



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:42 AM BST

PDB ID : 6GPB  
Title : REFINED CRYSTAL STRUCTURE OF THE PHOSPHORYLASE-HEPTULOSE 2-PHOSPHATE-OLIGOSACCHARIDE-AMP COMPLEX  
Authors : Acharya, K.R.; Johnson, L.N.  
Deposited on : 1990-06-04  
Resolution : 2.86 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

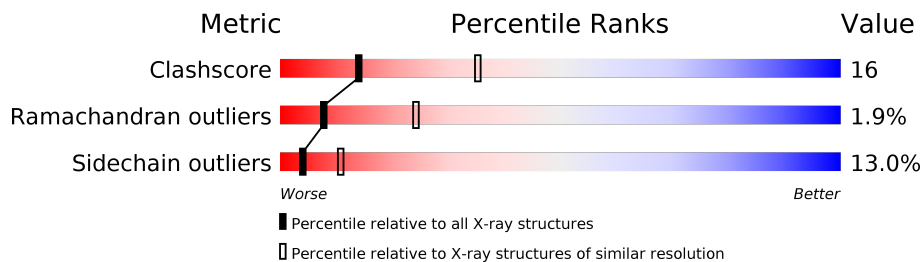
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	
2	B	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	H2P	A	998	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7469 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	0	0	0

There is a discrepancy between the modelled and reference sequences:

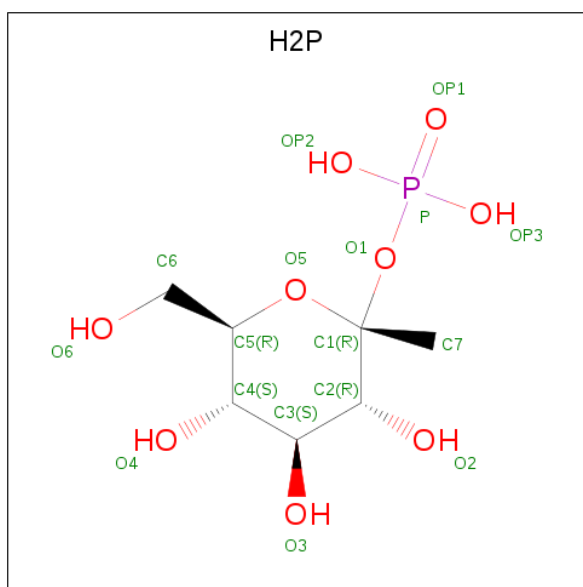
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



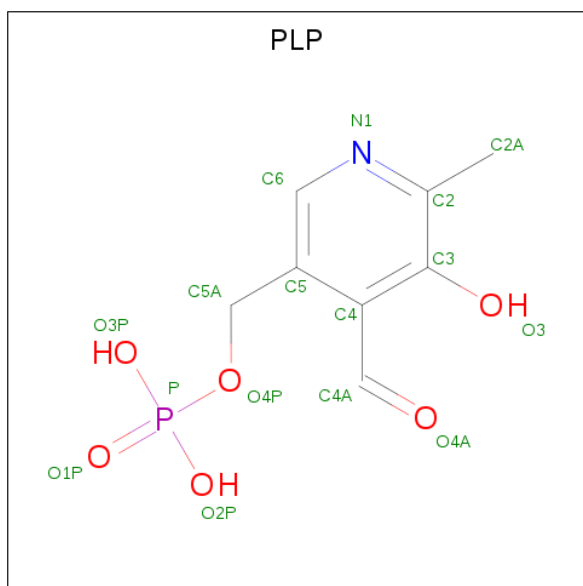
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	5	56	30	26	0	0	0

- Molecule 3 is 1-deoxy-2-O-phosphono-alpha-D-gluco-hept-2-ulopyranose (three-letter code: H2P) (formula: C<sub>7</sub>H<sub>15</sub>O<sub>9</sub>P).



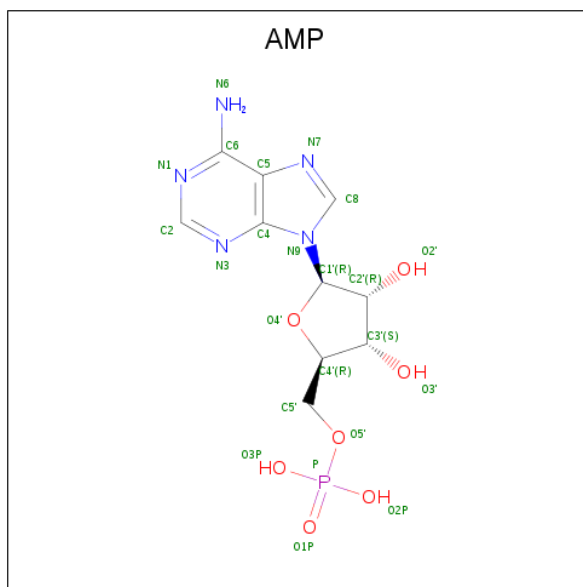
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			17	7	9	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



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

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
5	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 6 is water.

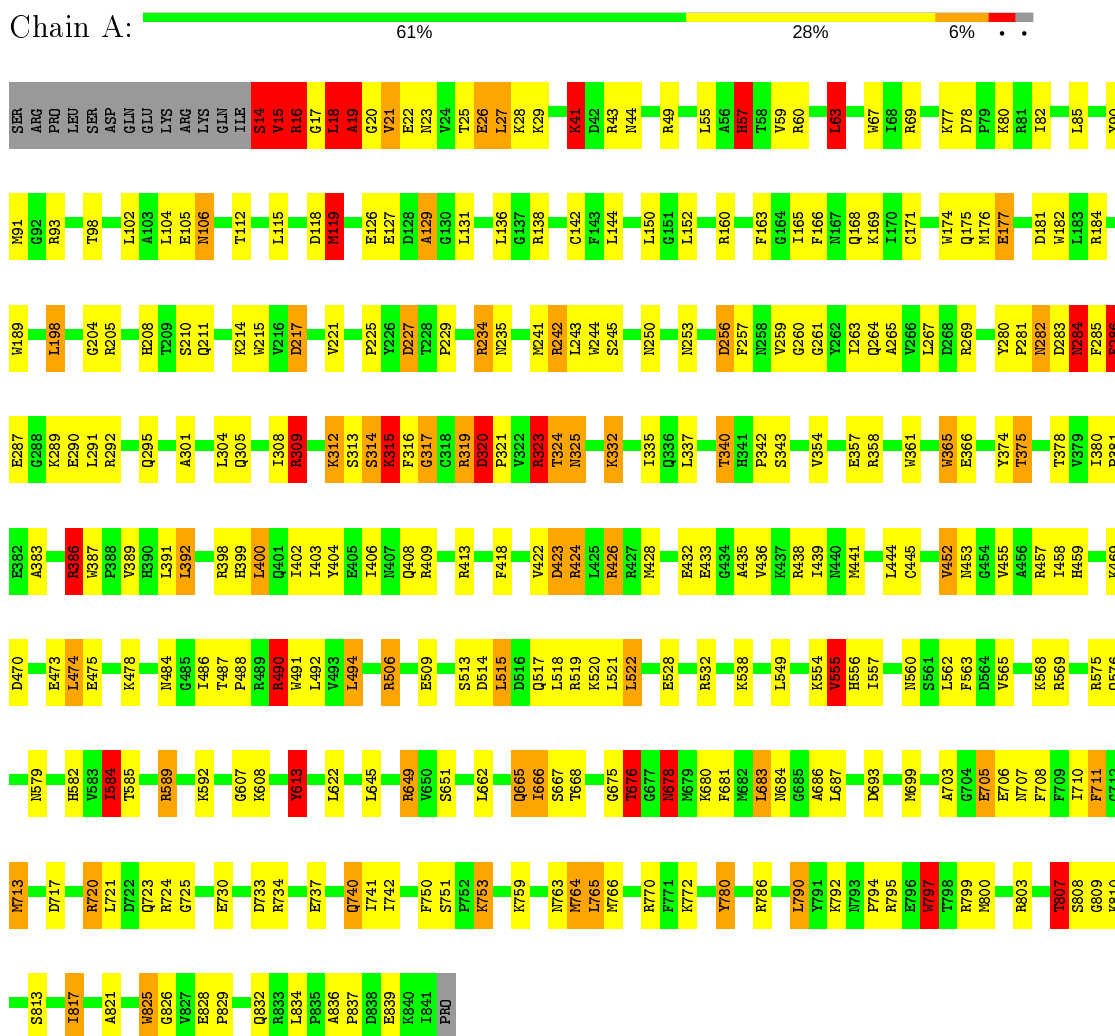
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	608	Total	O	0	0
			608	608		

