



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:00 AM UTC

PDB ID : 5GPB / pdb_00005gpb
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

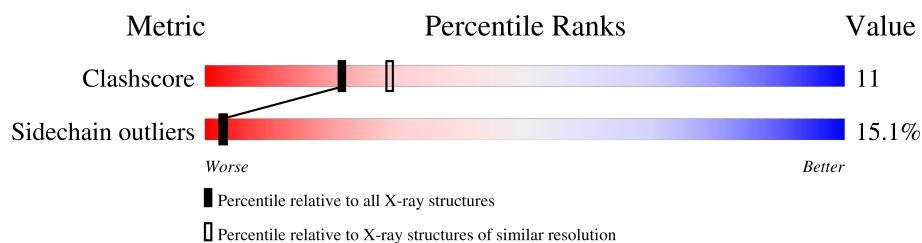
1 Overall quality at a glance

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)
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	
2	B	5	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7477 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.

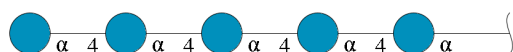
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

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

There is a discrepancy between the modelled and reference sequences:

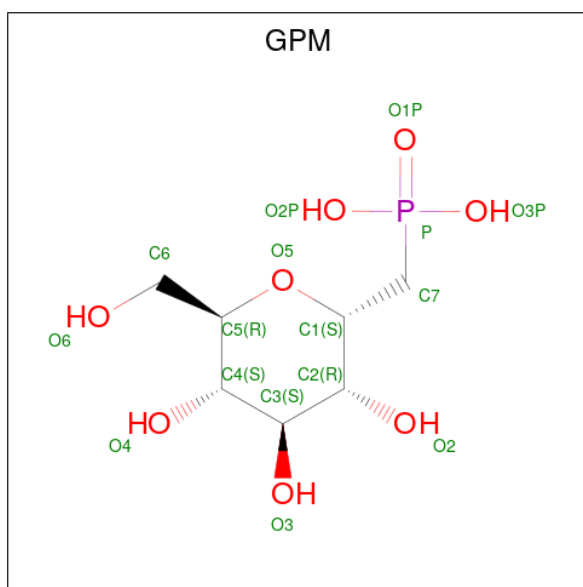
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

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



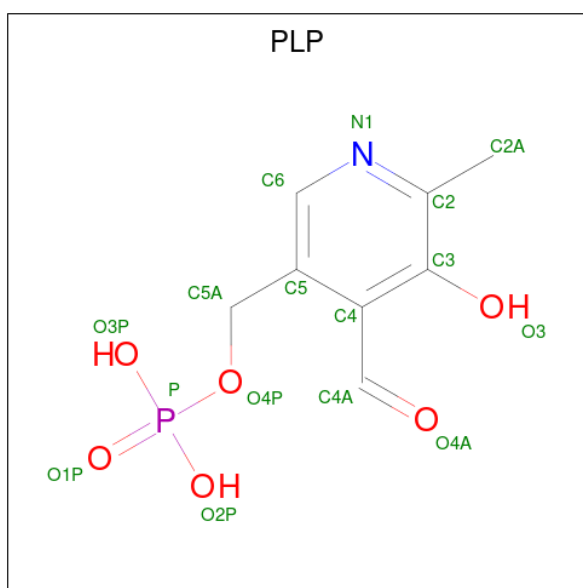
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is (1S)-1,5-anhydro-1-(phosphonomethyl)-D-glucitol (CCD ID: GPM) (formula: $C_7H_{15}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	7	8	1		
3	A	1	Total	C	O	P	0	0
			16	7	8	1		

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



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

- Molecule 5 is water.

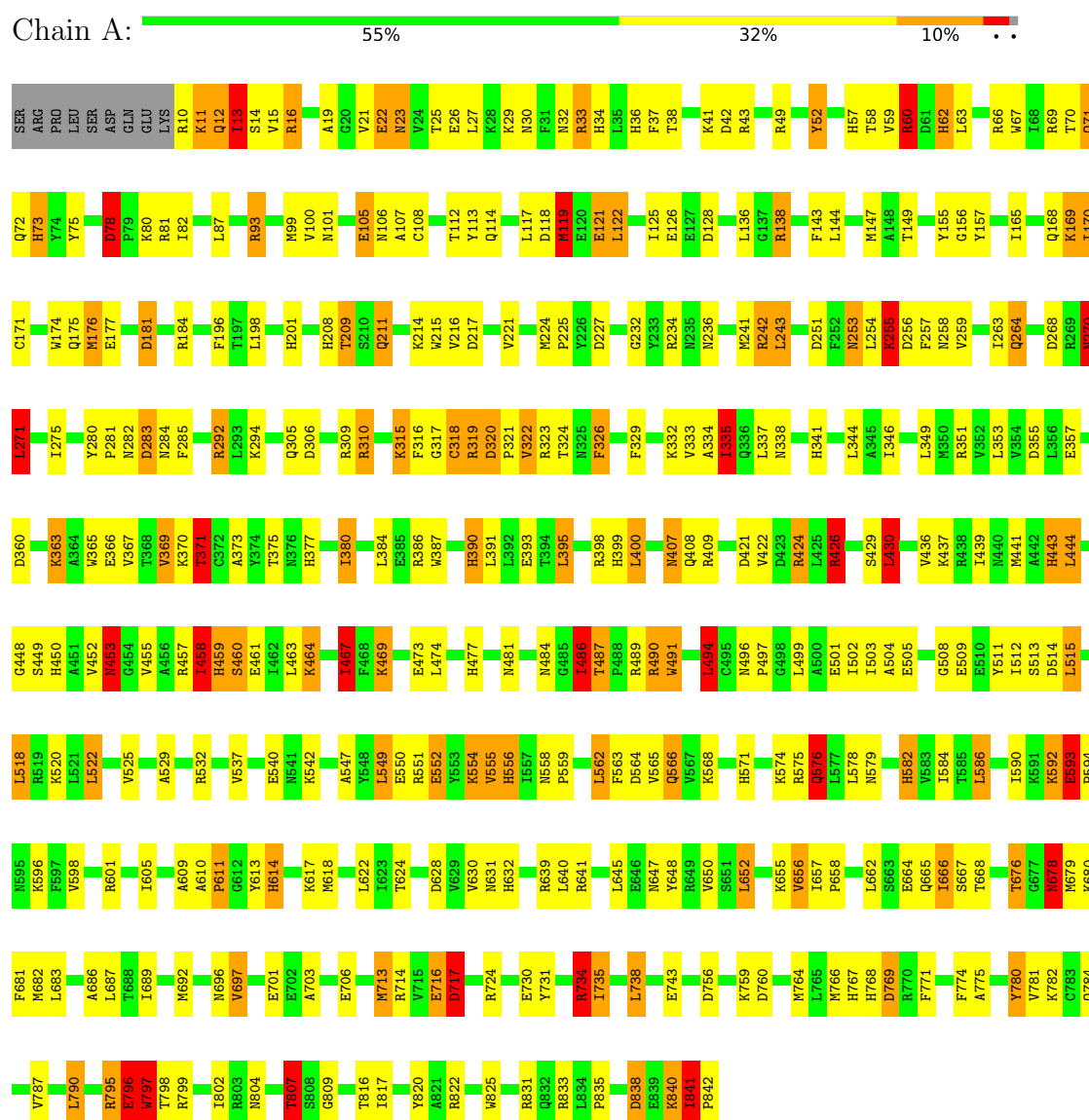
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	595	Total 595	O 595	0	0

