



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:46 PM GMT

PDB ID : 1H5U
Title : THE 1.76 Å RESOLUTION CRYSTAL STRUCTURE OF GLYCOGEN PHOSPHORYLASE B COMPLEXED WITH GLUCOSE AND CP320626, A POTENTIAL ANTIDIABETIC DRUG
Authors : Oikonomakos, N.G.; Zographos, S.E.; Skamnaki, V.T.; Archontis, G.
Deposited on : 2001-05-25
Resolution : 1.76 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

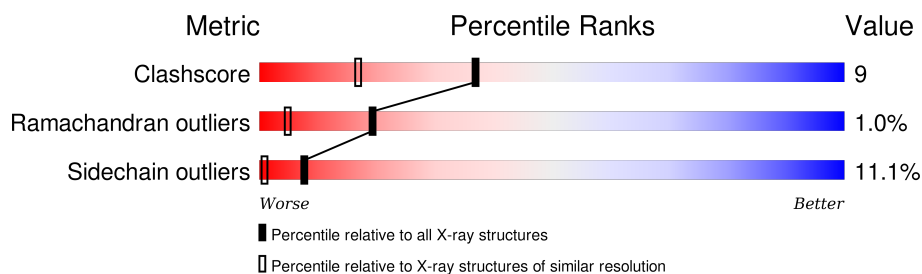
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	 74% 17% 5% •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7004 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.

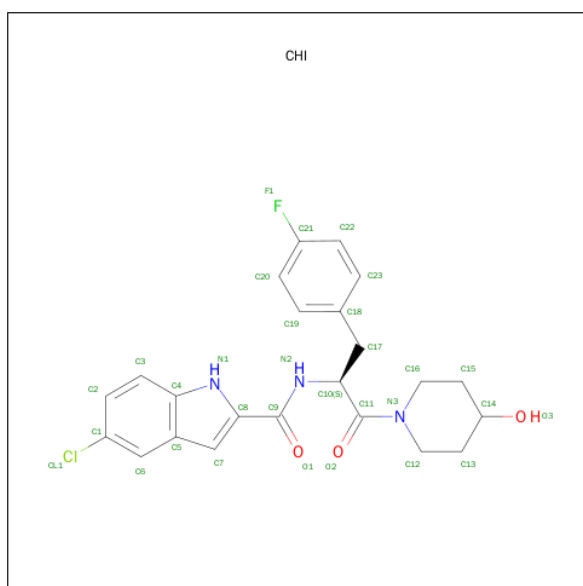
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	811	6591	4203	1160	1199	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

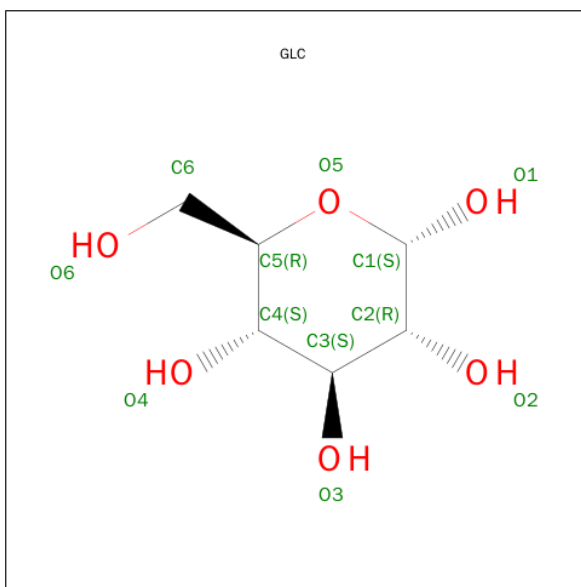
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489

- Molecule 2 is 5-CHLORO-1H-INDOLE-2-CARBOXYLIC ACID [1-(4-FLUOROBENZYL)-2-(4-HYDROXYPIPERIDIN-1YL)-2-OXOETHYL]AMIDE (three-letter code: CHI) (formula: $C_{23}H_{23}ClFN_3O_3$).



