



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:52 AM GMT

PDB ID : 2C2G  
Title : Crystal structure of Threonine Synthase from Arabidopsis thaliana in complex with its cofactor pyridoxal phosphate  
Authors : Mas-Droux, C.; Biou, V.; Dumas, R.  
Deposited on : 2005-09-29  
Resolution : 2.61 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

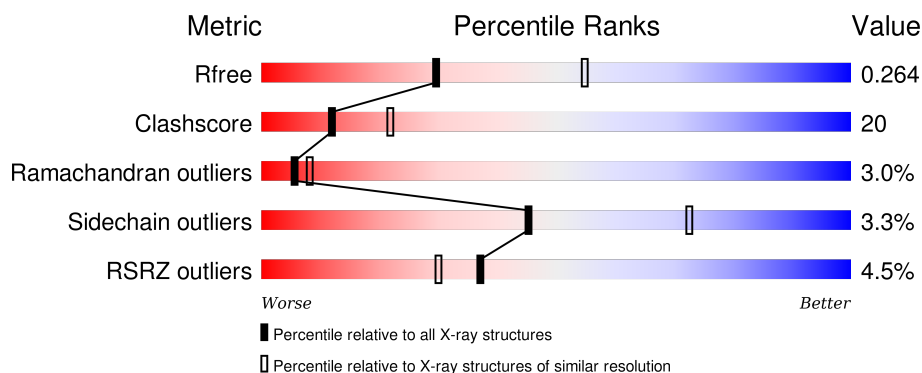
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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.

Mol	Chain	Length	Quality of chain
1	A	486	<div> <div>5%</div> <div>57%</div> <div>30%</div> <div>5%</div> <div>8%</div> </div>
1	B	486	<div> <div>3%</div> <div>58%</div> <div>27%</div> <div>• •</div> <div>10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	A	1163	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7015 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 THREONINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3474	2211	595	646	22			
1	B	437	Total	C	N	O	S	0	0	0
			3390	2161	575	632	22			

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



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		

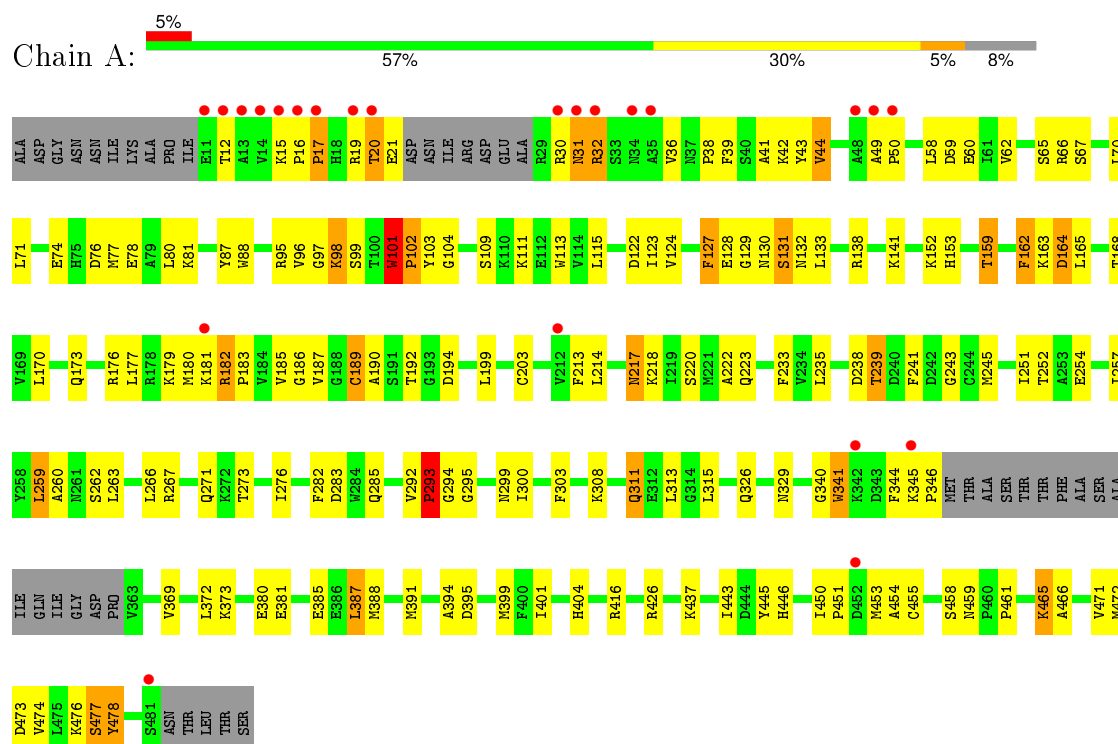
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	49	Total 49	O 49	0	0

