



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:14 am BST

PDB ID : 1CJ0  
Title : CRYSTAL STRUCTURE OF RABBIT CYTOSOLIC SERINE HYDROXY  
METHYLTRANSFERASE AT 2.8 ANGSTROM RESOLUTION  
Authors : Scarsdale, J.N.; Kazanina, G.; Radaev, S.; Schirch, V.; Wright, H.T.  
Deposited on : 1999-04-20  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

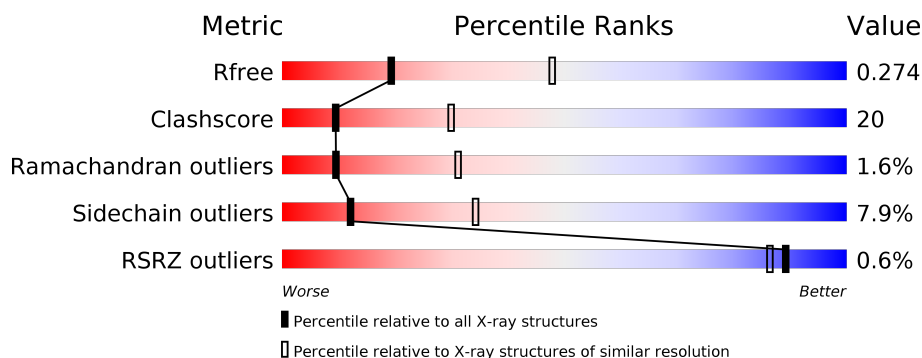
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>63%</span> <span>31%</span> <span>5% ..</span> </div> </div>
1	B	470	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span></span> <span>70%</span> <span>25%</span> <span>.. ..</span> </div> </div>

## 2 Entry composition [i](#)

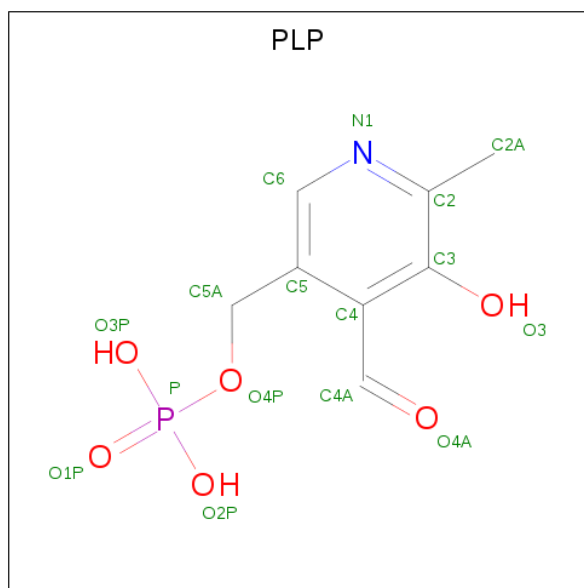
There are 3 unique types of molecules in this entry. The entry contains 7024 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (SERINE HYDROXYMETHYLTRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3494	2196	615	665	18			
1	B	466	Total	C	N	O	S	0	0	0
			3488	2186	614	670	18			

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

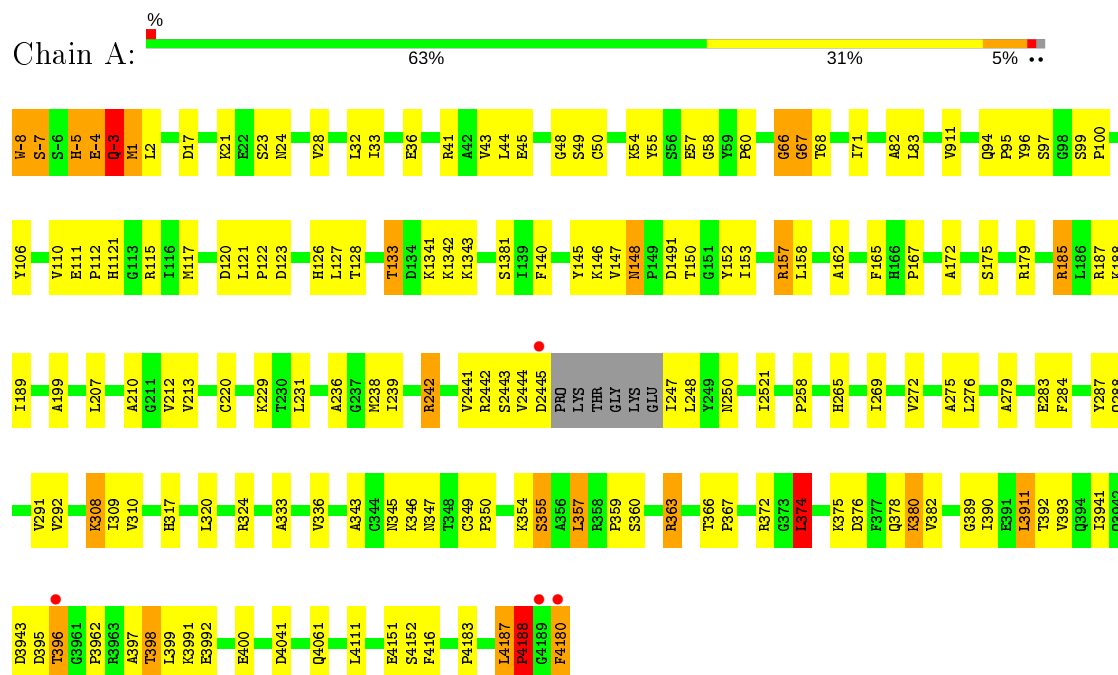
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	4	Total 4	O 4	0	0

