



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2025 – 05:09 AM EDT

PDB ID : 3GPB  
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

<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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

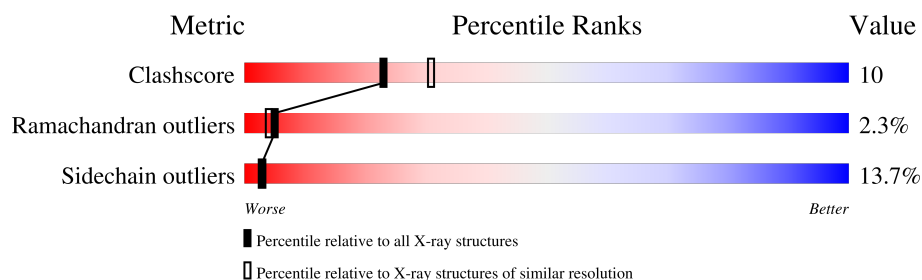
# 1 Overall quality at a glance

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	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (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  $\geq 3$ , 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	 62% 26% 8% . .

## 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.

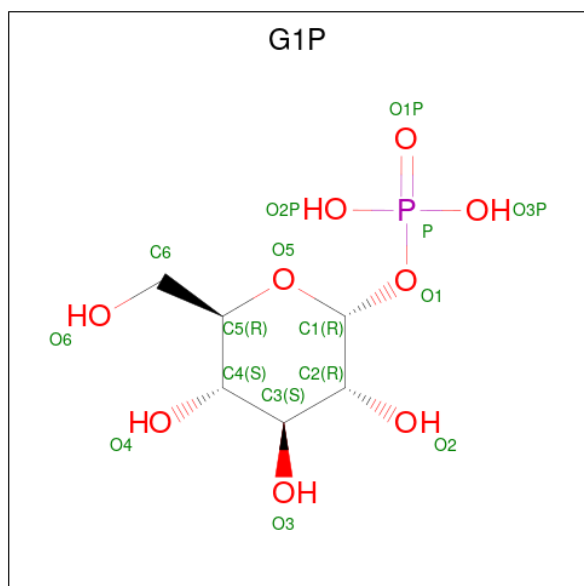
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

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:

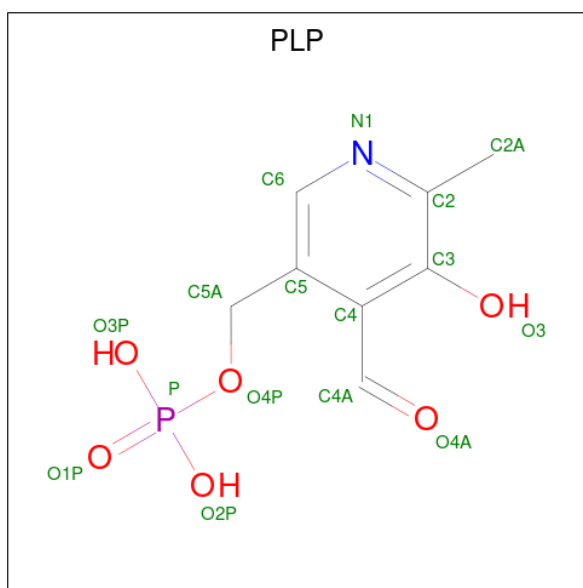
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is 1-O-phosphono-alpha-D-glucopyranose (three-letter code: G1P) (formula:  $C_6H_{13}O_9P$ ).