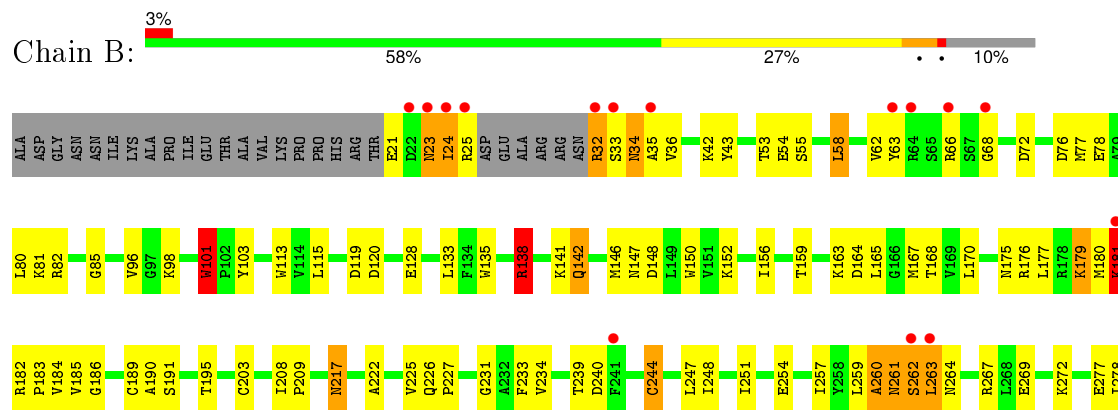
### 3 Residue-property plots

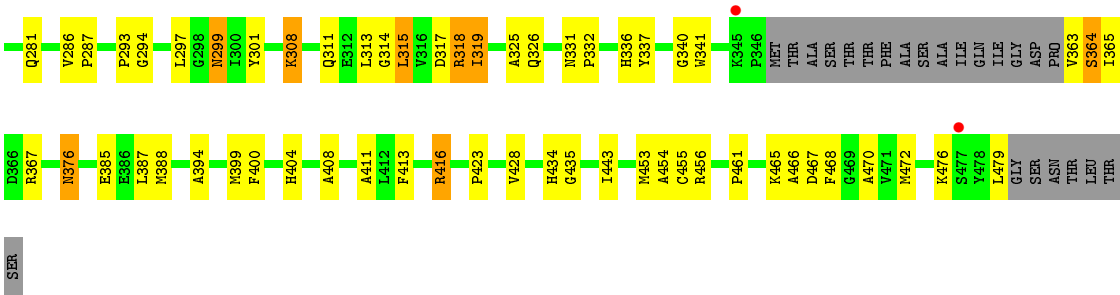
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: THREONINE SYNTHASE



#### • Molecule 1: THREONINE SYNTHASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.63Å 61.01Å 76.68Å 108.96° 102.00° 107.36°	Depositor
Resolution (Å)	20.63 – 2.61 20.62 – 2.61	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.63-2.61) 80.8 (20.62-2.61)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.187 , 0.264 0.188 , 0.264	Depositor DCC
$R_{free}$ test set	1311 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.1	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25741 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 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: 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	1.13	8/3554 (0.2%)	1.29	21/4817 (0.4%)
1	B	0.96	2/3467 (0.1%)	1.25	18/4699 (0.4%)
All	All	1.05	10/7021 (0.1%)	1.27	39/9516 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	CYS	CB-SG	-10.31	1.64	1.82
1	A	203	CYS	CB-SG	-7.98	1.68	1.82
1	A	127	PHE	CG-CD1	7.57	1.50	1.38
1	A	127	PHE	CE2-CZ	6.94	1.50	1.37
1	A	162	PHE	CE2-CZ	5.75	1.48	1.37
1	A	41	ALA	CA-CB	-5.28	1.41	1.52
1	B	138	ARG	CG-CD	5.27	1.65	1.51
1	A	213	PHE	CE1-CZ	5.11	1.47	1.37
1	B	244	CYS	CB-SG	-5.11	1.73	1.81
1	A	341	TRP	CB-CG	5.08	1.59	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	VAL	N-CA-C	-12.53	77.16	111.00
1	B	58	LEU	CB-CG-CD2	-9.57	94.72	111.00
1	B	101	TRP	C-N-CD	8.06	145.32	128.40
1	A	266	LEU	CA-CB-CG	8.01	133.73	115.30
1	A	101	TRP	C-N-CD	6.99	143.09	128.40
1	A	111	LYS	CD-CE-NZ	-6.84	95.97	111.70
1	B	259	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	182	ARG	C-N-CD	6.65	142.36	128.40
1	A	437	LYS	CD-CE-NZ	6.53	126.72	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	LEU	CB-CG-CD2	-6.45	100.04	111.00
1	B	319	ILE	N-CA-C	-6.28	94.05	111.00
1	A	295	GLY	N-CA-C	-6.04	97.99	113.10
1	B	308	LYS	CA-CB-CG	5.94	126.47	113.40
1	B	133	LEU	N-CA-C	-5.83	95.25	111.00
1	A	283	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	164	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	131	SER	N-CA-CB	-5.58	102.12	110.50
1	A	98	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	A	267	ARG	CB-CA-C	-5.51	99.38	110.40
1	A	311	GLN	CA-CB-CG	-5.45	101.40	113.40
1	B	262	SER	N-CA-C	-5.45	96.28	111.00
1	A	387	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	B	148	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	162	PHE	N-CA-CB	-5.39	100.90	110.60
1	B	176	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	101	TRP	C-N-CA	-5.29	99.80	122.00
1	A	239	THR	N-CA-CB	5.26	120.30	110.30
1	A	115	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	68	GLY	N-CA-C	-5.21	100.06	113.10
1	A	138	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	259	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	80	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	115	LEU	N-CA-C	-5.16	97.08	111.00
1	B	456	ARG	CB-CA-C	-5.15	100.11	110.40
1	A	251	ILE	CB-CA-C	-5.14	101.31	111.60
1	B	315	LEU	CA-CB-CG	5.12	127.08	115.30
1	B	400	PHE	N-CA-C	-5.08	97.30	111.00
1	B	103	TYR	N-CA-C	5.06	124.66	111.00
1	A	293	PRO	C-N-CA	-5.06	111.68	122.30

