



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 AM UTC

PDB ID : 3GPB / pdb_00003gpb
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

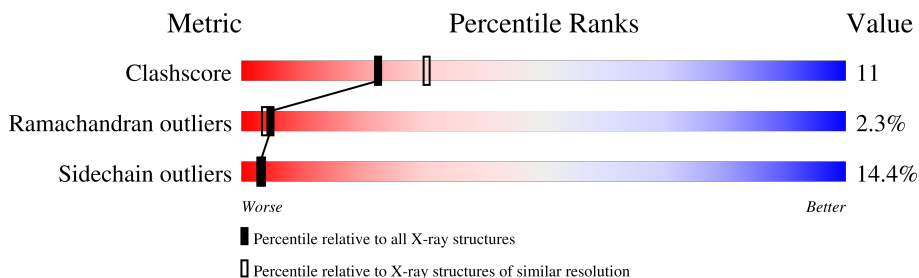
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	 52% 35% 10% . .

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.

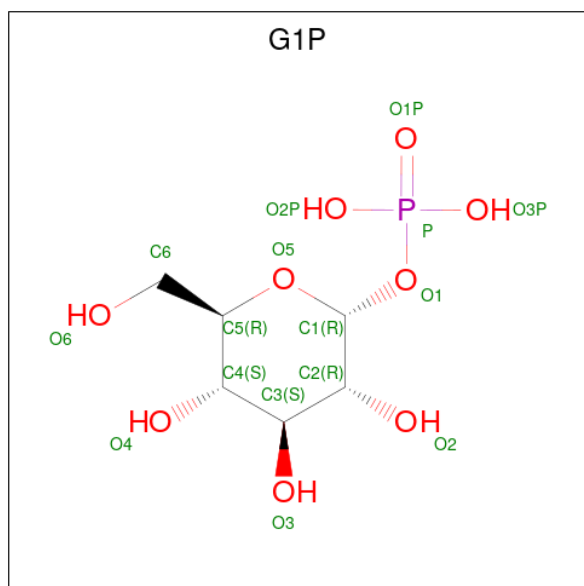
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

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:

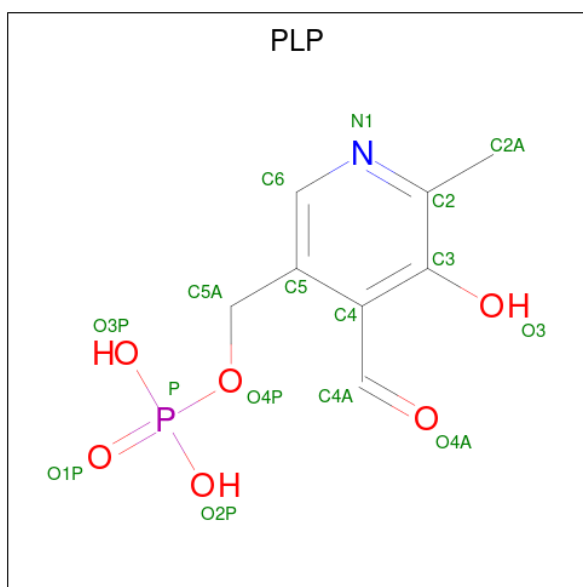
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is 1-O-phosphono-alpha-D-glucopyranose (CCD ID: 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 (CCD ID: 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.

