



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 06:11 PM BST

PDB ID : 5GPB
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 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

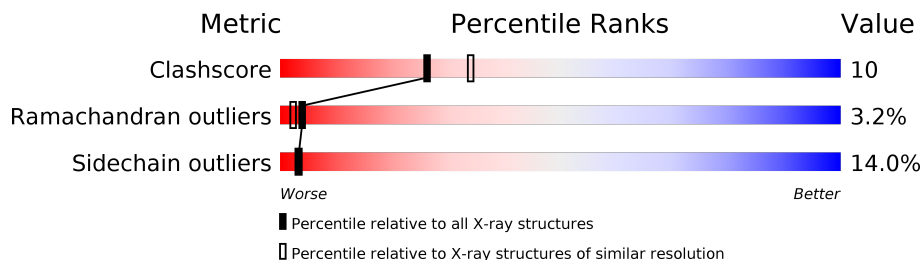
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 on 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
			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:

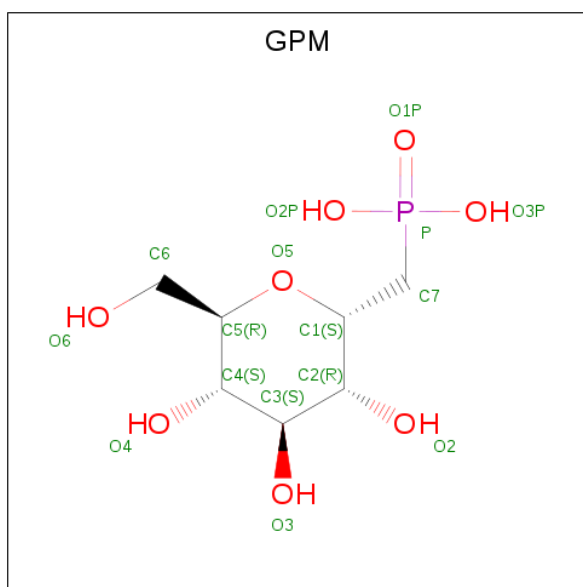
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

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



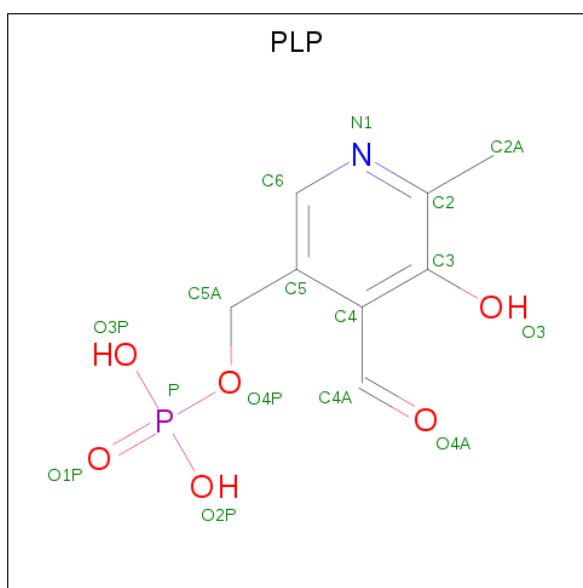
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	5	56	30	26	0	0	0

- Molecule 3 is (1S)-1,5-anhydro-1-(phosphonomethyl)-D-glucitol (three-letter code: GPM) (formula: C₇H₁₅O₈P).



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 (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 5 is water.

