



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:44 PM GMT

PDB ID : 1C8L  
Title : SYNERGISTIC INHIBITION OF GLYCOGEN PHOSPHORYLASE A BY A  
POTENTIAL ANTIDIABETIC DRUG AND CAFFEINE  
Authors : Tsitsanou, K.E.; Skamnaki, V.T.; Oikonomakos, N.G.  
Deposited on : 2000-05-16  
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](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.

---

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

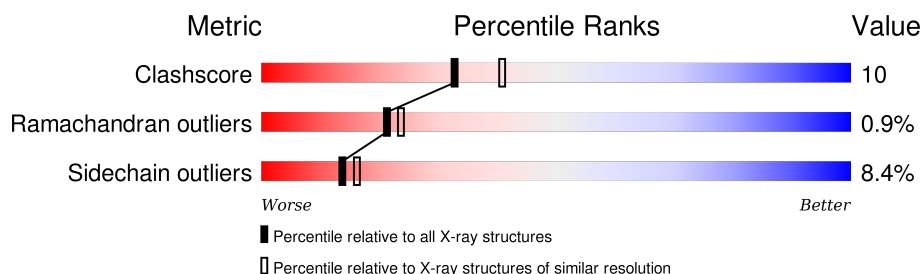
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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  $\geq 3$ , 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	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7378 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.

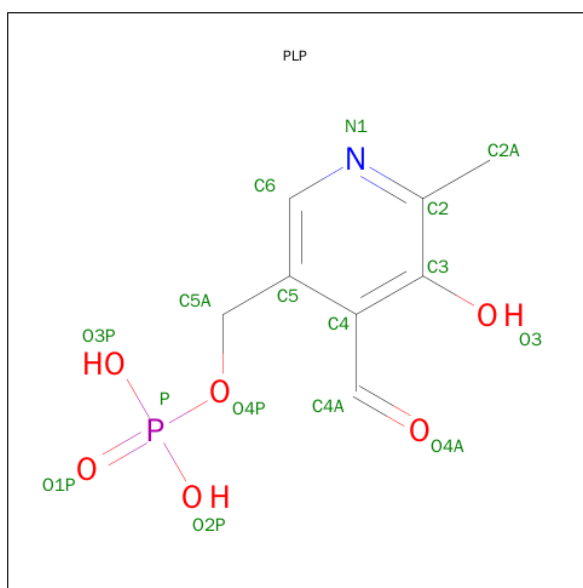
- Molecule 1 is a protein called PROTEIN (GLYCOGEN PHOSPHORYLASE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	812	6611	4208	1167	1206	1	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

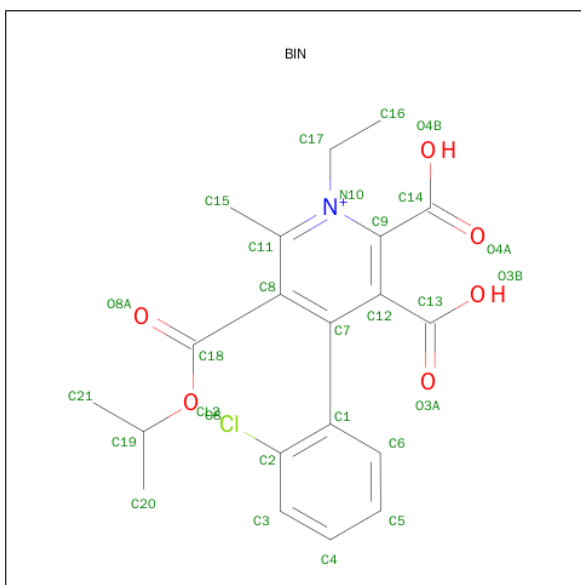
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SEP	SER	MODIFIED RESIDUE	UNP P00489