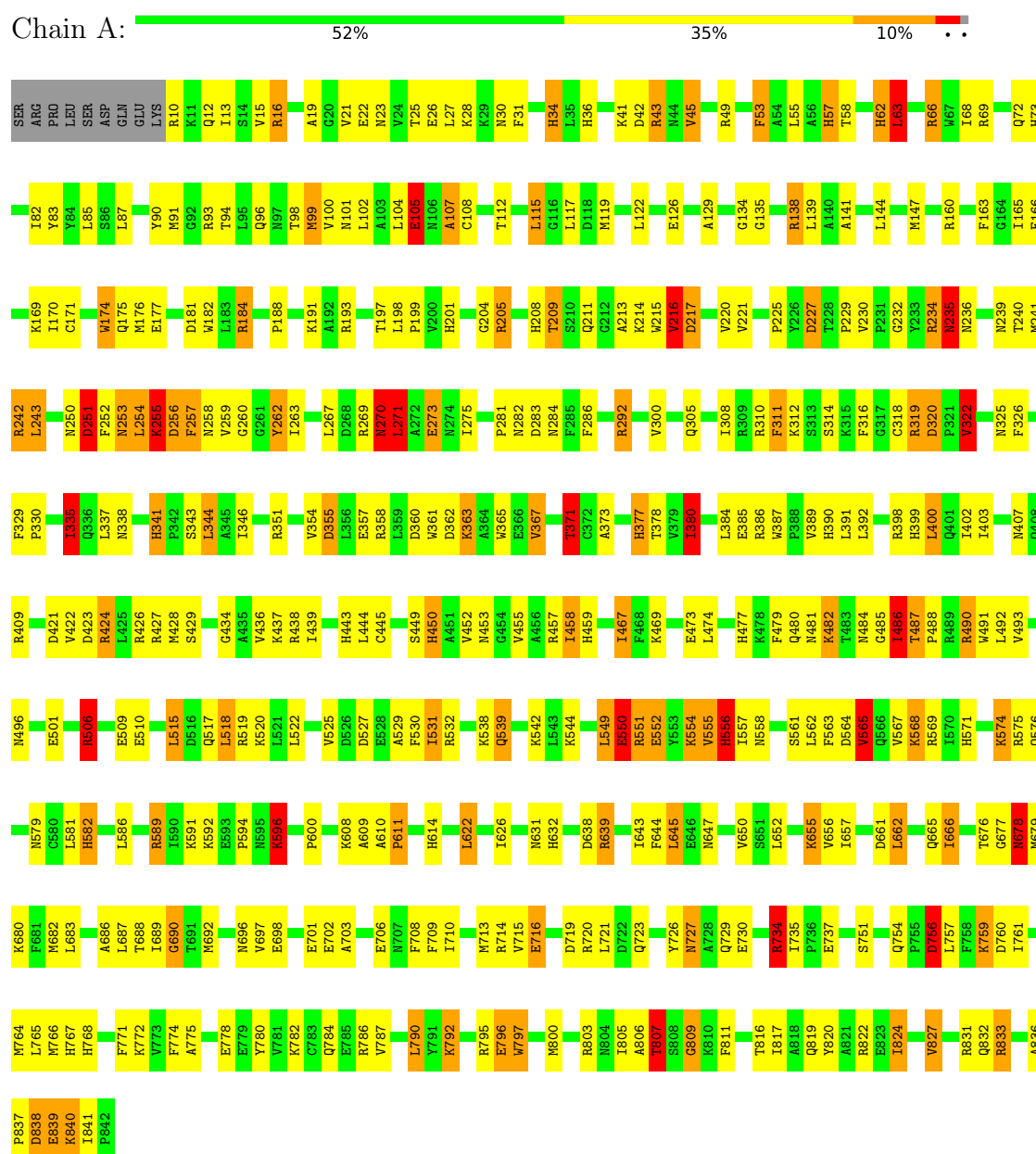
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	604	Total	O	0	0
			604	604		

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, α , β , γ	128.50Å 128.50Å 116.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7430	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: 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	1.20	40/6933 (0.6%)	2.10	256/9381 (2.7%)