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

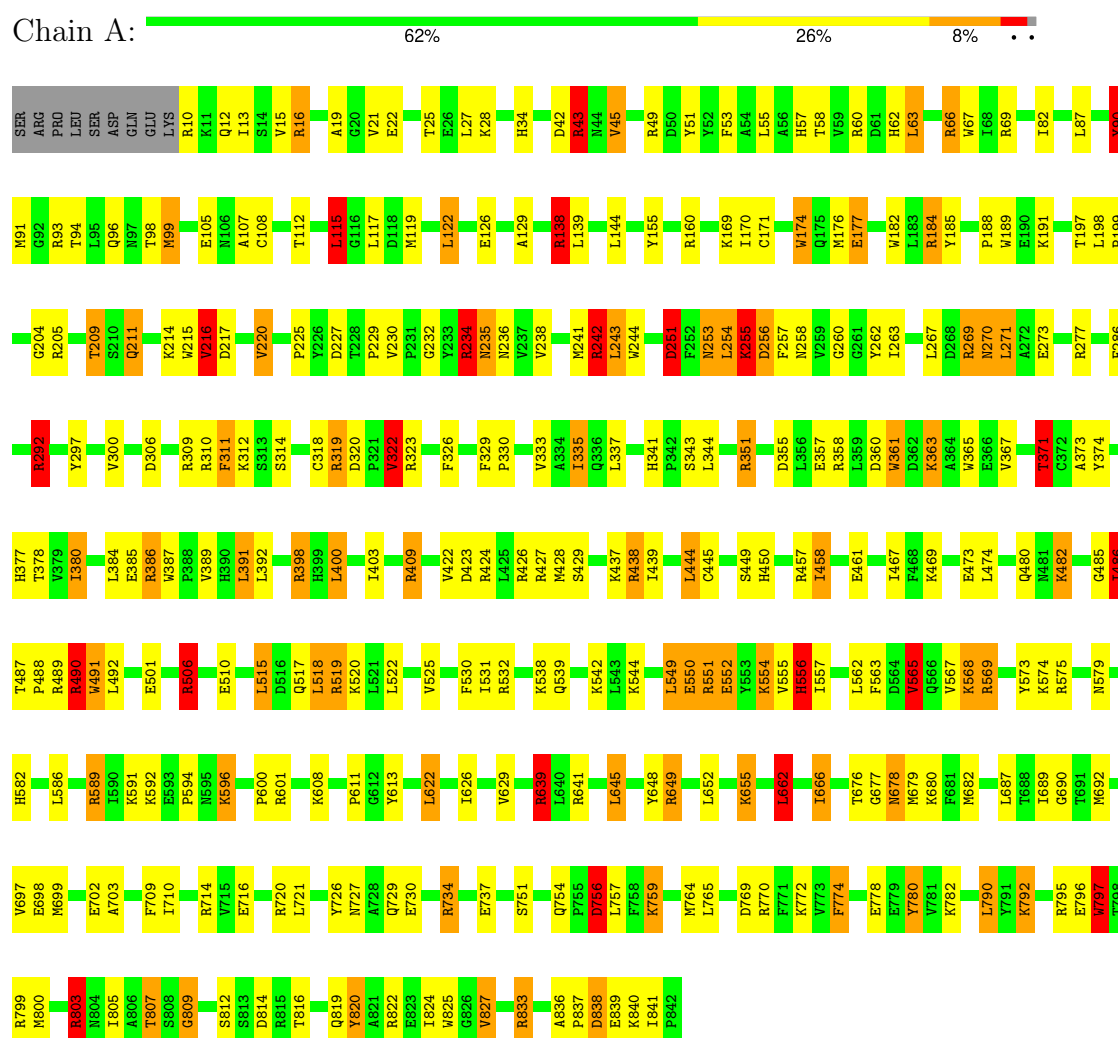
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	604	Total	O	0	0
			604	604		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 is therefore 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)	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	7430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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: PLP, G1P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.93	2/6933 (0.0%)	1.80	167/9381 (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	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	THR	CA-CB	6.37	1.70	1.53
1	A	812	SER	CB-OG	5.51	1.49	1.42