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



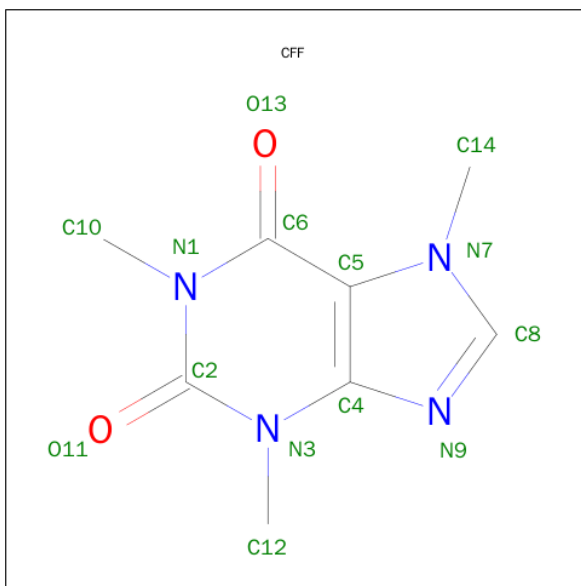
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

- Molecule 3 is 2,3-DICARBOXY-4-(2-CHLORO-PHENYL)-1-ETHYL-5-ISOPROPOXYCARBONYL-6-METHYL-PYRIDINIUM (three-letter code: BIN) (formula:  $C_{20}H_{21}ClNO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			28	20	1	1	6		

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula:  $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	4	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



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

- Molecule 6 is water.

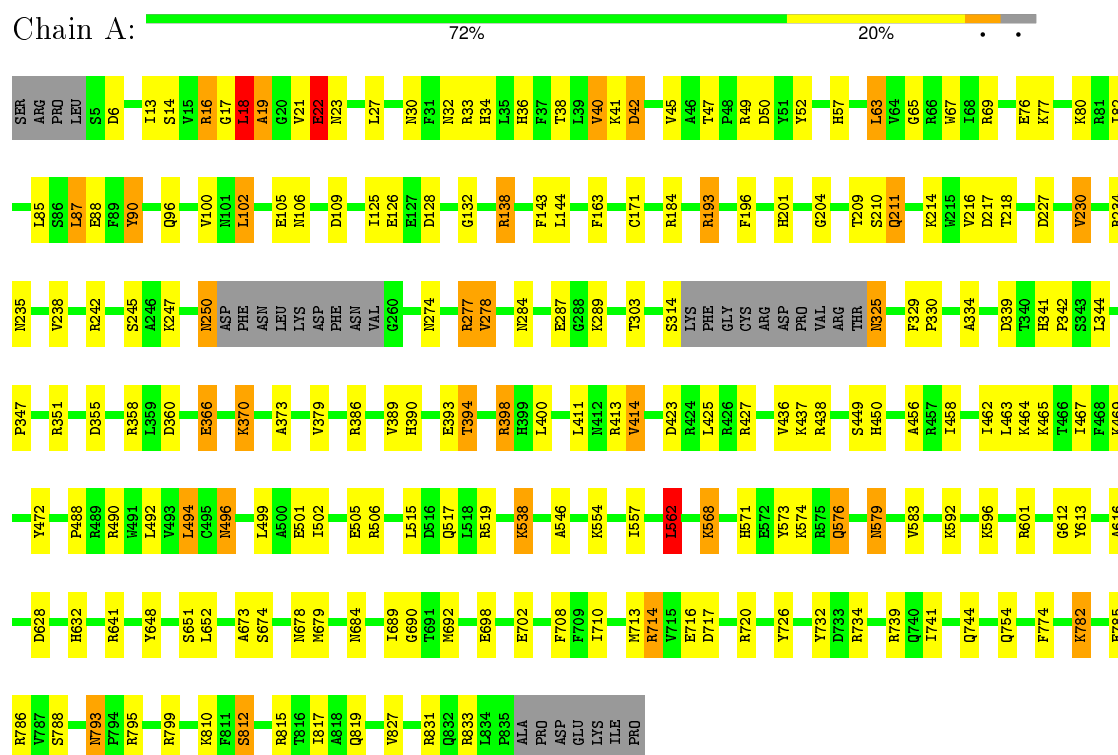
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	704	Total	O	0	0
			704	704		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: PROTEIN (GLYCOGEN PHOSPHORYLASE)