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 (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	THR	CA-CB	10.19	1.70	1.53
1	A	335	ILE	CA-CB	8.89	1.65	1.54
1	A	34	HIS	CG-ND1	-8.20	1.29	1.38
1	A	36	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	632	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	787	VAL	CA-CB	6.95	1.64	1.54
1	A	450	HIS	CD2-NE2	-6.87	1.30	1.37
1	A	34	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	443	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	62	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	556	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	201	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	322	VAL	CA-CB	6.60	1.63	1.54
1	A	582	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	399	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	208	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	565	VAL	CA-CB	6.35	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	208	HIS	CG-ND1	-6.21	1.31	1.38
1	A	767	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	262	TYR	CA-CB	6.08	1.62	1.53
1	A	768	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	614	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	57	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	346	ILE	CA-CB	5.89	1.61	1.54
1	A	377	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	824	ILE	CA-CB	5.84	1.62	1.54
1	A	477	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	165	ILE	CA-CB	5.56	1.60	1.54
1	A	459	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	367	VAL	CA-CB	5.54	1.60	1.54
1	A	632	HIS	CG-ND1	-5.47	1.32	1.38
1	A	341	HIS	CG-ND1	-5.47	1.32	1.38
1	A	83	TYR	CA-CB	-5.35	1.45	1.53
1	A	390	HIS	CD2-NE2	-5.24	1.32	1.37
1	A	450	HIS	CG-ND1	-5.21	1.32	1.38
1	A	827	VAL	CA-CB	5.17	1.63	1.54
1	A	643	ILE	CA-CB	5.15	1.61	1.54
1	A	201	HIS	CG-ND1	-5.07	1.32	1.38