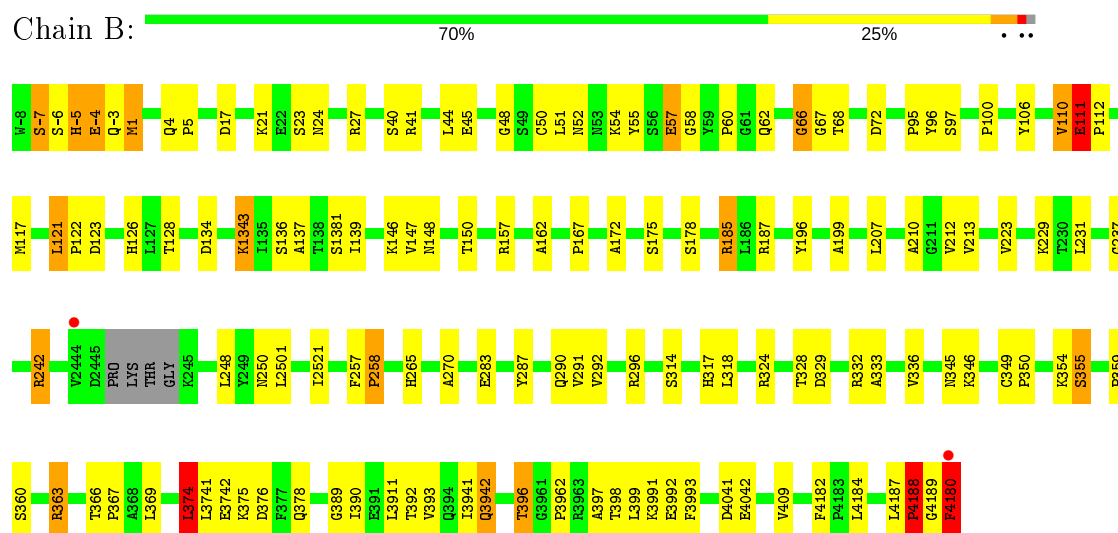
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

#### • Molecule 1: PROTEIN (SERINE HYDROXYMETHYLTRANSFERASE)



#### • Molecule 1: PROTEIN (SERINE HYDROXYMETHYLTRANSFERASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.38Å 116.38Å 165.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.98 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.80) 98.7 (19.98-2.61)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.59Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.214 , 0.280 0.207 , 0.274	Depositor DCC
$R_{free}$ test set	3531 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.77	6/3565 (0.2%)	0.93	7/4839 (0.1%)
1	B	0.76	5/3558 (0.1%)	0.93	7/4831 (0.1%)
All	All	0.76	11/7123 (0.2%)	0.93	14/9670 (0.1%)

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	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4180	PHE	CE1-CZ	7.58	1.51	1.37
1	B	4180	PHE	CE2-CZ	6.23	1.49	1.37
1	A	4180	PHE	N-CA	6.15	1.58	1.46
1	B	4180	PHE	C-OXT	5.95	1.34	1.23
1	B	4180	PHE	CE1-CZ	5.81	1.48	1.37
1	A	4180	PHE	C-OXT	5.66	1.34	1.23
1	A	4180	PHE	CD2-CE2	5.66	1.50	1.39
1	B	4180	PHE	CG-CD1	5.50	1.47	1.38
1	A	4180	PHE	CD1-CE1	5.48	1.50	1.39
1	A	4180	PHE	CG-CD2	5.44	1.47	1.38
1	B	4180	PHE	CD1-CE1	5.01	1.49	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	-7	SER	N-CA-C	-6.43	93.65	111.00
1	B	66	GLY	N-CA-C	6.03	128.18	113.10
1	A	66	GLY	N-CA-C	5.61	127.12	113.10
1	B	374	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	-3	GLN	N-CA-C	-5.47	96.23	111.00
1	B	-7	SER	N-CA-C	-5.45	96.28	111.00
1	B	-5	HIS	N-CA-C	-5.39	96.45	111.00
1	A	1	MET	N-CA-C	-5.32	96.64	111.00
1	B	1	MET	N-CA-C	-5.29	96.70	111.00
1	A	374	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	3962	PRO	N-CA-CB	5.21	109.55	103.30
1	B	111	GLU	C-N-CD	5.13	139.18	128.40
1	B	110	VAL	N-CA-C	-5.12	97.17	111.00
1	A	-5	HIS	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	4180	PHE	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3494	0	3355	164	1
1	B	3488	0	3316	128	0
2	A	15	0	6	2	0
2	B	15	0	6	1	0
3	A	8	0	0	0	0
3	B	4	0	0	1	0
All	All	7024	0	6683	268	1

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 20.