### 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



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose





## 4 Data and refinement statistics

Xtrriage (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 – 2.86	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.86)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, GLC, H2P, 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	1.41	29/6880 (0.4%)	1.73	148/9313 (1.6%)

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	1	9

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	ARG	C-O	49.23	2.16	1.23
1	A	18	LEU	CG-CD1	38.26	2.93	1.51
1	A	312	LYS	CE-NZ	34.45	2.35	1.49
1	A	18	LEU	CA-C	18.30	2.00	1.52
1	A	282	ASN	C-N	-17.31	0.94	1.34
1	A	14	SER	CA-CB	15.88	1.76	1.52
1	A	317	GLY	CA-C	-15.39	1.27	1.51
1	A	19	ALA	N-CA	-14.20	1.18	1.46
1	A	15	VAL	CA-C	12.97	1.86	1.52
1	A	17	GLY	N-CA	-12.77	1.26	1.46
1	A	18	LEU	CB-CG	-12.21	1.17	1.52
1	A	286	PHE	C-N	10.91	1.59	1.34
1	A	332	LYS	CE-NZ	10.22	1.74	1.49
1	A	41	LYS	C-N	-9.07	1.13	1.34
1	A	18	LEU	CG-CD2	8.74	1.84	1.51
1	A	319	ARG	CB-CG	-8.51	1.29	1.52
1	A	15	VAL	N-CA	-7.62	1.31	1.46
1	A	16	ARG	CZ-NH2	7.54	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	PRO	C-N	-7.45	1.17	1.34
1	A	14	SER	CA-C	-7.17	1.34	1.52
1	A	284	ASN	N-CA	6.50	1.59	1.46
1	A	14	SER	N-CA	6.22	1.58	1.46
1	A	14	SER	C-O	6.04	1.34	1.23
1	A	14	SER	C-N	6.03	1.48	1.34
1	A	319	ARG	CZ-NH1	-6.00	1.25	1.33
1	A	16	ARG	CB-CG	-5.84	1.36	1.52
1	A	19	ALA	CA-CB	-5.37	1.41	1.52
1	A	15	VAL	CA-CB	5.23	1.65	1.54
1	A	20	GLY	CA-C	5.14	1.60	1.51