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	A	613	TYR	CB-CG-CD2	-12.32	113.61	121.00
1	A	795	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	A	310	ARG	NE-CZ-NH2	-12.15	114.22	120.30
1	A	506	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	A	242	ARG	NE-CZ-NH2	-10.77	114.91	120.30
1	A	90	TYR	CB-CG-CD2	-10.26	114.84	121.00
1	A	387	TRP	CD1-CG-CD2	10.08	114.36	106.30
1	A	639	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	A	138	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	A	365	TRP	CD1-CG-CD2	9.46	113.87	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	A	309	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	A	734	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	16	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	A	613	TYR	CB-CG-CD1	8.77	126.26	121.00
1	A	244	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	A	138	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	A	803	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	714	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	374	TYR	CB-CG-CD2	-8.45	115.93	121.00
1	A	256	ASP	CA-CB-CG	-8.32	95.11	113.40
1	A	174	TRP	CE2-CD2-CG	-8.27	100.69	107.30
1	A	387	TRP	CE2-CD2-CG	-8.26	100.69	107.30
1	A	365	TRP	CE2-CD2-CG	-8.21	100.73	107.30
1	A	649	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	A	253	ASN	CA-C-N	-8.06	99.46	117.20
1	A	428	MET	CA-CB-CG	-8.02	99.67	113.30
1	A	174	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	A	67	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	A	255	LYS	N-CA-C	7.83	132.13	111.00
1	A	234	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	51	TYR	CB-CG-CD2	-7.82	116.31	121.00
1	A	189	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	A	822	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	182	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A	486	ILE	CA-CB-CG1	-7.55	96.65	111.00
1	A	807	THR	N-CA-CB	-7.52	96.01	110.30
1	A	386	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	361	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	A	174	TRP	CG-CD2-CE3	7.39	140.55	133.90
1	A	185	TYR	CB-CG-CD1	-7.39	116.57	121.00
1	A	361	TRP	CE2-CD2-CG	-7.37	101.40	107.30
1	A	734	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	792	LYS	CA-CB-CG	7.32	129.50	113.40
1	A	184	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	409	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	387	TRP	CG-CD2-CE3	7.23	140.41	133.90
1	A	398	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	444	LEU	CA-CB-CG	7.18	131.82	115.30
1	A	99	MET	CG-SD-CE	-7.13	88.78	100.20
1	A	457	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	795	ARG	NE-CZ-NH1	7.12	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	LEU	CA-CB-CG	7.06	131.55	115.30
1	A	244	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	A	15	VAL	CA-C-N	-6.89	102.03	117.20
1	A	234	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	457	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	189	TRP	CE2-CD2-CG	-6.77	101.89	107.30
1	A	182	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	277	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	67	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	A	825	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	A	639	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	209	THR	CA-C-N	-6.69	102.48	117.20
1	A	309	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	575	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	323	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	351	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	491	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	A	306	ASP	CB-CG-OD1	6.58	124.23	118.30
1	A	215	TRP	CD1-CG-CD2	6.53	111.52	106.30
1	A	458	ILE	CB-CA-C	-6.44	98.72	111.60
1	A	666	ILE	N-CA-CB	-6.40	96.07	110.80
1	A	365	TRP	CB-CG-CD1	-6.39	118.69	127.00
1	A	666	ILE	CA-CB-CG1	-6.37	98.90	111.00
1	A	797	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	A	365	TRP	CG-CD2-CE3	6.35	139.62	133.90
1	A	565	VAL	CG1-CB-CG2	-6.34	100.75	110.90
1	A	424	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	489	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	814	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	253	ASN	O-C-N	6.31	132.79	122.70
1	A	662	LEU	CA-CB-CG	6.29	129.78	115.30
1	A	322	VAL	CA-CB-CG1	6.28	120.32	110.90
1	A	387	TRP	CG-CD1-NE1	-6.27	103.83	110.10
1	A	629	VAL	CG1-CB-CG2	-6.21	100.96	110.90
1	A	825	TRP	CD1-CG-CD2	6.19	111.25	106.30
1	A	827	VAL	CG1-CB-CG2	-6.19	101.00	110.90
1	A	648	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	A	769	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	461	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	A	255	LYS	CA-CB-CG	6.13	126.89	113.40
1	A	365	TRP	CG-CD1-NE1	-6.09	104.01	110.10
1	A	197	THR	N-CA-CB	-6.08	98.75	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	489	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	601	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	387	TRP	CB-CG-CD1	-6.02	119.17	127.00
1	A	486	ILE	CA-CB-CG2	6.01	122.92	110.90
1	A	575	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	220	VAL	CG1-CB-CG2	-5.99	101.32	110.90
1	A	556	HIS	CA-CB-CG	5.96	123.73	113.60
1	A	215	TRP	CE2-CD2-CG	-5.95	102.54	107.30
1	A	490	ARG	CG-CD-NE	-5.92	99.38	111.80
1	A	491	TRP	CD1-CG-CD2	5.88	111.00	106.30
1	A	174	TRP	CB-CG-CD1	-5.86	119.39	127.00
1	A	774	PHE	CB-CG-CD2	-5.85	116.71	120.80
1	A	756	ASP	N-CA-CB	-5.83	100.12	110.60
1	A	189	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	A	770	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	666	ILE	CA-CB-CG2	5.79	122.49	110.90
1	A	333	VAL	CG1-CB-CG2	-5.77	101.66	110.90
1	A	94	THR	CA-C-N	5.71	129.75	117.20
1	A	358	ARG	CG-CD-NE	-5.70	99.83	111.80
1	A	277	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	322	VAL	CA-CB-CG2	-5.67	102.39	110.90
1	A	45	VAL	CB-CA-C	-5.64	100.69	111.40
1	A	319	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	63	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	312	LYS	CA-CB-CG	-5.61	101.05	113.40
1	A	297	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	A	244	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	A	797	TRP	NE1-CE2-CZ2	-5.61	124.23	130.40
1	A	67	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	A	184	ARG	CA-CB-CG	5.59	125.71	113.40
1	A	655	LYS	CA-CB-CG	5.58	125.68	113.40
1	A	799	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	311	PHE	N-CA-C	-5.53	96.08	111.00
1	A	820	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	216	VAL	N-CA-CB	-5.50	99.40	111.50
1	A	438	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	322	VAL	CA-C-N	-5.43	105.25	117.20
1	A	554	LYS	N-CA-C	5.43	125.66	111.00
1	A	520	LYS	CB-CG-CD	-5.41	97.55	111.60
1	A	253	ASN	C-N-CA	5.37	135.13	121.70
1	A	43	ARG	NE-CZ-NH2	-5.36	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	VAL	CA-CB-CG2	-5.33	102.90	110.90
1	A	122	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	155	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	800	MET	CG-SD-CE	-5.29	91.74	100.20
1	A	15	VAL	CA-C-O	5.28	131.18	120.10
1	A	519	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	189	TRP	CB-CG-CD1	-5.27	120.14	127.00
1	A	645	LEU	CA-C-N	-5.27	105.60	117.20
1	A	13	ILE	N-CA-C	5.26	125.21	111.00
1	A	238	VAL	CG1-CB-CG2	-5.25	102.49	110.90
1	A	251	ASP	CA-C-N	5.21	128.67	117.20
1	A	491	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	A	458	ILE	N-CA-CB	5.20	122.77	110.80
1	A	833	ARG	CB-CG-CD	-5.20	98.07	111.60
1	A	424	ARG	CA-CB-CG	-5.20	101.96	113.40
1	A	271	LEU	N-CA-C	-5.18	97.00	111.00
1	A	827	VAL	CA-CB-CG2	5.16	118.64	110.90
1	A	115	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	838	ASP	C-N-CA	5.08	134.41	121.70
1	A	699	MET	CG-SD-CE	5.07	108.31	100.20
1	A	780	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	A	300	VAL	CA-CB-CG2	-5.05	103.33	110.90
1	A	797	TRP	CB-CG-CD1	-5.05	120.44	127.00
1	A	386	ARG	CG-CD-NE	-5.04	101.21	111.80
1	A	215	TRP	N-CA-C	-5.03	97.42	111.00
1	A	215	TRP	CG-CD2-CE3	5.03	138.43	133.90
1	A	255	LYS	N-CA-CB	-5.02	101.57	110.60
1	A	770	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	177	GLU	OE1-CD-OE2	-5.01	117.29	123.30
1	A	292	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	ARG	Sidechain
1	A	255	LYS	Peptide
1	A	262	TYR	Sidechain
1	A	506	ARG	Sidechain

