD2	2.38	0.54
1:A:458:ILE:O	1:A:462:ILE:HG12	2.07	0.54
1:A:285:PHE:HE1	1:A:382:GLU:HB2	1.73	0.54
1:A:285:PHE:CE1	1:A:382:GLU:HB2	2.43	0.53
1:A:355:ASP:OD2	1:A:398:ARG:HD2	2.08	0.53
1:A:255:LYS:HZ2	1:A:255:LYS:HB3	1.74	0.53
1:A:711:PHE:CE2	1:A:780:TYR:HB2	2.44	0.53
1:A:532:ARG:O	1:A:536:LYS:HG3	2.09	0.53
1:A:308:ILE:HG22	1:A:312:LYS:HD2	1.91	0.53
1:A:178:GLU:HG2	4:A:1584:HOH:O	2.10	0.52
1:A:516:ASP:HA	1:A:809:GLY:HA3	1.90	0.52
1:A:183:LEU:CD2	1:A:187:ASN:HB2	2.40	0.52
1:A:312:LYS:HE2	4:A:1090:HOH:O	2.11	0.51
1:A:69:ARG:NH2	1:A:834:LEU:HD11	2.25	0.51
1:A:166:PHE:CE2	1:A:611:PRO:HD3	2.46	0.51
1:A:375:THR:HG23	1:A:453:ASN:HD21	1.75	0.51
1:A:753:LYS:HB3	4:A:1094:HOH:O	2.11	0.51
1:A:47:THR:O	1:A:50:ASP:HB2	2.11	0.51
1:A:166:PHE:HE2	1:A:611:PRO:HD3	1.76	0.51
1:A:319:ARG:O	1:A:319:ARG:NE	2.43	0.51
1:A:532:ARG:HG3	1:A:532:ARG:HH11	1.76	0.50
1:A:544:LYS:HD2	4:A:1222:HOH:O	2.09	0.50
1:A:482:LYS:HE2	1:A:824:ILE:HD11	1.92	0.50
1:A:569:ARG:HD2	1:A:608:LYS:O	2.11	0.50
1:A:497:PRO:HB3	4:A:1416:HOH:O	2.12	0.50
1:A:43:ARG:CZ	4:A:1002:HOH:O	2.59	0.50
1:A:831:ARG:HG3	4:A:1268:HOH:O	2.10	0.50
1:A:490:ARG:HA	1:A:494:LEU:HB3	1.93	0.50
1:A:647:ASN:O	1:A:649:ARG:HG2	2.11	0.50
1:A:529:ALA:HA	1:A:532:ARG:HD2	1.94	0.50
1:A:455:VAL:H	1:A:459:HIS:HD2	1.58	0.50
1:A:93:ARG:HD3	1:A:126:GLU:O	2.12	0.50
1:A:361:TRP:CZ3	1:A:409:ARG:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:CD1	1:A:827:VAL:HG21	2.41	0.49
1:A:157:TYR:OH	1:A:310:ARG:NH2	2.44	0.49
1:A:569:ARG:O	1:A:574:LYS:HD3	2.13	0.49
1:A:117:LEU:HD11	4:A:1002:HOH:O	2.11	0.49
1:A:93:ARG:HD2	1:A:126:GLU:HB3	1.95	0.49
1:A:754:GLN:NE2	1:A:757:LEU:HD13	2.28	0.49
1:A:386:ARG:NH2	4:A:1180:HOH:O	2.45	0.49
1:A:706:GLU:H	1:A:706:GLU:CD	2.16	0.48
1:A:365:TRP:CH2	1:A:448:GLY:HA2	2.47	0.48
1:A:405:GLU:HA	1:A:408:GLN:NE2	2.29	0.48
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.48	0.48
1:A:250:ASN:HA	1:A:269:ARG:NH1	2.27	0.48
1:A:110:GLU:OE2	1:A:114:GLN:NE2	2.46	0.48
1:A:486:ILE:CD1	1:A:676:THR:HB	2.44	0.48
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.96	0.48
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.95	0.48
1:A:490:ARG:HD2	4:A:1385:HOH:O	2.13	0.48
1:A:834:LEU:HD12	1:A:835:PRO:HD3	1.96	0.47
1:A:193:ARG:NH2	2:A:998:G6P:H2	2.29	0.47
1:A:316:PHE:O	1:A:320:ASP:HA	2.14	0.47
1:A:254:LEU:N	1:A:254:LEU:HD12	2.29	0.47
1:A:565:VAL:HG23	1:A:567:VAL:HG13	1.95	0.47
1:A:20:GLY:C	4:A:1204:HOH:O	2.53	0.47
1:A:511:TYR:HA	1:A:514:ASP:O	2.14	0.47
1:A:698:GLU:O	1:A:702:GLU:HB2	2.15	0.46
1:A:66:ARG:HD2	1:A:837:PRO:HB3	1.97	0.46
1:A:558:ASN:HB2	1:A:638:ASP:OD2	2.16	0.46
1:A:592:LYS:NZ	1:A:593:GLU:OE2	2.48	0.46
1:A:593:GLU:O	1:A:596:LYS:HG2	2.15	0.46
1:A:184:ARG:HB3	1:A:184:ARG:HH11	1.81	0.46
1:A:36:HIS:O	1:A:40:VAL:HA	2.16	0.46
1:A:723:GLN:HB2	4:A:1518:HOH:O	2.16	0.46
1:A:698:GLU:HB3	1:A:810:LYS:NZ	2.31	0.46
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.16	0.46
1:A:338:ASN:OD1	1:A:377:HIS:NE2	2.49	0.46
1:A:322:VAL:C	1:A:323:ARG:HD2	2.37	0.45
1:A:146:SER:O	1:A:150:LEU:HG	2.17	0.45
1:A:20:GLY:O	1:A:24:VAL:HG23	2.17	0.45
1:A:358:ARG:HH11	1:A:358:ARG:HG2	1.82	0.45
1:A:236:ASN:HB3	1:A:836:ALA:HB3	1.98	0.45
1:A:33:ARG:HA	4:A:1560:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:H	1:A:459:HIS:CD2	2.34	0.45