## 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, $\alpha$ , $\beta$ , $\gamma$	126.69 Å   126.69 Å   115.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	26.50 – 2.30	Depositor
% Data completeness (in resolution range)	98.4 (26.50-2.30)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.210 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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: BIN, GOL, PLP, CFF, 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	0/6746	0.64	2/9123 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LEU	CA-CB-CG	8.33	134.47	115.30
1	A	562	LEU	CA-CB-CG	6.17	129.48	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	6611	0	6554	137	0
2	A	15	0	7	0	0
3	A	28	0	19	2	0
4	A	14	0	10	2	0
5	A	6	0	8	1	0
6	A	704	0	0	15	0
All	All	7378	0	6598	138	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 (138) 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:18:LEU:CD2	1:A:19:ALA:H	1.58	1.17
1:A:18:LEU:HD22	1:A:19:ALA:N	1.60	1.15
1:A:211:GLN:HB3	1:A:358:ARG:NH2	1.76	1.01
1:A:18:LEU:HD22	1:A:19:ALA:H	0.80	0.96
1:A:250:ASN:HD22	1:A:250:ASN:H	1.10	0.94
1:A:389:VAL:O	1:A:393:GLU:HG2	1.69	0.91
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.33	0.90
1:A:211:GLN:HB3	1:A:358:ARG:HH21	1.43	0.81
1:A:63:LEU:HD13	1:A:102:LEU:HD21	1.63	0.81
1:A:250:ASN:H	1:A:250:ASN:ND2	1.77	0.80
1:A:714:ARG:HD3	6:A:1233:HOH:O	1.83	0.77
1:A:393:GLU:OE1	6:A:1561:HOH:O	2.05	0.74
1:A:325:ASN:HB3	6:A:1544:HOH:O	1.88	0.74
1:A:82:ILE:HD11	1:A:827:VAL:HG11	1.69	0.73
1:A:250:ASN:HD22	1:A:250:ASN:N	1.81	0.72
1:A:250:ASN:ND2	1:A:250:ASN:N	2.36	0.72
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.53	0.72
1:A:138:ARG:O	1:A:138:ARG:HD3	1.88	0.72
1:A:390:HIS:O	1:A:394:THR:HG23	1.89	0.72
1:A:464:LYS:HG2	1:A:472:TYR:CD1	2.26	0.71
1:A:413:ARG:HD2	6:A:1674:HOH:O	1.93	0.68
1:A:568:LYS:HD3	1:A:574:LYS:HD3	1.75	0.68
1:A:314:SER:HA	6:A:1662:HOH:O	1.92	0.68
1:A:786:ARG:HD3	6:A:1363:HOH:O	1.93	0.67
1:A:506:ARG:HH11	1:A:506:ARG:HG2	1.61	0.66
1:A:18:LEU:HD22	1:A:19:ALA:CB	2.25	0.65
1:A:19:ALA:HB1	1:A:30:ASN:ND2	2.12	0.65
1:A:16:ARG:HG3	1:A:17:GLY:H	1.66	0.61
1:A:171:CYS:SG	6:A:1699:HOH:O	2.37	0.60
1:A:36:HIS:HB3	6:A:1694:HOH:O	2.00	0.60
1:A:386:ARG:HD3	6:A:1427:HOH:O	2.02	0.59
1:A:732:TYR:O	1:A:739:ARG:HG3	2.01	0.59
1:A:351:ARG:O	1:A:355:ASP:HB2	2.04	0.58
1:A:562:LEU:C	1:A:562:LEU:HD12	2.24	0.58
1:A:163:PHE:HB2	1:A:278:VAL:HG13	1.86	0.57
1:A:138:ARG:HB3	6:A:1034:HOH:O	2.03	0.57
1:A:414:VAL:HG22	1:A:425:LEU:CD2	2.35	0.57
1:A:810:LYS:O	1:A:810:LYS:HG3	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HD22	1:A:812:SER:HB2	1.87	0.57
1:A:344:LEU:C	1:A:347:PRO:HD2	2.24	0.57
1:A:414:VAL:HG22	1:A:425:LEU:HD23	1.86	0.56
1:A:36:HIS:O	1:A:40:VAL:HA	2.05	0.56
1:A:18:LEU:HD22	1:A:19:ALA:CA	2.34	0.55
1:A:36:HIS:CE1	1:A:42:ASP:HA	2.42	0.55
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.11	0.54
1:A:502:ILE:HA	1:A:505:GLU:HG2	1.89	0.54
1:A:734:ARG:HD2	6:A:1257:HOH:O	2.08	0.53
1:A:67:TRP:HA	1:A:238:VAL:HB	1.90	0.53
1:A:393:GLU:HB3	1:A:400:LEU:HD23	1.92	0.52
1:A:128:ASP:OD1	1:A:651:SER:HB3	2.10	0.52
1:A:52:TYR:CZ	1:A:126:GLU:HB2	2.45	0.52
1:A:436:VAL:O	1:A:438:ARG:HG3	2.10	0.51
1:A:14:SEP:HB2	1:A:16:ARG:HG2	1.92	0.51
1:A:678:ASN:OD1	1:A:679:MET:HG3	2.11	0.51
1:A:21:VAL:C	1:A:22:GLU:HG2	2.31	0.51
1:A:366:GLU:HG3	1:A:370:LYS:HD2	1.93	0.51
1:A:274:ASN:OD1	1:A:277:ARG:HD2	2.11	0.51
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.11	0.50
1:A:344:LEU:O	1:A:347:PRO:HD2	2.11	0.50
1:A:501:GLU:HG3	1:A:502:ILE:N	2.27	0.50