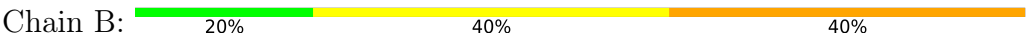
3 Residue-property plots

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}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7477	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: GPM, PLP, GLC

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	1.19	36/6933 (0.5%)	2.05	232/9381 (2.5%)

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	2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ILE	CA-CB	9.21	1.65	1.54
1	A	13	ILE	CA-CB	8.56	1.66	1.54
1	A	371	THR	CA-CB	7.97	1.66	1.53
1	A	571	HIS	CD2-NE2	-7.38	1.29	1.37
1	A	377	HIS	CG-ND1	-7.07	1.30	1.38
1	A	57	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	632	HIS	CD2-NE2	-6.99	1.30	1.37
1	A	459	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	399	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	377	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	201	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	34	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	36	HIS	CD2-NE2	-6.52	1.30	1.37
1	A	443	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	399	HIS	CG-ND1	-6.30	1.31	1.38
1	A	208	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	369	VAL	CA-CB	6.26	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	767	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	390	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	62	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	768	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	477	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	571	HIS	CG-ND1	-5.99	1.31	1.38
1	A	614	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	556	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	582	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	450	HIS	CG-ND1	-5.74	1.31	1.38
1	A	632	HIS	CG-ND1	-5.51	1.32	1.38
1	A	34	HIS	CG-ND1	-5.38	1.32	1.38
1	A	689	ILE	CA-CB	5.35	1.60	1.54
1	A	165	ILE	CA-CB	5.32	1.61	1.54
1	A	341	HIS	CD2-NE2	-5.15	1.32	1.37
1	A	100	VAL	CA-CB	5.10	1.60	1.54
1	A	841	ILE	CA-CB	5.05	1.60	1.54
1	A	341	HIS	CG-ND1	-5.00	1.32	1.38