All (268) 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:23:SER:HB2	1:A:4180:PHE:C	1.48	1.33
1:B:398:THR:HG22	1:B:3991:LYS:H	1.21	1.04
1:A:212:VAL:HG11	1:A:292:VAL:HG21	1.42	1.00
1:A:308:LYS:HE3	1:A:308:LYS:HA	1.44	0.99
1:A:23:SER:CB	1:A:4180:PHE:C	2.32	0.98
1:A:23:SER:HB2	1:A:4180:PHE:OXT	1.62	0.97
1:B:212:VAL:HG11	1:B:292:VAL:HG21	1.46	0.93
1:A:123:ASP:OD2	1:A:146:LYS:HB3	1.69	0.92
1:B:389:GLY:O	1:B:392:THR:HG23	1.70	0.90
1:A:50:CYS:H	1:B:4180:PHE:HE2	1.20	0.89
1:A:389:GLY:O	1:A:392:THR:HG23	1.73	0.88
1:A:4187:LEU:HB3	1:A:4188:PRO:HD2	1.56	0.87
1:A:50:CYS:N	1:B:4180:PHE:HE2	1.73	0.85
1:B:290:GLN:NE2	1:B:3741:LEU:HD13	1.91	0.85
1:A:336:VAL:HB	1:A:392:THR:HG22	1.60	0.84
1:A:133:THR:HG22	1:A:1341:LYS:H	1.41	0.84
1:A:41:ARG:HG3	1:A:4187:LEU:HD23	1.58	0.83
1:B:52:ASN:HB3	3:B:509:HOH:O	1.78	0.83
1:A:242:ARG:HH11	1:A:242:ARG:HG3	1.45	0.81
1:A:23:SER:HB3	1:B:50:CYS:SG	2.21	0.81
1:A:133:THR:CG2	1:A:1341:LYS:H	1.94	0.79
1:A:336:VAL:CB	1:A:392:THR:HG22	2.13	0.79
1:B:3941:ILE:O	1:B:396:THR:HB	1.82	0.78
1:A:23:SER:HB2	1:A:4180:PHE:O	1.83	0.77
1:A:346:LYS:HD2	1:A:359:PRO:HG3	1.66	0.77
1:B:346:LYS:HD2	1:B:359:PRO:HG3	1.67	0.77
1:A:148:ASN:HD22	1:A:1491:ASP:H	1.31	0.77
1:B:336:VAL:HB	1:B:392:THR:HG22	1.68	0.76
1:B:126:HIS:CD2	1:B:128:THR:H	2.04	0.76
1:A:133:THR:HG22	1:A:1341:LYS:N	2.01	0.75
1:B:336:VAL:CB	1:B:392:THR:HG22	2.17	0.75
1:B:242:ARG:HG3	1:B:242:ARG:HH11	1.52	0.75
1:B:398:THR:HG22	1:B:3991:LYS:N	2.00	0.74
1:A:4187:LEU:HB3	1:A:4188:PRO:CD	2.17	0.74
1:A:287:TYR:O	1:A:291:VAL:HG23	1.87	0.73
1:B:117:MET:HE3	1:B:167:PRO:HG3	1.70	0.73
1:B:95:PRO:HD2	1:B:237:GLY:O	1.89	0.73
1:A:23:SER:CB	1:A:4180:PHE:O	2.38	0.71
1:A:3911:LEU:O	1:A:3941:ILE:HG13	1.90	0.71
1:A:3941:ILE:O	1:A:396:THR:HB	1.90	0.71
1:B:146:LYS:HB3	1:B:146:LYS:HZ3	1.56	0.71
1:B:123:ASP:OD2	1:B:146:LYS:HB3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:LYS:HD3	1:A:1381:SER:O	1.91	0.70
1:A:308:LYS:CE	1:A:309:ILE:H	2.04	0.70
1:A:97:SER:OG	1:B:265:HIS:HE1	1.76	0.69
1:A:99:SER:HB2	1:A:100:PRO:HD3	1.75	0.69
1:A:185:ARG:HH11	1:A:185:ARG:HG3	1.58	0.68
1:A:97:SER:OG	1:B:265:HIS:CE1	2.46	0.68
1:A:308:LYS:HE2	1:A:309:ILE:H	1.58	0.67
1:B:290:GLN:NE2	1:B:3741:LEU:CD1	2.58	0.66
1:B:398:THR:HB	1:B:3992:GLU:HG3	1.78	0.66
1:A:-8:TRP:CE3	1:A:-7:SER:N	2.64	0.66
1:A:41:ARG:HG3	1:A:4187:LEU:CD2	2.27	0.65