## 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	138	0
2	A	32	0	22	0	0
3	A	15	0	7	0	0
4	A	604	0	0	16	0
All	All	7430	0	6758	138	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 10.

All (138) 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:482:LYS:HE2	1:A:819:GLN:HB3	1.66	0.77
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.69	0.74
1:A:253:ASN:HB3	1:A:269:ARG:HG2	1.70	0.73
1:A:363:LYS:HE2	1:A:367:VAL:HG23	1.73	0.71
1:A:677:GLY:HA2	1:A:680:LYS:HE2	1.73	0.70
1:A:486:ILE:HG12	1:A:680:LYS:HG2	1.75	0.68
1:A:551:ARG:HG3	1:A:552:GLU:H	1.60	0.67
1:A:170:ILE:HA	1:A:174:TRP:O	1.96	0.65
1:A:568:LYS:HE2	4:A:1500:HOH:O	1.97	0.64
1:A:703:ALA:CA	1:A:807:THR:HG21	2.28	0.62
1:A:171:CYS:SG	1:A:176:MET:HG3	2.40	0.62
1:A:236:ASN:HB3	1:A:836:ALA:HB3	1.80	0.62
1:A:169:LYS:HB3	1:A:176:MET:HB2	1.83	0.61
1:A:93:ARG:HD3	1:A:126:GLU:O	2.01	0.60
1:A:486:ILE:CD1	1:A:676:THR:HB	2.33	0.58
1:A:569:ARG:HD3	4:A:1390:HOH:O	2.01	0.58
1:A:703:ALA:HA	1:A:807:THR:HG21	1.85	0.58
1:A:58:THR:O	1:A:62:HIS:HD2	1.87	0.58
1:A:386:ARG:HB3	1:A:438:ARG:HD3	1.86	0.57
1:A:351:ARG:O	1:A:355:ASP:HB2	2.05	0.57
1:A:790:LEU:HD13	1:A:797:TRP:CD1	2.41	0.56
1:A:639:ARG:HG3	1:A:639:ARG:HH11	1.70	0.56
1:A:525:VAL:O	1:A:531:ILE:HD11	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LEU:HD21	1:A:662:LEU:HB2	1.88	0.55
1:A:105:GLU:HB2	4:A:1019:HOH:O	2.07	0.54
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.89	0.54
1:A:326:PHE:CE2	1:A:357:GLU:HG2	2.43	0.53
1:A:488:PRO:O	1:A:492:LEU:HB3	2.09	0.53
1:A:112:THR:HG23	1:A:117:LEU:HB2	1.90	0.52
1:A:816:THR:O	1:A:820:TYR:HD2	1.91	0.52
1:A:96:GLN:HA	1:A:99:MET:HG3	1.92	0.51
1:A:177:GLU:HG2	1:A:611:PRO:HG3	1.90	0.51
1:A:450:HIS:HE1	4:A:1568:HOH:O	1.93	0.51
1:A:692:MET:SD	1:A:710:ILE:HD13	2.50	0.51
1:A:34:HIS:CD2	1:A:57:HIS:HB3	2.46	0.51
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.91	0.51
1:A:209:THR:HB	1:A:214:LYS:HE2	1.92	0.51
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.92	0.51
1:A:676:THR:O	1:A:680:LYS:HG3	2.11	0.51
1:A:569:ARG:HD2	1:A:608:LYS:O	2.11	0.50
1:A:389:VAL:HG13	1:A:400:LEU:HD11	1.94	0.50
1:A:550:GLU:HB3	4:A:1497:HOH:O	2.11	0.50
1:A:690:GLY:O	1:A:710:ILE:HA	2.12	0.50
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.76	0.49
1:A:596:LYS:HE2	4:A:1508:HOH:O	2.13	0.49
1:A:16:ARG:HB3	1:A:105:GLU:HB3	1.94	0.49
1:A:756:ASP:O	1:A:759:LYS:HB2	2.13	0.49
1:A:816:THR:HG22	1:A:820:TYR:HE2	1.78	0.49
1:A:199:PRO:HB2	1:A:220:VAL:HG13	1.94	0.49
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.93	0.49
1:A:251:ASP:O	1:A:255:LYS:N	2.46	0.49
1:A:698:GLU:O	1:A:702:GLU:HB2	2.13	0.49
1:A:569:ARG:O	1:A:574:LYS:HD2	2.13	0.48
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.48	0.48
1:A:423:ASP:O	1:A:427:ARG:HG3	2.14	0.48
1:A:703:ALA:HB2	1:A:807:THR:HG21	1.95	0.48
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.13	0.48
1:A:139:LEU:HD22	1:A:377:HIS:HE1	1.78	0.48
1:A:790:LEU:HB3	1:A:797:TRP:CD1	2.49	0.47
1:A:28:LYS:HD2	1:A:115:LEU:HD13	1.96	0.47
1:A:63:LEU:HD21	1:A:229:PRO:CB	2.44	0.47
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.96	0.47
1:A:716:GLU:OE2	1:A:720:ARG:HD3	2.15	0.47
1:A:591:LYS:HA	1:A:591:LYS:HD2	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:LYS:HB3	1:A:655:LYS:HE2	1.57	0.46