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	838	ASP	N-CA-C	12.21	128.25	110.42
1	A	656	VAL	CB-CA-C	-11.32	97.66	111.81
1	A	258	ASN	CA-CB-CG	11.05	123.65	112.60
1	A	555	VAL	N-CA-C	10.77	131.73	109.34
1	A	255	LYS	N-CA-C	10.58	125.56	108.63
1	A	484	ASN	OD1-CG-ND2	-10.22	112.38	122.60
1	A	270	ASN	OD1-CG-ND2	-9.98	112.62	122.60
1	A	490	ARG	CB-CA-C	-9.75	94.27	110.85
1	A	23	ASN	CA-CB-CG	-9.69	102.91	112.60
1	A	841	ILE	N-CA-C	-9.68	96.93	107.77
1	A	838	ASP	O-C-N	9.15	133.36	123.11
1	A	575	ARG	N-CA-C	9.05	124.19	111.52
1	A	666	ILE	N-CA-CB	-8.82	96.68	111.23
1	A	285	PHE	CA-CB-CG	8.81	122.61	113.80
1	A	656	VAL	N-CA-C	8.73	118.77	110.30
1	A	490	ARG	N-CA-CB	8.67	123.00	110.16
1	A	686	ALA	N-CA-C	-8.64	96.74	110.14
1	A	181	ASP	CA-CB-CG	8.57	121.17	112.60
1	A	270	ASN	CB-CG-ND2	8.48	129.12	116.40
1	A	256	ASP	N-CA-C	-8.44	94.00	107.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ILE	CB-CA-C	-8.36	101.06	112.02
1	A	263	ILE	N-CA-C	-8.34	102.69	110.53
1	A	15	VAL	CA-C-O	8.33	131.19	120.78
1	A	458	ILE	N-CA-CB	8.33	121.23	110.57
1	A	121	GLU	CB-CA-C	-8.21	97.99	110.88
1	A	338	ASN	OD1-CG-ND2	-8.20	114.40	122.60
1	A	807	THR	N-CA-CB	-8.11	98.15	110.73
1	A	575	ARG	CB-CG-CD	-8.05	92.80	111.30
1	A	767	HIS	CB-CG-CD2	-7.80	121.06	131.20
1	A	780	TYR	CA-C-O	-7.78	112.89	120.90
1	A	489	ARG	CA-C-O	-7.55	113.12	120.90
1	A	734	ARG	CA-CB-CG	7.55	129.19	114.10
1	A	121	GLU	CA-CB-CG	7.54	129.18	114.10
1	A	656	VAL	N-CA-CB	7.53	118.83	110.62
1	A	469	LYS	CA-CB-CG	7.51	129.13	114.10
1	A	259	VAL	N-CA-C	7.50	124.93	109.34
1	A	453	ASN	OD1-CG-ND2	-7.34	115.25	122.60
1	A	624	THR	N-CA-C	-7.33	103.32	111.82
1	A	822	ARG	N-CA-C	7.31	119.25	111.28
1	A	78	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	365	TRP	CG-CD2-CE3	7.24	141.14	133.90
1	A	797	TRP	CG-CD2-CE3	7.11	141.01	133.90
1	A	270	ASN	CA-CB-CG	7.02	119.62	112.60
1	A	436	VAL	N-CA-C	-7.01	97.06	107.51
1	A	650	VAL	CA-C-O	-7.01	113.98	121.27
1	A	16	ARG	N-CA-C	-6.99	103.21	112.72
1	A	713	MET	CA-CB-CG	6.99	128.07	114.10
1	A	128	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	804	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	A	796	GLU	CB-CG-CD	6.88	124.30	112.60
1	A	19	ALA	N-CA-C	-6.86	98.86	108.54
1	A	421	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	255	LYS	CA-C-O	6.78	128.82	121.02
1	A	323	ARG	N-CA-C	-6.74	96.44	110.80
1	A	453	ASN	CB-CG-ND2	6.74	126.51	116.40
1	A	486	ILE	CA-CB-CG1	-6.74	98.94	110.40
1	A	611	PRO	N-CA-C	6.72	126.31	112.47
1	A	576	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	784	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	A	62	HIS	CB-CG-ND1	6.60	132.59	122.70
1	A	170	ILE	N-CA-CB	-6.59	103.20	111.31
1	A	566	GLN	OE1-CD-NE2	-6.55	116.05	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	A	121	GLU	N-CA-CB	6.53	119.47	110.01
1	A	578	LEU	N-CA-C	-6.51	104.11	111.14
1	A	601	ARG	CA-CB-CG	6.43	126.96	114.10
1	A	655	LYS	CA-C-O	-6.42	114.06	120.80
1	A	216	VAL	N-CA-CB	-6.42	103.54	112.52
1	A	264	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	A	505	GLU	N-CA-C	6.36	118.21	111.28
1	A	264	GLN	CG-CD-NE2	6.36	125.94	116.40
1	A	838	ASP	CA-CB-CG	-6.36	106.24	112.60
1	A	59	VAL	CA-C-O	-6.35	114.12	120.85
1	A	315	LYS	N-CA-C	-6.35	104.76	114.16
1	A	282	ASN	N-CA-CB	-6.30	99.58	110.17
1	A	797	TRP	CB-CG-CD1	-6.25	117.52	126.90
1	A	631	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	A	283	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	390	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	60	ARG	CA-CB-CG	6.18	126.46	114.10
1	A	610	ALA	CA-C-N	6.18	127.56	119.84
1	A	610	ALA	C-N-CA	6.18	127.56	119.84
1	A	452	VAL	N-CA-C	-6.17	99.60	108.48
1	A	258	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	A	280	TYR	CA-C-N	6.14	127.52	119.84
1	A	280	TYR	C-N-CA	6.14	127.52	119.84
1	A	682	MET	CA-C-O	-6.12	113.94	120.42
1	A	365	TRP	CB-CG-CD1	-6.11	117.73	126.90
1	A	767	HIS	CB-CG-ND1	6.11	131.87	122.70
1	A	713	MET	N-CA-CB	-6.10	100.36	109.69
1	A	208	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	735	ILE	CA-C-N	6.09	125.81	119.05
1	A	735	ILE	C-N-CA	6.09	125.81	119.05
1	A	107	ALA	N-CA-C	-6.08	104.73	111.36
1	A	321	PRO	CA-C-N	6.04	132.84	121.97
1	A	321	PRO	C-N-CA	6.04	132.84	121.97
1	A	838	ASP	CA-C-O	6.02	126.97	120.95
1	A	486	ILE	CA-CB-CG2	6.01	120.72	110.50
1	A	215	TRP	N-CA-C	-6.00	98.95	108.73
1	A	338	ASN	CB-CG-ND2	5.96	125.33	116.40
1	A	119	MET	CB-CA-C	-5.95	101.29	110.81
1	A	562	LEU	CA-CB-CG	5.93	137.07	116.30
1	A	668	THR	CA-C-O	-5.93	114.00	120.81
1	A	464	LYS	CB-CG-CD	-5.92	97.69	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	678	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	37	PHE	CA-C-O	-5.88	114.19	120.42
1	A	484	ASN	CB-CG-ND2	5.88	125.21	116.40
1	A	697	VAL	CA-C-O	-5.87	114.95	121.17
1	A	57	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	A	833	ARG	CA-CB-CG	5.86	125.82	114.10
1	A	424	ARG	NE-CZ-NH2	-5.84	113.94	119.20
1	A	817	ILE	CA-C-O	-5.84	114.56	121.05
1	A	840	LYS	CA-C-N	-5.84	116.95	123.02
1	A	840	LYS	C-N-CA	-5.84	116.95	123.02
1	A	305	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	529	ALA	N-CA-C	-5.80	104.33	111.40
1	A	556	HIS	N-CA-C	5.79	123.14	110.80
1	A	113	TYR	N-CA-C	-5.78	104.67	110.97
1	A	614	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	A	459	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	A	558	ASN	O-C-N	-5.76	116.57	121.23
1	A	563	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	93	ARG	CB-CG-CD	-5.73	98.12	111.30
1	A	576	GLN	CG-CD-NE2	5.70	124.95	116.40
1	A	652	LEU	N-CA-C	-5.69	104.69	111.69
1	A	584	ILE	CA-C-O	-5.68	115.04	120.95
1	A	630	VAL	N-CA-C	5.68	115.87	110.42
1	A	324	THR	CA-C-O	5.67	128.62	120.51
1	A	579	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	666	ILE	CB-CA-C	5.63	120.53	111.29
1	A	407	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	A	491	TRP	CG-CD2-CE3	5.59	139.49	133.90
1	A	477	HIS	CB-CG-CD2	-5.59	123.94	131.20
1	A	696	ASN	CB-CA-C	-5.58	101.19	110.68
1	A	201	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	A	21	VAL	N-CA-C	5.57	120.93	109.34
1	A	655	LYS	CA-C-N	5.57	127.66	120.70
1	A	655	LYS	C-N-CA	5.57	127.66	120.70
1	A	181	ASP	N-CA-C	-5.56	101.28	109.62
1	A	30	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	332	LYS	N-CA-C	-5.54	107.53	114.56
1	A	264	GLN	CA-C-O	-5.52	115.00	120.90
1	A	380	ILE	CA-C-N	5.51	125.13	119.56
1	A	380	ILE	C-N-CA	5.51	125.13	119.56
1	A	310	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	835	PRO	O-C-N	5.49	129.86	122.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	LEU	CA-C-N	5.48	127.57	120.44
1	A	400	LEU	C-N-CA	5.48	127.57	120.44
1	A	253	ASN	O-C-N	5.48	129.56	122.71
1	A	547	ALA	N-CA-C	-5.47	104.96	111.03
1	A	52	TYR	O-C-N	-5.46	116.44	122.07
1	A	317	GLY	N-CA-C	-5.45	100.26	113.18
1	A	666	ILE	CA-CB-CG2	5.45	119.77	110.50
1	A	840	LYS	CA-CB-CG	5.42	124.94	114.10
1	A	632	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	A	497	PRO	N-CA-C	-5.41	106.16	113.40
1	A	628	ASP	CA-C-O	-5.39	115.16	120.82
1	A	236	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	72	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	A	487	THR	CA-CB-OG1	-5.38	101.54	109.60
1	A	255	LYS	CA-CB-CG	5.37	124.83	114.10
1	A	322	VAL	CA-C-N	5.36	131.78	121.54
1	A	322	VAL	C-N-CA	5.36	131.78	121.54
1	A	657	ILE	O-C-N	-5.34	115.01	121.10
1	A	324	THR	N-CA-C	5.33	122.16	110.80
1	A	494	LEU	N-CA-CB	-5.33	101.93	110.19
1	A	605	ILE	O-C-N	-5.32	117.59	123.18
1	A	496	ASN	CA-C-N	5.31	124.64	118.85
1	A	496	ASN	C-N-CA	5.31	124.64	118.85
1	A	647	ASN	N-CA-C	5.30	118.71	111.39
1	A	676	THR	CA-C-O	5.30	124.59	118.55
1	A	334	ALA	N-CA-C	-5.30	99.81	108.76
1	A	283	ASP	N-CA-C	-5.29	101.07	109.96
1	A	769	ASP	CA-C-O	5.29	126.69	120.98
1	A	681	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	666	ILE	O-C-N	-5.27	115.98	122.57
1	A	256	ASP	N-CA-CB	5.27	119.02	110.32
1	A	768	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	A	209	THR	O-C-N	5.26	129.27	123.33
1	A	724	ARG	CA-CB-CG	5.25	124.61	114.10
1	A	114	GLN	CA-CB-CG	5.25	124.61	114.10
1	A	271	LEU	N-CA-C	-5.25	99.62	110.80
1	A	822	ARG	CB-CA-C	-5.24	102.08	110.79
1	A	63	LEU	N-CA-CB	-5.24	103.06	110.81
1	A	322	VAL	O-C-N	5.24	129.12	122.57
1	A	365	TRP	CE2-CD2-CG	-5.24	100.92	107.20
1	A	520	LYS	N-CA-C	-5.22	106.75	113.01
1	A	38	THR	CA-C-O	5.20	126.12	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	717	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	196	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	80	LYS	N-CA-C	-5.17	102.62	110.28
1	A	609	ALA	O-C-N	-5.17	117.26	123.06
1	A	22	GLU	N-CA-C	5.16	116.59	111.07
1	A	253	ASN	CA-C-N	5.16	131.39	121.54
1	A	253	ASN	C-N-CA	5.16	131.39	121.54
1	A	558	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	564	ASP	O-C-N	-5.14	116.77	122.93
1	A	426	ARG	CG-CD-NE	5.13	123.30	112.00
1	A	326	PHE	CA-C-N	5.13	127.47	120.54
1	A	326	PHE	C-N-CA	5.13	127.47	120.54
1	A	579	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	36	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	A	395	LEU	N-CA-C	5.12	118.68	112.23
1	A	12	GLN	CA-CB-CG	-5.11	103.88	114.10
1	A	387	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	A	430	LEU	N-CA-C	-5.11	107.00	113.18
1	A	696	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	501	GLU	CA-C-O	-5.10	115.02	120.42
1	A	593	GLU	CA-C-N	5.09	125.38	119.47
1	A	593	GLU	C-N-CA	5.09	125.38	119.47
1	A	467	ILE	CB-CA-C	5.09	119.01	112.14
1	A	119	MET	N-CA-CB	5.08	117.51	109.94
1	A	487	THR	CA-CB-CG2	5.07	119.12	110.50
1	A	650	VAL	O-C-N	-5.07	116.87	121.94
1	A	346	ILE	CA-C-O	-5.07	113.16	119.95
1	A	771	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	552	GLU	N-CA-C	5.06	118.22	111.75
1	A	407	ASN	CB-CG-ND2	5.05	123.98	116.40
1	A	114	GLN	CB-CA-C	-5.05	104.23	111.91
1	A	678	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	156	GLY	O-C-N	-5.04	119.62	123.35
1	A	460	SER	N-CA-C	5.04	116.77	111.28
1	A	825	TRP	N-CA-C	-5.04	106.99	113.23
1	A	477	HIS	CB-CG-ND1	5.03	130.25	122.70
1	A	71	GLN	N-CA-C	5.03	116.84	111.36
1	A	365	TRP	CG-CD1-NE1	-5.02	103.68	110.20
1	A	532	ARG	CA-CB-CG	5.02	124.13	114.10
1	A	592	LYS	CB-CG-CD	5.02	122.84	111.30
1	A	551	ARG	CA-CB-CG	5.01	124.13	114.10
1	A	655	LYS	CA-CB-CG	-5.01	104.07	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	CYS	N-CA-C	-5.01	100.12	110.80
1	A	714	ARG	N-CA-C	-5.00	103.45	110.35