1:B:398:THR:CG2	1:B:3991:LYS:H	2.02	0.65
1:A:126:HIS:HD2	1:A:128:THR:OG1	1.79	0.65
1:A:212:VAL:CG1	1:A:292:VAL:HG21	2.22	0.65
1:A:50:CYS:SG	1:B:23:SER:HB3	2.37	0.65
1:A:66:GLY:O	1:A:68:THR:N	2.31	0.64
1:B:-4:GLU:O	1:B:1:MET:N	2.31	0.63
1:A:54:LYS:HE2	1:A:67:GLY:O	1.99	0.63
1:B:-4:GLU:HG2	1:B:-4:GLU:O	1.97	0.63
1:B:117:MET:HG3	1:B:167:PRO:HB3	1.80	0.63
1:A:150:THR:HB	1:A:152:TYR:HD2	1.63	0.62
1:B:148:ASN:HB3	1:B:150:THR:OG1	2.00	0.62
1:A:242:ARG:NH1	1:A:242:ARG:HG3	2.11	0.62
1:A:28:VAL:HB	1:A:4151:GLU:HB3	1.82	0.62
1:B:1343:LYS:HG2	1:B:1381:SER:O	2.00	0.61
1:A:212:VAL:HG11	1:A:292:VAL:CG2	2.24	0.61
1:A:308:LYS:CE	1:A:308:LYS:HA	2.26	0.61
1:A:145:TYR:CG	1:A:158:LEU:HD13	2.36	0.60
1:A:41:ARG:O	1:A:45:GLU:HG3	2.02	0.60
1:A:188:LYS:NZ	1:A:188:LYS:HB3	2.16	0.60
1:A:374:LEU:HD23	1:A:374:LEU:H	1.65	0.59
1:B:96:TYR:O	1:B:97:SER:HB2	2.01	0.59
1:A:398:THR:CG2	1:A:399:LEU:N	2.65	0.59
1:B:126:HIS:HD2	1:B:128:THR:H	1.50	0.59
1:A:106:TYR:O	1:A:110:VAL:O	2.19	0.59
1:A:308:LYS:CA	1:A:308:LYS:HE3	2.25	0.59
1:A:126:HIS:CD2	1:A:128:THR:H	2.21	0.59
1:A:376:ASP:O	1:A:380:LYS:HB3	2.03	0.58
1:A:50:CYS:HB3	1:B:4180:PHE:CZ	2.38	0.58
1:A:333:ALA:HA	1:A:392:THR:HG21	1.85	0.58
1:A:283:GLU:HB3	1:B:-4:GLU:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:HIS:NE2	1:B:128:THR:HG23	2.19	0.58
1:A:111:GLU:HB3	1:A:112:PRO:CD	2.34	0.58
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.68	0.57
1:B:374:LEU:HD22	1:B:4182:PHE:CE2	2.39	0.57
1:B:287:TYR:O	1:B:291:VAL:HG23	2.04	0.57
1:B:41:ARG:O	1:B:45:GLU:HG3	2.03	0.57
1:A:390:ILE:O	1:A:393:VAL:HG23	2.05	0.57
1:B:4189:GLY:O	1:B:4180:PHE:HB2	2.06	0.56
1:A:97:SER:HB3	2:A:2291:PLP:O3P	2.05	0.56
1:A:140:PHE:CE1	1:B:112:PRO:HG3	2.40	0.56
1:B:121:LEU:HB3	1:B:122:PRO:CD	2.36	0.56
1:A:-8:TRP:CD2	1:A:-7:SER:N	2.74	0.55
1:B:398:THR:CG2	1:B:399:LEU:N	2.70	0.55
1:A:345:ASN:HD21	1:A:363:ARG:NH1	2.04	0.55
1:B:157:ARG:HH11	1:B:157:ARG:HG3	1.71	0.55
1:A:148:ASN:HD22	1:A:1491:ASP:N	2.03	0.55
1:A:148:ASN:HB3	1:A:150:THR:OG1	2.07	0.55
1:A:308:LYS:HE2	1:A:309:ILE:N	2.21	0.55
1:A:50:CYS:HB3	1:B:4180:PHE:CE2	2.42	0.54
1:A:117:MET:HE1	1:A:162:ALA:HB2	1.89	0.54
1:A:147:VAL:HA	1:A:153:ILE:HA	1.89	0.54
1:A:2441:VAL:HG12	1:A:2442:ARG:N	2.23	0.54
1:B:-7:SER:C	1:B:-5:HIS:H	2.10	0.54
1:A:363:ARG:HG2	1:A:363:ARG:HH11	1.71	0.54