1:A:571:HIS:H	1:A:576:GLN:HE22	1.60	0.49
1:A:230:VAL:HG22	1:A:230:VAL:O	2.11	0.49
1:A:538:LYS:NZ	1:A:684:ASN:O	2.45	0.49
1:A:450:HIS:HD2	6:A:1202:HOH:O	1.96	0.49
1:A:138:ARG:C	1:A:138:ARG:HD3	2.30	0.49
1:A:373:ALA:HA	1:A:449:SER:HB3	1.95	0.48
1:A:34:HIS:CE1	1:A:57:HIS:HB3	2.48	0.48
1:A:612:GLY:C	4:A:940:CFF:H142	2.34	0.48
1:A:613:TYR:CD2	1:A:616:ALA:HB2	2.49	0.47
1:A:184:ARG:NH2	6:A:1087:HOH:O	2.47	0.47
1:A:204:GLY:HA2	1:A:217:ASP:O	2.14	0.47
1:A:795:ARG:O	1:A:799:ARG:HG3	2.14	0.47
1:A:689:ILE:HG23	1:A:689:ILE:O	2.15	0.47
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.96	0.47
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.94	0.47
1:A:628:ASP:O	1:A:632:HIS:HD2	1.97	0.47
1:A:143:PHE:CG	1:A:817:ILE:HD11	2.49	0.47
1:A:456:ALA:HB2	1:A:674:SER:HB2	1.97	0.47
1:A:414:VAL:CG2	1:A:425:LEU:HD23	2.43	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HH11	1:A:398:ARG:CG	2.14	0.47
1:A:235:ASN:HA	1:A:833:ARG:HG2	1.97	0.47
1:A:793:ASN:C	1:A:793:ASN:HD22	2.17	0.47
1:A:458:ILE:O	1:A:462:ILE:HG13	2.15	0.46
1:A:355:ASP:OD2	1:A:398:ARG:NE	2.45	0.46
1:A:716:GLU:CD	1:A:716:GLU:H	2.17	0.46
1:A:698:GLU:O	1:A:702:GLU:HG2	2.16	0.46
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.97	0.46
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.45	0.46
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.98	0.46
1:A:214:LYS:HE2	1:A:216:VAL:HG12	1.98	0.45
1:A:47:THR:O	1:A:50:ASP:HB2	2.17	0.45
1:A:227:ASP:CG	1:A:242:ARG:HH21	2.19	0.45
1:A:579:ASN:O	1:A:583:VAL:HG13	2.17	0.45
1:A:490:ARG:HA	1:A:494:LEU:HB2	1.97	0.45
1:A:546:ALA:HA	1:A:557:ILE:HD11	1.99	0.45
1:A:690:GLY:O	1:A:710:ILE:HA	2.17	0.45
1:A:65:GLY:O	1:A:69:ARG:HD3	2.17	0.44
1:A:568:LYS:CD	1:A:574:LYS:HD3	2.46	0.44
1:A:562:LEU:HG	1:A:601:ARG:HG2	1.99	0.44
1:A:496:ASN:HB2	1:A:684:ASN:ND2	2.32	0.44
1:A:18:LEU:CD2	1:A:19:ALA:N	2.43	0.44
1:A:517:GLN:HE21	1:A:517:GLN:HB3	1.63	0.44
1:A:741:ILE:HA	1:A:744:GLN:NE2	2.26	0.44
1:A:815:ARG:O	1:A:819:GLN:HG3	2.18	0.43
1:A:465:LYS:O	1:A:469:LYS:HD3	2.17	0.43
1:A:90:TYR:HE1	6:A:1529:HOH:O	2.01	0.43
1:A:782:LYS:O	1:A:785:GLU:HB2	2.19	0.43
1:A:18:LEU:CG	1:A:19:ALA:H	2.16	0.43
1:A:411:LEU:HA	1:A:414:VAL:HG13	2.01	0.42
1:A:571:HIS:CE1	4:A:940:CFF:C12	3.02	0.42
1:A:40:VAL:O	1:A:41:LYS:HG2	2.19	0.42
1:A:227:ASP:OD2	1:A:242:ARG:NH2	2.42	0.42
1:A:423:ASP:O	1:A:427:ARG:HG3	2.19	0.42
1:A:673:ALA:HB3	5:A:998:GOL:C1	2.50	0.42
1:A:579:ASN:HD22	1:A:579:ASN:C	2.22	0.41
1:A:193:ARG:NH1	3:A:930:BIN:CL2	2.90	0.41
1:A:100:VAL:HG11	1:A:494:LEU:HD12	2.03	0.41
1:A:554:LYS:HA	1:A:554:LYS:HD3	1.86	0.41
1:A:506:ARG:CG	1:A:506:ARG:HH11	2.29	0.41
1:A:34:HIS:O	1:A:38:THR:HB	2.19	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.02	0.41
1:A:42:ASP:OD1	1:A:45:VAL:HG22	2.20	0.41
1:A:201:HIS:HD2	1:A:218:THR:OG1	2.02	0.41
1:A:106:ASN:HA	1:A:106:ASN:HD22	1.62	0.41
1:A:562:LEU:C	1:A:562:LEU:CD1	2.89	0.41
1:A:576:GLN:HB2	1:A:576:GLN:HE21	1.61	0.41
1:A:720:ARG:HG2	6:A:1436:HOH:O	2.20	0.41
1:A:648:TYR:HA	1:A:652:LEU:HD23	2.03	0.41
1:A:678:ASN:OD1	1:A:679:MET:N	2.53	0.41
1:A:287:GLU:HG2	1:A:289:LYS:HG2	2.03	0.41
1:A:488:PRO:O	1:A:492:LEU:HB3	2.21	0.41
1:A:88:GLU:HB3	1:A:132:GLY:HA2	2.02	0.40
3:A:930:BIN:H171	3:A:930:BIN:H151	1.90	0.40
1:A:85:LEU:HD11	1:A:303:THR:HG21	2.03	0.40
1:A:49:ARG:HA	1:A:125:ILE:HG21	2.02	0.40
1:A:105:GLU:O	1:A:109:ASP:HB2	2.22	0.40
1:A:19:ALA:HB1	1:A:30:ASN:HD21	1.85	0.40
1:A:692:MET:HG2	1:A:710:ILE:HG21	2.02	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%)	767 (95%)	31 (4%)	7 (1%)	21 24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	22	GLU
1	A	6	ASP