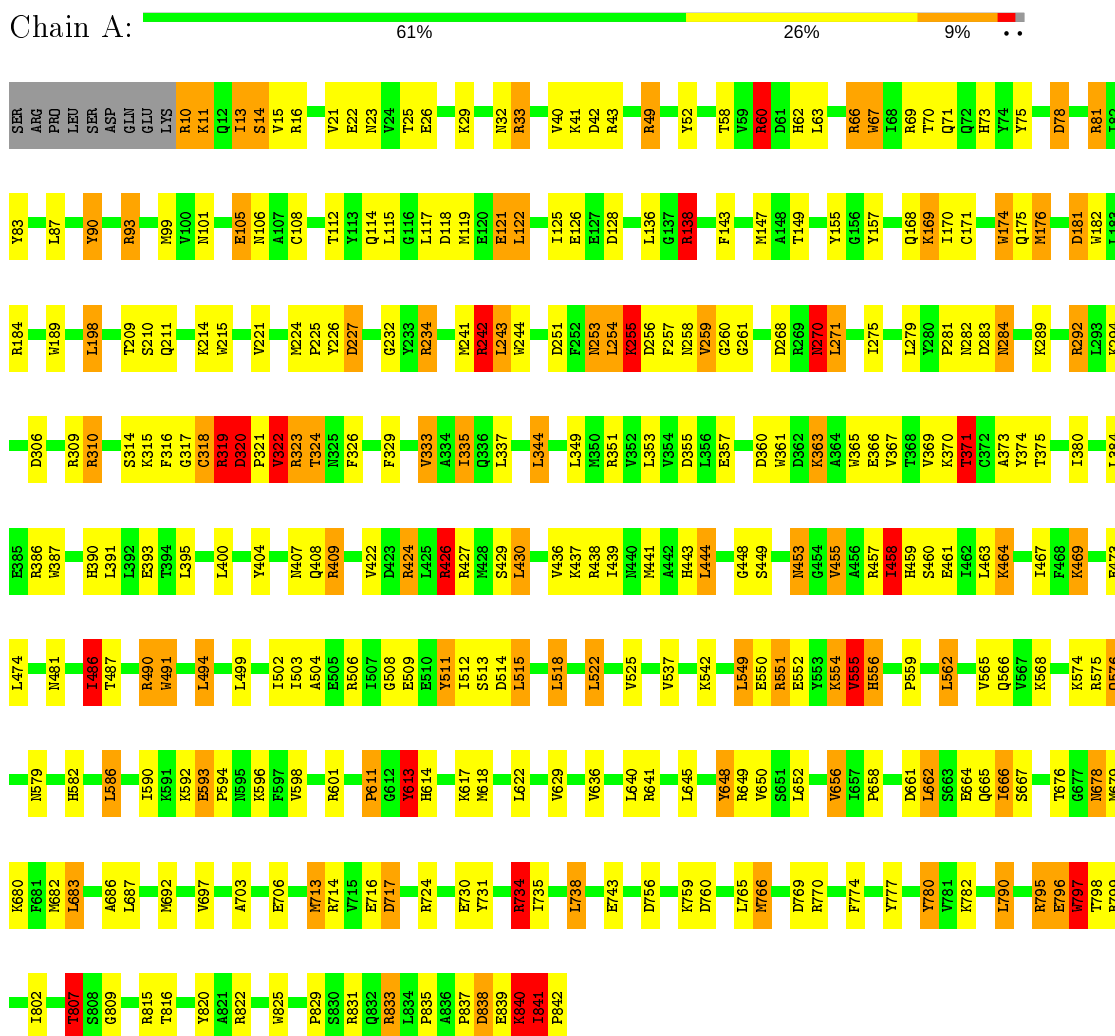
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	595	Total 595	O 595	0	0

3 Residue-property plots

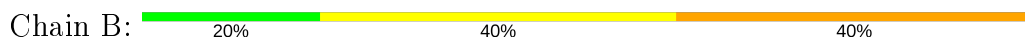
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



- 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, 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.	Xtrriage
Total number of atoms	7477	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: GPM, GLC, 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	0.92	1/6933 (0.0%)	1.77	157/9381 (1.7%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	THR	CA-CB	5.02	1.66	1.53