1:B:117:MET:HE1	1:B:162:ALA:HB2	1.89	0.54
1:A:366:THR:N	1:A:367:PRO:HD3	2.23	0.53
1:A:239:ILE:HG21	1:A:2521:ILE:HD13	1.90	0.53
1:A:366:THR:N	1:A:367:PRO:CD	2.72	0.53
1:B:242:ARG:NH1	1:B:242:ARG:HG3	2.20	0.53
1:B:106:TYR:O	1:B:110:VAL:O	2.27	0.52
1:B:212:VAL:CG1	1:B:292:VAL:HG21	2.31	0.52
1:A:50:CYS:CB	1:B:4180:PHE:CE2	2.93	0.52
1:B:97:SER:O	1:B:100:PRO:HG2	2.08	0.52
1:B:332:ARG:HD2	1:B:3942:GLN:OE1	2.09	0.52
1:A:308:LYS:HE3	1:A:309:ILE:H	1.75	0.52
1:A:308:LYS:CE	1:A:309:ILE:N	2.72	0.52
1:A:17:ASP:O	1:A:21:LYS:HG3	2.09	0.52
1:A:2443:SER:H	1:A:247:ILE:HG23	1.74	0.52
1:B:2501:LEU:O	1:B:2521:ILE:HG13	2.09	0.52
1:B:375:LYS:HA	1:B:378:GLN:HG3	1.92	0.52
1:A:117:MET:CE	1:A:162:ALA:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PHE:CD1	1:B:258:PRO:HA	2.45	0.51
1:A:50:CYS:SG	1:B:4180:PHE:CE2	3.03	0.51
1:A:398:THR:HG22	1:A:3991:LYS:N	2.25	0.51
1:A:49:SER:HB2	1:B:4180:PHE:HD2	1.76	0.51
1:A:120:ASP:OD2	1:A:146:LYS:HE3	2.11	0.51
1:B:374:LEU:HD13	1:B:376:ASP:HB3	1.93	0.51
1:A:41:ARG:NH1	1:B:5:PRO:HG3	2.26	0.51
1:A:94:GLN:N	1:A:95:PRO:CD	2.74	0.51
1:A:1:MET:HE1	1:B:283:GLU:HB2	1.92	0.51
1:B:66:GLY:O	1:B:68:THR:N	2.40	0.51
1:A:111:GLU:HB3	1:A:112:PRO:HD2	1.93	0.50
1:A:121:LEU:HB3	1:A:122:PRO:CD	2.42	0.50
1:A:238:MET:HE3	1:A:272:VAL:CG1	2.41	0.50
1:A:363:ARG:CG	1:A:363:ARG:HH11	2.24	0.50
1:A:112:PRO:O	1:A:1121:HIS:HB2	2.10	0.50
1:A:158:LEU:HD23	1:A:189:ILE:CD1	2.42	0.50
1:A:310:VAL:HG21	1:A:320:LEU:HG	1.94	0.50
1:A:-8:TRP:CE3	1:A:-8:TRP:C	2.85	0.50
1:B:354:LYS:O	1:B:355:SER:CB	2.60	0.50
1:B:366:THR:N	1:B:367:PRO:CD	2.74	0.50
1:B:3942:GLN:O	1:B:396:THR:HG22	2.11	0.50
1:B:146:LYS:HB3	1:B:146:LYS:NZ	2.23	0.50
1:A:50:CYS:N	1:B:4180:PHE:CE2	2.59	0.50
1:A:363:ARG:HG2	1:A:363:ARG:NH1	2.27	0.50
1:A:2:LEU:HA	1:B:40:SER:HB2	1.94	0.49
1:B:333:ALA:HA	1:B:392:THR:HG21	1.92	0.49
1:A:94:GLN:N	1:A:95:PRO:HD3	2.28	0.49
1:A:336:VAL:HB	1:A:392:THR:CG2	2.38	0.49
1:A:3943:ASP:C	1:A:396:THR:H	2.15	0.49
1:B:62:GLN:HG2	1:B:62:GLN:O	2.13	0.49
1:A:317:HIS:H	1:A:317:HIS:HD1	1.60	0.48
1:B:3911:LEU:HD21	1:B:409:VAL:HG22	1.93	0.48
1:B:126:HIS:CD2	1:B:128:THR:HG23	2.49	0.48
1:A:48:GLY:O	1:B:44:LEU:HD22	2.14	0.47
1:A:4187:LEU:CB	1:A:4188:PRO:CD	2.90	0.47
1:A:380:LYS:HG2	1:A:416:PHE:CZ	2.50	0.47
1:B:185:ARG:CG	1:B:185:ARG:HH11	2.27	0.47
1:A:96:TYR:O	1:A:236:ALA:HA	2.14	0.47