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LEU	C-N-CA	16.65	163.32	121.70
1	A	16	ARG	CA-CB-CG	16.62	149.96	113.40
1	A	15	VAL	CA-C-N	-15.55	82.98	117.20
1	A	19	ALA	N-CA-CB	15.31	131.53	110.10
1	A	14	SER	N-CA-CB	14.19	131.78	110.50
1	A	19	ALA	C-N-CA	12.27	148.06	122.30
1	A	16	ARG	NE-CZ-NH2	12.10	126.35	120.30
1	A	14	SER	O-C-N	-11.47	104.34	122.70
1	A	18	LEU	CA-CB-CG	-11.41	89.05	115.30
1	A	284	ASN	CA-C-O	11.19	143.61	120.10
1	A	286	PHE	O-C-N	-11.17	104.82	122.70
1	A	323	ARG	N-CA-C	-10.38	82.98	111.00
1	A	281	PRO	O-C-N	-9.97	106.75	122.70
1	A	20	GLY	CA-C-O	-9.60	103.32	120.60
1	A	18	LEU	CB-CG-CD1	-9.24	95.30	111.00
1	A	309	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	A	215	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	A	234	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	67	TRP	CD1-CG-CD2	8.53	113.13	106.30
1	A	284	ASN	CA-C-N	-8.51	98.48	117.20
1	A	257	PHE	N-CA-C	-8.41	88.29	111.00
1	A	807	THR	N-CA-CB	-8.32	94.48	110.30
1	A	387	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	A	361	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	A	174	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	A	799	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	A	649	ARG	NE-CZ-NH2	-7.71	116.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	GLY	CA-C-N	-7.58	100.52	117.20
1	A	319	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	825	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	A	825	TRP	CD1-CG-CD2	7.41	112.23	106.30
1	A	387	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	386	ARG	N-CA-C	-7.39	91.05	111.00
1	A	324	THR	N-CA-C	-7.37	91.09	111.00
1	A	215	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	A	67	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	491	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	A	317	GLY	O-C-N	7.27	134.34	122.70
1	A	189	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	A	797	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	A	409	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	365	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	A	16	ARG	CD-NE-CZ	7.12	133.57	123.60
1	A	361	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A	14	SER	CB-CA-C	-7.10	96.62	110.10
1	A	174	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	189	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	365	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	A	15	VAL	CA-CB-CG1	-7.05	100.33	110.90
1	A	259	VAL	N-CA-C	-7.01	92.07	111.00
1	A	182	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	A	244	TRP	CD1-CG-CD2	6.98	111.89	106.30
1	A	15	VAL	CB-CA-C	-6.90	98.28	111.40
1	A	491	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	A	764	MET	CA-CB-CG	6.88	125.00	113.30
1	A	683	LEU	N-CA-C	-6.85	92.50	111.00
1	A	324	THR	O-C-N	-6.79	111.83	122.70
1	A	18	LEU	CD1-CG-CD2	-6.75	90.25	110.50
1	A	78	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	490	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	15	VAL	O-C-N	6.59	133.24	122.70
1	A	182	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	A	724	ARG	CA-CB-CG	6.56	127.83	113.40
1	A	63	LEU	CA-CB-CG	6.55	130.37	115.30
1	A	205	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	332	LYS	CD-CE-NZ	-6.53	96.67	111.70
1	A	554	LYS	N-CA-C	-6.51	93.43	111.00
1	A	797	TRP	CD1-CG-CD2	6.48	111.48	106.30
1	A	324	THR	CA-C-N	6.47	131.44	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ALA	CB-CA-C	-6.41	100.49	110.10
1	A	281	PRO	CA-C-N	6.39	131.26	117.20
1	A	678	ASN	CA-CB-CG	6.37	127.42	113.40
1	A	215	TRP	N-CA-C	-6.36	93.83	111.00
1	A	17	GLY	N-CA-C	6.35	128.97	113.10
1	A	260	GLY	N-CA-C	-6.32	97.30	113.10
1	A	244	TRP	CE2-CD2-CG	-6.24	102.31	107.30
1	A	19	ALA	N-CA-C	6.21	127.76	111.00
1	A	314	SER	O-C-N	6.20	132.62	122.70
1	A	424	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	227	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	519	ARG	CA-CB-CG	6.12	126.88	113.40
1	A	119	MET	CG-SD-CE	-6.11	90.43	100.20
1	A	825	TRP	CG-CD2-CE3	6.11	139.39	133.90
1	A	386	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	261	GLY	N-CA-C	-6.06	97.96	113.10
1	A	221	VAL	N-CA-C	-6.03	94.71	111.00
1	A	292	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	A	494	LEU	O-C-N	-5.98	113.13	122.70
1	A	14	SER	CA-CB-OG	5.90	127.14	111.20
1	A	478	LYS	N-CA-CB	-5.90	99.97	110.60
1	A	584	ILE	CA-CB-CG2	-5.90	99.10	110.90
1	A	676	THR	N-CA-CB	-5.88	99.14	110.30
1	A	651	SER	CA-CB-OG	-5.82	95.49	111.20
1	A	366	GLU	CA-CB-CG	5.76	126.06	113.40
1	A	780	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	563	PHE	N-CA-C	-5.73	95.54	111.00
1	A	613	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	A	675	GLY	N-CA-C	-5.70	98.85	113.10
1	A	176	MET	N-CA-C	-5.69	95.63	111.00
1	A	770	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	562	LEU	N-CA-C	-5.64	95.77	111.00
1	A	312	LYS	CD-CE-NZ	5.63	124.65	111.70
1	A	795	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	797	TRP	CB-CG-CD1	-5.59	119.73	127.00
1	A	786	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	A	18	LEU	CB-CA-C	-5.56	99.64	110.20
1	A	57	HIS	CA-CB-CG	-5.56	104.15	113.60
1	A	834	LEU	N-CA-C	-5.55	96.02	111.00
1	A	286	PHE	CA-C-N	-5.54	105.00	117.20
1	A	215	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	436	VAL	N-CA-C	-5.53	96.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	678	ASN	CA-C-N	-5.52	105.05	117.20
1	A	693	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	584	ILE	CA-CB-CG1	5.50	121.45	111.00
1	A	129	ALA	N-CA-C	-5.43	96.34	111.00
1	A	668	THR	N-CA-C	-5.42	96.36	111.00
1	A	15	VAL	CA-C-O	5.39	131.42	120.10
1	A	67	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	575	ARG	CB-CG-CD	-5.32	97.78	111.60
1	A	184	ARG	CA-CB-CG	5.31	125.09	113.40
1	A	16	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
1	A	452	VAL	N-CA-C	-5.30	96.70	111.00
1	A	711	PHE	N-CA-C	-5.27	96.76	111.00
1	A	720	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	169	LYS	N-CA-C	-5.25	96.83	111.00
1	A	319	ARG	NH1-CZ-NH2	-5.25	113.63	119.40
1	A	491	TRP	CG-CD2-CE3	5.24	138.62	133.90
1	A	181	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	506	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	387	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	387	TRP	CG-CD2-CE3	5.17	138.56	133.90
1	A	241	MET	N-CA-C	-5.16	97.06	111.00
1	A	575	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	713	MET	CA-CB-CG	5.14	122.04	113.30
1	A	365	TRP	CG-CD2-CE3	5.14	138.52	133.90
1	A	361	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	A	725	GLY	N-CA-C	-5.12	100.31	113.10
1	A	733	ASP	O-C-N	-5.07	114.58	122.70
1	A	163	PHE	N-CA-C	-5.06	97.34	111.00
1	A	67	TRP	CB-CG-CD1	-5.05	120.44	127.00
1	A	287	GLU	N-CA-C	-5.04	97.41	111.00
1	A	404	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	A	315	LYS	N-CA-CB	-5.03	101.54	110.60
1	A	69	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	666	ILE	N-CA-CB	-5.01	99.27	110.80
1	A	282	ASN	C-N-CA	5.01	134.23	121.70
1	A	171	CYS	N-CA-C	-5.01	97.48	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	19	ALA	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	SER	Mainchain
1	A	15	VAL	Mainchain
1	A	16	ARG	Sidechain
1	A	18	LEU	Peptide
1	A	286	PHE	Mainchain
1	A	320	ASP	Peptide
1	A	57	HIS	Sidechain,Mainchain
1	A	836	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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	6652	203	1
2	B	56	0	48	11	0
3	A	17	0	13	9	0
4	A	15	0	7	2	0
5	A	46	0	22	1	0
6	A	608	0	0	27	1
All	All	7469	0	6742	212	1