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ASP	CA-CB-CG	-17.49	95.11	112.60
1	A	756	ASP	CA-CB-CG	11.25	123.85	112.60
1	A	555	VAL	N-CA-C	10.84	123.07	111.58
1	A	320	ASP	CA-CB-CG	10.69	123.29	112.60
1	A	484	ASN	OD1-CG-ND2	-10.36	112.24	122.60
1	A	576	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	A	458	ILE	CB-CA-C	-10.15	98.72	112.02
1	A	255	LYS	N-CA-C	10.01	132.13	110.80
1	A	571	HIS	CB-CG-CD2	-9.94	118.28	131.20
1	A	556	HIS	CA-CB-CG	9.93	123.73	113.80
1	A	15	VAL	CA-C-O	9.82	131.18	122.63
1	A	257	PHE	N-CA-C	9.72	124.06	108.41
1	A	458	ILE	N-CA-CB	9.53	122.77	110.57
1	A	575	ARG	N-CA-C	9.52	124.13	111.28
1	A	807	THR	N-CA-CB	-9.49	96.01	110.73
1	A	719	ASP	CA-CB-CG	-9.22	103.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	ILE	N-CA-CB	-9.19	96.07	111.23
1	A	15	VAL	N-CA-C	9.17	116.02	106.21
1	A	16	ARG	N-CA-C	-8.78	102.65	112.57
1	A	216	VAL	N-CA-CB	-8.69	99.40	112.35
1	A	239	ASN	OD1-CG-ND2	-8.48	114.12	122.60
1	A	760	ASP	CA-CB-CG	8.42	121.02	112.60
1	A	338	ASN	OD1-CG-ND2	-8.39	114.21	122.60
1	A	735	ILE	CB-CA-C	-8.19	103.30	111.08
1	A	529	ALA	N-CA-C	-8.16	101.45	111.40
1	A	571	HIS	CB-CG-ND1	8.15	134.92	122.70
1	A	486	ILE	CA-CB-CG1	-8.09	96.65	110.40
1	A	227	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	270	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	A	792	LYS	CA-CB-CG	7.70	129.50	114.10
1	A	101	ASN	OD1-CG-ND2	-7.69	114.91	122.60
1	A	197	THR	N-CA-CB	-7.63	98.75	109.97
1	A	13	ILE	N-CA-C	7.63	125.21	109.34
1	A	250	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	A	141	ALA	N-CA-C	7.61	119.58	111.28
1	A	253	ASN	O-C-N	7.61	132.79	122.83
1	A	767	HIS	CB-CG-CD2	-7.39	121.60	131.20
1	A	213	ALA	N-CA-C	-7.38	98.29	110.17
1	A	486	ILE	CA-CB-CG2	7.31	122.92	110.50
1	A	175	GLN	OE1-CD-NE2	-7.31	115.29	122.60
1	A	579	ASN	CA-CB-CG	7.30	119.90	112.60
1	A	259	VAL	O-C-N	7.29	130.55	122.75
1	A	215	TRP	N-CA-C	-7.26	97.42	109.46
1	A	221	VAL	O-C-N	-7.22	115.47	122.98
1	A	428	MET	CA-CB-CG	-7.22	99.67	114.10
1	A	458	ILE	N-CA-C	-7.15	103.81	110.53
1	A	250	ASN	CB-CG-ND2	7.15	127.13	116.40
1	A	579	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	A	101	ASN	CB-CG-ND2	7.15	127.12	116.40
1	A	609	ALA	O-C-N	-7.14	115.08	123.22
1	A	253	ASN	CA-C-N	7.12	135.13	121.54
1	A	253	ASN	C-N-CA	7.12	135.13	121.54
1	A	579	ASN	CB-CG-ND2	7.06	126.98	116.40
1	A	666	ILE	CA-CB-CG2	7.05	122.49	110.50
1	A	678	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	554	LYS	N-CA-C	6.98	125.66	110.80
1	A	197	THR	CB-CA-C	6.94	121.52	109.65
1	A	311	PHE	N-CA-C	-6.91	96.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	817	ILE	CA-C-O	-6.83	113.41	120.71
1	A	284	ASN	N-CA-C	6.80	120.76	111.17
1	A	310	ARG	N-CA-CB	-6.78	102.27	110.53
1	A	300	VAL	N-CA-CB	-6.77	102.63	110.55
1	A	666	ILE	CA-CB-CG1	-6.76	98.90	110.40
1	A	407	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	A	775	ALA	N-CA-C	6.74	120.77	112.54
1	A	822	ARG	N-CA-C	6.74	118.70	111.36
1	A	838	ASP	CA-C-N	6.74	134.41	121.54
1	A	838	ASP	C-N-CA	6.74	134.41	121.54
1	A	723	GLN	N-CA-C	-6.67	103.93	111.14
1	A	174	TRP	CG-CD2-CE3	6.65	140.55	133.90
1	A	270	ASN	CB-CG-ND2	6.65	126.37	116.40
1	A	201	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	A	756	ASP	N-CA-CB	-6.59	100.12	110.46
1	A	251	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	63	LEU	N-CA-CB	-6.56	100.89	110.47
1	A	312	LYS	CA-CB-CG	-6.52	101.05	114.10
1	A	576	GLN	CG-CD-NE2	6.51	126.17	116.40
1	A	387	TRP	CG-CD2-CE3	6.50	140.41	133.90
1	A	62	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	A	734	ARG	N-CA-C	6.48	120.45	112.54
1	A	657	ILE	O-C-N	-6.48	113.71	121.10
1	A	271	LEU	N-CA-C	-6.48	97.00	110.80
1	A	481	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	678	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	358	ARG	N-CA-C	6.44	120.44	112.58