1:A:211:GLN:NE2	4:A:1563:HOH:O	2.49	0.46
1:A:816:THR:HG22	1:A:820:TYR:CE2	2.51	0.46
1:A:49:ARG:NH1	4:A:1579:HOH:O	2.48	0.46
1:A:99:MET:HE1	1:A:108:CYS:SG	2.56	0.46
1:A:99:MET:CE	1:A:108:CYS:SG	3.04	0.46
1:A:292:ARG:NH2	4:A:1421:HOH:O	2.49	0.45
1:A:205:ARG:HB2	1:A:216:VAL:HG12	1.98	0.45
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.98	0.45
1:A:803:ARG:O	1:A:807:THR:HB	2.17	0.45
1:A:727:ASN:OD1	1:A:729:GLN:HB3	2.17	0.45
1:A:263:ILE:O	1:A:267:LEU:HG	2.17	0.45
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.16	0.45
1:A:378:THR:OG1	1:A:380:ILE:HG13	2.17	0.45
1:A:343:SER:HB3	1:A:445:CYS:SG	2.58	0.44
1:A:490:ARG:HD2	4:A:1396:HOH:O	2.18	0.44
1:A:386:ARG:HA	1:A:439:ILE:O	2.17	0.44
1:A:480:GLN:OE1	1:A:482:LYS:NZ	2.50	0.44
1:A:751:SER:HB3	1:A:757:LEU:HD23	1.99	0.44
1:A:703:ALA:CB	1:A:807:THR:HG21	2.48	0.44
1:A:355:ASP:OD1	1:A:398:ARG:NH1	2.51	0.44
1:A:43:ARG:HA	1:A:43:ARG:HD2	1.82	0.44
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.99	0.44
1:A:437:LYS:HE2	4:A:1553:HOH:O	2.16	0.44
1:A:485:GLY:O	1:A:486:ILE:HD12	2.18	0.44
1:A:565:VAL:HG23	1:A:567:VAL:HG13	1.98	0.44
1:A:678:ASN:HD22	1:A:679:MET:H	1.65	0.44
1:A:230:VAL:HG13	4:A:1427:HOH:O	2.17	0.44
1:A:329:PHE:CD2	1:A:371:THR:HG21	2.53	0.44
1:A:392:LEU:HD12	1:A:439:ILE:HG13	1.99	0.44
1:A:487:THR:O	1:A:491:TRP:HB2	2.18	0.44
1:A:10:ARG:HG2	4:A:1324:HOH:O	2.18	0.44
1:A:235:ASN:H	1:A:235:ASN:HD22	1.66	0.44
1:A:682:MET:CE	1:A:807:THR:HG22	2.48	0.44
1:A:53:PHE:CD1	1:A:188:PRO:HG3	2.53	0.43
1:A:589:ARG:HD3	1:A:737:GLU:OE2	2.18	0.43
1:A:551:ARG:HG3	1:A:552:GLU:N	2.32	0.43
1:A:138:ARG:O	1:A:138:ARG:HD3	2.18	0.43
1:A:225:PRO:CB	1:A:242:ARG:HD2	2.49	0.43
1:A:716:GLU:HB2	4:A:1115:HOH:O	2.18	0.43
1:A:594:PRO:O	1:A:639:ARG:NH2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LEU:HD23	1:A:772:LYS:HD3	2.01	0.43
1:A:204:GLY:HA2	1:A:217:ASP:O	2.19	0.42
1:A:270:ASN:HA	1:A:273:GLU:HB2	2.00	0.42
1:A:469:LYS:NZ	1:A:473:GLU:OE2	2.52	0.42
1:A:600:PRO:HB3	1:A:639:ARG:HA	2.01	0.42
1:A:90:TYR:HE1	4:A:1598:HOH:O	2.03	0.42
1:A:363:LYS:HE2	1:A:367:VAL:CG2	2.47	0.42
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.54	0.42
1:A:538:LYS:O	1:A:542:LYS:HG3	2.20	0.42
1:A:689:ILE:HA	1:A:709:PHE:HB2	2.02	0.42
1:A:63:LEU:HD12	1:A:98:THR:HG23	2.01	0.42
1:A:557:ILE:HD12	1:A:563:PHE:CZ	2.55	0.41
1:A:790:LEU:HB3	1:A:797:TRP:NE1	2.35	0.41
1:A:93:ARG:HD3	1:A:93:ARG:HH11	1.66	0.41
1:A:335:ILE:O	1:A:335:ILE:HG13	2.21	0.41
1:A:337:LEU:HD13	1:A:373:ALA:O	2.21	0.41
1:A:652:LEU:HD12	1:A:655:LYS:HG3	2.01	0.41
1:A:361:TRP:CH2	1:A:409:ARG:HD2	2.55	0.41
1:A:805:ILE:HD13	1:A:805:ILE:HG21	1.89	0.41
1:A:66:ARG:H	1:A:66:ARG:HG2	1.59	0.41
1:A:515:LEU:HB3	1:A:809:GLY:HA2	2.03	0.41
1:A:373:ALA:HA	1:A:449:SER:HB3	2.02	0.41
1:A:487:THR:HA	1:A:488:PRO:HD2	1.77	0.41
1:A:622:LEU:O	1:A:626:ILE:HG13	2.21	0.41
1:A:329:PHE:HD2	1:A:371:THR:HG21	1.86	0.41
1:A:501:GLU:HG3	4:A:1162:HOH:O	2.20	0.40
1:A:730:GLU:O	1:A:734:ARG:HD3	2.21	0.40
1:A:19:ALA:HA	1:A:107:ALA:HA	2.03	0.40
1:A:403:ILE:HD13	1:A:403:ILE:HG21	1.92	0.40
1:A:682:MET:HE1	1:A:807:THR:HG22	2.03	0.40
1:A:549:LEU:HG	1:A:555:VAL:HG21	2.03	0.40
1:A:824:ILE:HG21	1:A:824:ILE:HD13	1.78	0.40
1:A:241:MET:HG2	1:A:243:LEU:HD13	2.03	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%)	761 (92%)	51 (6%)	19 (2%)	5 4