1:A:521:LEU:HB2	1:A:806:ALA:HB2	1.99	0.45
1:A:408:GLN:HG2	4:A:1189:HOH:O	2.16	0.45
1:A:795:ARG:O	1:A:799:ARG:HG3	2.17	0.45
1:A:170:ILE:HA	1:A:174:TRP:O	2.17	0.45
1:A:793:ASN:HA	1:A:794:PRO:HD3	1.60	0.44
1:A:181:ASP:HB3	1:A:184:ARG:NH2	2.32	0.44
1:A:502:ILE:O	1:A:506:ARG:HD3	2.17	0.44
1:A:423:ASP:O	1:A:427:ARG:HG3	2.17	0.44
1:A:417:ALA:C	1:A:419:PRO:HD3	2.38	0.44
1:A:561:SER:HB2	1:A:601:ARG:HA	1.98	0.44
1:A:547:ALA:O	1:A:550:GLU:N	2.51	0.44
1:A:343:SER:HB3	1:A:445:CYS:SG	2.58	0.44
1:A:461:GLU:OE1	1:A:465:LYS:NZ	2.51	0.44
1:A:21:VAL:HG13	1:A:22:GLU:N	2.33	0.44
1:A:593:GLU:HB3	1:A:596:LYS:HG2	1.98	0.44
1:A:515:LEU:O	1:A:518:LEU:HB2	2.18	0.44
1:A:424:ARG:NH2	1:A:470:ASP:HA	2.32	0.44
1:A:483:THR:O	1:A:816:THR:HG23	2.17	0.44
1:A:57:HIS:HE1	4:A:1007:HOH:O	2.01	0.44
1:A:502:ILE:HD13	1:A:533:ASP:HB3	2.00	0.43
1:A:562:LEU:HD21	1:A:662:LEU:HB2	2.00	0.43
1:A:566:GLN:HA	4:A:1364:HOH:O	2.17	0.43
1:A:166:PHE:CD1	1:A:177:GLU:HB3	2.54	0.43
1:A:205:ARG:HG3	1:A:216:VAL:HG12	2.01	0.43
1:A:373:ALA:HB1	4:A:1255:HOH:O	2.18	0.43
1:A:118:ASP:HA	4:A:1419:HOH:O	2.18	0.43
1:A:678:ASN:HB2	1:A:699:MET:SD	2.58	0.43
1:A:589:ARG:NH1	1:A:737:GLU:OE1	2.52	0.43
1:A:817:ILE:HA	1:A:817:ILE:HD13	1.91	0.43
1:A:605:ILE:O	1:A:644:PHE:HA	2.18	0.43
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.99	0.43
1:A:251:ASP:HB2	1:A:255:LYS:HZ2	1.83	0.43
1:A:177:GLU:OE1	1:A:611:PRO:HG3	2.18	0.43
1:A:375:THR:HG23	1:A:453:ASN:ND2	2.33	0.43
1:A:767:HIS:HB2	1:A:768:HIS:CE1	2.54	0.43
1:A:328:ALA:HB2	4:A:1446:HOH:O	2.19	0.43
1:A:501:GLU:O	1:A:505:GLU:HG3	2.19	0.42
1:A:234:ARG:NH1	4:A:1570:HOH:O	2.45	0.42
1:A:459:HIS:O	1:A:463:LEU:HG	2.19	0.42
1:A:517:GLN:O	1:A:520:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:LYS:O	1:A:763:ASN:HB2	2.18	0.42
1:A:487:THR:HG23	1:A:490:ARG:HB3	2.02	0.42
1:A:533:ASP:HA	1:A:536:LYS:HE2	2.02	0.42
1:A:421:ASP:O	1:A:425:LEU:HD13	2.19	0.42
1:A:591:LYS:HD3	1:A:633:ASP:OD2	2.20	0.42
1:A:486:ILE:HG12	1:A:680:LYS:HG2	2.02	0.42
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.82	0.42
1:A:263:ILE:O	1:A:267:LEU:HG	2.20	0.42
1:A:309:ARG:HE	1:A:309:ARG:HB3	1.24	0.41
1:A:340:THR:HG23	1:A:441:MET:HB3	2.01	0.41
1:A:484:ASN:ND2	4:A:1046:HOH:O	2.52	0.41
1:A:648:TYR:HA	1:A:652:LEU:HD23	2.01	0.41
1:A:549:LEU:HB3	1:A:550:GLU:OE1	2.20	0.41
1:A:803:ARG:O	1:A:807:THR:HB	2.20	0.41
1:A:330:PRO:HD3	1:A:367:VAL:HG13	2.01	0.41
1:A:256:ASP:HB3	1:A:258:ASN:HD21	1.86	0.41
1:A:379:VAL:HG12	4:A:1649:HOH:O	2.20	0.41
1:A:275:ILE:HD12	1:A:294:LYS:HB3	2.01	0.41
1:A:103:ALA:HB2	1:A:234:ARG:HD2	2.02	0.41
1:A:754:GLN:OE1	1:A:757:LEU:HB2	2.20	0.41
1:A:344:LEU:HD22	4:A:1609:HOH:O	2.20	0.41
1:A:242:ARG:NH2	2:A:998:G6P:O3P	2.49	0.40
1:A:593:GLU:HG2	1:A:596:LYS:CE	2.45	0.40
1:A:292:ARG:NH2	4:A:1408:HOH:O	2.53	0.40
1:A:353:LEU:HB3	1:A:359:LEU:HD12	2.02	0.40
1:A:685:GLY:HA2	4:A:1650:HOH:O	2.21	0.40
1:A:553:TYR:O	1:A:554:LYS:HG3	2.21	0.40
1:A:323:ARG:N	1:A:323:ARG:HD2	2.36	0.40
1:A:117:LEU:HD21	4:A:1002:HOH:O	2.21	0.40
1:A:172:GLY:O	1:A:621:LYS:NZ	2.55	0.40
1:A:251:ASP:HB2	1:A:255:LYS:HZ1	1.85	0.40
1:A:445:CYS:O	1:A:449:SER:HB2	2.21	0.40
1:A:83:TYR:CE2	1:A:333:VAL:HG13	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ALA:O	4:A:1064:HOH:O[7_556]	1.76	0.44
1:A:111:ALA:CB	4:A:1064:HOH:O[7_556]	2.13	0.07

