



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:46 am GMT

PDB ID : 1LWO  
Title : Crystal structure of rabbit muscle glycogen phosphorylase a in complex with a potential hypoglycaemic drug at 2.0 Å resolution  
Authors : Oikonomakos, N.G.; Chrysina, E.D.; Kosmopoulou, M.N.; Leonidas, D.D.  
Deposited on : 2002-06-01  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

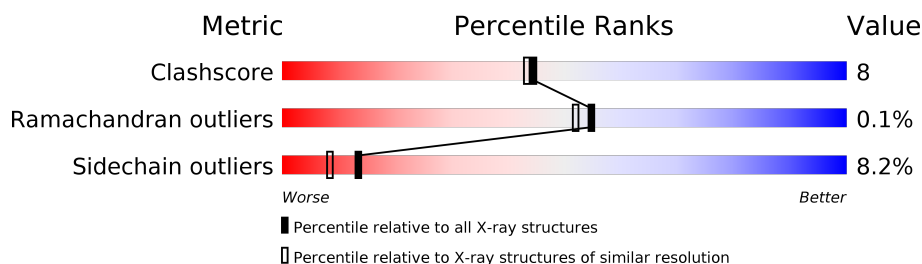
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	 78% 16% . .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7002 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.

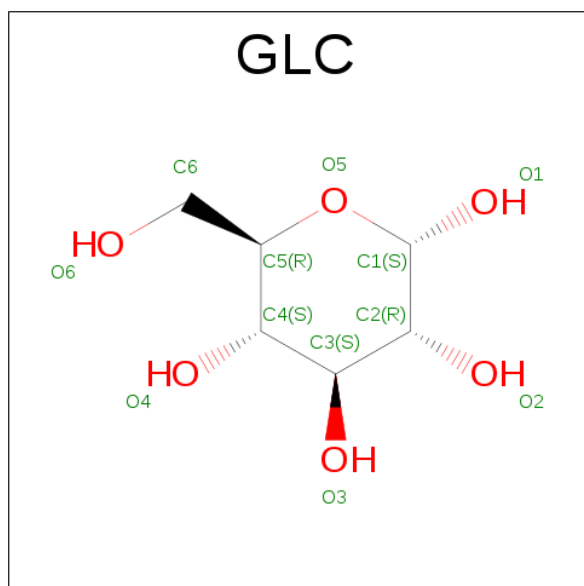
- Molecule 1 is a protein called glycogen phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	815	6635	4222	1170	1213	1	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SEP	SER	MODIFIED RESIDUE	UNP P00489

- Molecule 2 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



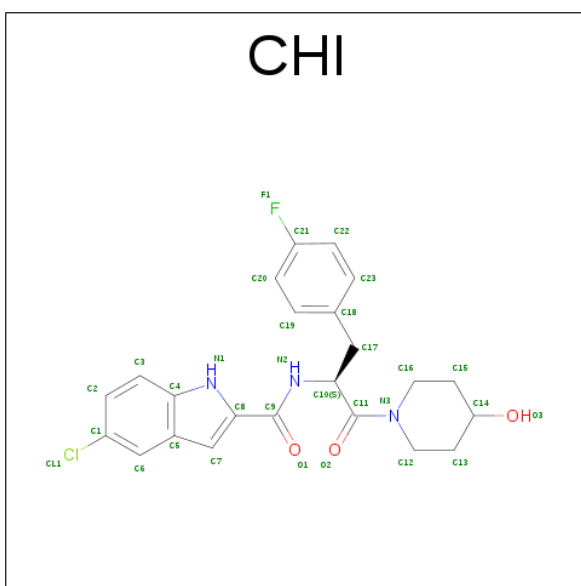
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

- Molecule 4 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
4	A	1	Total	C	Cl	F	N	O	0	0
			31	23	1	1	3	3		

- Molecule 5 is water.