1	A	305	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	A	255	LYS	CA-CB-CG	6.40	126.89	114.10
1	A	479	PHE	O-C-N	6.39	130.49	123.27
1	A	708	PHE	O-C-N	-6.38	115.39	123.24
1	A	209	THR	CA-C-O	6.35	127.19	120.33
1	A	94	THR	O-C-N	-6.34	114.81	122.48
1	A	453	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	A	380	ILE	CA-C-N	6.27	126.18	119.28
1	A	380	ILE	C-N-CA	6.27	126.18	119.28
1	A	784	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	A	390	HIS	CA-CB-CG	6.23	120.03	113.80
1	A	316	PHE	N-CA-C	-6.23	103.79	112.45
1	A	283	ASP	N-CA-C	-6.23	99.50	109.96
1	A	217	ASP	N-CA-C	6.21	119.96	111.39
1	A	319	ARG	CA-C-O	-6.19	112.77	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	PHE	N-CA-C	6.18	118.01	111.28
1	A	325	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	A	235	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	A	239	ASN	CB-CG-ND2	6.13	125.59	116.40
1	A	216	VAL	CB-CA-C	6.12	120.12	110.52
1	A	796	GLU	CB-CG-CD	6.10	122.97	112.60
1	A	434	GLY	N-CA-C	-6.09	102.39	110.74
1	A	539	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	A	565	VAL	N-CA-C	6.08	116.87	108.12
1	A	424	ARG	CA-CB-CG	-6.07	101.96	114.10
1	A	647	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	A	362	ASP	CA-CB-CG	-6.05	106.55	112.60
1	A	644	PHE	CA-CB-CG	-6.04	107.75	113.80
1	A	735	ILE	CA-C-N	6.04	125.52	119.24
1	A	735	ILE	C-N-CA	6.04	125.52	119.24
1	A	100	VAL	N-CA-C	-6.03	104.76	110.42
1	A	556	HIS	CB-CG-CD2	-6.01	123.38	131.20
1	A	422	VAL	CA-C-O	-5.99	114.16	120.57
1	A	520	LYS	CB-CG-CD	-5.98	97.55	111.30
1	A	656	VAL	N-CA-C	5.98	116.62	110.82
1	A	325	ASN	CA-CB-CG	5.97	118.57	112.60
1	A	322	VAL	CA-C-O	5.96	128.23	120.78
1	A	57	HIS	CB-CG-CD2	-5.95	123.47	131.20
1	A	201	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	316	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	611	PRO	N-CA-C	5.92	122.57	113.75
1	A	273	GLU	CB-CG-CD	5.90	122.63	112.60
1	A	193	ARG	CA-C-N	5.89	125.76	119.28
1	A	193	ARG	C-N-CA	5.89	125.76	119.28
1	A	766	MET	N-CA-C	5.87	117.68	111.28
1	A	807	THR	CB-CA-C	5.87	120.64	110.72
1	A	831	ARG	CA-C-O	5.86	125.23	119.08
1	A	496	ASN	CA-C-N	5.85	125.71	119.28
1	A	496	ASN	C-N-CA	5.85	125.71	119.28
1	A	322	VAL	CA-CB-CG1	5.83	120.32	110.40
1	A	72	GLN	CB-CG-CD	5.83	122.51	112.60
1	A	163	PHE	CA-CB-CG	-5.81	107.99	113.80
1	A	270	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	325	ASN	CB-CG-ND2	5.81	125.11	116.40
1	A	184	ARG	CA-CB-CG	5.80	125.71	114.10
1	A	655	LYS	CA-CB-CG	5.79	125.68	114.10
1	A	833	ARG	CB-CG-CD	-5.75	98.07	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ARG	CG-CD-NE	-5.74	99.38	112.00
1	A	459	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	817	ILE	N-CA-C	-5.73	104.75	111.00
1	A	582	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	A	574	LYS	CA-C-N	5.72	130.87	122.63
1	A	574	LYS	C-N-CA	5.72	130.87	122.63
1	A	107	ALA	CA-C-O	-5.72	114.82	120.82
1	A	365	TRP	CG-CD2-CE3	5.71	139.62	133.90
1	A	696	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	105	GLU	N-CA-C	5.70	117.16	111.07
1	A	493	VAL	CB-CA-C	-5.70	104.68	111.97
1	A	490	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	45	VAL	CB-CA-C	-5.67	100.69	110.94
1	A	354	VAL	N-CA-CB	-5.63	102.41	110.52
1	A	62	HIS	CB-CG-ND1	5.63	131.14	122.70
1	A	727	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	795	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	A	344	LEU	CA-C-N	5.60	128.05	120.38
1	A	344	LEU	C-N-CA	5.60	128.05	120.38
1	A	436	VAL	N-CA-C	-5.60	99.66	108.23
1	A	761	ILE	N-CA-C	-5.59	104.90	111.00
1	A	610	ALA	CA-C-N	5.58	125.69	119.32
1	A	610	ALA	C-N-CA	5.58	125.69	119.32
1	A	811	PHE	CA-CB-CG	-5.58	108.22	113.80
1	A	338	ASN	CB-CG-ND2	5.56	124.74	116.40
1	A	678	ASN	CA-C-N	5.56	128.18	120.29
1	A	678	ASN	C-N-CA	5.56	128.18	120.29
1	A	399	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	A	310	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	A	358	ARG	CG-CD-NE	-5.53	99.83	112.00