## 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	826/842 (98%)	746 (90%)	62 (8%)	18 (2%)	<b>8</b> <b>9</b>

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLY
1	A	321	PRO
1	A	322	VAL
1	A	324	THR
1	A	555	VAL
1	A	837	PRO
1	A	312	LYS
1	A	320	ASP
1	A	436	VAL
1	A	705	GLU
1	A	203	TYR
1	A	435	ALA
1	A	611	PRO
1	A	260	GLY
1	A	319	ARG
1	A	489	ARG
1	A	15	VAL
1	A	835	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	715/731 (98%)	592 (83%)	123 (17%)	<b>2</b> <b>3</b>

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	18	LEU
1	A	22	GLU
1	A	26	GLU
1	A	38	THR
1	A	43	ARG
1	A	55	LEU
1	A	60	ARG
1	A	63	LEU
1	A	69	ARG
1	A	76	GLU
1	A	77	LYS
1	A	82	ILE
1	A	85	LEU
1	A	90	TYR
1	A	102	LEU
1	A	110	GLU
1	A	113	TYR
1	A	114	GLN
1	A	127	GLU
1	A	138	ARG
1	A	144	LEU
1	A	152	LEU
1	A	159	ILE
1	A	165	ILE
1	A	169	LYS
1	A	170	ILE
1	A	176	MET
1	A	177	GLU
1	A	191	LYS
1	A	198	LEU
1	A	209	THR
1	A	214	LYS
1	A	216	VAL
1	A	217	ASP
1	A	224	MET
1	A	235	ASN
1	A	242	ARG