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	3474	0	3428	164	0
1	B	3390	0	3341	133	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
3	A	72	0	0	6	0
3	B	49	0	0	2	0
All	All	7015	0	6781	273	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 20.

All (273) 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:252:THR:HG21	1:A:259:LEU:CD1	1.74	1.17
1:B:138:ARG:HH11	1:B:138:ARG:CG	1.60	1.14
1:B:261:ASN:HB2	1:B:264:ASN:HB2	1.09	1.05
1:A:252:THR:HG21	1:A:259:LEU:HD11	1.02	1.00
1:B:32:ARG:HD3	1:B:33:SER:H	1.26	0.99
1:B:182:ARG:HG3	1:B:183:PRO:HD2	1.46	0.97
1:B:317:ASP:HB2	1:B:318:ARG:NH1	1.80	0.95
1:B:138:ARG:HG2	1:B:138:ARG:HH11	1.32	0.92
1:B:263:LEU:HD12	1:B:364:SER:OG	1.72	0.88
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.39	0.87
1:A:252:THR:CG2	1:A:259:LEU:HD11	1.97	0.87
1:A:32:ARG:HB2	1:A:38:PRO:HD2	1.58	0.86
1:A:31:ASN:O	1:A:31:ASN:ND2	2.07	0.86
1:A:238:ASP:OD2	1:B:465:LYS:NZ	2.09	0.85
1:B:78:GLU:HA	1:B:78:GLU:OE2	1.78	0.84
1:B:261:ASN:HB2	1:B:264:ASN:CB	2.03	0.82
1:A:32:ARG:CB	1:A:38:PRO:HD2	2.10	0.81
1:A:113:TRP:CZ2	1:A:313:LEU:HD12	2.16	0.80
1:B:152:LYS:NZ	1:B:277:GLU:OE1	2.14	0.78
1:B:142:GLN:HA	1:B:142:GLN:HE21	1.47	0.78
1:A:141:LYS:HB3	1:A:141:LYS:NZ	1.99	0.77
1:B:138:ARG:NH1	1:B:138:ARG:CG	2.36	0.77
1:A:446:HIS:HD2	1:A:459:ASN:H	1.33	0.77
1:A:472:MET:O	1:A:476:LYS:HG2	1.85	0.76
1:A:159:THR:HB	1:A:164:ASP:OD1	1.86	0.75
1:B:180:MET:O	1:B:182:ARG:N	2.18	0.75
1:A:49:ALA:HB1	1:A:50:PRO:HD2	1.69	0.75
1:A:326:GLN:NE2	1:A:326:GLN:HA	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:CD	1:B:33:SER:H	2.00	0.74
1:A:15:LYS:HB2	1:A:19:ARG:HE	1.52	0.73
1:B:175:ASN:O	1:B:179:LYS:HG2	1.89	0.73
1:A:326:GLN:CA	1:A:326:GLN:HE21	2.00	0.73
1:A:466:ALA:CB	1:B:239:THR:HG23	2.19	0.73
1:B:217:ASN:HD22	1:B:217:ASN:H	1.37	0.72
1:B:262:SER:HB2	1:B:263:LEU:HD22	1.71	0.72
1:B:416:ARG:NH2	1:B:423:PRO:HD3	2.06	0.71
1:B:311:GLN:NE2	1:B:319:ILE:HG23	2.05	0.70
1:B:299:ASN:N	1:B:299:ASN:HD22	1.89	0.70
1:A:32:ARG:HB2	1:A:38:PRO:CD	2.21	0.70
1:A:31:ASN:HD22	1:A:31:ASN:C	1.93	0.69
1:A:466:ALA:HB2	1:B:239:THR:HG23	1.73	0.69
1:A:127:PHE:CE1	3:A:2028:HOH:O	2.44	0.69
1:B:472:MET:O	1:B:476:LYS:HG2	1.93	0.69
1:B:180:MET:O	1:B:181:LYS:C	2.31	0.69
1:A:141:LYS:HB3	1:A:141:LYS:HZ3	1.56	0.68
1:A:477:SER:O	1:A:478:TYR:C	2.31	0.68
1:A:173:GLN:OE1	1:A:173:GLN:HA	1.93	0.68
1:A:391:MET:HA	1:A:401:ILE:HD11	1.76	0.67
1:B:32:ARG:HD3	1:B:33:SER:N	2.06	0.67
1:A:241:PHE:CZ	1:A:245:MET:HE3	2.30	0.67
1:A:326:GLN:HE21	1:A:326:GLN:HA	1.58	0.67
1:A:88:TRP:HB2	1:A:315:LEU:HD21	1.75	0.66
1:B:299:ASN:HD22	1:B:299:ASN:H	1.42	0.66
1:A:128:GLU:CD	1:A:128:GLU:H	1.98	0.66
1:B:465:LYS:HE2	1:B:465:LYS:HA	1.77	0.65
1:B:189:CYS:SG	1:B:191:SER:HB3	2.36	0.65
1:A:99:SER:HB3	1:B:281:GLN:O	1.95	0.65
1:A:443:ILE:HD11	1:B:222:ALA:HA	1.78	0.65
1:B:77:MET:O	1:B:81:LYS:HG3	1.96	0.65
1:A:473:ASP:O	1:A:474:VAL:C	2.36	0.65
1:B:138:ARG:NH1	1:B:138:ARG:HG3	2.07	0.64
1:A:31:ASN:OD1	1:A:87:TYR:HE2	1.80	0.64
1:A:39:PHE:CD1	1:A:80:LEU:HD23	2.34	0.63