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	254	LEU
1	A	255	LYS
1	A	556	HIS
1	A	837	PRO
1	A	839	GLU
1	A	234	ARG
1	A	260	GLY
1	A	271	LEU
1	A	318	CYS
1	A	840	LYS
1	A	12	GLN
1	A	311	PHE
1	A	838	ASP
1	A	258	ASN
1	A	314	SER
1	A	517	GLN
1	A	809	GLY
1	A	322	VAL

### 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	722/731 (99%)	623 (86%)	99 (14%)	<b>3</b> <b>3</b>

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	25	THR
1	A	27	LEU
1	A	42	ASP
1	A	43	ARG
1	A	45	VAL
1	A	55	LEU
1	A	60	ARG
1	A	66	ARG
1	A	69	ARG
1	A	90	TYR
1	A	115	LEU
1	A	119	MET
1	A	122	LEU
1	A	138	ARG
1	A	144	LEU
1	A	191	LYS
1	A	198	LEU
1	A	211	GLN
1	A	216	VAL
1	A	234	ARG
1	A	235	ASN
1	A	242	ARG
1	A	243	LEU
1	A	251	ASP
1	A	254	LEU
1	A	255	LYS
1	A	256	ASP
1	A	257	PHE
1	A	270	ASN
1	A	292	ARG
1	A	319	ARG
1	A	320	ASP
1	A	322	VAL
1	A	335	ILE
1	A	344	LEU
1	A	360	ASP
1	A	363	LYS

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Mol	Chain	Res	Type
1	A	371	THR
1	A	380	ILE
1	A	384	LEU
1	A	391	LEU
1	A	400	LEU
1	A	429	SER
1	A	444	LEU
1	A	458	ILE
1	A	467	ILE
1	A	474	LEU
1	A	482	LYS
1	A	486	ILE
1	A	490	ARG
1	A	506	ARG
1	A	510	GLU
1	A	515	LEU
1	A	518	LEU
1	A	519	ARG
1	A	522	LEU
1	A	530	PHE
1	A	532	ARG
1	A	539	GLN
1	A	544	LYS
1	A	549	LEU
1	A	550	GLU
1	A	551	ARG
1	A	552	GLU
1	A	554	LYS
1	A	556	HIS
1	A	565	VAL
1	A	568	LYS
1	A	569	ARG
1	A	573	TYR
1	A	579	ASN
1	A	586	LEU
1	A	589	ARG
1	A	592	LYS
1	A	596	LYS
1	A	622	LEU
1	A	639	ARG
1	A	641	ARG
1	A	645	LEU

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Mol	Chain	Res	Type
1	A	649	ARG
1	A	662	LEU
1	A	666	ILE
1	A	678	ASN
1	A	687	LEU
1	A	754	GLN
1	A	756	ASP
1	A	759	LYS
1	A	764	MET
1	A	765	LEU
1	A	778	GLU
1	A	782	LYS
1	A	790	LEU
1	A	792	LYS
1	A	796	GLU
1	A	797	TRP
1	A	803	ARG
1	A	833	ARG
1	A	841	ILE