1:A:133:THR:HG22	1:A:1342:LYS:H	1.78	0.47
1:A:354:LYS:O	1:A:355:SER:CB	2.63	0.47
1:A:374:LEU:HD13	1:A:376:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ASP:O	1:B:21:LYS:HG3	2.14	0.47
1:A:1:MET:CE	1:B:283:GLU:HB2	2.44	0.47
1:B:117:MET:HE3	1:B:167:PRO:CG	2.44	0.47
1:B:172:ALA:O	1:B:199:ALA:HA	2.15	0.47
1:B:328:THR:OG1	1:B:329:ASP:N	2.47	0.47
1:A:336:VAL:CG1	1:A:392:THR:HG22	2.45	0.46
1:A:265:HIS:O	1:A:269:ILE:HG13	2.16	0.46
1:A:283:GLU:HB3	1:B:-4:GLU:CG	2.46	0.46
1:A:376:ASP:O	1:A:382:VAL:HG23	2.15	0.46
1:A:380:LYS:HG2	1:A:416:PHE:CE1	2.51	0.46
1:B:374:LEU:HD22	1:B:4182:PHE:CD2	2.51	0.46
1:A:2443:SER:OG	1:A:247:ILE:HG21	2.14	0.46
1:A:398:THR:HG23	1:A:399:LEU:N	2.31	0.46
1:A:115:ARG:HB3	1:A:165:PHE:CE2	2.51	0.46
1:A:210:ALA:HB3	1:A:212:VAL:HG23	1.97	0.46
1:B:210:ALA:HB3	1:B:212:VAL:HG23	1.98	0.46
1:B:296:ARG:HG3	1:B:296:ARG:HH11	1.80	0.46
1:B:3741:LEU:HD12	1:B:3742:GLU:OE1	2.15	0.45
1:A:375:LYS:HA	1:A:378:GLN:HG3	1.99	0.45
1:A:54:LYS:HG2	1:A:71:ILE:HG13	1.97	0.45
1:A:396:THR:HG23	1:A:397:ALA:CB	2.47	0.45
1:A:172:ALA:O	1:A:199:ALA:HA	2.16	0.45
1:B:111:GLU:HB3	1:B:112:PRO:CD	2.46	0.45
1:B:345:ASN:HD21	1:B:363:ARG:NH1	2.13	0.45
1:A:3992:GLU:O	1:A:400:GLU:N	2.49	0.45
1:A:44:LEU:HD22	1:B:48:GLY:O	2.16	0.45
1:B:212:VAL:HG11	1:B:292:VAL:CG2	2.32	0.45
1:B:324:ARG:HG3	1:B:360:SER:HB3	1.99	0.45
1:B:137:ALA:HA	1:B:139:ILE:HD12	1.98	0.45
1:B:123:ASP:HB3	1:B:147:VAL:HG13	1.99	0.45
1:A:28:VAL:O	1:A:4151:GLU:HA	2.15	0.45
1:B:363:ARG:HG2	1:B:363:ARG:HH11	1.81	0.45
1:A:33:ILE:HB	1:A:36:GLU:HG3	2.00	0.44
1:B:374:LEU:HD23	1:B:374:LEU:H	1.81	0.44
1:B:366:THR:N	1:B:367:PRO:HD3	2.33	0.44
1:A:185:ARG:CG	1:A:185:ARG:NH1	2.81	0.44
1:A:207:LEU:HB3	1:A:213:VAL:HG13	2.00	0.44
1:A:-8:TRP:HE3	1:A:-8:TRP:C	2.21	0.44
1:B:207:LEU:HB3	1:B:213:VAL:HG13	2.01	0.43
1:B:27:ARG:HB2	1:B:4184:LEU:HD22	2.01	0.43
1:B:196:TYR:CE1	1:B:2501:LEU:HD21	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:VAL:CG1	1:B:392:THR:HG22	2.48	0.43
1:A:324:ARG:HG3	1:A:360:SER:HB3	2.00	0.43
1:B:51:LEU:CD1	1:B:270:ALA:HB2	2.48	0.43
1:A:23:SER:OG	1:A:4180:PHE:O	2.31	0.43
1:B:336:VAL:CG2	1:B:392:THR:HG22	2.48	0.43
1:A:336:VAL:CG2	1:A:392:THR:HG22	2.49	0.43
1:B:117:MET:CE	1:B:167:PRO:HG3	2.45	0.43
1:B:3741:LEU:O	1:B:3742:GLU:C	2.57	0.43
1:A:-8:TRP:CG	1:A:-7:SER:N	2.84	0.43