1:B:311:GLN:NE2	1:B:319:ILE:CG2	2.62	0.63
1:A:192:THR:HG22	1:A:214:LEU:HD11	1.81	0.63
1:B:182:ARG:HG3	1:B:183:PRO:CD	2.25	0.63
1:A:177:LEU:O	1:A:182:ARG:HB3	1.99	0.63
1:B:317:ASP:HB2	1:B:318:ARG:HH11	1.63	0.62
1:B:138:ARG:HG2	1:B:138:ARG:NH1	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:N	1:A:263:LEU:HD22	2.14	0.62
1:A:445:TYR:CE1	1:A:455:CYS:HA	2.35	0.61
1:A:88:TRP:HB2	1:A:315:LEU:CD2	2.29	0.61
1:A:326:GLN:CA	1:A:326:GLN:NE2	2.58	0.61
1:A:16:PRO:O	1:A:17:PRO:C	2.37	0.61
1:A:62:VAL:HG12	1:A:71:LEU:CD1	2.31	0.60
1:A:217:ASN:ND2	1:A:218:LYS:HG2	2.16	0.60
1:A:30:ARG:CB	1:A:32:ARG:HD2	2.31	0.60
1:A:385:GLU:HG3	1:A:453:MET:HG3	1.82	0.60
1:A:380:GLU:HG3	1:A:381:GLU:N	2.17	0.59
1:A:465:LYS:HE3	1:A:465:LYS:HA	1.85	0.59
1:A:239:THR:HG23	1:B:466:ALA:CB	2.32	0.59
1:A:65:SER:O	1:A:67:SER:N	2.35	0.59
1:A:162:PHE:CZ	1:A:271:GLN:HB3	2.38	0.58
1:A:19:ARG:O	1:A:20:THR:OG1	2.21	0.58
1:B:203:CYS:HB3	1:B:208:ILE:O	2.04	0.58
1:A:122:ASP:OD1	1:A:179:LYS:HD2	2.02	0.57
1:B:135:TRP:HB2	1:B:150:TRP:CZ3	2.38	0.57
1:B:364:SER:HB3	1:B:367:ARG:HD2	1.87	0.57
1:A:170:LEU:C	1:A:170:LEU:HD23	2.25	0.57
1:B:185:VAL:O	1:B:209:PRO:HG2	2.05	0.56
1:B:240:ASP:O	1:B:244:CYS:HB2	2.05	0.56
1:A:133:LEU:HD21	1:A:282:PHE:CE2	2.40	0.56
1:A:388:MET:CE	1:A:391:MET:CE	2.83	0.56
1:A:97:GLY:C	3:A:2022:HOH:O	2.43	0.56
1:A:222:ALA:HA	1:B:443:ILE:HD11	1.88	0.56
1:A:233:PHE:CE2	1:A:235:LEU:HD21	2.41	0.56
1:B:177:LEU:O	1:B:182:ARG:HB3	2.06	0.56
1:B:293:PRO:HA	1:B:325:ALA:HB3	1.88	0.55
1:B:53:THR:O	1:B:53:THR:HG22	2.06	0.55
1:B:263:LEU:HD22	1:B:263:LEU:H	1.70	0.55
1:B:85:GLY:HA3	1:B:314:GLY:O	2.06	0.55
1:B:385:GLU:HG3	1:B:453:MET:HG3	1.88	0.55
1:B:34:ASN:OD1	1:B:35:ALA:N	2.39	0.55
1:A:345:LYS:HD2	1:A:346:PRO:HD2	1.89	0.55
1:B:119:ASP:OD1	1:B:120:ASP:N	2.39	0.55
1:B:195:THR:OG1	1:B:267:ARG:NH2	2.37	0.55
1:B:62:VAL:HG12	1:B:63:TYR:H	1.71	0.54
1:A:387:LEU:HD12	1:A:387:LEU:C	2.29	0.54
1:A:220:SER:OG	1:A:223:GLN:HG3	2.09	0.53
1:B:297:LEU:HD11	1:B:331:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:PHE:HE2	1:A:235:LEU:HD21	1.73	0.53
1:A:30:ARG:HB2	1:A:32:ARG:HD2	1.90	0.53
1:A:446:HIS:HA	1:A:458:SER:HB2	1.89	0.53
1:B:376:ASN:C	1:B:376:ASN:HD22	2.11	0.53
1:A:454:ALA:O	1:A:455:CYS:HB2	2.08	0.53
1:A:78:GLU:OE2	1:A:78:GLU:HA	2.08	0.53
1:A:243:GLY:HA2	3:A:2046:HOH:O	2.09	0.53
1:A:241:PHE:CZ	1:A:245:MET:CE	2.92	0.53
1:A:292:VAL:O	1:A:293:PRO:O	2.26	0.53
1:A:131:SER:HB3	1:A:152:LYS:NZ	2.23	0.53
1:B:159:THR:HB	1:B:164:ASP:OD1	2.09	0.53
1:A:163:LYS:HE3	1:A:194:ASP:HB2	1.90	0.53
1:A:466:ALA:HB1	1:B:239:THR:HG23	1.91	0.52
1:A:132:ASN:HB3	1:A:153:HIS:HB2	1.91	0.52
1:A:299:ASN:O	1:A:303:PHE:HD1	1.92	0.52
1:A:101:TRP:HZ3	3:A:2028:HOH:O	1.93	0.52
1:A:43:TYR:CE1	1:A:58:LEU:HA	2.44	0.52
1:A:446:HIS:HD2	1:A:459:ASN:N	2.06	0.52
1:A:59:ASP:HA	1:A:177:LEU:HD21	1.91	0.52
1:A:70:LEU:CD2	1:A:263:LEU:HD12	2.40	0.52
1:B:128:GLU:CD	1:B:128:GLU:H	2.13	0.52
1:A:459:ASN:HD22	1:B:231:GLY:HA2	1.74	0.51
1:A:185:VAL:HG12	1:B:479:LEU:HD22	1.92	0.51
1:B:394:ALA:HB1	1:B:399:MET:CE	2.39	0.51