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	19	ALA
1	A	339	ASP
1	A	13	ILE
1	A	40	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	702/730 (96%)	643 (92%)	59 (8%)	14	16

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	22	GLU
1	A	23	ASN
1	A	27	LEU
1	A	32	ASN
1	A	33	ARG
1	A	42	ASP
1	A	63	LEU
1	A	76	GLU
1	A	77	LYS
1	A	87	LEU
1	A	90	TYR
1	A	96	GLN
1	A	102	LEU
1	A	138	ARG
1	A	144	LEU
1	A	193	ARG
1	A	196	PHE
1	A	209	THR
1	A	210	SER
1	A	211	GLN
1	A	230	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	234	ARG
1	A	245	SER
1	A	247	LYS
1	A	250	ASN
1	A	277	ARG
1	A	278	VAL
1	A	284	ASN
1	A	325	ASN
1	A	360	ASP
1	A	366	GLU
1	A	370	LYS
1	A	379	VAL
1	A	394	THR
1	A	398	ARG
1	A	414	VAL
1	A	437	LYS
1	A	494	LEU
1	A	496	ASN
1	A	499	LEU
1	A	519	ARG
1	A	538	LYS
1	A	562	LEU
1	A	568	LYS
1	A	573	TYR
1	A	576	GLN
1	A	579	ASN
1	A	592	LYS
1	A	596	LYS
1	A	641	ARG
1	A	708	PHE
1	A	714	ARG
1	A	754	GLN
1	A	782	LYS
1	A	788	SER
1	A	793	ASN
1	A	812	SER
1	A	831	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	57	HIS
1	A	71	GLN
1	A	72	GLN
1	A	106	ASN
1	A	201	HIS
1	A	250	ASN
1	A	282	ASN
1	A	325	ASN
1	A	408	GLN
1	A	412	ASN
1	A	450	HIS
1	A	484	ASN
1	A	496	ASN
1	A	517	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	8,9,10	1.14	1 (12%)	8,12,14	4.43	2 (25%)