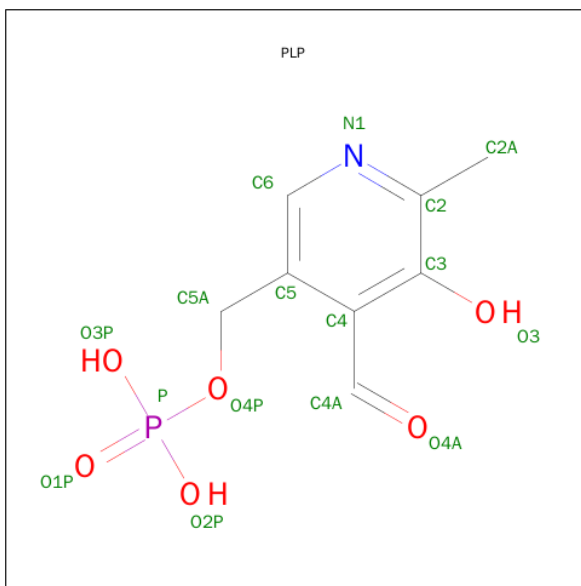
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
2	A	1	31	23	1	1	3	3	0	0

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	355	Total 355	O 355	0	0

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.97Å 128.97Å 116.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.25 – 1.76	Depositor
% Data completeness (in resolution range)	95.8 (26.25-1.76)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.211 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7004	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: CHI, 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	0.36	0/6739	0.60	0/9121

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6591	0	6535	124	0
2	A	31	0	23	0	0
3	A	12	0	12	0	0
4	A	15	0	7	0	0
5	A	355	0	0	14	0
All	All	7004	0	6577	124	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 9.