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 (212) 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:14:SER:CB	1:A:14:SER:CA	1.76	1.57
1:A:18:LEU:CD2	1:A:18:LEU:CG	1.84	1.51
1:A:332:LYS:CE	1:A:332:LYS:NZ	1.74	1.46
1:A:15:VAL:CA	1:A:15:VAL:C	1.86	1.41
1:A:18:LEU:C	1:A:18:LEU:CA	2.00	1.30
1:A:18:LEU:CD2	6:A:1376:HOH:O	1.86	1.19
1:A:309:ARG:NH1	1:A:309:ARG:HG2	1.53	1.10
1:A:15:VAL:CA	1:A:16:ARG:N	2.17	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:HIS:CE1	6:A:1431:HOH:O	2.09	1.06
1:A:18:LEU:CG	6:A:1376:HOH:O	2.03	1.05
1:A:309:ARG:CG	1:A:309:ARG:HH11	1.69	1.04
1:A:309:ARG:NE	6:A:1249:HOH:O	1.85	1.02
1:A:14:SER:CB	1:A:14:SER:C	2.33	0.96
1:A:18:LEU:CD1	6:A:1376:HOH:O	2.14	0.95
1:A:14:SER:HB2	1:A:16:ARG:HG2	1.49	0.94
1:A:312:LYS:NZ	1:A:357:GLU:OE2	2.01	0.94
1:A:15:VAL:HG23	6:A:1160:HOH:O	1.66	0.94
1:A:312:LYS:NZ	1:A:312:LYS:CE	2.35	0.90
1:A:286:PHE:CD1	1:A:286:PHE:C	2.46	0.89
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.57	0.85
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.58	0.85
1:A:309:ARG:C	1:A:309:ARG:O	2.16	0.84
1:A:15:VAL:CA	1:A:16:ARG:H	1.88	0.84
1:A:426:ARG:HB2	2:B:1:GLC:O2	1.78	0.83
1:A:19:ALA:HB2	1:A:106:ASN:O	1.79	0.83
1:A:332:LYS:CD	1:A:332:LYS:NZ	2.45	0.78
2:B:1:GLC:O3	2:B:2:GLC:C1	2.31	0.78
1:A:309:ARG:CD	6:A:1249:HOH:O	2.25	0.78
2:B:2:GLC:C4	2:B:3:GLC:C1	2.62	0.77
1:A:18:LEU:CB	1:A:18:LEU:CD2	2.58	0.77
3:A:998:H2P:O2	3:A:998:H2P:OP3	2.02	0.77
1:A:290:GLU:HG3	1:A:391:LEU:HD11	1.70	0.73
1:A:309:ARG:HG2	1:A:309:ARG:HH11	0.74	0.73
1:A:283:ASP:HB3	1:A:569:ARG:HD2	1.71	0.72
1:A:569:ARG:NH1	3:A:998:H2P:P	2.64	0.70
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.75	0.68
1:A:730:GLU:O	1:A:734:ARG:HG2	1.93	0.68
1:A:314:SER:C	1:A:316:PHE:H	1.97	0.67
1:A:316:PHE:CD1	1:A:319:ARG:HD3	2.30	0.66
1:A:282:ASN:ND2	1:A:285:PHE:HD2	1.94	0.66
1:A:166:PHE:O	1:A:608:LYS:HE2	1.96	0.66
1:A:312:LYS:NZ	1:A:357:GLU:CD	2.50	0.65
1:A:16:ARG:NH1	1:A:105:GLU:OE2	2.30	0.65
1:A:312:LYS:NZ	1:A:357:GLU:OE1	2.30	0.65
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.79	0.64
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.79	0.64
1:A:315:LYS:C	1:A:317:GLY:H	1.98	0.64
1:A:569:ARG:NH1	3:A:998:H2P:OP3	2.30	0.64
1:A:18:LEU:HD21	6:A:1376:HOH:O	1.68	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:O	1:A:313:SER:N	2.31	0.63
1:A:316:PHE:CE1	1:A:319:ARG:HD3	2.34	0.63
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.34	0.63
1:A:15:VAL:CB	1:A:15:VAL:C	2.66	0.61
3:A:998:H2P:OP1	3:A:998:H2P:H3	2.01	0.61
1:A:250:ASN:HA	1:A:269:ARG:HH12	1.64	0.60
1:A:320:ASP:HB3	1:A:321:PRO:HD3	1.83	0.60
1:A:15:VAL:HA	1:A:16:ARG:H	1.66	0.60
1:A:665:GLN:HG2	1:A:678:ASN:HD22	1.66	0.60
1:A:666:ILE:HG23	1:A:711:PHE:HZ	1.67	0.60
1:A:18:LEU:O	6:A:1576:HOH:O	2.15	0.60
1:A:665:GLN:HG2	1:A:678:ASN:ND2	2.16	0.59
1:A:263:ILE:O	1:A:267:LEU:HG	2.02	0.59
1:A:584:ILE:HG21	1:A:750:PHE:CZ	2.38	0.59
1:A:713:MET:HB2	1:A:717:ASP:HB2	1.84	0.59
1:A:790:LEU:HD12	1:A:797:TRP:HD1	1.68	0.58
1:A:569:ARG:NH1	3:A:998:H2P:OP2	2.34	0.58
1:A:314:SER:O	1:A:316:PHE:N	2.27	0.58
3:A:998:H2P:HO2	3:A:998:H2P:P	2.27	0.58
1:A:584:ILE:HG21	1:A:750:PHE:HZ	1.68	0.57
1:A:378:THR:HG22	1:A:380:ILE:HB	1.87	0.57
1:A:589:ARG:HG3	1:A:589:ARG:HH11	1.69	0.57
1:A:549:LEU:HB3	1:A:555:VAL:HG11	1.86	0.56
1:A:21:VAL:HG13	1:A:22:GLU:N	2.20	0.56
1:A:424:ARG:HH21	1:A:470:ASP:HA	1.71	0.56
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.88	0.56
1:A:15:VAL:HB	1:A:509:GLU:OE2	2.04	0.56
1:A:408:GLN:HE21	2:B:4:GLC:H61	1.71	0.56
1:A:16:ARG:NH1	6:A:1419:HOH:O	2.35	0.56
1:A:49:ARG:HD2	6:A:1566:HOH:O	2.06	0.55
1:A:343:SER:HB3	1:A:445:CYS:SG	2.46	0.55
1:A:742:ILE:HG21	1:A:766:MET:HE3	1.88	0.55
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.06	0.55
1:A:250:ASN:HA	1:A:269:ARG:NH1	2.22	0.55
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.72	0.54
1:A:314:SER:C	1:A:316:PHE:N	2.60	0.54
1:A:18:LEU:CB	1:A:18:LEU:C	2.75	0.54
1:A:432:GLU:HB3	1:A:438:ARG:HG3	1.90	0.54
1:A:225:PRO:CB	1:A:242:ARG:HD2	2.33	0.54
1:A:428:MET:SD	1:A:470:ASP:HB3	2.48	0.53
1:A:392:LEU:HD13	1:A:439:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:LYS:NZ	6:A:1450:HOH:O	2.41	0.53
1:A:280:TYR:OH	1:A:291:LEU:HB3	2.08	0.53
2:B:2:GLC:O4	2:B:3:GLC:O5	2.21	0.53
3:A:998:H2P:OP1	4:A:999:PLP:O3P	2.26	0.53
1:A:320:ASP:HB3	1:A:321:PRO:CD	2.37	0.53
1:A:55:LEU:HD23	1:A:55:LEU:O	2.09	0.52
1:A:204:GLY:HA2	1:A:217:ASP:O	2.08	0.52
1:A:792:LYS:O	1:A:794:PRO:HD3	2.10	0.52
1:A:283:ASP:HB3	1:A:569:ARG:CD	2.39	0.52
1:A:569:ARG:HH11	3:A:998:H2P:P	2.30	0.52
1:A:102:LEU:HB3	1:A:104:LEU:HD23	1.91	0.52
1:A:408:GLN:HG3	2:B:4:GLC:H61	1.92	0.52
1:A:424:ARG:HH22	1:A:473:GLU:CD	2.13	0.51
1:A:375:THR:HG23	1:A:453:ASN:HD21	1.76	0.51