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ASP	Peptide
1	A	52	TYR	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	149	0
2	B	56	0	48	3	0
3	A	32	0	26	3	0
4	A	15	0	7	0	0
5	A	595	0	0	12	0
All	All	7477	0	6810	149	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 (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.57	0.86
1:A:593:GLU:HB2	1:A:596:LYS:HD2	1.62	0.82
1:A:764:MET:HE2	1:A:769:ASP:HA	1.64	0.79
1:A:78:ASP:HB3	1:A:315:LYS:NZ	2.01	0.74
1:A:294:LYS:HE3	1:A:395:LEU:HD11	1.69	0.74
1:A:122:LEU:HA	1:A:125:ILE:HD12	1.70	0.74
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.71	0.72
1:A:81:ARG:HG3	1:A:155:TYR:HE1	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLU:O	1:A:734:ARG:HG2	1.91	0.70
1:A:841:ILE:HD13	1:A:842:PRO:HD2	1.76	0.68
1:A:554:LYS:HE2	5:A:1332:HOH:O	1.95	0.66
1:A:16:ARG:HB3	1:A:105:GLU:HB3	1.78	0.64
1:A:329:PHE:O	1:A:333:VAL:HG12	1.98	0.63
1:A:490:ARG:HA	1:A:494:LEU:HD23	1.81	0.63
1:A:143:PHE:HB3	1:A:147:MET:HE2	1.81	0.62
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.81	0.62
1:A:441:MET:HE3	1:A:444:LEU:HD12	1.83	0.61
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.84	0.60
1:A:422:VAL:HG22	2:B:1:GLC:O2	2.03	0.59
1:A:367:VAL:O	1:A:371:THR:HG23	2.04	0.58
1:A:504:ALA:HA	1:A:508:GLY:O	2.04	0.58
1:A:315:LYS:O	1:A:318:CYS:HB2	2.04	0.58
1:A:486:ILE:CD1	1:A:676:THR:HB	2.35	0.57
1:A:713:MET:HE1	1:A:775:ALA:HB3	1.87	0.56
1:A:716:GLU:HB2	5:A:1115:HOH:O	2.05	0.56
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.40	0.56
1:A:463:LEU:HA	1:A:467:ILE:HG23	1.88	0.56
1:A:713:MET:HG3	1:A:717:ASP:HB2	1.87	0.56
1:A:60:ARG:HG2	1:A:60:ARG:HH11	1.70	0.56
1:A:678:ASN:HD22	1:A:679:MET:H	1.52	0.55
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.06	0.55
1:A:756:ASP:HB2	1:A:759:LYS:HD3	1.88	0.55
1:A:58:THR:O	1:A:62:HIS:HD2	1.90	0.55
1:A:225:PRO:CB	1:A:242:ARG:HD2	2.35	0.54
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.71	0.54
1:A:316:PHE:HA	1:A:319:ARG:O	2.07	0.53
1:A:566:GLN:HG3	1:A:664:GLU:HB2	1.89	0.53
1:A:386:ARG:HA	1:A:439:ILE:O	2.09	0.53
1:A:486:ILE:HG12	1:A:680:LYS:HG2	1.92	0.52
1:A:487:THR:O	1:A:491:TRP:HB2	2.10	0.52
1:A:66:ARG:HA	1:A:69:ARG:HG2	1.93	0.51
1:A:590:ILE:O	1:A:594:PRO:HA	2.11	0.51
1:A:33:ARG:HH11	1:A:33:ARG:HG3	1.75	0.51
1:A:409:ARG:HD3	5:A:1469:HOH:O	2.10	0.51
1:A:790:LEU:HD22	1:A:797:TRP:HD1	1.76	0.51
1:A:798:THR:O	1:A:802:ILE:HG13	2.11	0.51
1:A:268:ASP:O	1:A:271:LEU:HB2	2.11	0.50
1:A:349:LEU:O	1:A:353:LEU:HG	2.11	0.50
1:A:157:TYR:OH	1:A:310:ARG:NH2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HG12	5:A:1304:HOH:O	2.11	0.50
1:A:703:ALA:HB2	1:A:807:THR:HG21	1.92	0.50
1:A:430:LEU:HD13	1:A:444:LEU:HA	1.95	0.49
1:A:430:LEU:HD22	1:A:443:HIS:HB3	1.93	0.49
1:A:81:ARG:HG3	1:A:155:TYR:CE1	2.43	0.48
1:A:549:LEU:HG	1:A:555:VAL:HG21	1.95	0.48
1:A:75:TYR:HB2	5:A:1009:HOH:O	2.13	0.48
1:A:67:TRP:O	1:A:71:GLN:HG2	2.13	0.48
1:A:574:LYS:NZ	3:A:901:GPM:O1P	2.46	0.48
1:A:614:HIS:O	1:A:618:MET:HG2	2.14	0.48
1:A:486:ILE:HG12	1:A:680:LYS:CG	2.44	0.47
1:A:461:GLU:OE2	1:A:464:LYS:NZ	2.48	0.47
1:A:366:GLU:HG2	1:A:370:LYS:HE3	1.96	0.47
1:A:441:MET:CE	1:A:444:LEU:HD12	2.43	0.47
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.80	0.47
1:A:99:MET:HE2	1:A:108:CYS:SG	2.54	0.47
1:A:369:VAL:HG12	1:A:448:GLY:HA2	1.97	0.47
1:A:329:PHE:CD2	1:A:371:THR:HG21	2.50	0.47
1:A:375:THR:HG23	1:A:453:ASN:HD21	1.78	0.47
1:A:251:ASP:O	1:A:255:LYS:N	2.48	0.46
1:A:486:ILE:HD11	1:A:676:THR:HB	1.95	0.46
1:A:16:ARG:HB2	1:A:106:ASN:CG	2.40	0.46
1:A:426:ARG:HG3	5:A:1186:HOH:O	2.13	0.46
1:A:703:ALA:CB	1:A:807:THR:HG21	2.44	0.46
1:A:99:MET:HE1	1:A:119:MET:SD	2.55	0.46
1:A:796:GLU:OE2	1:A:799:ARG:NH1	2.48	0.46
1:A:181:ASP:O	1:A:184:ARG:HG3	2.16	0.46
1:A:490:ARG:HD2	5:A:1396:HOH:O	2.14	0.46
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.97	0.46
1:A:703:ALA:HA	1:A:807:THR:HG21	1.96	0.46
1:A:93:ARG:NH1	1:A:126:GLU:O	2.49	0.45
1:A:181:ASP:O	1:A:184:ARG:NH1	2.50	0.45
1:A:32:ASN:OD1	1:A:43:ARG:NH1	2.48	0.45
1:A:11:LYS:HD2	5:A:1226:HOH:O	2.15	0.45
1:A:170:ILE:HA	1:A:174:TRP:O	2.17	0.45
1:A:169:LYS:HG3	1:A:176:MET:HB3	1.99	0.45
1:A:703:ALA:CA	1:A:807:THR:HG21	2.47	0.45
1:A:144:LEU:HD12	1:A:147:MET:HE3	1.98	0.45
1:A:319:ARG:HA	1:A:322:VAL:CG2	2.47	0.45
1:A:502:ILE:HD13	1:A:537:VAL:HG21	1.98	0.44
1:A:118:ASP:HB3	1:A:121:GLU:HG3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:SER:CB	1:A:481:ASN:HB2	2.46	0.44
1:A:112:THR:HG23	1:A:117:LEU:HB2	1.99	0.44
1:A:437:LYS:NZ	2:B:3:GLC:O2	2.50	0.44
1:A:373:ALA:HA	1:A:449:SER:HB3	2.00	0.44
1:A:360:ASP:OD1	1:A:363:LYS:HB2	2.18	0.43
1:A:257:PHE:CD1	1:A:257:PHE:N	2.86	0.43
1:A:731:TYR:O	1:A:735:ILE:HD12	2.18	0.43
1:A:795:ARG:O	1:A:799:ARG:HG3	2.18	0.43
1:A:326:PHE:CE2	1:A:357:GLU:HG2	2.54	0.43
1:A:509:GLU:HB3	1:A:512:ILE:HD12	2.01	0.43
1:A:11:LYS:HA	1:A:11:LYS:HD3	1.85	0.43
1:A:43:ARG:NH2	5:A:1002:HOH:O	2.51	0.43
1:A:678:ASN:ND2	1:A:679:MET:HG3	2.33	0.43
1:A:329:PHE:HD2	1:A:371:THR:HG21	1.84	0.43
1:A:499:LEU:O	1:A:503:ILE:HG13	2.19	0.42
1:A:241:MET:HG2	1:A:243:LEU:HD13	2.01	0.42
1:A:816:THR:HG22	1:A:820:TYR:HE1	1.84	0.42
1:A:171:CYS:HB2	1:A:176:MET:SD	2.59	0.42
1:A:221:VAL:HG11	1:A:275:ILE:HD12	2.01	0.42
1:A:550:GLU:CD	1:A:556:HIS:HB3	2.44	0.42
1:A:665:GLN:HG3	1:A:678:ASN:HB3	2.01	0.42
1:A:319:ARG:HA	1:A:322:VAL:HG23	2.01	0.42
1:A:550:GLU:OE1	1:A:554:LYS:NZ	2.52	0.42
1:A:522:LEU:O	1:A:525:VAL:HG12	2.20	0.42
1:A:101:ASN:HB3	1:A:232:GLY:O	2.20	0.42
1:A:138:ARG:HB3	5:A:1520:HOH:O	2.19	0.41
1:A:143:PHE:O	1:A:147:MET:HG3	2.20	0.41
1:A:511:TYR:HA	1:A:514:ASP:O	2.20	0.41
1:A:390:HIS:HA	1:A:393:GLU:HG2	2.02	0.41
1:A:455:VAL:H	1:A:459:HIS:HD2	1.68	0.41
1:A:550:GLU:O	1:A:554:LYS:HA	2.20	0.41
1:A:25:THR:O	1:A:29:LYS:HG3	2.20	0.41
1:A:70:THR:O	1:A:73:HIS:HB3	2.20	0.41
1:A:309:ARG:HH12	3:A:909:GPM:P	2.43	0.41
1:A:10:ARG:HH21	1:A:540:GLU:CD	2.28	0.41
1:A:437:LYS:HE2	5:A:1553:HOH:O	2.21	0.41
1:A:458:ILE:HG21	1:A:458:ILE:HD13	1.81	0.41
1:A:26:GLU:HA	1:A:29:LYS:HE2	2.02	0.41
1:A:590:ILE:HG22	1:A:598:VAL:HG11	2.03	0.41
1:A:168:GLN:HG3	1:A:175:GLN:HG3	2.03	0.41
1:A:270:ASN:O	1:A:271:LEU:HD12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HD12	1:A:337:LEU:N	2.35	0.41
1:A:457:ARG:HH22	1:A:701:GLU:CD	2.28	0.41
1:A:550:GLU:OE1	1:A:556:HIS:HB3	2.20	0.41
1:A:586:LEU:HD23	1:A:640:LEU:HD13	2.03	0.41
1:A:738:LEU:HD21	1:A:774:PHE:CE1	2.56	0.41
1:A:284:ASN:ND2	3:A:901:GPM:O3P	2.54	0.41
1:A:292:ARG:NH2	5:A:1421:HOH:O	2.53	0.40
1:A:351:ARG:O	1:A:355:ASP:HB2	2.22	0.40
1:A:613:TYR:O	1:A:617:LYS:HG2	2.20	0.40
1:A:149:THR:O	1:A:831:ARG:HD2	2.21	0.40
1:A:335:ILE:O	1:A:335:ILE:HG13	2.21	0.40
1:A:424:ARG:NH2	1:A:473:GLU:OE1	2.55	0.40
1:A:542:LYS:HE2	1:A:559:PRO:O	2.22	0.40
1:A:169:LYS:HE2	1:A:169:LYS:HB3	1.78	0.40
1:A:209:THR:O	1:A:211:GLN:N	2.55	0.40
1:A:407:ASN:HB3	2:B:3:GLC:O6	2.22	0.40
1:A:319:ARG:NE	1:A:320:ASP:H	2.20	0.40
1:A:459:HIS:O	1:A:463:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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%)	613 (85%)	109 (15%)	3 3