1:B:413:PHE:HD1	3:B:2036:HOH:O	1.94	0.51
1:A:388:MET:CE	1:A:391:MET:HE1	2.41	0.51
1:A:344:PHE:CE2	1:A:369:VAL:HG21	2.46	0.51
1:B:21:GLU:HG2	1:B:101:TRP:CD1	2.45	0.51
1:B:260:ALA:O	1:B:261:ASN:C	2.50	0.51
1:A:199:LEU:HD22	1:A:260:ALA:HB3	1.91	0.51
1:B:299:ASN:ND2	1:B:299:ASN:H	2.06	0.50
1:B:299:ASN:N	1:B:299:ASN:ND2	2.59	0.50
1:A:62:VAL:HG12	1:A:71:LEU:HD11	1.93	0.50
1:B:363:VAL:O	1:B:365:ILE:HG13	2.11	0.50
1:A:153:HIS:HE1	3:A:2035:HOH:O	1.95	0.50
1:A:60:GLU:HB2	1:A:62:VAL:HG23	1.93	0.50
1:A:199:LEU:HD22	1:A:260:ALA:CB	2.42	0.50
1:A:446:HIS:CD2	1:A:459:ASN:H	2.20	0.49
1:A:388:MET:HE1	1:A:391:MET:HE1	1.93	0.49
1:A:31:ASN:OD1	1:A:87:TYR:CE2	2.63	0.49
1:B:78:GLU:OE2	1:B:78:GLU:CA	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HB3	1:A:38:PRO:HD2	1.91	0.49
1:A:141:LYS:NZ	1:A:141:LYS:CB	2.73	0.49
1:A:19:ARG:H	1:B:147:ASN:ND2	2.10	0.49
1:A:32:ARG:CB	1:A:38:PRO:CD	2.84	0.49
1:A:466:ALA:CB	1:B:239:THR:CG2	2.91	0.49
1:B:43:TYR:CE1	1:B:58:LEU:HA	2.48	0.49
1:A:395:ASP:HA	1:A:399:MET:O	2.13	0.48
1:B:261:ASN:CB	1:B:264:ASN:HB2	2.05	0.48
1:A:478:TYR:CD1	1:B:233:PHE:CD1	3.02	0.48
1:B:317:ASP:CB	1:B:318:ARG:NH1	2.64	0.48
1:A:466:ALA:HB1	1:B:239:THR:CG2	2.42	0.48
1:B:293:PRO:CB	1:B:404:HIS:HB3	2.44	0.48
1:A:254:GLU:HG2	1:B:468:PHE:HZ	1.78	0.48
1:B:364:SER:HB3	1:B:367:ARG:CD	2.44	0.48
1:A:30:ARG:HB3	1:A:32:ARG:HD2	1.94	0.48
1:A:98:LYS:HD2	1:A:98:LYS:N	2.29	0.48
1:B:62:VAL:HG12	1:B:63:TYR:N	2.30	0.47
1:A:217:ASN:HD22	1:A:218:LYS:HG2	1.79	0.47
1:A:187:VAL:HG11	1:A:199:LEU:HD11	1.96	0.47
1:B:311:GLN:HE21	1:B:319:ILE:CG2	2.27	0.47
1:B:434:HIS:ND1	1:B:435:GLY:N	2.63	0.47
1:B:170:LEU:HD23	1:B:170:LEU:C	2.35	0.47
1:B:180:MET:C	1:B:182:ARG:N	2.69	0.47
1:A:293:PRO:HB3	1:A:404:HIS:HB3	1.97	0.47
1:A:113:TRP:CZ2	1:A:313:LEU:CD1	2.92	0.47
1:A:162:PHE:HZ	1:A:271:GLN:HB3	1.80	0.47
1:B:76:ASP:OD1	1:B:78:GLU:HB3	2.15	0.46
1:B:190:ALA:HB2	1:B:248:ILE:HD11	1.97	0.46
1:B:24:ILE:O	1:B:25:ARG:HB2	2.15	0.46
1:B:454:ALA:O	1:B:455:CYS:HB2	2.14	0.46
1:A:263:LEU:N	1:A:263:LEU:CD2	2.79	0.46
1:B:226:GLN:O	1:B:227:PRO:C	2.53	0.46
1:B:387:LEU:HD12	1:B:388:MET:N	2.30	0.46
1:A:31:ASN:CG	1:A:87:TYR:OH	2.54	0.46
1:A:292:VAL:C	1:A:293:PRO:O	2.52	0.46
1:B:167:MET:CE	1:B:170:LEU:HD13	2.46	0.46
1:A:102:PRO:O	1:A:104:GLY:N	2.48	0.46
1:A:31:ASN:OD1	1:A:88:TRP:CZ3	2.68	0.46
1:B:53:THR:O	1:B:53:THR:CG2	2.65	0.45
1:A:131:SER:HB3	1:A:152:LYS:HZ2	1.81	0.45
1:B:225:VAL:HG13	1:B:226:GLN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:TRP:CE3	1:A:373:LYS:HE2	2.51	0.45
1:B:142:GLN:HA	1:B:142:GLN:NE2	2.25	0.45
1:A:263:LEU:HD22	1:A:263:LEU:H	1.79	0.45
1:A:380:GLU:HG3	1:A:381:GLU:H	1.80	0.45
1:A:345:LYS:HA	1:A:346:PRO:HD3	1.81	0.45
1:B:163:LYS:NZ	2:B:1163:PLP:O3	2.48	0.45
1:A:44:VAL:HG21	1:A:74:GLU:OE1	2.17	0.45
1:A:472:MET:CE	1:B:254:GLU:HG2	2.47	0.45
1:B:387:LEU:C	1:B:387:LEU:HD12	2.37	0.45
1:B:269:GLU:O	1:B:272:LYS:HG2	2.17	0.45
1:B:260:ALA:C	1:B:261:ASN:O	2.55	0.44
1:A:394:ALA:HB1	1:A:399:MET:CE	2.48	0.44
1:A:129:GLY:O	1:A:130:ASN:HB2	2.17	0.44
1:A:96:VAL:HG12	1:B:96:VAL:HG12	1.99	0.44