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	ARG	NE-CZ-NH2	-12.71	113.94	120.30
1	A	310	ARG	NE-CZ-NH2	-12.07	114.26	120.30
1	A	490	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	A	409	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	A	60	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	A	822	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	A	242	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	A	562	LEU	CA-CB-CG	9.46	137.07	115.30
1	A	138	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	365	TRP	CD1-CG-CD2	9.25	113.70	106.30
1	A	67	TRP	CD1-CG-CD2	8.93	113.44	106.30
1	A	387	TRP	CD1-CG-CD2	8.91	113.43	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	215	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	A	10	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	244	TRP	CD1-CG-CD2	8.72	113.27	106.30
1	A	713	MET	CA-CB-CG	8.69	128.07	113.30
1	A	506	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	234	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	10	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	242	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	649	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	A	613	TYR	CB-CG-CD2	-8.30	116.02	121.00
1	A	838	ASP	CA-C-N	-8.16	99.25	117.20
1	A	234	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	490	ARG	CB-CA-C	-8.06	94.27	110.40
1	A	365	TRP	CG-CD2-CE3	8.05	141.14	133.90
1	A	90	TYR	CB-CG-CD2	-8.04	116.17	121.00
1	A	138	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	457	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	365	TRP	CE2-CD2-CG	-7.98	100.92	107.30
1	A	797	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	A	182	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	A	387	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	555	VAL	N-CA-C	7.68	131.73	111.00
1	A	601	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	361	TRP	CD1-CG-CD2	7.56	112.35	106.30
1	A	244	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	A	67	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	374	TYR	CB-CG-CD2	-7.38	116.58	121.00
1	A	601	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	457	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	494	LEU	CA-CB-CG	7.35	132.21	115.30
1	A	797	TRP	CB-CG-CD1	-7.29	117.52	127.00
1	A	575	ARG	CB-CG-CD	-7.23	92.80	111.60
1	A	656	VAL	CB-CA-C	-7.23	97.66	111.40
1	A	189	TRP	CD1-CG-CD2	7.23	112.08	106.30
1	A	438	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	734	ARG	CA-CB-CG	7.18	129.19	113.40
1	A	121	GLU	CA-CB-CG	7.17	129.18	113.40
1	A	469	LYS	CA-CB-CG	7.15	129.13	113.40
1	A	365	TRP	CB-CG-CD1	-7.13	117.73	127.00
1	A	797	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	A	215	TRP	CE2-CD2-CG	-7.12	101.61	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	174	TRP	CD1-CG-CD2	6.94	111.85	106.30
1	A	174	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	A	182	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	A	60	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	83	TYR	CB-CG-CD1	-6.89	116.87	121.00
1	A	490	ARG	N-CA-CB	6.89	123.00	110.60
1	A	361	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	490	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	780	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	A	838	ASP	O-C-N	6.66	133.36	122.70
1	A	255	LYS	CA-C-N	-6.63	102.61	117.20
1	A	344	LEU	CA-CB-CG	6.62	130.52	115.30
1	A	661	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	189	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	A	766	MET	CG-SD-CE	6.53	110.65	100.20
1	A	181	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	322	VAL	CG1-CB-CG2	-6.48	100.53	110.90
1	A	815	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	404	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	A	365	TRP	CG-CD1-NE1	-6.42	103.68	110.10
1	A	807	THR	N-CA-CB	-6.39	98.15	110.30
1	A	511	TYR	CB-CG-CD1	-6.39	117.17	121.00
1	A	838	ASP	N-CA-C	6.39	128.25	111.00
1	A	427	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	486	ILE	CA-CB-CG1	-6.35	98.94	111.00
1	A	256	ASP	N-CA-C	-6.30	94.00	111.00
1	A	683	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	491	TRP	CG-CD2-CE3	6.21	139.49	133.90
1	A	310	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	121	GLU	CB-CA-C	-6.21	97.99	110.40
1	A	67	TRP	CG-CD1-NE1	-6.20	103.90	110.10
1	A	601	ARG	CA-CB-CG	6.16	126.96	113.40
1	A	648	TYR	CB-CG-CD1	-6.16	117.31	121.00
1	A	666	ILE	N-CA-CB	-6.14	96.68	110.80
1	A	282	ASN	N-CA-CB	-6.12	99.58	110.60
1	A	777	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	682	MET	CG-SD-CE	6.10	109.96	100.20
1	A	40	VAL	CG1-CB-CG2	-6.00	101.30	110.90
1	A	629	VAL	CG1-CB-CG2	-6.00	101.30	110.90
1	A	60	ARG	CA-CB-CG	5.94	126.46	113.40
1	A	797	TRP	NE1-CE2-CZ2	-5.93	123.88	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	A	333	VAL	CG1-CB-CG2	-5.81	101.61	110.90
1	A	455	VAL	CA-CB-CG1	-5.76	102.26	110.90
1	A	825	TRP	CD1-CG-CD2	5.76	110.91	106.30
1	A	825	TRP	CE2-CD2-CG	-5.71	102.73	107.30
1	A	713	MET	N-CA-CB	-5.69	100.36	110.60
1	A	575	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	833	ARG	CA-CB-CG	5.64	125.82	113.40
1	A	835	PRO	CA-C-N	-5.55	104.99	117.20
1	A	90	TYR	CB-CG-CD1	5.52	124.31	121.00
1	A	215	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	A	244	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	A	426	ARG	CG-CD-NE	5.47	123.30	111.80
1	A	611	PRO	N-CA-C	5.46	126.31	112.10
1	A	387	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	491	TRP	CE2-CD2-CG	-5.45	102.94	107.30
1	A	189	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	A	324	THR	CA-C-N	-5.42	105.29	117.20
1	A	227	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	255	LYS	N-CA-C	5.39	125.56	111.00
1	A	323	ARG	N-CA-C	-5.39	96.44	111.00
1	A	464	LYS	CB-CG-CD	-5.35	97.69	111.60
1	A	270	ASN	CA-C-N	-5.30	105.55	117.20
1	A	491	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	A	226	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	A	15	VAL	CA-C-O	5.28	131.19	120.10
1	A	686	ALA	N-CA-C	-5.28	96.74	111.00
1	A	458	ILE	CB-CA-C	-5.27	101.06	111.60
1	A	387	TRP	CG-CD2-CE3	5.26	138.63	133.90
1	A	253	ASN	CA-C-N	-5.26	105.63	117.20
1	A	322	VAL	CA-CB-CG2	-5.25	103.03	110.90
1	A	840	LYS	CA-CB-CG	5.25	124.94	113.40
1	A	387	TRP	CB-CG-CD1	-5.24	120.19	127.00
1	A	198	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	841	ILE	N-CA-C	-5.21	96.93	111.00
1	A	255	LYS	CA-CB-CG	5.20	124.83	113.40
1	A	770	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	649	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	714	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	93	ARG	CB-CG-CD	-5.18	98.12	111.60
1	A	63	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	270	ASN	CB-CG-ND2	5.17	129.12	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	VAL	N-CA-C	-5.16	97.06	111.00
1	A	650	VAL	CA-C-N	5.16	128.56	117.20
1	A	259	VAL	N-CA-C	5.16	124.93	111.00
1	A	765	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	317	GLY	N-CA-C	-5.14	100.26	113.10
1	A	258	ASN	CA-C-N	-5.13	105.91	117.20
1	A	49	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	769	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	551	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	114	GLN	CA-CB-CG	5.09	124.61	113.40
1	A	724	ARG	CA-CB-CG	5.09	124.61	113.40
1	A	66	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	797	TRP	CD1-CG-CD2	5.06	110.35	106.30
1	A	734	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	822	ARG	CG-CD-NE	-5.05	101.18	111.80
1	A	60	ARG	CG-CD-NE	5.03	122.36	111.80
1	A	636	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	A	565	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	A	613	TYR	CB-CG-CD1	5.01	124.01	121.00