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	12	GLN
1	A	13	ILE
1	A	14	SER
1	A	22	GLU
1	A	23	ASN
1	A	27	LEU
1	A	33	ARG
1	A	41	LYS
1	A	42	ASP
1	A	49	ARG
1	A	60	ARG
1	A	78	ASP
1	A	82	ILE
1	A	87	LEU
1	A	105	GLU
1	A	119	MET
1	A	122	LEU
1	A	136	LEU
1	A	138	ARG
1	A	169	LYS
1	A	176	MET
1	A	177	GLU
1	A	198	LEU
1	A	211	GLN
1	A	214	LYS
1	A	217	ASP
1	A	224	MET
1	A	234	ARG
1	A	242	ARG
1	A	243	LEU
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	264	GLN
1	A	270	ASN
1	A	271	LEU
1	A	281	PRO
1	A	283	ASP
1	A	292	ARG
1	A	306	ASP
1	A	319	ARG
1	A	335	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	344	LEU
1	A	363	LYS
1	A	371	THR
1	A	380	ILE
1	A	384	LEU
1	A	391	LEU
1	A	398	ARG
1	A	400	LEU
1	A	408	GLN
1	A	426	ARG
1	A	429	SER
1	A	430	LEU
1	A	444	LEU
1	A	453	ASN
1	A	458	ILE
1	A	467	ILE
1	A	469	LYS
1	A	474	LEU
1	A	486	ILE
1	A	494	LEU
1	A	513	SER
1	A	515	LEU
1	A	518	LEU
1	A	522	LEU
1	A	549	LEU
1	A	552	GLU
1	A	554	LYS
1	A	562	LEU
1	A	565	VAL
1	A	568	LYS
1	A	576	GLN
1	A	586	LEU
1	A	592	LYS
1	A	593	GLU
1	A	611	PRO
1	A	622	LEU
1	A	639	ARG
1	A	641	ARG
1	A	645	LEU
1	A	656	VAL
1	A	658	PRO
1	A	662	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	666	ILE
1	A	667	SER
1	A	678	ASN
1	A	683	LEU
1	A	687	LEU
1	A	706	GLU
1	A	716	GLU
1	A	717	ASP
1	A	734	ARG
1	A	738	LEU
1	A	743	GLU
1	A	760	ASP
1	A	766	MET
1	A	781	VAL
1	A	782	LYS
1	A	787	VAL
1	A	790	LEU
1	A	795	ARG
1	A	796	GLU
1	A	797	TRP
1	A	807	THR
1	A	838	ASP
1	A	840	LYS
1	A	841	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	34	HIS
1	A	57	HIS
1	A	62	HIS
1	A	187	ASN
1	A	253	ASN
1	A	258	ASN
1	A	284	ASN
1	A	453	ASN
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	566	GLN
1	A	571	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	579	ASN
1	A	678	ASN
1	A	768	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	1.75	3 (25%)	17,17,17	1.63	4 (23%)
2	GLC	B	2	2	11,11,12	0.87	0	15,15,17	0.71	0
2	GLC	B	3	2	11,11,12	0.68	0	15,15,17	1.81	2 (13%)
2	GLC	B	4	2	11,11,12	1.13	1 (9%)	15,15,17	1.43	3 (20%)
2	GLC	B	5	2	11,11,12	0.95	0	15,15,17	1.31	2 (13%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLC	C4-C5	3.62	1.60	1.53
2	B	1	GLC	C4-C3	2.91	1.59	1.52
2	B	4	GLC	C4-C5	2.60	1.58	1.53
2	B	1	GLC	O4-C4	2.23	1.48	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	GLC	C1-O5-C5	4.68	118.45	112.19
2	B	1	GLC	C1-O5-C5	4.35	122.07	113.65
2	B	3	GLC	O4-C4-C3	-3.30	102.59	110.38
2	B	5	GLC	C1-O5-C5	3.27	116.57	112.19
2	B	4	GLC	C1-O5-C5	3.11	116.35	112.19
2	B	5	GLC	O4-C4-C3	-2.59	104.26	110.38
2	B	4	GLC	C6-C5-C4	2.50	119.16	113.02
2	B	1	GLC	O3-C3-C2	-2.41	104.70	110.38
2	B	4	GLC	O4-C4-C3	-2.40	104.73	110.38
2	B	1	GLC	O5-C1-C2	2.27	114.29	110.30
2	B	1	GLC	O2-C2-C3	-2.01	105.64	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