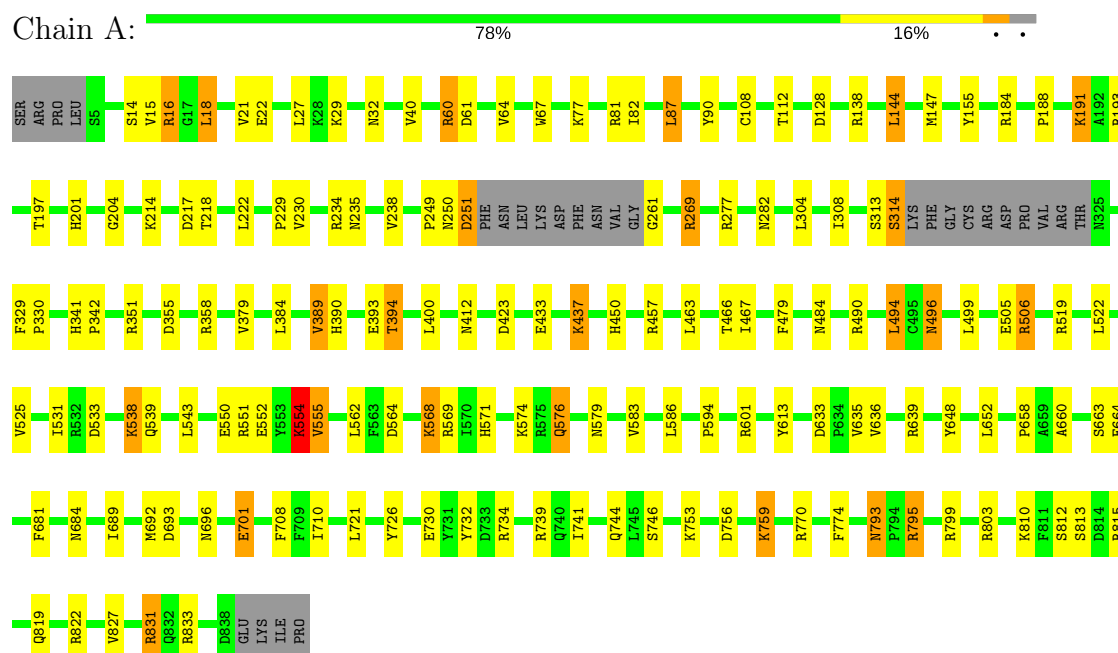
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	309	Total 309	O 309	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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



## 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, $\alpha$ , $\beta$ , $\gamma$	128.65Å 128.65Å 116.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 2.00	Depositor
% Data completeness (in resolution range)	97.6 (29.36-2.00)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.207 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	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, SEP

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	0.37	0/6771	0.60	0/9159

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	6635	0	6571	100	0
2	A	12	0	12	0	0
3	A	15	0	7	0	0
4	A	31	0	23	3	0
5	A	309	0	0	12	0
All	All	7002	0	6613	100	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 8.