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

Mol	Chain	Res	Type
1	A	34	HIS
1	A	62	HIS
1	A	97	ASN
1	A	187	ASN
1	A	235	ASN
1	A	253	ASN
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	767	HIS

### 5.3.3 RNA ⓘ

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 oligosaccharides 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$
3	PLP	A	999	1	15,15,16	1.52	3 (20%)	21,22,23	1.17	2 (9%)
2	G1P	A	901	-	15,16,16	2.63	8 (53%)	24,24,24	2.17	7 (29%)
2	G1P	A	900	-	15,16,16	1.71	2 (13%)	24,24,24	1.85	8 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	999	1	-	1/6/6/8	0/1/1/1
2	G1P	A	901	-	-	4/7/27/27	0/1/1/1
2	G1P	A	900	-	-	2/7/27/27	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	G1P	P-O1	4.80	1.67	1.59
2	A	900	G1P	O5-C1	4.43	1.53	1.41
2	A	901	G1P	O5-C5	4.27	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	G1P	O5-C1	4.04	1.52	1.41
2	A	901	G1P	C1-C2	3.72	1.63	1.52
3	A	999	PLP	C3-C2	-3.07	1.37	1.41
2	A	900	G1P	P-O1	2.96	1.64	1.59
2	A	901	G1P	C6-C5	2.43	1.60	1.51
2	A	901	G1P	C4-C5	2.33	1.58	1.53
3	A	999	PLP	C3-C4	-2.28	1.35	1.40
3	A	999	PLP	P-O3P	2.27	1.63	1.54
2	A	901	G1P	O4-C4	2.07	1.48	1.43
2	A	901	G1P	P-O1P	2.02	1.56	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	G1P	O2-C2-C1	5.42	122.99	110.08
2	A	901	G1P	C4-C3-C2	-4.75	102.49	110.83
2	A	900	G1P	O5-C1-O1	-3.94	106.22	111.36
2	A	900	G1P	O2-C2-C1	3.36	118.07	110.08
2	A	900	G1P	O5-C1-C2	-3.29	103.61	110.37
2	A	901	G1P	O5-C1-C2	-3.21	103.77	110.37
2	A	901	G1P	C6-C5-C4	-2.75	106.26	113.02
2	A	901	G1P	O5-C5-C6	2.71	113.14	106.44
2	A	900	G1P	O3P-P-O2P	2.56	117.42	107.80
2	A	901	G1P	O3-C3-C4	2.45	116.14	110.38
2	A	901	G1P	O1-C1-C2	2.44	112.86	108.38
2	A	900	G1P	O4-C4-C3	-2.43	104.64	110.38
2	A	900	G1P	C1-O5-C5	-2.36	109.12	113.72
3	A	999	PLP	C6-C5-C4	2.25	119.94	118.10
3	A	999	PLP	C5-C6-N1	-2.19	120.27	123.83
2	A	900	G1P	P-O1-C1	2.12	129.23	123.54
2	A	900	G1P	O1-P-O1P	-2.03	102.09	109.33

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	G1P	O5-C1-O1-P
2	A	901	G1P	C2-C1-O1-P
2	A	901	G1P	O5-C1-O1-P
3	A	999	PLP	C4-C5-C5A-O4P
2	A	901	G1P	C1-O1-P-O3P
2	A	900	G1P	C1-O1-P-O3P