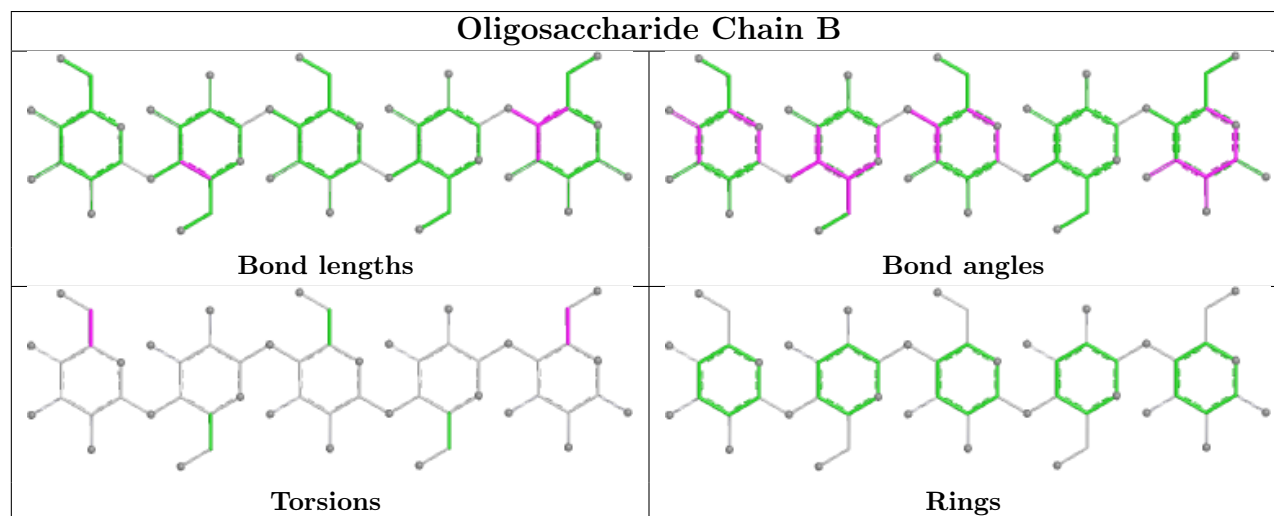
Mol	Chain	Res	Type	Atoms
2	B	1	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6
2	B	5	GLC	C4-C5-C6-O6
2	B	5	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	GLC	2	0
2	B	1	GLC	1	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](#)