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Mol	Chain	Res	Type
1	A	243	LEU
1	A	250	ASN
1	A	252	PHE
1	A	255	LYS
1	A	259	VAL
1	A	285	PHE
1	A	292	ARG
1	A	305	GLN
1	A	309	ARG
1	A	316	PHE
1	A	318	CYS
1	A	319	ARG
1	A	320	ASP
1	A	321	PRO
1	A	335	ILE
1	A	337	LEU
1	A	344	LEU
1	A	360	ASP
1	A	361	TRP
1	A	363	LYS
1	A	384	LEU
1	A	390	HIS
1	A	398	ARG
1	A	400	LEU
1	A	405	GLU
1	A	426	ARG
1	A	430	LEU
1	A	433	GLU
1	A	444	LEU
1	A	467	ILE
1	A	469	LYS
1	A	474	LEU
1	A	486	ILE
1	A	490	ARG
1	A	501	GLU
1	A	506	ARG
1	A	513	SER
1	A	515	LEU
1	A	519	ARG
1	A	522	LEU
1	A	526	ASP
1	A	539	GLN

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Mol	Chain	Res	Type
1	A	548	TYR
1	A	549	LEU
1	A	550	GLU
1	A	556	HIS
1	A	565	VAL
1	A	576	GLN
1	A	579	ASN
1	A	586	LEU
1	A	593	GLU
1	A	596	LYS
1	A	601	ARG
1	A	611	PRO
1	A	613	TYR
1	A	622	LEU
1	A	638	ASP
1	A	641	ARG
1	A	649	ARG
1	A	655	LYS
1	A	662	LEU
1	A	687	LEU
1	A	702	GLU
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	710	ILE
1	A	720	ARG
1	A	729	GLN
1	A	734	ARG
1	A	735	ILE
1	A	740	GLN
1	A	753	LYS
1	A	754	GLN
1	A	764	MET
1	A	765	LEU
1	A	790	LEU
1	A	795	ARG
1	A	797	TRP
1	A	800	MET
1	A	807	THR
1	A	827	VAL
1	A	831	ARG
1	A	838	ASP

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Mol	Chain	Res	Type
1	A	839	GLU

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	72	GLN
1	A	97	ASN
1	A	187	ASN
1	A	219	GLN
1	A	235	ASN
1	A	408	GLN
1	A	453	ASN
1	A	459	HIS
1	A	477	HIS
1	A	481	ASN
1	A	484	ASN
1	A	576	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 ⓘ

There are no carbohydrates 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	G6P	A	998	-	16,16,16	1.81	5 (31%)	23,24,24	2.46	9 (39%)
3	PLP	A	999	1	15,15,16	2.45	5 (33%)	21,22,23	1.50	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	G6P	A	998	-	-	0/6/26/26	0/1/1/1
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C3-C2	-7.19	1.35	1.40
3	A	999	PLP	C5-C4	-3.10	1.36	1.40
2	A	998	G6P	C1-C2	-2.93	1.47	1.52
3	A	999	PLP	P-O2P	-2.88	1.44	1.54
2	A	998	G6P	C4-C3	-2.86	1.44	1.52
2	A	998	G6P	C3-C2	-2.67	1.45	1.52
3	A	999	PLP	P-O4P	-2.53	1.51	1.60
2	A	998	G6P	O5-C5	2.10	1.49	1.44
3	A	999	PLP	C4A-C4	2.18	1.56	1.51
2	A	998	G6P	O5-C1	2.80	1.48	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	G6P	O4-C4-C3	-4.85	99.41	110.34
3	A	999	PLP	O4P-C5A-C5	-4.44	101.66	108.99
2	A	998	G6P	O1-C1-C2	-3.97	98.58	109.21
2	A	998	G6P	O2-C2-C3	-3.75	101.89	110.34
2	A	998	G6P	O3-C3-C4	-2.27	105.23	110.34
3	A	999	PLP	C4A-C4-C5	-2.26	118.53	120.88
3	A	999	PLP	C5-C6-N1	-2.20	120.04	123.86
2	A	998	G6P	C4-C3-C2	2.58	115.60	110.79
3	A	999	PLP	O2P-P-O1P	2.69	119.24	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	G6P	O5-C5-C6	2.88	112.49	106.61
2	A	998	G6P	O6-C6-C5	3.12	120.60	109.12
2	A	998	G6P	C1-C2-C3	3.72	115.96	110.43
2	A	998	G6P	O1-C1-O5	4.69	123.07	110.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	998	G6P	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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.