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 [\(i\)](#)

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	6779	0	6729	142	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	142	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (142) 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:294:LYS:HE3	1:A:395:LEU:HD11	1.69	0.74
1:A:78:ASP:HB3	1:A:315:LYS:NZ	2.01	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
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:648:TYR:HA	1:A:652:LEU:HD23	1.81	0.62
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:441:MET:HE3	1:A:444:LEU:HD12	1.85	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: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:HH11	1:A:60:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:549:LEU:HG	1:A:555:VAL:HG21	1.95	0.48
1:A:81:ARG:HG3	1:A:155:TYR:CE1	2.43	0.48
1:A:75:TYR:HB2	5:A:1009:HOH:O	2.13	0.48
1:A:574:LYS:NZ	3:A:901:GPM:O1P	2.46	0.48
1:A:67:TRP:O	1:A:71:GLN:HG2	2.13	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: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:143:PHE:HB3	1:A:147:MET:HE2	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:N	1:A:257:PHE:CD1	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:HD3	1:A:11:LYS:HA	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:437:LYS:NZ	2:B:3:GLC:O2	2.50	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:16:ARG:HB2	1:A:106:ASN:CG	2.40	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:99:MET:HE1	1:A:108:CYS:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:337:LEU:HD12	1:A:337:LEU:N	2.35	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: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:149:THR:O	1:A:831:ARG:HD2	2.21	0.40
1:A:169:LYS:HB3	1:A:169:LYS:HE2	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](#)