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	GPM	A	909	-	16,16,16	1.97	3 (18%)	19,24,24	1.28	2 (10%)
3	GPM	A	901	-	16,16,16	1.34	1 (6%)	19,24,24	1.75	3 (15%)
4	PLP	A	999	1	15,15,16	1.53	3 (20%)	21,22,23	1.27	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GPM	A	909	-	-	1/7/27/27	0/1/1/1
3	GPM	A	901	-	-	1/7/27/27	0/1/1/1
4	PLP	A	999	1	-	3/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	909	GPM	P-C7	5.13	1.84	1.79
3	A	909	GPM	C4-C5	3.79	1.61	1.53
4	A	999	PLP	C3-C2	-3.41	1.37	1.41
3	A	901	GPM	C2-C1	3.33	1.60	1.53
4	A	999	PLP	P-O2P	-2.44	1.45	1.54
3	A	909	GPM	C7-C1	2.41	1.59	1.53
4	A	999	PLP	C2A-C2	-2.11	1.47	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	GPM	O1P-P-C7	-4.22	103.66	111.56
3	A	901	GPM	O2-C2-C1	3.51	117.98	109.32
3	A	909	GPM	O2-C2-C1	2.82	116.27	109.32
4	A	999	PLP	O4P-C5A-C5	2.67	114.37	109.36
3	A	901	GPM	O3P-P-O2P	2.56	115.25	107.96
4	A	999	PLP	O2P-P-O1P	2.50	120.56	110.83
4	A	999	PLP	C5-C6-N1	-2.29	120.10	123.83
3	A	909	GPM	O4-C4-C3	-2.12	105.39	110.38
4	A	999	PLP	C6-C5-C4	2.11	119.83	118.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