1:B:138:ARG:NH1	3:B:2010:HOH:O	2.49	0.44
1:A:77:MET:O	1:A:81:LYS:HG3	2.18	0.44
1:A:20:THR:OG1	1:B:141:LYS:NZ	2.45	0.44
1:A:70:LEU:HD22	1:A:263:LEU:HD12	2.00	0.44
1:A:273:THR:HG22	1:A:276:ILE:HD12	2.00	0.43
1:B:54:GLU:OE1	1:B:66:ARG:N	2.49	0.43
1:A:192:THR:HG22	1:A:214:LEU:CD1	2.48	0.43
1:A:153:HIS:CE1	3:A:2035:HOH:O	2.71	0.43
1:B:23:ASN:O	1:B:25:ARG:N	2.50	0.43
1:A:30:ARG:O	1:A:32:ARG:HG3	2.18	0.43
1:B:294:GLY:O	1:B:326:GLN:OE1	2.37	0.43
1:B:247:LEU:O	1:B:251:ILE:HG12	2.18	0.43
1:A:15:LYS:HB2	1:A:16:PRO:HD2	1.99	0.43
1:A:39:PHE:CE1	1:A:80:LEU:HD23	2.52	0.43
1:B:101:TRP:O	1:B:101:TRP:CE3	2.72	0.43
1:A:186:GLY:O	1:A:257:ILE:HA	2.18	0.43
1:A:21:GLU:HB2	1:A:101:TRP:HB2	1.99	0.43
1:B:156:ILE:HG21	1:B:156:ILE:HD13	1.78	0.43
1:B:113:TRP:CZ2	1:B:313:LEU:HD12	2.53	0.43
1:B:317:ASP:HB2	1:B:318:ARG:CZ	2.46	0.43
1:B:286:VAL:HA	1:B:287:PRO:HD3	1.97	0.43
1:A:180:MET:O	1:A:181:LYS:HB3	2.17	0.43
1:A:450:ILE:HA	1:A:451:PRO:HD3	1.88	0.43
1:B:165:LEU:O	1:B:168:THR:HG22	2.19	0.43
1:A:443:ILE:CD1	1:B:222:ALA:HA	2.47	0.42
1:B:293:PRO:HB2	1:B:404:HIS:HB3	2.01	0.42
1:A:15:LYS:HD2	1:A:19:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:SER:OG	1:A:478:TYR:N	2.52	0.42
1:A:263:LEU:H	1:A:263:LEU:CD2	2.32	0.42
1:B:408:ALA:O	1:B:411:ALA:HB3	2.20	0.42
1:A:461:PRO:HA	1:B:234:VAL:HB	2.02	0.42
1:A:252:THR:HG21	1:A:259:LEU:HD12	1.86	0.42
1:A:471:VAL:HG21	1:B:247:LEU:HD13	2.01	0.42
1:B:467:ASP:O	1:B:470:ALA:HB3	2.20	0.42
1:B:337:TYR:HD1	1:B:341:TRP:CZ2	2.38	0.42
1:A:43:TYR:CD1	1:A:58:LEU:HD23	2.54	0.42
1:A:187:VAL:HG12	1:A:199:LEU:HD21	2.02	0.42
1:B:337:TYR:HD1	1:B:341:TRP:CH2	2.38	0.41
1:A:123:ILE:HG22	1:A:124:VAL:N	2.34	0.41
1:A:311:GLN:HG2	1:A:311:GLN:O	2.04	0.41
1:A:252:THR:CG2	1:A:259:LEU:CD1	2.69	0.41
1:B:217:ASN:HD22	1:B:217:ASN:N	2.03	0.41
1:A:262:SER:HB2	1:A:263:LEU:HD22	2.02	0.41
1:B:186:GLY:O	1:B:257:ILE:HA	2.20	0.41
1:A:60:GLU:HB2	1:A:62:VAL:CG2	2.49	0.41
1:A:222:ALA:HA	1:B:443:ILE:CD1	2.50	0.41
1:B:394:ALA:HB1	1:B:399:MET:HE3	2.02	0.41
1:B:43:TYR:O	1:B:55:SER:HA	2.20	0.41
1:B:332:PRO:HB2	1:B:336:HIS:HD2	1.85	0.41
1:A:189:CYS:SG	1:A:190:ALA:N	2.93	0.41
1:B:278:ILE:HD13	1:B:428:VAL:HG11	2.02	0.41
1:A:20:THR:O	1:A:20:THR:HG22	2.21	0.41
1:A:21:GLU:CG	1:A:101:TRP:HB2	2.51	0.41
1:A:43:TYR:CE1	1:A:58:LEU:HD23	2.56	0.41
1:A:173:GLN:O	1:A:176:ARG:HB3	2.20	0.41
1:A:472:MET:SD	1:B:251:ILE:HD12	2.60	0.41
1:A:465:LYS:CE	1:A:465:LYS:HA	2.51	0.41
1:B:72:ASP:OD2	1:B:301:TYR:OH	2.25	0.41
1:A:385:GLU:HA	1:A:453:MET:CE	2.51	0.41
1:A:76:ASP:OD1	1:A:78:GLU:HB3	2.21	0.41
1:B:146:MET:SD	1:B:416:ARG:HD2	2.61	0.40
1:A:95:ARG:NH1	1:A:109:SER:O	2.48	0.40
1:A:300:ILE:CD1	1:A:372:LEU:HD21	2.51	0.40
1:A:285:GLN:HB2	1:A:426:ARG:HH12	1.86	0.40
1:A:459:ASN:ND2	1:B:231:GLY:HA2	2.36	0.40
1:B:98:LYS:HA	1:B:98:LYS:HD3	1.70	0.40
1:A:165:LEU:O	1:A:168:THR:HG22	2.21	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	442/486 (91%)	391 (88%)	36 (8%)	15 (3%)		
1	B	431/486 (89%)	377 (88%)	43 (10%)	11 (3%)		
All	All	873/972 (90%)	768 (88%)	79 (9%)	26 (3%)		