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%)	755 (91%)	49 (6%)	27 (3%)	4 2

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	210	SER
1	A	254	LEU
1	A	259	VAL
1	A	318	CYS
1	A	320	ASP
1	A	321	PRO
1	A	322	VAL
1	A	323	ARG
1	A	324	THR
1	A	555	VAL
1	A	556	HIS
1	A	839	GLU
1	A	840	LYS
1	A	115	LEU
1	A	284	ASN
1	A	319	ARG
1	A	14	SER
1	A	261	GLY
1	A	271	LEU
1	A	314	SER
1	A	554	LYS
1	A	234	ARG
1	A	551	ARG
1	A	829	PRO
1	A	260	GLY
1	A	837	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	722/731 (99%)	621 (86%)	101 (14%)	3 3

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	11	LYS
1	A	13	ILE
1	A	14	SER
1	A	22	GLU
1	A	23	ASN
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	81	ARG
1	A	87	LEU
1	A	90	TYR
1	A	105	GLU
1	A	119	MET
1	A	122	LEU
1	A	128	ASP
1	A	136	LEU
1	A	138	ARG
1	A	169	LYS
1	A	176	MET
1	A	198	LEU
1	A	214	LYS
1	A	224	MET
1	A	242	ARG
1	A	243	LEU
1	A	253	ASN
1	A	254	LEU
1	A	255	LYS
1	A	270	ASN
1	A	279	LEU
1	A	281	PRO
1	A	283	ASP
1	A	289	LYS
1	A	292	ARG
1	A	306	ASP
1	A	319	ARG
1	A	320	ASP
1	A	335	ILE
1	A	344	LEU
1	A	363	LYS

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Mol	Chain	Res	Type
1	A	371	THR
1	A	380	ILE
1	A	384	LEU
1	A	391	LEU
1	A	400	LEU
1	A	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	469	LYS
1	A	474	LEU
1	A	486	ILE
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	562	LEU
1	A	568	LYS
1	A	576	GLN
1	A	579	ASN
1	A	586	LEU
1	A	592	LYS
1	A	593	GLU
1	A	611	PRO
1	A	613	TYR
1	A	622	LEU
1	A	641	ARG
1	A	645	LEU
1	A	656	VAL
1	A	658	PRO
1	A	662	LEU
1	A	666	ILE
1	A	667	SER
1	A	678	ASN
1	A	683	LEU
1	A	687	LEU
1	A	706	GLU

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Mol	Chain	Res	Type
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	782	LYS
1	A	790	LEU
1	A	795	ARG
1	A	796	GLU
1	A	797	TRP
1	A	807	THR
1	A	833	ARG
1	A	838	ASP
1	A	840	LYS
1	A	841	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) 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	253	ASN
1	A	284	ASN
1	A	408	GLN
1	A	459	HIS
1	A	481	ASN
1	A	566	GLN
1	A	571	HIS
1	A	576	GLN
1	A	579	ASN
1	A	678	ASN
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](#)