1:A:737:GLU:O	1:A:740:GLN:HG2	2.11	0.51
1:A:568:LYS:O	1:A:607:GLY:HA3	2.11	0.51
1:A:285:PHE:HA	1:A:383:ALA:HA	1.92	0.50
1:A:455:VAL:H	1:A:459:HIS:HD2	1.59	0.50
1:A:555:VAL:HG13	1:A:557:ILE:HG23	1.93	0.50
1:A:803:ARG:O	1:A:807:THR:HB	2.11	0.50
1:A:469:LYS:NZ	6:A:1168:HOH:O	2.45	0.50
1:A:41:LYS:NZ	6:A:1565:HOH:O	2.45	0.49
1:A:399:HIS:O	1:A:403:ILE:HG13	2.12	0.49
1:A:380:ILE:HA	1:A:381:PRO:HD3	1.67	0.49
1:A:490:ARG:HA	1:A:494:LEU:HB3	1.94	0.49
1:A:55:LEU:HD23	1:A:59:VAL:HG23	1.94	0.49
1:A:422:VAL:HG12	2:B:1:GLC:H2	1.94	0.48
1:A:707:ASN:HA	1:A:800:MET:SD	2.53	0.48
1:A:142:CYS:SG	1:A:487:THR:HG22	2.53	0.48
1:A:286:PHE:HD1	1:A:286:PHE:C	2.10	0.48
1:A:474:LEU:HD12	1:A:475:GLU:HG3	1.95	0.48
1:A:289:LYS:NZ	6:A:1557:HOH:O	2.47	0.48
1:A:678:ASN:HB3	1:A:699:MET:SD	2.54	0.48
1:A:315:LYS:N	1:A:315:LYS:HD2	2.28	0.48
1:A:208:HIS:HB2	6:A:1264:HOH:O	2.12	0.48
1:A:538:LYS:HD2	1:A:538:LYS:HA	1.68	0.47
1:A:282:ASN:HD21	1:A:285:PHE:HD2	1.62	0.47
3:A:998:H2P:H3	3:A:998:H2P:P	2.54	0.47
1:A:63:LEU:HD21	1:A:229:PRO:HG3	1.96	0.47
1:A:93:ARG:HD3	1:A:126:GLU:O	2.14	0.47
1:A:18:LEU:CD1	1:A:18:LEU:CG	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:O	1:A:406:ILE:HG12	2.15	0.47
1:A:764:MET:SD	1:A:765:LEU:HD13	2.54	0.47
1:A:301:ALA:O	1:A:305:GLN:HG3	2.14	0.47
1:A:705:GLU:HG2	1:A:710:ILE:HD12	1.97	0.47
1:A:681:PHE:HB3	1:A:686:ALA:HB3	1.97	0.47
1:A:335:ILE:HD13	1:A:335:ILE:HG21	1.51	0.46
1:A:354:VAL:O	1:A:358:ARG:HA	2.15	0.46
1:A:790:LEU:HB3	1:A:797:TRP:CD1	2.49	0.46
1:A:82:ILE:HD13	1:A:825:TRP:CE3	2.50	0.46
1:A:433:GLU:CD	2:B:3:GLC:HO2	2.18	0.46
1:A:378:THR:HG22	1:A:380:ILE:H	1.79	0.46
1:A:389:VAL:HG23	1:A:400:LEU:HD21	1.97	0.46
1:A:759:LYS:NZ	6:A:1535:HOH:O	2.47	0.46
1:A:723:GLN:HB2	6:A:1528:HOH:O	2.15	0.46
1:A:455:VAL:HB	1:A:484:ASN:ND2	2.31	0.46
1:A:579:ASN:HB2	6:A:1332:HOH:O	2.16	0.46
1:A:23:ASN:HA	1:A:26:GLU:HG2	1.96	0.45
1:A:14:SER:CB	1:A:14:SER:HA	2.18	0.45
1:A:375:THR:HG23	1:A:453:ASN:ND2	2.31	0.45
1:A:175:GLN:HG2	1:A:177:GLU:OE1	2.17	0.45
1:A:392:LEU:HB3	1:A:400:LEU:HG	1.98	0.45
1:A:532:ARG:HH11	1:A:532:ARG:HD3	1.66	0.45
1:A:488:PRO:O	1:A:492:LEU:HB3	2.17	0.45
1:A:309:ARG:NH1	1:A:309:ARG:CG	2.39	0.45
1:A:426:ARG:NH2	6:A:1182:HOH:O	2.47	0.44
1:A:332:LYS:HD3	1:A:332:LYS:NZ	2.29	0.44
1:A:676:THR:HG22	4:A:999:PLP:H5A1	1.98	0.44
1:A:93:ARG:HD2	1:A:126:GLU:HB3	1.99	0.44
1:A:21:VAL:CG1	1:A:22:GLU:N	2.80	0.44
2:B:1:GLC:H3	2:B:2:GLC:O2	2.17	0.44
1:A:55:LEU:HD13	1:A:119:MET:CE	2.48	0.43
1:A:517:GLN:OE1	1:A:520:LYS:NZ	2.52	0.43
1:A:522:LEU:HA	1:A:522:LEU:HD12	1.78	0.43
1:A:721:LEU:HD23	1:A:772:LYS:HD3	2.00	0.43
1:A:358:ARG:HD3	6:A:1597:HOH:O	2.18	0.43
1:A:418:PHE:HE2	1:A:474:LEU:HD23	1.82	0.43
1:A:568:LYS:NZ	6:A:1498:HOH:O	2.51	0.43
1:A:408:GLN:CG	2:B:4:GLC:H61	2.48	0.43
1:A:469:LYS:HD2	6:A:1167:HOH:O	2.16	0.43
1:A:765:LEU:HA	1:A:765:LEU:HD12	1.81	0.43
1:A:538:LYS:NZ	1:A:684:ASN:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ILE:HD12	1:A:817:ILE:HA	1.79	0.43
1:A:316:PHE:HD1	1:A:319:ARG:HD3	1.81	0.43
1:A:457:ARG:HG3	1:A:458:ILE:N	2.34	0.42
1:A:386:ARG:NH2	6:A:1181:HOH:O	2.52	0.42
1:A:323:ARG:HB2	1:A:324:THR:H	1.53	0.42
1:A:389:VAL:HG22	1:A:400:LEU:HD11	2.01	0.42
1:A:198:LEU:HA	1:A:198:LEU:HD12	1.82	0.42
1:A:214:LYS:NZ	6:A:1595:HOH:O	2.52	0.42
1:A:666:ILE:HD13	1:A:780:TYR:CE1	2.55	0.42
1:A:703:ALA:CA	1:A:807:THR:HG21	2.50	0.42
1:A:282:ASN:ND2	1:A:285:PHE:CD2	2.82	0.41
1:A:365:TRP:CZ3	1:A:406:ILE:HD12	2.55	0.41
1:A:253:ASN:O	1:A:265:ALA:HB1	2.19	0.41
1:A:423:ASP:O	1:A:426:ARG:HB3	2.21	0.41
1:A:319:ARG:NH2	6:A:1275:HOH:O	2.53	0.41
1:A:408:GLN:CG	2:B:4:GLC:C6	2.99	0.41
1:A:592:LYS:HD2	1:A:592:LYS:HA	1.89	0.41
1:A:374:TYR:HD2	1:A:452:VAL:HG13	1.86	0.41
1:A:400:LEU:HA	1:A:400:LEU:HD23	1.86	0.41
1:A:753:LYS:HD2	1:A:753:LYS:H	1.86	0.41
1:A:304:LEU:O	1:A:308:ILE:HG12	2.20	0.41
1:A:613:TYR:CZ	5:A:913:AMP:H3'	2.55	0.41
1:A:821:ALA:O	1:A:826:GLY:N	2.53	0.41
1:A:832:GLN:HG3	6:A:1037:HOH:O	2.21	0.41
1:A:309:ARG:O	1:A:313:SER:CB	2.69	0.41
1:A:15:VAL:N	1:A:15:VAL:C	2.57	0.41
1:A:27:LEU:HA	1:A:27:LEU:HD12	1.88	0.41
1:A:325:ASN:HA	1:A:325:ASN:HD22	1.61	0.41
1:A:585:THR:OG1	1:A:741:ILE:HD11	2.20	0.41
1:A:486:ILE:HD11	1:A:680:LYS:HE3	2.03	0.41
1:A:828:GLU:HA	1:A:829:PRO:HD2	1.79	0.41
1:A:487:THR:HA	1:A:488:PRO:HD2	1.87	0.41
1:A:742:ILE:HD13	1:A:742:ILE:HA	1.86	0.41
1:A:98:THR:O	1:A:102:LEU:HB2	2.21	0.41
1:A:340:THR:HG23	1:A:374:TYR:CE1	2.55	0.41
1:A:683:LEU:O	1:A:684:ASN:HB2	2.21	0.40
1:A:589:ARG:HH12	1:A:737:GLU:CD	2.24	0.40
1:A:93:ARG:HB3	1:A:126:GLU:OE1	2.21	0.40
1:A:25:THR:HA	1:A:28:LYS:HE2	2.01	0.40
1:A:291:LEU:O	1:A:295:GLN:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:NH1	6:A:1229:HOH:O[5_545]	1.79	0.41