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	66	ARG
1	A	103	TYR
1	A	478	TYR
1	B	23	ASN
1	B	34	ASN
1	B	181	LYS
1	A	36	VAL
1	A	102	PRO
1	A	293	PRO
1	A	340	GLY
1	B	179	LYS
1	B	184	VAL
1	B	260	ALA
1	B	340	GLY
1	A	329	ASN
1	B	364	SER
1	A	12	THR
1	A	17	PRO
1	B	101	TRP
1	A	477	SER
1	B	261	ASN
1	A	294	GLY
1	B	24	ILE
1	A	101	TRP

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Mol	Chain	Res	Type
1	A	183	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	373/403 (93%)	364 (98%)	9 (2%)	57	81
1	B	364/403 (90%)	349 (96%)	15 (4%)	37	65
All	All	737/806 (91%)	713 (97%)	24 (3%)	45	72

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	32	ARG
1	A	42	LYS
1	A	44	VAL
1	A	159	THR
1	A	217	ASN
1	A	308	LYS
1	A	416	ARG
1	A	465	LYS
1	B	32	ARG
1	B	42	LYS
1	B	82	ARG
1	B	138	ARG
1	B	142	GLN
1	B	181	LYS
1	B	217	ASN
1	B	263	LEU
1	B	299	ASN
1	B	308	LYS
1	B	315	LEU
1	B	318	ARG
1	B	376	ASN