All (124) 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:519:ARG:HH22	1:A:807:THR:HG22	1.14	1.08
1:A:251:ASP:CG	1:A:252:PHE:H	1.57	1.04
1:A:252:PHE:C	1:A:254:LEU:H	1.61	1.02
1:A:15:VAL:HG23	5:A:2002:HOH:O	1.64	0.97
1:A:252:PHE:O	1:A:254:LEU:N	1.96	0.96
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.52	0.89
1:A:227:ASP:OD2	1:A:242:ARG:HD3	1.75	0.85
1:A:519:ARG:NH2	1:A:807:THR:HG22	1.91	0.85
1:A:739:ARG:O	1:A:743:GLU:HG3	1.79	0.81
1:A:251:ASP:CG	1:A:252:PHE:N	2.32	0.81
1:A:678:ASN:HD22	1:A:679:MET:H	1.27	0.80
1:A:252:PHE:C	1:A:254:LEU:N	2.30	0.79
1:A:225:PRO:CB	1:A:242:ARG:HD2	2.12	0.78
1:A:65:GLY:O	1:A:69:ARG:HG2	1.84	0.78
1:A:261:GLY:HA3	5:A:2122:HOH:O	1.85	0.76
1:A:15:VAL:CG2	5:A:2002:HOH:O	2.29	0.75
1:A:719:ASP:O	1:A:723:GLN:HG2	1.87	0.74
1:A:455:VAL:H	1:A:459:HIS:HD2	1.35	0.74
1:A:795:ARG:O	1:A:799:ARG:HG3	1.89	0.72
1:A:545:PHE:CZ	1:A:656:VAL:HG13	2.25	0.70
1:A:13:ILE:O	1:A:14:SER:HB2	1.90	0.70
1:A:413:ARG:HG2	1:A:413:ARG:HH21	1.56	0.68
1:A:250:ASN:HA	1:A:269:ARG:HH21	1.58	0.67
1:A:266:VAL:O	1:A:269:ARG:HG3	1.95	0.67
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.76	0.66
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.78	0.66
1:A:235:ASN:HD22	1:A:235:ASN:H	1.43	0.65
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.77	0.65
1:A:16:ARG:HD3	1:A:105:GLU:HG2	1.77	0.65
1:A:678:ASN:HD22	1:A:679:MET:N	1.96	0.63
1:A:555:VAL:HG23	1:A:556:HIS:N	2.17	0.60
1:A:65:GLY:O	1:A:69:ARG:CG	2.51	0.59
1:A:592:LYS:O	1:A:592:LYS:HD2	2.03	0.59
1:A:730:GLU:O	1:A:734:ARG:HG2	2.02	0.59
1:A:34:HIS:HE1	1:A:61:ASP:OD1	1.85	0.58
1:A:379:VAL:HG22	5:A:2171:HOH:O	2.03	0.58
1:A:678:ASN:ND2	1:A:679:MET:H	1.99	0.58
1:A:16:ARG:HB3	1:A:105:GLU:HB3	1.87	0.56
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.86	0.56
1:A:367:VAL:O	1:A:371:THR:HG23	2.06	0.55
1:A:386:ARG:HH21	1:A:386:ARG:HB2	1.71	0.55
1:A:450:HIS:HE1	5:A:2169:HOH:O	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ARG:NH2	1:A:413:ARG:HG2	2.22	0.54
1:A:718:VAL:HG13	1:A:772:LYS:HE2	1.90	0.54
1:A:571:HIS:HB2	1:A:574:LYS:HG3	1.90	0.53
1:A:360:ASP:OD1	1:A:363:LYS:HB2	2.09	0.53
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.93	0.52
1:A:463:LEU:HA	1:A:467:ILE:HG22	1.92	0.51
1:A:355:ASP:OD1	1:A:398:ARG:HD3	2.09	0.51
1:A:191:LYS:HG3	1:A:193:ARG:HE	1.75	0.51
1:A:94:THR:CG2	5:A:2036:HOH:O	2.60	0.50
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.11	0.50
1:A:636:VAL:O	1:A:639:ARG:HD3	2.11	0.50
1:A:378:THR:OG1	1:A:380:ILE:HG12	2.11	0.50
1:A:835:PRO:O	1:A:836:ALA:O	2.30	0.50
1:A:836:ALA:HB1	1:A:837:PRO:CD	2.42	0.49
1:A:191:LYS:HG2	1:A:193:ARG:HH21	1.76	0.49
1:A:282:ASN:HB2	5:A:2134:HOH:O	2.12	0.49
1:A:555:VAL:CG2	1:A:556:HIS:N	2.75	0.49
1:A:386:ARG:NH2	1:A:386:ARG:HB2	2.27	0.49
1:A:122:LEU:HA	1:A:125:ILE:HD12	1.94	0.48
1:A:536:LYS:HE2	1:A:540:GLU:OE1	2.13	0.48
1:A:810:LYS:O	1:A:810:LYS:HG2	2.13	0.48