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	1.78	3 (25%)	17,17,17	1.65	4 (23%)
2	GLC	B	2	2	11,11,12	0.89	0	15,15,17	0.75	0
2	GLC	B	3	2	11,11,12	0.70	0	15,15,17	1.88	4 (26%)
2	GLC	B	4	2	11,11,12	1.16	1 (9%)	15,15,17	1.49	4 (26%)
2	GLC	B	5	2	11,11,12	0.95	1 (9%)	15,15,17	1.32	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
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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLC	C4-C5	3.66	1.60	1.53
2	B	1	GLC	C4-C3	2.97	1.59	1.52
2	B	4	GLC	C4-C5	2.63	1.58	1.53
2	B	1	GLC	O4-C4	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GLC	C4-C5	2.01	1.57	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	GLC	C1-O5-C5	4.62	118.45	112.19
2	B	1	GLC	C1-O5-C5	4.46	122.07	113.66
2	B	3	GLC	O4-C4-C3	-3.36	102.59	110.35
2	B	5	GLC	C1-O5-C5	3.23	116.57	112.19
2	B	4	GLC	C1-O5-C5	3.07	116.35	112.19
2	B	5	GLC	O4-C4-C3	-2.63	104.26	110.35
2	B	4	GLC	C6-C5-C4	2.63	119.16	113.00
2	B	1	GLC	O3-C3-C2	-2.44	104.70	110.35
2	B	4	GLC	O4-C4-C3	-2.43	104.73	110.35
2	B	1	GLC	O5-C1-C2	2.25	114.29	110.28
2	B	3	GLC	C1-C2-C3	2.21	112.38	109.67
2	B	4	GLC	O5-C5-C6	-2.09	103.93	107.20
2	B	3	GLC	O5-C1-C2	2.04	113.92	110.77
2	B	1	GLC	O2-C2-C3	-2.04	105.64	110.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

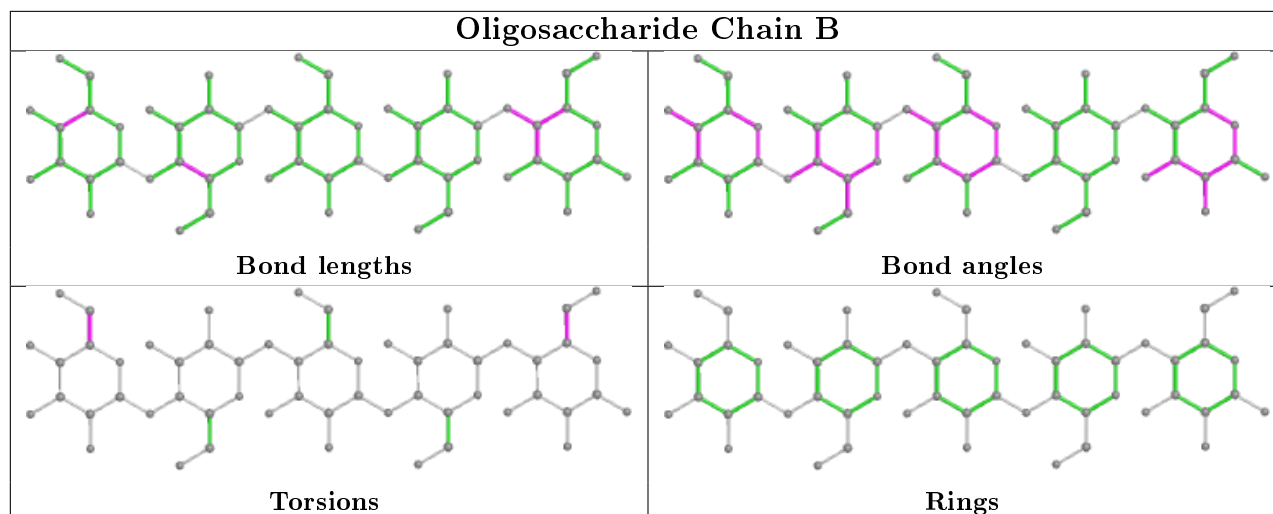
Mol	Chain	Res	Type	Atoms
2	B	1	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6
2	B	5	GLC	C4-C5-C6-O6
2	B	5	GLC	O5-C5-C6-O6