1	A	434	GLY	O-C-N	-5.53	118.63	123.88
1	A	596	LYS	N-CA-C	-5.53	100.69	109.76
1	A	576	GLN	N-CA-C	-5.51	105.81	112.54
1	A	99	MET	CG-SD-CE	-5.51	88.78	100.90
1	A	426	ARG	CB-CG-CD	-5.48	98.69	111.30
1	A	786	ARG	N-CA-C	5.48	118.01	111.71
1	A	365	TRP	CB-CG-CD1	-5.47	118.69	126.90
1	A	134	GLY	CA-C-N	5.47	126.01	119.94
1	A	134	GLY	C-N-CA	5.47	126.01	119.94
1	A	487	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	402	ILE	N-CA-C	-5.45	105.41	110.53
1	A	666	ILE	N-CA-C	5.43	120.64	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	TRP	CE2-CD2-CG	-5.43	100.69	107.20
1	A	387	TRP	CE2-CD2-CG	-5.43	100.69	107.20
1	A	30	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	556	HIS	N-CA-C	5.42	122.34	110.80
1	A	661	ASP	N-CA-C	-5.42	105.47	112.68
1	A	564	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	135	GLY	N-CA-C	5.41	118.78	112.50
1	A	31	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	467	ILE	N-CA-C	5.41	116.18	110.72
1	A	771	PHE	CA-CB-CG	-5.40	108.40	113.80
1	A	665	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	A	527	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	839	GLU	CA-C-N	5.39	131.84	121.54
1	A	839	GLU	C-N-CA	5.39	131.84	121.54
1	A	365	TRP	CE2-CD2-CG	-5.39	100.73	107.20
1	A	716	GLU	CB-CG-CD	5.38	121.75	112.60
1	A	839	GLU	N-CA-C	-5.38	99.34	110.80
1	A	558	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	493	VAL	N-CA-C	5.38	115.58	110.42
1	A	714	ARG	N-CA-C	-5.36	102.82	110.59
1	A	209	THR	O-C-N	5.35	130.18	123.12
1	A	688	THR	CA-C-O	-5.33	114.65	120.36
1	A	23	ASN	N-CA-C	5.33	117.17	111.36
1	A	614	HIS	CA-C-O	-5.32	114.91	120.55
1	A	650	VAL	CA-C-O	-5.31	115.75	121.27
1	A	275	ILE	CA-C-O	-5.30	115.43	120.95
1	A	767	HIS	CB-CG-ND1	5.29	130.64	122.70
1	A	355	ASP	N-CA-C	5.28	118.19	111.69
1	A	193	ARG	O-C-N	-5.28	116.64	121.34
1	A	281	PRO	N-CA-C	5.28	123.35	112.47
1	A	255	LYS	N-CA-CB	-5.28	101.57	110.49
1	A	421	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	575	ARG	CB-CG-CD	-5.25	99.22	111.30
1	A	181	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	175	GLN	CG-CD-NE2	5.21	124.22	116.40
1	A	614	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	A	800	MET	CA-C-N	5.21	127.13	120.56
1	A	800	MET	C-N-CA	5.21	127.13	120.56
1	A	531	ILE	CA-C-O	-5.21	115.53	120.95
1	A	558	ASN	CA-C-N	5.20	124.91	119.82
1	A	558	ASN	C-N-CA	5.20	124.91	119.82
1	A	686	ALA	N-CA-C	-5.20	101.69	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ILE	CA-C-O	-5.18	115.30	121.05
1	A	452	VAL	N-CA-C	-5.18	100.74	108.46
1	A	282	ASN	N-CA-C	5.17	117.40	109.07
1	A	832	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	72	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	182	TRP	CA-C-O	5.17	125.94	120.10
1	A	645	LEU	CA-C-O	5.16	126.58	120.70
1	A	387	TRP	CB-CG-CD1	-5.15	119.17	126.90
1	A	506	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	A	690	GLY	N-CA-C	5.14	118.79	110.87
1	A	455	VAL	N-CA-C	5.12	117.11	112.29
1	A	205	ARG	CA-CB-CG	5.12	124.34	114.10
1	A	631	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	253	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	A	715	VAL	CA-C-O	-5.08	115.78	121.17
1	A	665	GLN	CB-CG-CD	5.08	121.24	112.60
1	A	240	THR	CA-C-O	-5.07	114.88	120.36
1	A	550	GLU	O-C-N	-5.07	116.75	122.12
1	A	166	PHE	N-CA-C	5.06	116.81	110.24
1	A	666	ILE	CB-CA-C	5.05	119.57	111.29
1	A	387	TRP	CD1-CG-CD2	5.04	114.36	106.30
1	A	85	LEU	O-C-N	-5.03	116.28	122.82
1	A	638	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	509	GLU	CA-CB-CG	5.02	124.13	114.10
1	A	840	LYS	N-CA-C	5.02	121.48	110.80
1	A	561	SER	CA-CB-OG	5.01	121.12	111.10
1	A	205	ARG	N-CA-C	-5.01	101.67	109.24
1	A	506	ARG	N-CA-C	5.01	116.59	111.03
1	A	174	TRP	CB-CG-CD1	-5.01	119.39	126.90
1	A	806	ALA	CA-C-O	5.00	125.55	119.05