1:A:254:LEU:HD21	1:A:266:VAL:HG23	1.95	0.48
1:A:564:ASP:OD1	1:A:601:ARG:NH1	2.47	0.48
1:A:191:LYS:HE2	1:A:192:ALA:O	2.14	0.48
1:A:251:ASP:O	1:A:254:LEU:CB	2.62	0.48
1:A:678:ASN:HD22	1:A:678:ASN:N	2.12	0.47
1:A:351:ARG:O	1:A:355:ASP:HB2	2.14	0.47
1:A:367:VAL:O	1:A:371:THR:CG2	2.63	0.47
1:A:313:SER:O	1:A:314:SER:C	2.54	0.47
1:A:81:ARG:HG2	1:A:155:TYR:HE2	1.79	0.47
1:A:251:ASP:O	1:A:254:LEU:HB3	2.16	0.46
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.51	0.46
1:A:214:LYS:HB3	1:A:214:LYS:HE2	1.72	0.46
1:A:510:GLU:HB2	5:A:2221:HOH:O	2.16	0.46
1:A:21:VAL:HG23	1:A:22:GLU:N	2.31	0.45
1:A:209:THR:O	1:A:211:GLN:N	2.49	0.45
1:A:144:LEU:HD12	1:A:147:MET:CE	2.46	0.45
1:A:467:ILE:HG23	1:A:468:PHE:CG	2.53	0.44
1:A:308:ILE:O	1:A:312:LYS:HG3	2.18	0.44
1:A:678:ASN:ND2	1:A:679:MET:N	2.62	0.44
1:A:13:ILE:O	1:A:14:SER:CB	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ARG:HG2	5:A:2262:HOH:O	2.18	0.44
1:A:457:ARG:HH12	1:A:701:GLU:CD	2.21	0.43
1:A:519:ARG:HG2	1:A:519:ARG:HH21	1.83	0.43
1:A:81:ARG:HG2	1:A:155:TYR:CE2	2.54	0.43
1:A:488:PRO:O	1:A:492:LEU:HB3	2.18	0.43
1:A:128:ASP:OD2	1:A:651:SER:HB3	2.19	0.43
1:A:304:LEU:HD12	1:A:348:GLU:CG	2.49	0.43
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.86	0.43
1:A:466:THR:OG1	1:A:467:ILE:N	2.48	0.43
1:A:648:TYR:HA	1:A:652:LEU:HD23	2.01	0.42
1:A:519:ARG:NH2	1:A:519:ARG:HG2	2.34	0.42
1:A:21:VAL:CG2	1:A:22:GLU:N	2.82	0.42
1:A:42:ASP:OD2	1:A:45:VAL:HG22	2.19	0.42
1:A:737:GLU:HG3	5:A:2302:HOH:O	2.18	0.42
1:A:423:ASP:O	1:A:426:ARG:HG3	2.19	0.42
1:A:692:MET:HE1	1:A:697:VAL:HG13	2.02	0.42
1:A:678:ASN:ND2	1:A:678:ASN:N	2.66	0.42
1:A:836:ALA:HB1	1:A:837:PRO:HD2	2.00	0.42
1:A:338:ASN:OD1	1:A:377:HIS:NE2	2.53	0.42
1:A:663:SER:HB2	1:A:681:PHE:CG	2.55	0.42
1:A:181:ASP:OD2	1:A:184:ARG:CZ	2.68	0.41
1:A:641:ARG:HG3	5:A:2249:HOH:O	2.18	0.41
1:A:522:LEU:HA	1:A:522:LEU:HD12	1.84	0.41
1:A:834:LEU:O	1:A:836:ALA:N	2.54	0.41
1:A:363:LYS:O	1:A:367:VAL:HG23	2.20	0.41
1:A:519:ARG:O	1:A:522:LEU:HB2	2.20	0.41
1:A:66:ARG:NH2	1:A:837:PRO:HG3	2.35	0.41
1:A:522:LEU:HD13	1:A:806:ALA:CB	2.50	0.41
1:A:571:HIS:ND1	5:A:2232:HOH:O	2.37	0.41
1:A:234:ARG:NH1	5:A:2112:HOH:O	2.32	0.41
1:A:592:LYS:C	1:A:592:LYS:HD2	2.41	0.41
1:A:693:ASP:O	1:A:696:ASN:HB2	2.21	0.41
1:A:405:GLU:O	1:A:409:ARG:HG3	2.21	0.41
1:A:225:PRO:HB3	1:A:242:ARG:HD2	1.98	0.41
1:A:592:LYS:HG3	1:A:593:GLU:HG2	2.02	0.41
1:A:834:LEU:HD12	1:A:834:LEU:HA	1.78	0.41
1:A:380:ILE:HG12	1:A:380:ILE:H	1.68	0.40
1:A:689:ILE:O	1:A:689:ILE:HG23	2.21	0.40
1:A:549:LEU:HA	1:A:549:LEU:HD12	1.79	0.40
1:A:94:THR:HG22	5:A:2036:HOH:O	2.19	0.40
1:A:601:ARG:HH11	1:A:601:ARG:HD3	1.76	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	805/842 (96%)	765 (95%)	32 (4%)	8 (1%)	19 5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	210	SER
1	A	253	ASN
1	A	836	ALA
1	A	554	LYS
1	A	835	PRO
1	A	555	VAL
1	A	556	HIS