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
4	PLP	A	999	1	15,15,16	1.49	2 (13%)	20,22,23	1.29	4 (20%)
3	GPM	A	901	-	15,16,16	1.32	1 (6%)	21,24,24	1.71	3 (14%)
3	GPM	A	909	-	15,16,16	1.99	2 (13%)	21,24,24	1.23	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
4	PLP	A	999	1	-	3/6/6/8	0/1/1/1
3	GPM	A	901	-	-	1/7/27/27	0/1/1/1
3	GPM	A	909	-	-	1/7/27/27	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	909	GPM	P-C7	5.40	1.84	1.78
3	A	909	GPM	C4-C5	3.83	1.61	1.53
4	A	999	PLP	C3-C2	-3.47	1.37	1.40
3	A	901	GPM	C2-C1	3.36	1.60	1.53
4	A	999	PLP	P-O2P	-2.36	1.45	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	GPM	O1P-P-C7	-4.25	103.66	111.54
3	A	901	GPM	O2-C2-C1	3.50	117.98	109.30
3	A	909	GPM	O2-C2-C1	2.81	116.27	109.30
4	A	999	PLP	O4P-C5A-C5	2.63	114.37	109.35
4	A	999	PLP	O2P-P-O1P	2.52	120.56	110.68
3	A	901	GPM	O3P-P-O2P	2.46	115.25	108.08
4	A	999	PLP	C5-C6-N1	-2.23	120.10	123.82
3	A	909	GPM	O4-C4-C3	-2.14	105.39	110.35
4	A	999	PLP	C6-C5-C4	2.12	119.83	118.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

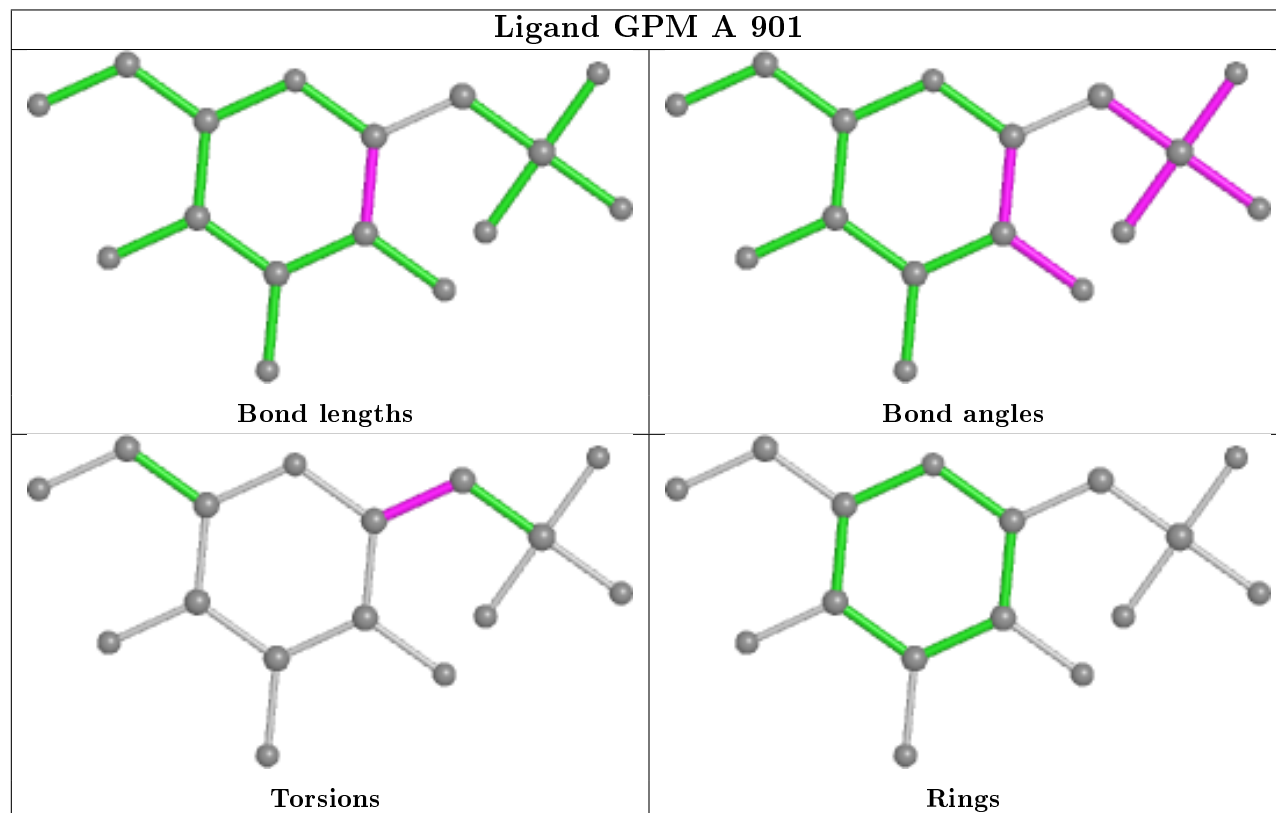
There are no ring outliers.