### 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%)	766 (93%)	44 (5%)	16 (2%)	<b>8</b> <b>24</b>

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	284	ASN
1	A	320	ASP
1	A	323	ARG
1	A	315	LYS
1	A	435	ALA
1	A	556	HIS
1	A	837	PRO
1	A	21	VAL
1	A	118	ASP
1	A	210	SER
1	A	555	VAL
1	A	256	ASP
1	A	678	ASN
1	A	514	ASP
1	A	342	PRO

#### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	715/731 (98%)	622 (87%)	93 (13%)	4 11

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	26	GLU
1	A	27	LEU
1	A	29	LYS
1	A	41	LYS
1	A	43	ARG
1	A	44	ASN
1	A	57	HIS
1	A	60	ARG
1	A	63	LEU
1	A	77	LYS
1	A	80	LYS
1	A	85	LEU
1	A	90	TYR
1	A	106	ASN
1	A	112	THR
1	A	115	LEU
1	A	119	MET
1	A	127	GLU
1	A	131	LEU
1	A	136	LEU
1	A	138	ARG
1	A	144	LEU
1	A	152	LEU
1	A	165	ILE
1	A	177	GLU
1	A	198	LEU
1	A	211	GLN
1	A	217	ASP
1	A	234	ARG
1	A	235	ASN
1	A	242	ARG
1	A	243	LEU
1	A	245	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	256	ASP
1	A	264	GLN
1	A	284	ASN
1	A	286	PHE
1	A	309	ARG
1	A	315	LYS
1	A	320	ASP
1	A	325	ASN
1	A	337	LEU
1	A	340	THR
1	A	375	THR
1	A	386	ARG
1	A	392	LEU
1	A	398	ARG
1	A	400	LEU
1	A	413	ARG
1	A	423	ASP
1	A	426	ARG
1	A	441	MET
1	A	444	LEU
1	A	474	LEU
1	A	490	ARG
1	A	506	ARG
1	A	513	SER
1	A	515	LEU
1	A	521	LEU
1	A	522	LEU
1	A	528	GLU
1	A	555	VAL
1	A	560	ASN
1	A	565	VAL
1	A	576	GLN
1	A	584	ILE
1	A	589	ARG
1	A	613	TYR
1	A	622	LEU
1	A	645	LEU
1	A	649	ARG
1	A	662	LEU
1	A	665	GLN
1	A	667	SER
1	A	676	THR

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Mol	Chain	Res	Type
1	A	687	LEU
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	720	ARG
1	A	740	GLN
1	A	751	SER
1	A	753	LYS
1	A	763	ASN
1	A	765	LEU
1	A	790	LEU
1	A	797	TRP
1	A	807	THR
1	A	808	SER
1	A	813	SER
1	A	817	ILE
1	A	839	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	ASN
1	A	264	GLN
1	A	325	ASN
1	A	481	ASN
1	A	484	ASN
1	A	576	GLN
1	A	678	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

5 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	B	1	2	12,12,12	1.09	1 (8%)	17,17,17	1.72	2 (11%)
2	GLC	B	2	2	11,11,12	0.58	0	15,15,17	0.91	0
2	GLC	B	3	2	11,11,12	1.97	1 (9%)	15,15,17	1.59	2 (13%)
2	GLC	B	4	2	11,11,12	0.79	0	15,15,17	1.01	1 (6%)
2	GLC	B	5	2	11,11,12	0.48	0	15,15,17	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	1	2	-	2/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	0/2/19/22	0/1/1/1
2	GLC	B	4	2	-	0/2/19/22	0/1/1/1
2	GLC	B	5	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	GLC	O5-C1	-6.24	1.33	1.43
2	B	1	GLC	O1-C1	2.53	1.47	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	O1-C1-O5	5.36	126.45	110.38
2	B	3	GLC	O5-C1-C2	4.35	117.48	110.77
2	B	1	GLC	O3-C3-C2	-3.20	102.95	110.35
2	B	3	GLC	C1-O5-C5	2.54	115.63	112.19
2	B	4	GLC	C2-C3-C4	-2.27	106.96	110.89



There are no chirality outliers.