All (100) 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:756:ASP:HB2	1:A:759:LYS:HG3	1.45	0.97
1:A:313:SER:O	1:A:314:SER:HB2	1.77	0.83
1:A:390:HIS:O	1:A:394:THR:HG22	1.79	0.81
1:A:555:VAL:HB	5:A:1290:HOH:O	1.81	0.79
1:A:822:ARG:NH1	5:A:1238:HOH:O	2.14	0.79
1:A:554:LYS:O	1:A:554:LYS:HG2	1.86	0.75
1:A:795:ARG:O	1:A:799:ARG:HG3	1.90	0.72
1:A:250:ASN:HA	1:A:269:ARG:HH11	1.52	0.72
1:A:191:LYS:HD2	1:A:193:ARG:NH1	2.06	0.70
1:A:64:VAL:HB	4:A:920:CHI:CL1	2.29	0.69
1:A:304:LEU:O	1:A:308:ILE:HG12	1.94	0.68
1:A:191:LYS:C	1:A:191:LYS:HD3	2.14	0.68
1:A:506:ARG:NH1	1:A:533:ASP:OD1	2.27	0.68
1:A:261:GLY:HA3	5:A:1266:HOH:O	1.93	0.68
1:A:191:LYS:HE3	4:A:920:CHI:O2	1.96	0.65
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.81	0.63
1:A:379:VAL:HG22	5:A:1095:HOH:O	1.99	0.62
1:A:250:ASN:HA	1:A:269:ARG:NH1	2.14	0.62
1:A:15:VAL:HA	1:A:18:LEU:HD22	1.82	0.61
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.31	0.61
1:A:82:ILE:HD11	1:A:827:VAL:HG11	1.83	0.60
1:A:770:ARG:HD3	5:A:1284:HOH:O	2.01	0.60
1:A:522:LEU:O	1:A:525:VAL:HG23	2.02	0.59
1:A:393:GLU:HB3	1:A:400:LEU:CD2	2.33	0.58
1:A:550:GLU:HG3	1:A:551:ARG:N	2.20	0.57
1:A:351:ARG:O	1:A:355:ASP:HB2	2.04	0.57
1:A:793:ASN:C	1:A:793:ASN:HD22	2.09	0.56
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.88	0.56
1:A:531:ILE:HD13	1:A:795:ARG:HD2	1.88	0.54
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.89	0.54
1:A:250:ASN:ND2	1:A:269:ARG:NH1	2.56	0.54
1:A:61:ASP:O	1:A:64:VAL:HG12	2.07	0.54
1:A:689:ILE:O	1:A:689:ILE:HG23	2.07	0.53
1:A:734:ARG:HD2	5:A:1228:HOH:O	2.08	0.53
1:A:313:SER:O	1:A:314:SER:CB	2.54	0.53
1:A:732:TYR:O	1:A:739:ARG:HG3	2.08	0.53
1:A:250:ASN:HD22	1:A:269:ARG:NH1	2.08	0.52
1:A:490:ARG:HA	1:A:494:LEU:HB2	1.92	0.52
1:A:538:LYS:NZ	1:A:684:ASN:O	2.42	0.52
1:A:799:ARG:O	1:A:803:ARG:HG3	2.10	0.52
1:A:393:GLU:HB3	1:A:400:LEU:HD22	1.92	0.51
1:A:539:GLN:HE21	1:A:543:LEU:HD13	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:HG12	1:A:22:GLU:N	2.25	0.50
1:A:730:GLU:O	1:A:734:ARG:HD3	2.11	0.50
1:A:204:GLY:HA2	1:A:217:ASP:O	2.12	0.50
1:A:450:HIS:HE1	5:A:1010:HOH:O	1.94	0.49
1:A:463:LEU:HD22	1:A:467:ILE:HD11	1.94	0.49
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.11	0.49
1:A:14:SEP:OG	1:A:16:ARG:HB2	2.11	0.49
1:A:479:PHE:HB3	5:A:1111:HOH:O	2.11	0.49
1:A:496:ASN:HB2	1:A:684:ASN:ND2	2.28	0.48
1:A:67:TRP:HA	1:A:238:VAL:HB	1.96	0.48
1:A:144:LEU:HD12	1:A:147:MET:CE	2.43	0.48
1:A:81:ARG:HG2	1:A:155:TYR:HE1	1.77	0.47
1:A:692:MET:CE	1:A:710:ILE:HG12	2.45	0.47
1:A:594:PRO:O	1:A:639:ARG:NH1	2.47	0.47
1:A:450:HIS:HD2	5:A:1273:HOH:O	1.97	0.47
1:A:633:ASP:OD2	1:A:635:VAL:HG13	2.14	0.47
1:A:230:VAL:CG2	1:A:230:VAL:O	2.63	0.47
1:A:793:ASN:ND2	1:A:793:ASN:C	2.69	0.47
1:A:201:HIS:HD2	1:A:218:THR:OG1	1.98	0.46
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.97	0.46
1:A:251:ASP:OD1	1:A:251:ASP:C	2.54	0.45
1:A:663:SER:HB2	1:A:681:PHE:CG	2.51	0.45
1:A:389:VAL:HG13	1:A:437:LYS:HB3	1.99	0.45
1:A:191:LYS:HD2	1:A:193:ARG:HD3	1.99	0.45
1:A:191:LYS:HE2	5:A:1064:HOH:O	2.16	0.45
1:A:230:VAL:HG22	1:A:230:VAL:O	2.17	0.45
1:A:554:LYS:O	1:A:555:VAL:HG23	2.17	0.45
1:A:108:CYS:O	1:A:112:THR:HG23	2.17	0.44
1:A:564:ASP:OD2	1:A:664:GLU:OE2	2.35	0.44
1:A:61:ASP:O	1:A:64:VAL:CG1	2.65	0.44
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.98	0.44
1:A:538:LYS:HE3	1:A:658:PRO:O	2.16	0.44
1:A:538:LYS:HE2	1:A:660:ALA:O	2.18	0.44
1:A:815:ARG:O	1:A:819:GLN:HG3	2.18	0.44
1:A:810:LYS:O	1:A:810:LYS:HG2	2.17	0.43
1:A:60:ARG:HG2	1:A:60:ARG:NH1	2.34	0.43
1:A:457:ARG:NH1	1:A:701:GLU:OE2	2.43	0.43
1:A:433:GLU:OE2	1:A:437:LYS:HE2	2.18	0.43
1:A:235:ASN:HB3	1:A:831:ARG:NH1	2.34	0.43
1:A:496:ASN:HB2	1:A:684:ASN:HD21	1.84	0.43
1:A:60:ARG:HD2	1:A:188:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:HIS:CD2	1:A:218:THR:OG1	2.72	0.42
1:A:60:ARG:HH11	1:A:60:ARG:HG2	1.84	0.42
1:A:282:ASN:HB2	5:A:1076:HOH:O	2.19	0.42
1:A:191:LYS:HD2	1:A:193:ARG:HH11	1.82	0.42
1:A:15:VAL:HA	1:A:18:LEU:CD2	2.50	0.42
1:A:197:THR:CG2	1:A:222:LEU:HB3	2.50	0.42
1:A:569:ARG:O	1:A:574:LYS:HD2	2.20	0.42
1:A:412:ASN:HD22	1:A:412:ASN:HA	1.67	0.41
1:A:576:GLN:HB2	1:A:576:GLN:HE21	1.63	0.41
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.34	0.41
1:A:229:PRO:HG3	4:A:920:CHI:H21	2.03	0.41
1:A:466:THR:OG1	1:A:467:ILE:N	2.53	0.41
1:A:484:ASN:ND2	5:A:1115:HOH:O	2.54	0.40
1:A:636:VAL:O	1:A:639:ARG:HD3	2.21	0.40
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.86	0.40
1:A:138:ARG:HD2	1:A:138:ARG:HA	1.94	0.40
1:A:693:ASP:O	1:A:696:ASN:HB2	2.22	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	808/842 (96%)	776 (96%)	31 (4%)	1 (0%)	55	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	LYS