1:A:188:LYS:HZ2	1:A:188:LYS:HB3	1.81	0.43
1:A:398:THR:HG23	1:A:399:LEU:H	1.83	0.43
1:A:49:SER:HB2	1:B:4180:PHE:CD2	2.54	0.43
1:A:97:SER:HG	1:B:265:HIS:CE1	2.35	0.43
1:A:279:ALA:HA	1:A:284:PHE:CG	2.53	0.43
1:B:4189:GLY:O	1:B:4180:PHE:HD1	2.02	0.43
1:B:178:SER:HB3	1:B:314:SER:HA	2.00	0.42
1:B:398:THR:CB	1:B:3992:GLU:HG3	2.47	0.42
1:A:152:TYR:CE1	1:A:179:ARG:HG3	2.54	0.42
1:A:157:ARG:HA	1:A:157:ARG:HD3	1.70	0.42
1:A:82:ALA:N	1:A:276:LEU:HD13	2.34	0.42
1:A:2443:SER:N	1:A:247:ILE:HG23	2.34	0.42
1:B:332:ARG:HB3	1:B:3993:PHE:CZ	2.54	0.42
1:A:127:LEU:HD13	1:B:258:PRO:HB2	2.02	0.42
1:A:242:ARG:NH1	1:A:242:ARG:CG	2.79	0.42
1:A:32:LEU:HB2	1:A:343:ALA:O	2.20	0.42
1:A:398:THR:CG2	1:A:3991:LYS:H	2.33	0.42
1:B:123:ASP:OD1	1:B:146:LYS:NZ	2.53	0.42
1:B:57:GLU:HG2	1:B:257:PHE:CZ	2.55	0.42
1:B:396:THR:HG23	1:B:397:ALA:HB3	2.02	0.42
1:B:4187:LEU:O	1:B:4188:PRO:O	2.38	0.42
1:B:3911:LEU:O	1:B:3941:ILE:HG13	2.20	0.41
1:A:117:MET:HG3	1:A:167:PRO:HB3	2.02	0.41
1:A:229:LYS:NZ	2:A:2291:PLP:O3	2.52	0.41
1:A:-7:SER:C	1:A:-5:HIS:H	2.22	0.41
1:A:83:LEU:HG	1:A:911:VAL:CG2	2.50	0.41
1:A:308:LYS:CE	1:A:308:LYS:CA	2.94	0.41
1:A:4111:LEU:HD12	1:A:4111:LEU:O	2.20	0.41
1:B:68:THR:O	1:B:72:ASP:OD1	2.38	0.41
1:A:133:THR:HG23	1:A:1341:LYS:H	1.79	0.41
1:A:199:ALA:HB2	1:A:220:CYS:SG	2.60	0.41
1:A:207:LEU:HA	1:A:288:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:CYS:O	1:A:350:PRO:C	2.57	0.41
1:B:229:LYS:NZ	2:B:2291:PLP:O3	2.53	0.41
1:B:4189:GLY:O	1:B:4180:PHE:CB	2.69	0.41
1:A:185:ARG:HH11	1:A:185:ARG:CG	2.22	0.41
1:B:121:LEU:HB3	1:B:122:PRO:HD3	2.03	0.41
1:A:2443:SER:OG	1:A:247:ILE:HD13	2.20	0.41
1:B:54:LYS:HE2	1:B:67:GLY:O	2.21	0.41
1:A:4041:ASP:OD1	1:A:4041:ASP:C	2.59	0.41
1:B:117:MET:HE1	1:B:162:ALA:CB	2.51	0.41
1:B:390:ILE:O	1:B:393:VAL:HG23	2.21	0.41
1:B:-4:GLU:CG	1:B:-4:GLU:O	2.67	0.41
1:A:247:ILE:O	1:A:247:ILE:HG23	2.21	0.41
1:B:349:CYS:O	1:B:350:PRO:C	2.58	0.41
1:B:318:LEU:HD12	1:B:318:LEU:C	2.41	0.40
1:A:355:SER:C	1:A:357:LEU:H	2.25	0.40
1:A:372:ARG:O	1:A:4183:PRO:HD2	2.20	0.40
1:A:43:VAL:HG21	1:A:275:ALA:HB2	2.04	0.40
1:B:199:ALA:O	1:B:223:VAL:HA	2.22	0.40
1:B:317:HIS:HD1	1:B:317:HIS:H	1.69	0.40
1:B:369:LEU:HA	1:B:369:LEU:HD23	1.94	0.40
1:B:4:GLN:HA	1:B:5:PRO:HD3	1.88	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:NH2	1:A:157:ARG:NH2[7_556]	2.01	0.19