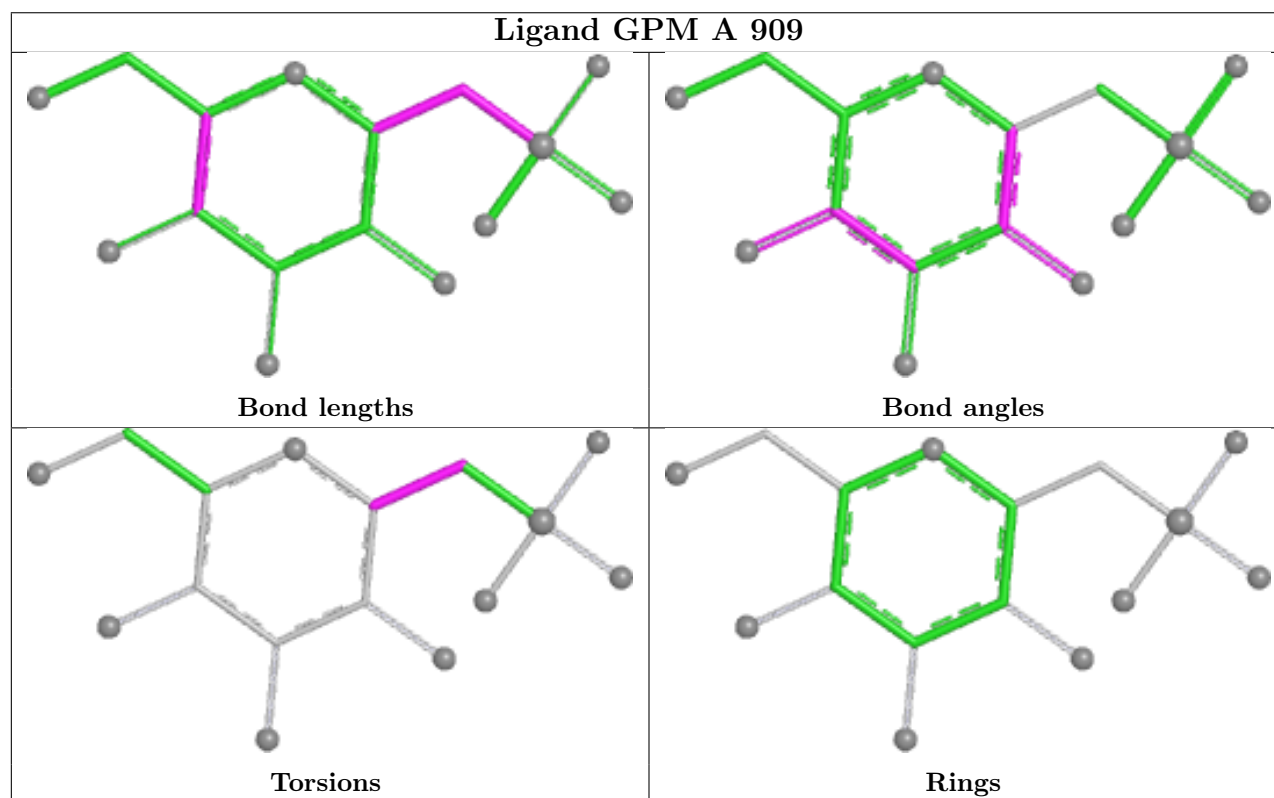
Mol	Chain	Res	Type	Atoms
3	A	901	GPM	O5-C1-C7-P
3	A	909	GPM	O5-C1-C7-P
4	A	999	PLP	C5A-O4P-P-O3P
4	A	999	PLP	C5A-O4P-P-O2P
4	A	999	PLP	C5A-O4P-P-O1P

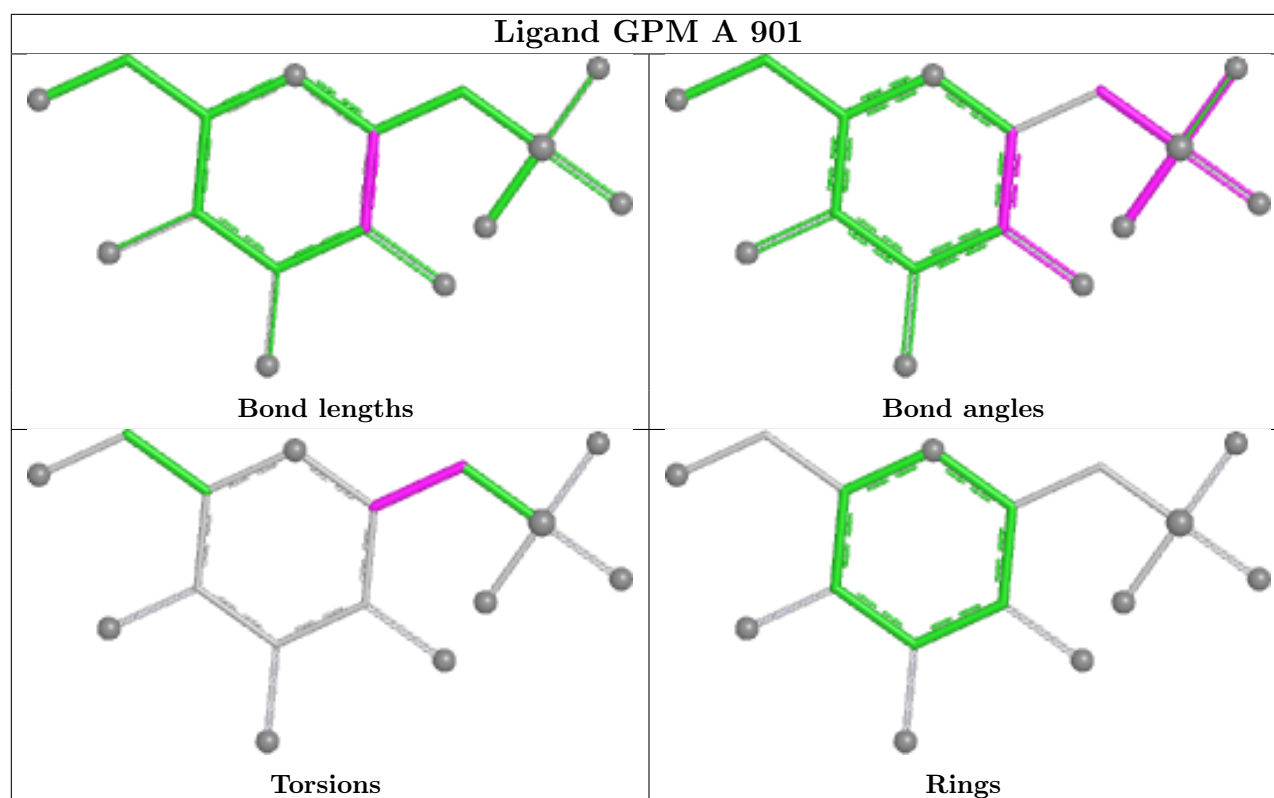
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	909	GPM	1	0
3	A	901	GPM	2	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](#)

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.