All (2) torsion outliers are listed below:

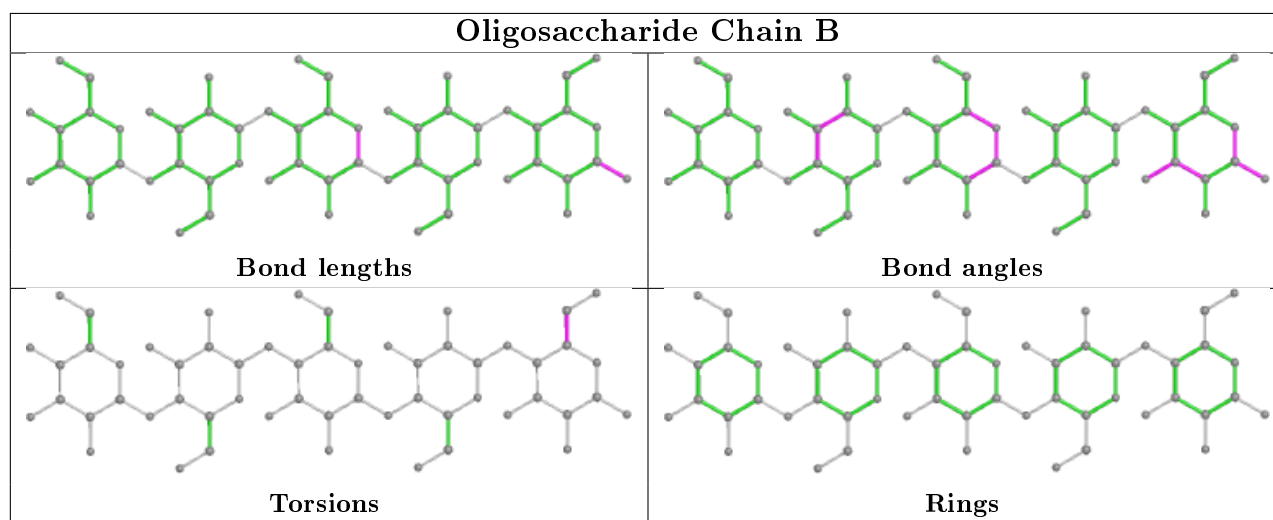
Mol	Chain	Res	Type	Atoms
2	B	1	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	GLC	4	0
2	B	3	GLC	3	0
2	B	2	GLC	4	0
2	B	1	GLC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

4 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
4	PLP	A	999	1	15,15,16	1.27	3 (20%)	20,22,23	1.01	1 (5%)
5	AMP	A	997	-	22,25,25	1.52	4 (18%)	25,38,38	1.95	9 (36%)
5	AMP	A	913	-	22,25,25	3.08	6 (27%)	25,38,38	2.45	11 (44%)
3	H2P	A	998	-	15,17,17	1.69	3 (20%)	19,27,27	1.03	1 (5%)

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
4	PLP	A	999	1	-	0/6/6/8	0/1/1/1
5	AMP	A	997	-	-	2/6/26/26	0/3/3/3
5	AMP	A	913	-	-	2/6/26/26	0/3/3/3
3	H2P	A	998	-	-	0/5/31/31	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	913	AMP	O4'-C1'	7.91	1.52	1.41
5	A	913	AMP	C2-N1	7.31	1.47	1.33
5	A	913	AMP	O4'-C4'	-5.11	1.33	1.45
5	A	913	AMP	C8-N7	4.97	1.43	1.34
5	A	913	AMP	C2-N3	4.13	1.38	1.32
5	A	997	AMP	C2-N3	3.98	1.38	1.32
3	A	998	H2P	O5-C1	3.93	1.47	1.42
5	A	997	AMP	C8-N7	2.88	1.39	1.34
3	A	998	H2P	P-OP1	2.74	1.59	1.50
5	A	997	AMP	C2-N1	2.64	1.38	1.33
4	A	999	PLP	C3-C2	-2.61	1.38	1.40
4	A	999	PLP	C5-C4	-2.40	1.37	1.40
5	A	997	AMP	C5-C4	-2.39	1.34	1.40
5	A	913	AMP	C5-C4	-2.21	1.35	1.40
3	A	998	H2P	O2-C2	2.15	1.47	1.42
4	A	999	PLP	C2-N1	2.12	1.37	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	913	AMP	O4'-C4'-C3'	5.64	116.27	105.11
5	A	913	AMP	C5-C6-N6	5.48	128.68	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	997	AMP	N3-C2-N1	-4.11	122.26	128.68
5	A	997	AMP	O3'-C3'-C4'	3.82	122.11	111.05
5	A	913	AMP	C5-C6-N1	-3.75	111.85	120.35
3	A	998	H2P	P-O1-C1	3.46	135.21	127.99
5	A	913	AMP	O2'-C2'-C1'	3.44	123.56	110.85
5	A	913	AMP	C4-C5-N7	-3.19	106.08	109.40
5	A	997	AMP	O4'-C4'-C3'	3.19	111.42	105.11
5	A	997	AMP	C1'-N9-C4	-3.06	121.27	126.64
5	A	913	AMP	N3-C2-N1	-2.86	124.21	128.68
5	A	913	AMP	C2'-C3'-C4'	-2.71	97.37	102.64
5	A	913	AMP	C3'-C2'-C1'	2.67	105.00	100.98
5	A	997	AMP	N6-C6-N1	2.62	124.01	118.57
5	A	913	AMP	O3'-C3'-C2'	2.35	119.42	111.82
5	A	997	AMP	C5'-C4'-C3'	2.27	123.70	115.18
5	A	997	AMP	O2P-P-O1P	2.27	119.56	110.68
4	A	999	PLP	C6-C5-C4	2.21	119.90	118.16
5	A	997	AMP	P-O5'-C5'	2.12	124.15	118.30
5	A	997	AMP	C2'-C3'-C4'	-2.10	98.56	102.64
5	A	913	AMP	C5'-C4'-C3'	2.06	122.90	115.18
5	A	913	AMP	O3'-C3'-C4'	2.06	117.00	111.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	997	AMP	C5'-O5'-P-O1P
5	A	913	AMP	C5'-O5'-P-O2P
5	A	913	AMP	C5'-O5'-P-O3P
5	A	997	AMP	O4'-C4'-C5'-O5'