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Mol	Chain	Res	Type
1	B	416	ARG
1	B	461	PRO

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	47	ASN
1	A	132	ASN
1	A	153	HIS
1	A	217	ASN
1	A	223	GLN
1	A	299	ASN
1	A	326	GLN
1	A	376	ASN
1	A	418	GLN
1	A	446	HIS
1	A	448	ASN
1	B	47	ASN
1	B	142	GLN
1	B	217	ASN
1	B	223	GLN
1	B	226	GLN
1	B	230	ASN
1	B	299	ASN
1	B	311	GLN
1	B	326	GLN
1	B	336	HIS
1	B	376	ASN
1	B	393	GLN
1	B	446	HIS

### 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	A	1163	1	15,15,16	1.79	4 (26%)	21,22,23	2.01	6 (28%)
2	PLP	B	1163	1	15,15,16	2.10	4 (26%)	21,22,23	2.61	3 (14%)

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	A	1163	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1163	1	-	0/6/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1163	PLP	O3-C3	-5.35	1.24	1.37
2	A	1163	PLP	O3-C3	-5.29	1.24	1.37
2	A	1163	PLP	P-O3P	-2.08	1.47	1.54
2	A	1163	PLP	C2-N1	2.11	1.38	1.34
2	A	1163	PLP	C6-N1	2.31	1.39	1.34
2	B	1163	PLP	C2-N1	2.88	1.40	1.34
2	B	1163	PLP	C6-N1	2.97	1.40	1.34
2	B	1163	PLP	C5-C4	3.08	1.44	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	1163	PLP	O3P-P-O4P	-2.88	98.26	106.56
2	A	1163	PLP	C4A-C4-C5	-2.39	118.39	120.88
2	B	1163	PLP	O4P-P-O1P	-2.25	101.42	107.14
2	A	1163	PLP	O3P-P-O2P	2.50	116.90	107.38
2	B	1163	PLP	C5A-C5-C4	2.60	125.09	121.65
2	A	1163	PLP	O3-C3-C2	2.63	122.23	117.66
2	A	1163	PLP	C3-C4-C5	2.63	121.65	118.78
2	A	1163	PLP	O4P-C5A-C5	5.57	118.20	108.99
2	B	1163	PLP	O4P-C5A-C5	10.05	125.60	108.99

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
2	B	1163	PLP	1	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 ⓘ

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	448/486 (92%)	-0.10	23 (5%)	32 25	6, 18, 37, 73	0
1	B	437/486 (89%)	-0.24	17 (3%)	43 36	7, 18, 34, 55	0
All	All	885/972 (91%)	-0.17	40 (4%)	37 30	6, 18, 36, 73	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	ALA	14.1
1	A	14	VAL	11.2
1	A	12	THR	8.4
1	B	32	ARG	7.0
1	B	24	ILE	6.7
1	A	11	GLU	6.6
1	A	15	LYS	5.5
1	A	49	ALA	5.1
1	B	35	ALA	4.9
1	A	30	ARG	4.8
1	A	32	ARG	4.4
1	B	25	ARG	4.2
1	B	23	ASN	4.0
1	A	34	ASN	3.9
1	B	263	LEU	3.9
1	B	68	GLY	3.8
1	A	50	PRO	3.6
1	B	33	SER	3.6
1	A	481	SER	3.5
1	B	64	ARG	3.1
1	B	181	LYS	2.9
1	B	66	ARG	2.8
1	A	452	ASP	2.8
1	A	20	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	181	LYS	2.8
1	B	262	SER	2.7
1	B	63	TYR	2.7
1	A	48	ALA	2.5
1	B	22	ASP	2.5
1	B	241	PHE	2.4
1	A	342	LYS	2.3
1	B	345	LYS	2.3
1	A	31	ASN	2.3
1	A	19	ARG	2.2
1	A	212	VAL	2.2
1	A	16	PRO	2.2
1	A	345	LYS	2.2
1	A	17	PRO	2.2
1	A	35	ALA	2.1
1	B	477	SER	2.1

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PLP	A	1163	15/16	0.93	0.29	3.54	47,52,53,55	0
2	PLP	B	1163	15/16	0.88	0.32	1.50	47,52,54,56	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.