### 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	705/730 (97%)	647 (92%)	58 (8%)	13 8

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	18	LEU
1	A	27	LEU
1	A	29	LYS
1	A	32	ASN
1	A	40	VAL
1	A	60	ARG
1	A	77	LYS
1	A	87	LEU
1	A	90	TYR
1	A	128	ASP
1	A	144	LEU
1	A	184	ARG
1	A	191	LYS
1	A	214	LYS
1	A	234	ARG
1	A	249	PRO
1	A	251	ASP
1	A	269	ARG
1	A	277	ARG
1	A	314	SER
1	A	358	ARG
1	A	384	LEU
1	A	389	VAL
1	A	394	THR
1	A	423	ASP
1	A	437	LYS
1	A	494	LEU
1	A	496	ASN
1	A	499	LEU

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Mol	Chain	Res	Type
1	A	505	GLU
1	A	506	ARG
1	A	519	ARG
1	A	538	LYS
1	A	552	GLU
1	A	554	LYS
1	A	555	VAL
1	A	562	LEU
1	A	568	LYS
1	A	571	HIS
1	A	576	GLN
1	A	579	ASN
1	A	583	VAL
1	A	586	LEU
1	A	601	ARG
1	A	613	TYR
1	A	701	GLU
1	A	708	PHE
1	A	721	LEU
1	A	746	SER
1	A	753	LYS
1	A	759	LYS
1	A	793	ASN
1	A	795	ARG
1	A	812	SER
1	A	813	SER
1	A	831	ARG
1	A	833	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	36	HIS
1	A	106	ASN
1	A	201	HIS
1	A	250	ASN
1	A	412	ASN
1	A	450	HIS
1	A	484	ASN
1	A	496	ASN
1	A	517	GLN