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	143	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	143	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 11.

All (143) 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:682:MET:HE2	1:A:807:THR:HG22	1.89	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LYS:HA	1:A:591:LYS:HD2	1.72	0.46
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: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:251:ASP:CG	1:A:252:PHE:N	2.75	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:99:MET:HE1	1:A:108:CYS:SG	2.58	0.43
1:A:457:ARG:HH22	1:A:701:GLU:CD	2.26	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:713:MET:HE1	1:A:772:LYS:HG3	2.02	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:424:ARG:HH22	1:A:473:GLU:CD	2.27	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:63:LEU:C	1:A:63:LEU:HD23	2.45	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: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

5.3.1 Protein backbone

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

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%)	618 (86%)	104 (14%)	3 3

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	25	THR
1	A	26	GLU
1	A	27	LEU
1	A	41	LYS
1	A	42	ASP
1	A	43	ARG
1	A	45	VAL
1	A	55	LEU
1	A	63	LEU
1	A	66	ARG
1	A	68	ILE
1	A	69	ARG
1	A	102	LEU
1	A	104	LEU
1	A	105	GLU
1	A	115	LEU
1	A	119	MET
1	A	122	LEU
1	A	138	ARG
1	A	144	LEU
1	A	147	MET
1	A	191	LYS
1	A	198	LEU
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	271	LEU
1	A	292	ARG
1	A	308	ILE

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Mol	Chain	Res	Type
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
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	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	581	LEU
1	A	586	LEU
1	A	589	ARG
1	A	592	LYS
1	A	596	LYS

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Mol	Chain	Res	Type
1	A	622	LEU
1	A	639	ARG
1	A	645	LEU
1	A	662	LEU
1	A	666	ILE
1	A	678	ASN
1	A	683	LEU
1	A	687	LEU
1	A	706	GLU
1	A	734	ARG
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	807	THR
1	A	833	ARG
1	A	841	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	62	HIS
1	A	96	GLN
1	A	97	ASN
1	A	187	ASN
1	A	235	ASN
1	A	253	ASN
1	A	270	ASN
1	A	282	ASN
1	A	376	ASN
1	A	390	HIS
1	A	566	GLN
1	A	576	GLN
1	A	595	ASN

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Mol	Chain	Res	Type
1	A	614	HIS
1	A	678	ASN
1	A	767	HIS
1	A	768	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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$
2	G1P	A	900	-	15,16,16	1.71	2 (13%)	24,24,24	1.85	8 (33%)
2	G1P	A	901	-	15,16,16	2.63	8 (53%)	24,24,24	2.17	7 (29%)
3	PLP	A	999	1	15,15,16	1.52	3 (20%)	21,22,23	1.17	2 (9%)