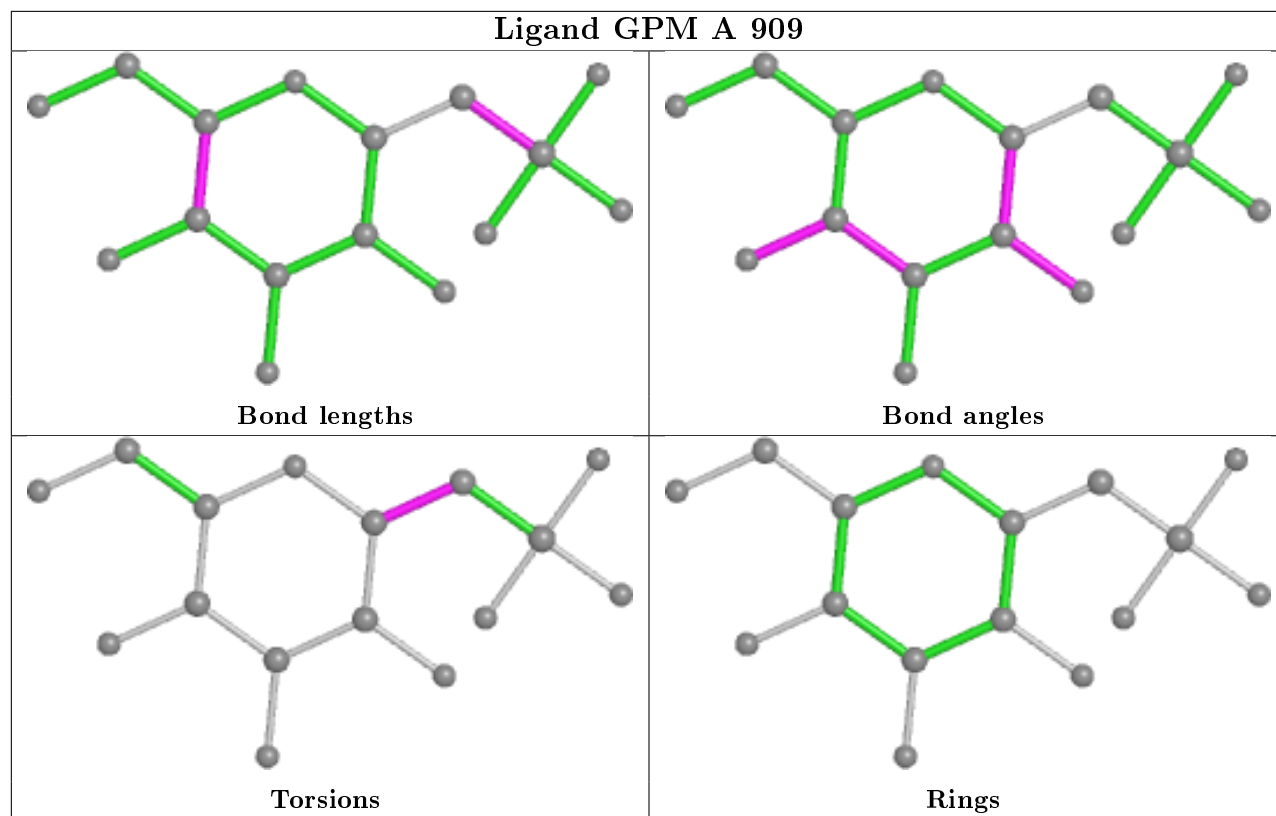
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	GPM	2	0
3	A	909	GPM	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 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.