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Mol	Chain	Res	Type
1	A	539	GLN
1	A	541	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	588	ASN
1	A	632	HIS
1	A	684	ASN
1	A	744	GLN
1	A	793	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	SEP	A	14	1	9,9,10	1.37	2 (22%)	9,12,14	5.27	2 (22%)

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
1	SEP	A	14	1	-	0/5/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	SEP	P-O2P	2.08	1.63	1.54
1	A	14	SEP	CA-C	2.62	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	SEP	O3P-P-O1P	2.55	120.49	110.50
1	A	14	SEP	OG-CB-CA	15.40	123.35	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	14	SEP	1	0

## 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	$\# Z  > 2$
4	CHI	A	920	-	32,34,34	3.38	20 (62%)	43,48,48	2.49	16 (37%)
2	GLC	A	998	-	12,12,12	1.32	1 (8%)	17,17,17	0.90	0
3	PLP	A	999	1	15,15,16	1.49	3 (20%)	20,22,23	1.03	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHI	A	920	-	-	0/17/30/30	0/4/4/4
2	GLC	A	998	-	-	0/2/22/22	0/1/1/1
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	920	CHI	C1-CL1	-3.95	1.65	1.74
3	A	999	PLP	C3-C2	-2.43	1.39	1.40
4	A	920	CHI	C4-N1	-2.33	1.31	1.39
4	A	920	CHI	C10-N2	2.03	1.50	1.45
3	A	999	PLP	C5A-C5	2.18	1.57	1.50
4	A	920	CHI	C10-C11	2.26	1.57	1.53
4	A	920	CHI	C9-N2	2.39	1.39	1.34
4	A	920	CHI	C11-N3	2.47	1.38	1.34
4	A	920	CHI	C20-C19	2.52	1.43	1.38
4	A	920	CHI	C13-C14	2.71	1.58	1.51
2	A	998	GLC	C4-C5	2.87	1.59	1.53
3	A	999	PLP	C4A-C4	2.92	1.57	1.51
4	A	920	CHI	C23-C18	3.13	1.45	1.38
4	A	920	CHI	C17-C10	3.37	1.62	1.54
4	A	920	CHI	C12-N3	3.46	1.53	1.47
4	A	920	CHI	C22-C21	3.51	1.44	1.37
4	A	920	CHI	C19-C18	3.73	1.46	1.38
4	A	920	CHI	C16-N3	3.85	1.53	1.47
4	A	920	CHI	C3-C2	4.74	1.46	1.36
4	A	920	CHI	C3-C4	4.85	1.50	1.41
4	A	920	CHI	C20-C21	4.92	1.46	1.37
4	A	920	CHI	C7-C8	6.41	1.51	1.39
4	A	920	CHI	C6-C1	6.61	1.49	1.36
4	A	920	CHI	O2-C11	8.05	1.36	1.22

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	920	CHI	C1-C6-C5	-7.78	113.87	119.18
4	A	920	CHI	C2-C3-C4	-4.95	114.77	120.84
4	A	920	CHI	O1-C9-C8	-4.36	111.79	121.13
4	A	920	CHI	C16-N3-C11	-4.27	107.62	123.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	920	CHI	C8-C7-C5	-3.55	102.12	106.55
4	A	920	CHI	O2-C11-N3	-3.08	118.00	121.68
4	A	920	CHI	O2-C11-C10	-2.56	114.98	119.65
4	A	920	CHI	C12-N3-C11	-2.55	113.95	123.28
4	A	920	CHI	C17-C18-C23	-2.50	115.86	120.91
4	A	920	CHI	C2-C1-CL1	-2.25	115.80	119.35
4	A	920	CHI	C3-C4-N1	-2.13	124.59	130.78
4	A	920	CHI	C6-C5-C4	2.14	122.86	119.87
4	A	920	CHI	C2-C1-C6	2.17	124.81	121.98
3	A	999	PLP	O3P-P-O1P	2.46	120.12	110.50
4	A	920	CHI	C8-N1-C4	3.44	111.55	104.47
4	A	920	CHI	C8-C9-N2	4.20	123.76	115.20
4	A	920	CHI	C10-C11-N3	5.21	127.00	118.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	920	CHI	3	0

## 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.