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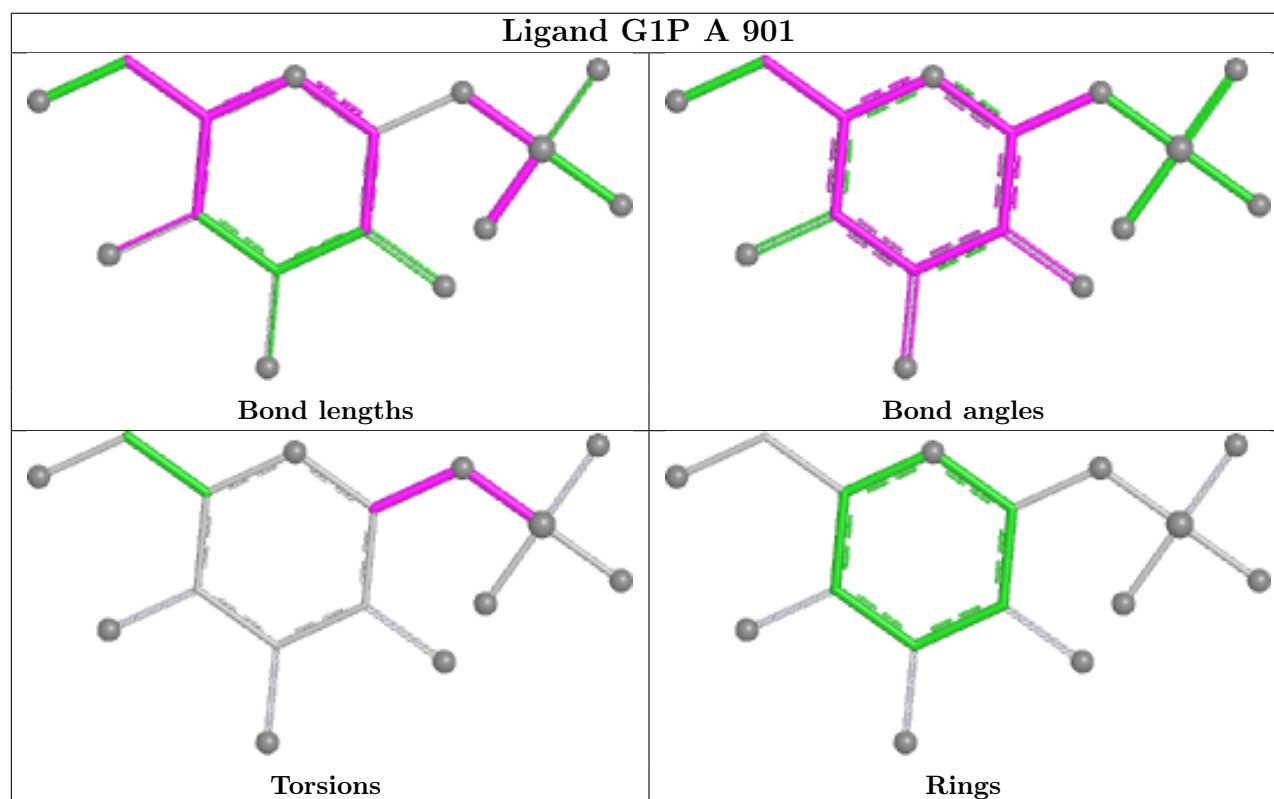
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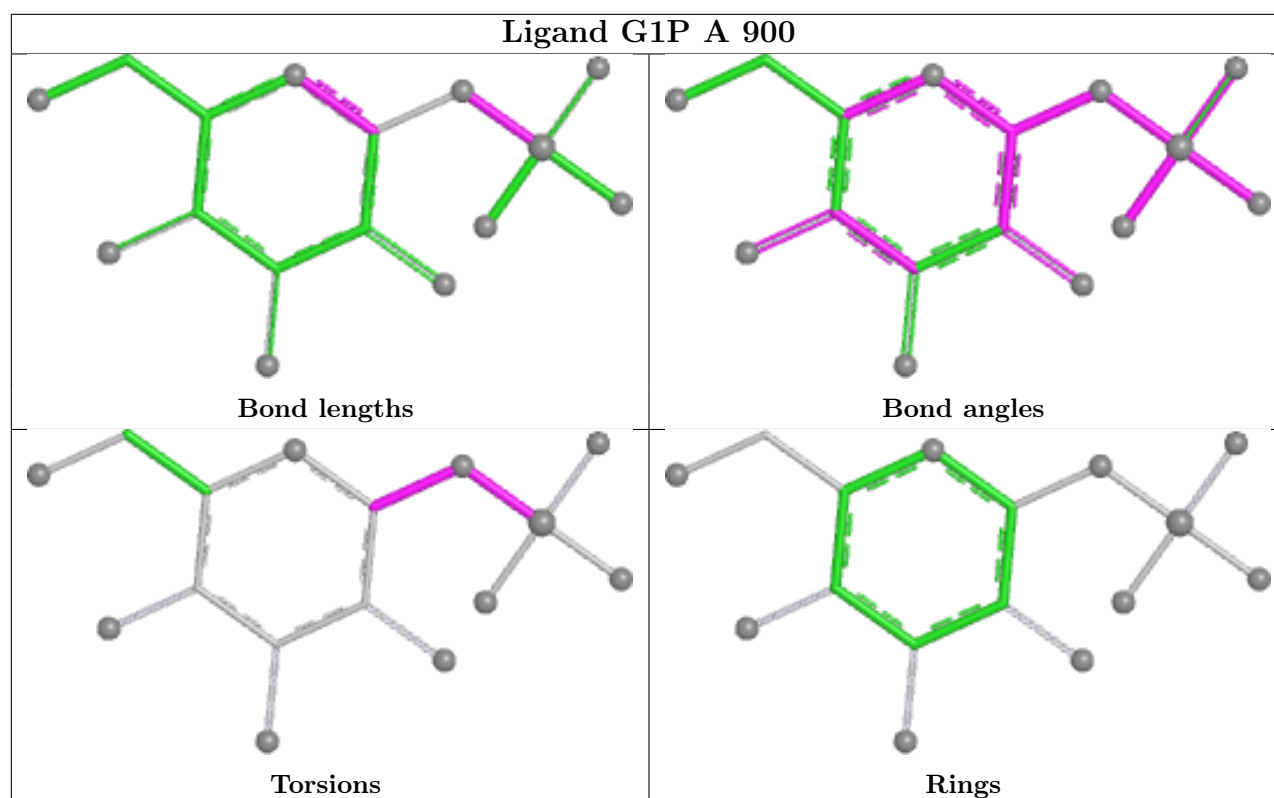
Mol	Chain	Res	Type	Atoms
2	A	901	G1P	C1-O1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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.