## 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	460/470 (98%)	407 (88%)	45 (10%)	8 (2%)	9	29
1	B	462/470 (98%)	426 (92%)	29 (6%)	7 (2%)	10	33
All	All	922/940 (98%)	833 (90%)	74 (8%)	15 (2%)	9	31

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-3	GLN
1	A	355	SER
1	B	355	SER
1	B	4188	PRO
1	A	58	GLY
1	B	58	GLY
1	A	4188	PRO
1	B	-6	SER
1	A	-4	GLU
1	A	395	ASP
1	A	4187	LEU
1	B	-3	GLN
1	A	67	GLY
1	B	111	GLU
1	B	3962	PRO

### 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	356/384 (93%)	324 (91%)	32 (9%)	9	28
1	B	352/384 (92%)	328 (93%)	24 (7%)	16	42
All	All	708/768 (92%)	652 (92%)	56 (8%)	12	34

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-8	TRP

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Mol	Chain	Res	Type
1	A	-4	GLU
1	A	-3	GLN
1	A	24	ASN
1	A	55	TYR
1	A	57	GLU
1	A	60	PRO
1	A	133	THR
1	A	148	ASN
1	A	157	ARG
1	A	175	SER
1	A	185	ARG
1	A	187	ARG
1	A	231	LEU
1	A	242	ARG
1	A	2444	VAL
1	A	2445	ASP
1	A	248	LEU
1	A	250	ASN
1	A	258	PRO
1	A	308	LYS
1	A	347	ASN
1	A	357	LEU
1	A	363	ARG
1	A	374	LEU
1	A	380	LYS
1	A	3911	LEU
1	A	396	THR
1	A	398	THR
1	A	4061	GLN
1	A	4152	SER
1	A	4188	PRO
1	B	-4	GLU
1	B	24	ASN
1	B	55	TYR
1	B	57	GLU
1	B	60	PRO
1	B	121	LEU
1	B	134	ASP
1	B	1343	LYS
1	B	136	SER
1	B	175	SER
1	B	185	ARG

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Mol	Chain	Res	Type
1	B	187	ARG
1	B	231	LEU
1	B	242	ARG
1	B	248	LEU
1	B	250	ASN
1	B	258	PRO
1	B	363	ARG
1	B	374	LEU
1	B	3942	GLN
1	B	396	THR
1	B	4041	ASP
1	B	4042	GLU
1	B	4188	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-3	GLN
1	A	53	ASN
1	A	70	HIS
1	A	126	HIS
1	A	148	ASN
1	A	203	HIS
1	A	250	ASN
1	B	53	ASN
1	B	126	HIS
1	B	203	HIS
1	B	250	ASN
1	B	265	HIS
1	B	290	GLN
1	B	4061	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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	PLP	B	2291	1	15,15,16	1.96	5 (33%)	20,22,23	2.77	9 (45%)
2	PLP	A	2291	1	15,15,16	1.74	4 (26%)	20,22,23	2.71	8 (40%)

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	PLP	B	2291	1	-	0/6/6/8	0/1/1/1
2	PLP	A	2291	1	-	0/6/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2291	PLP	C4A-C4	-3.90	1.43	1.51
2	B	2291	PLP	O3-C3	-3.07	1.29	1.37
2	A	2291	PLP	C4A-C4	-3.06	1.45	1.51
2	A	2291	PLP	O3-C3	-2.85	1.30	1.37
2	B	2291	PLP	C2A-C2	-2.64	1.45	1.50
2	A	2291	PLP	C5-C4	-2.53	1.37	1.40
2	B	2291	PLP	C6-C5	2.49	1.42	1.37
2	A	2291	PLP	C2A-C2	-2.20	1.46	1.50
2	B	2291	PLP	P-O4P	-2.19	1.53	1.60

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2291	PLP	O4P-C5A-C5	7.23	123.13	109.35
2	B	2291	PLP	O4P-C5A-C5	6.76	122.23	109.35
2	B	2291	PLP	C2A-C2-C3	5.61	127.82	120.89
2	A	2291	PLP	C2A-C2-C3	4.50	126.44	120.89
2	B	2291	PLP	C5A-C5-C6	-4.27	112.36	119.37
2	A	2291	PLP	C5A-C5-C6	-3.95	112.88	119.37
2	A	2291	PLP	O3P-P-O4P	3.90	117.10	106.73
2	B	2291	PLP	C6-N1-C2	3.27	125.22	119.17
2	A	2291	PLP	C6-N1-C2	2.96	124.65	119.17
2	A	2291	PLP	C3-C2-N1	-2.90	117.02	120.77
2	B	2291	PLP	O3P-P-O4P	2.88	114.39	106.73
2	B	2291	PLP	C3-C2-N1	-2.87	117.06	120.77
2	B	2291	PLP	C6-C5-C4	-2.71	116.02	118.16
2	B	2291	PLP	C3-C4-C5	2.60	121.55	118.74
2	A	2291	PLP	C3-C4-C5	2.45	121.38	118.74
2	B	2291	PLP	O4P-P-O1P	-2.30	100.03	106.47
2	A	2291	PLP	C6-C5-C4	-2.15	116.47	118.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2291	PLP	1	0
2	A	2291	PLP	2	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	464/470 (98%)	-0.53	4 (0%) 84 80	42, 73, 99, 99	0
1	B	466/470 (99%)	-0.68	2 (0%) 92 91	41, 65, 95, 99	0
All	All	930/940 (98%)	-0.60	6 (0%) 89 86	41, 68, 97, 99	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4189	GLY	4.3
1	B	4180	PHE	3.8
1	A	4180	PHE	3.1
1	B	2444	VAL	2.4
1	A	396	THR	2.2
1	A	2445	ASP	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	A	2291	15/16	0.96	0.13	62,62,62,62	0
2	PLP	B	2291	15/16	0.98	0.11	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.