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	701/731 (96%)	623 (89%)	78 (11%)	8 1

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	14	SER
1	A	18	LEU
1	A	22	GLU
1	A	27	LEU
1	A	33	ARG
1	A	39	LEU
1	A	69	ARG
1	A	90	TYR
1	A	94	THR
1	A	102	LEU
1	A	104	LEU
1	A	115	LEU
1	A	122	LEU
1	A	128	ASP
1	A	144	LEU
1	A	191	LYS
1	A	193	ARG
1	A	198	LEU
1	A	210	SER
1	A	211	GLN
1	A	214	LYS
1	A	235	ASN
1	A	243	LEU
1	A	250	ASN
1	A	252	PHE
1	A	253	ASN
1	A	254	LEU
1	A	314	SER
1	A	324	THR
1	A	325	ASN
1	A	358	ARG
1	A	363	LYS
1	A	371	THR
1	A	380	ILE
1	A	384	LEU
1	A	386	ARG
1	A	400	LEU
1	A	413	ARG
1	A	425	LEU
1	A	426	ARG
1	A	433	GLU
1	A	436	VAL

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Mol	Chain	Res	Type
1	A	444	LEU
1	A	467	ILE
1	A	474	LEU
1	A	510	GLU
1	A	518	LEU
1	A	522	LEU
1	A	528	GLU
1	A	544	LYS
1	A	549	LEU
1	A	552	GLU
1	A	565	VAL
1	A	568	LYS
1	A	571	HIS
1	A	579	ASN
1	A	596	LYS
1	A	603	VAL
1	A	613	TYR
1	A	622	LEU
1	A	643	ILE
1	A	645	LEU
1	A	656	VAL
1	A	662	LEU
1	A	678	ASN
1	A	687	LEU
1	A	706	GLU
1	A	708	PHE
1	A	721	LEU
1	A	734	ARG
1	A	742	ILE
1	A	763	ASN
1	A	765	LEU
1	A	768	HIS
1	A	790	LEU
1	A	830	SER
1	A	833	ARG

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	34	HIS
1	A	36	HIS
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	253	ASN
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	763	ASN
1	A	832	GLN

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 carbohydrates 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	CHI	A	920	-	32,34,34	2.41	15 (46%)	43,48,48	1.67	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	A	998	-	12,12,12	1.49	3 (25%)	17,17,17	0.70	0
4	PLP	A	999	1	15,15,16	1.56	2 (13%)	21,22,23	1.18	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	CHI	A	920	-	-	0/17/30/30	0/4/4/4
3	GLC	A	998	-	-	0/2/22/22	0/1/1/1
4	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	PLP	C3-C2	-4.42	1.37	1.40
2	A	920	CHI	C17-C10	2.21	1.59	1.54
2	A	920	CHI	C3-C4	2.24	1.45	1.41
2	A	920	CHI	C15-C14	2.29	1.57	1.51
2	A	920	CHI	C23-C22	2.31	1.42	1.38
2	A	920	CHI	C7-C5	2.32	1.50	1.41
4	A	999	PLP	C5A-C5	2.34	1.57	1.50
3	A	998	GLC	C4-C5	2.36	1.58	1.53
3	A	998	GLC	C3-C2	2.43	1.58	1.52
2	A	920	CHI	C10-C11	2.46	1.58	1.53
2	A	920	CHI	C19-C18	2.93	1.45	1.38
2	A	920	CHI	C20-C19	3.13	1.44	1.38
2	A	920	CHI	C22-C21	3.14	1.43	1.37
3	A	998	GLC	C1-C2	3.15	1.58	1.52
2	A	920	CHI	C23-C18	3.27	1.45	1.38
2	A	920	CHI	C2-C1	3.41	1.44	1.38
2	A	920	CHI	C6-C1	3.43	1.43	1.36
2	A	920	CHI	C3-C2	3.94	1.45	1.36
2	A	920	CHI	C20-C21	4.43	1.46	1.37
2	A	920	CHI	C11-N3	5.52	1.43	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	920	CHI	C2-C3-C4	-3.92	116.62	120.88
2	A	920	CHI	C7-C5-C4	-3.31	103.38	106.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	920	CHI	C1-C6-C5	-2.97	117.31	119.19
4	A	999	PLP	C5-C6-N1	-2.43	119.64	123.86
2	A	920	CHI	C13-C12-N3	-2.10	108.03	111.07
2	A	920	CHI	C8-C9-N2	2.41	120.47	115.10
2	A	920	CHI	C10-C11-N3	2.46	122.84	118.95
4	A	999	PLP	O3P-P-O1P	2.76	119.48	110.58
2	A	920	CHI	C16-C15-C14	3.00	113.58	110.93
2	A	920	CHI	C16-N3-C12	3.07	118.26	112.56
2	A	920	CHI	C8-N1-C4	3.59	111.86	104.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.