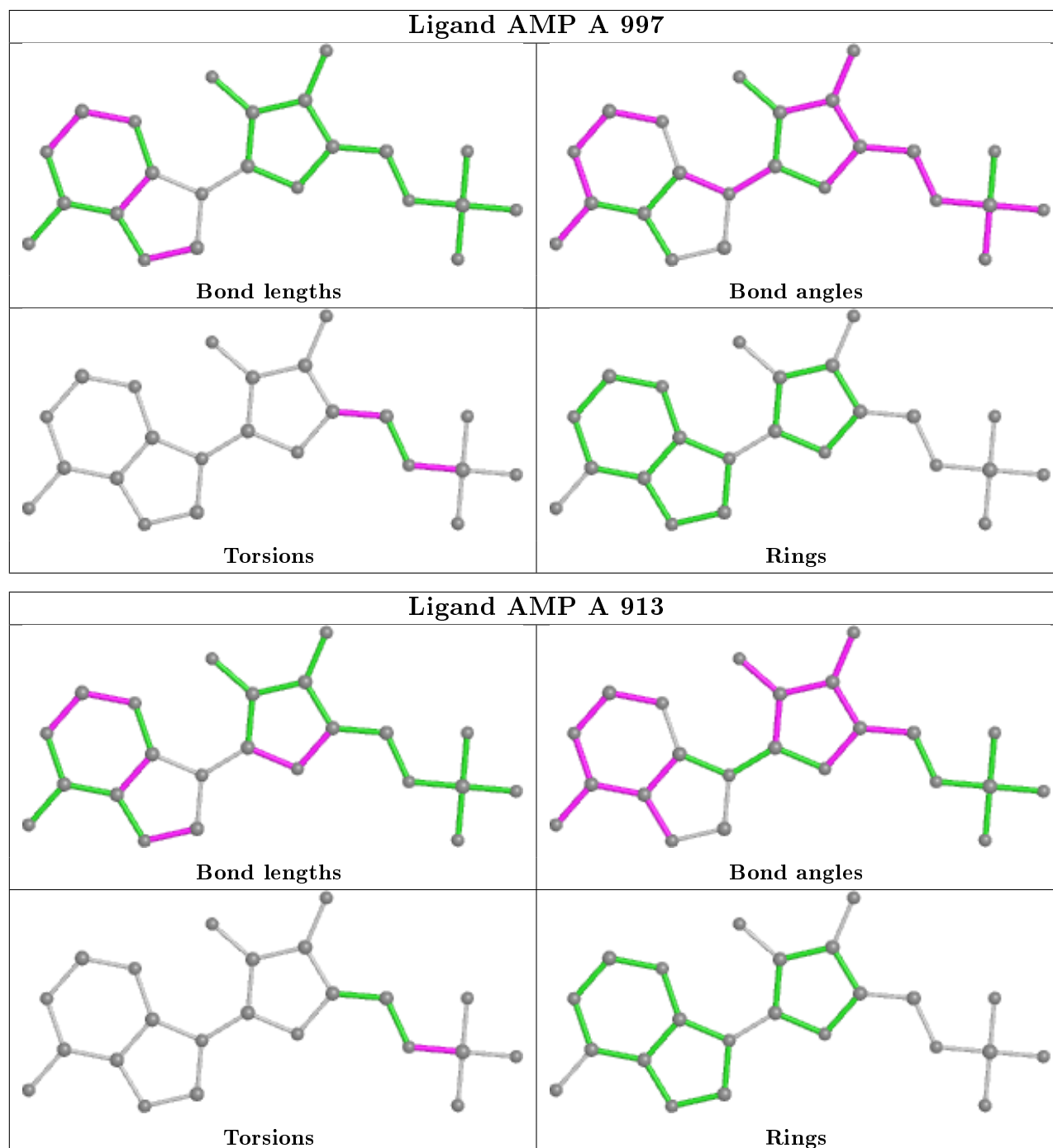
There are no ring outliers.

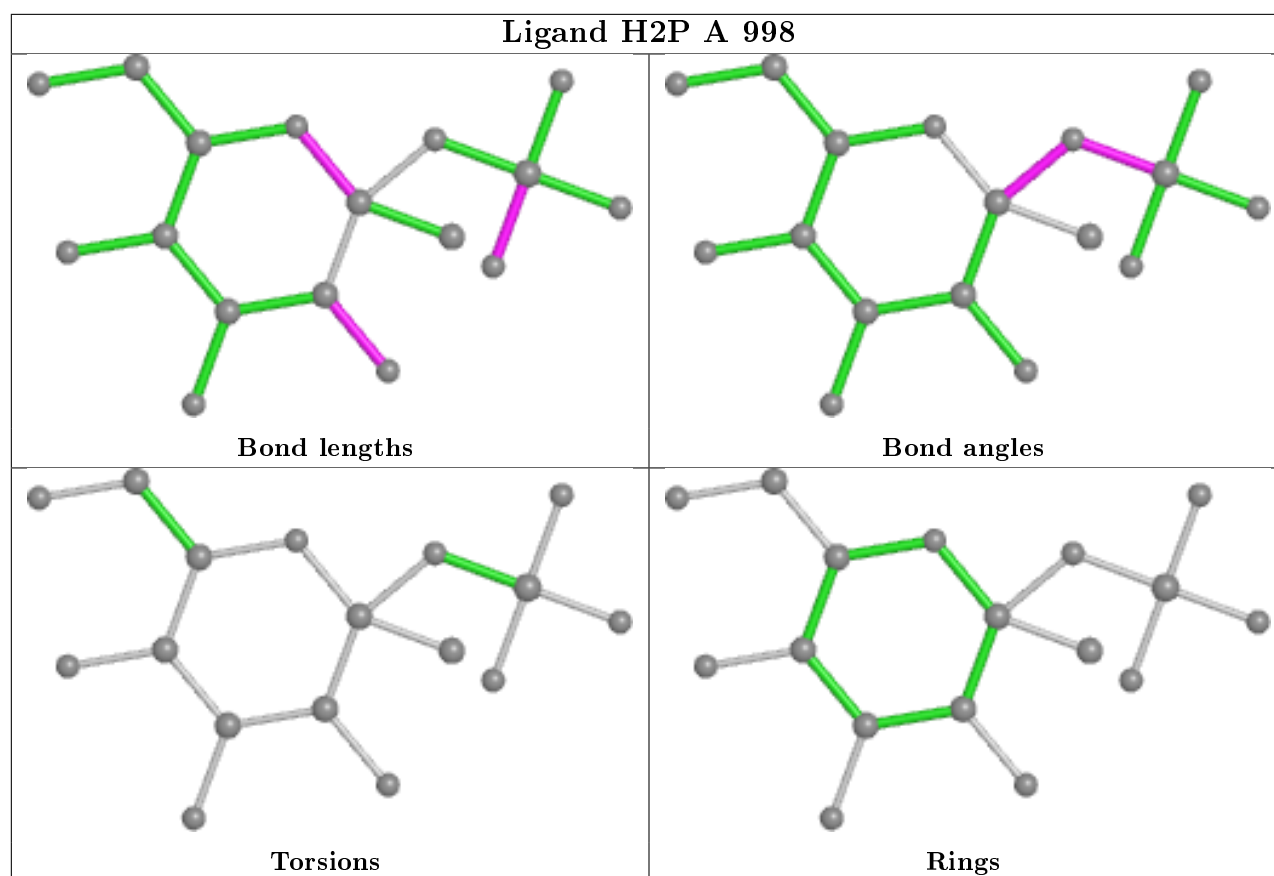
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	PLP	2	0
5	A	913	AMP	1	0
3	A	998	H2P	9	0

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 [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	281:PRO	C	282:ASN	N	1.16
1	A	41:LYS	C	42:ASP	N	1.13
1	A	282:ASN	C	283:ASP	N	0.94

## 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.