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	-	0/6/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	SEP	P-O2P	2.52	1.63	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	SEP	OG-CB-CA	-11.99	98.04	108.27
1	A	14	SEP	O3P-P-O1P	2.78	119.53	110.58

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](#)

4 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	BIN	A	930	-	21,29,29	6.93	14 (66%)	25,42,42	3.21	11 (44%)
4	CFF	A	940	-	8,15,15	1.82	4 (50%)	8,23,23	1.06	0
5	GOL	A	998	-	5,5,5	0.18	0	5,5,5	0.58	0
2	PLP	A	999	1	15,15,16	1.86	4 (26%)	21,22,23	1.15	1 (4%)

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	BIN	A	930	-	-	0/14/22/22	0/2/2/2
4	CFF	A	940	-	-	0/0/0/0	0/2/2/2
5	GOL	A	998	-	-	0/4/4/4	0/0/0/0
2	PLP	A	999	1	-	0/6/6/8	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	PLP	C3-C2	-4.41	1.37	1.40
3	A	930	BIN	C2-CL2	-2.33	1.67	1.73
4	A	940	CFF	C6-C5	2.05	1.44	1.41
4	A	940	CFF	O13-C6	2.06	1.29	1.24
2	A	999	PLP	P-O2P	2.11	1.62	1.54
3	A	930	BIN	C17-N10	2.17	1.52	1.47
2	A	999	PLP	C5A-C5	2.26	1.57	1.50
4	A	940	CFF	C6-N1	2.36	1.41	1.38
4	A	940	CFF	C4-N3	2.95	1.42	1.39
2	A	999	PLP	C4A-C4	3.39	1.58	1.51
3	A	930	BIN	C5-C6	4.46	1.48	1.38
3	A	930	BIN	C3-C2	4.64	1.49	1.39
3	A	930	BIN	C8-C18	5.14	1.63	1.50
3	A	930	BIN	O8-C19	5.41	1.60	1.47
3	A	930	BIN	C4-C3	6.13	1.51	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	930	BIN	C6-C1	6.62	1.51	1.39
3	A	930	BIN	C12-C9	6.73	1.49	1.41
3	A	930	BIN	C12-C7	7.35	1.55	1.41
3	A	930	BIN	C1-C2	8.92	1.57	1.40
3	A	930	BIN	C1-C7	10.54	1.63	1.50
3	A	930	BIN	C11-N10	12.65	1.55	1.35
3	A	930	BIN	C7-C8	19.13	1.70	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	930	BIN	C1-C7-C12	-9.99	105.24	120.26
3	A	930	BIN	C1-C7-C8	-6.74	110.71	120.80
3	A	930	BIN	C15-C11-N10	-3.57	116.88	119.92
3	A	930	BIN	C7-C8-C18	-2.76	115.33	120.43
3	A	930	BIN	C6-C1-C2	-2.69	113.93	117.50
3	A	930	BIN	C17-N10-C11	-2.40	117.72	119.39
3	A	930	BIN	C19-O8-C18	2.52	121.74	117.61
3	A	930	BIN	C5-C4-C3	2.56	123.94	120.19
3	A	930	BIN	C6-C1-C7	3.11	126.12	118.56
2	A	999	PLP	O3P-P-O1P	3.15	120.74	110.58
3	A	930	BIN	C15-C11-C8	4.61	128.16	122.68
3	A	930	BIN	C16-C17-N10	4.74	122.35	111.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	930	BIN	2	0
4	A	940	CFF	2	0
5	A	998	GOL	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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.