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

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

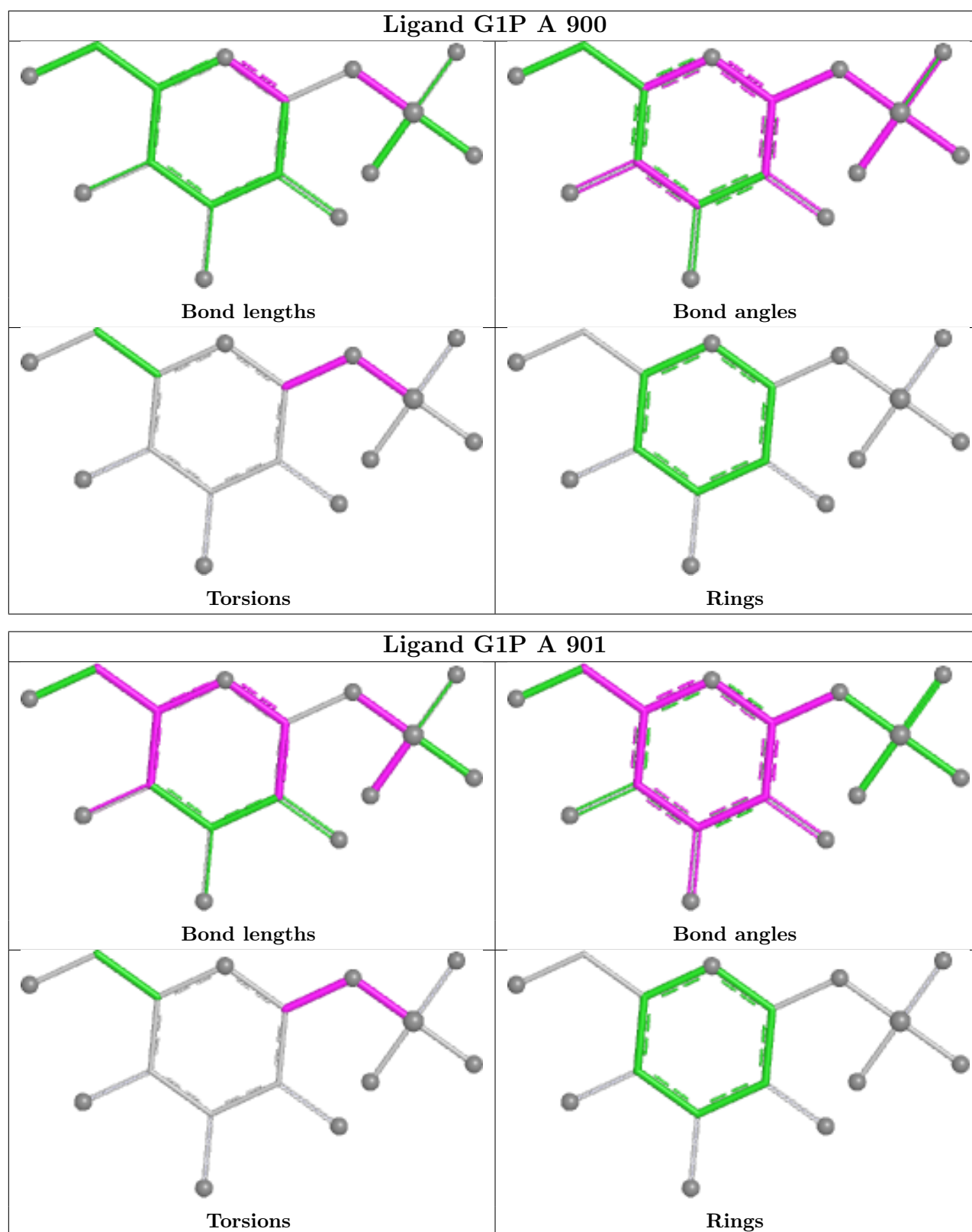
All (7) torsion outliers are listed below:

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
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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.