



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:28 PM GMT

PDB ID : 1C7G  
Title : TYROSINE PHENOL-LYASE FROM ERWINIA HERBICOLA  
Authors : Mikami, B.; Yamamoto, Y.; Katayama, T.; Suzuki, H.  
Deposited on : 2000-02-18  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

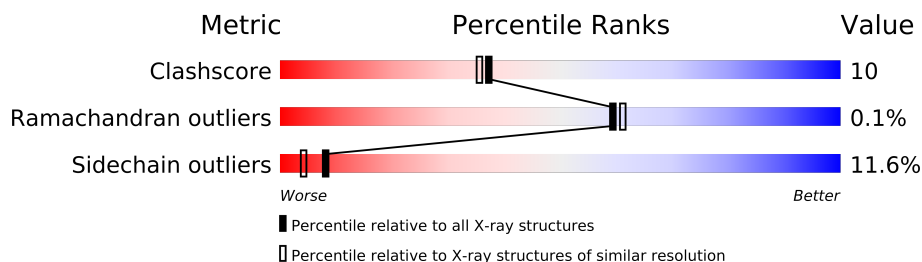
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 Å.



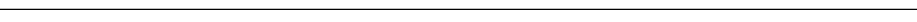

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	456	
1	B	456	
1	C	456	
1	D	456	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PLP	A	1000	X	-
2	PLP	B	1000	X	-

## 2 Entry composition i

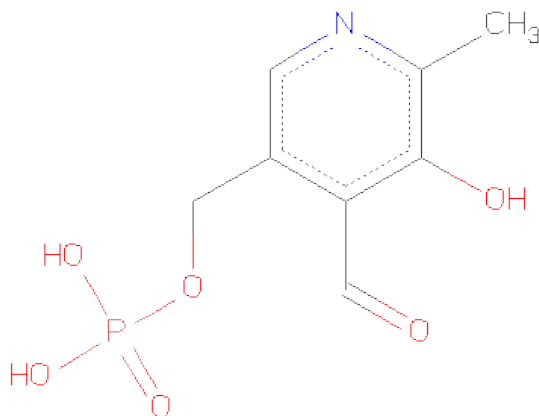
There are 3 unique types of molecules in this entry. The entry contains 14905 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TYROSINE PHENOL-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3605	2282	618	678	27			
1	B	456	Total	C	N	O	S	0	0	0
			3605	2282	618	678	27			
1	C	456	Total	C	N	O	S	0	0	0
			3605	2282	618	678	27			
1	D	456	Total	C	N	O	S	0	0	0
			3605	2282	618	678	27			

- 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		

*Continued on next page...*

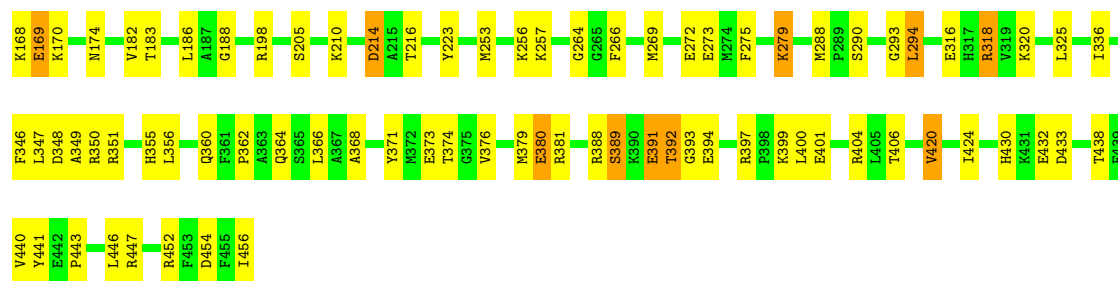
*Continued from previous page...*

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

- Molecule 3 is water.

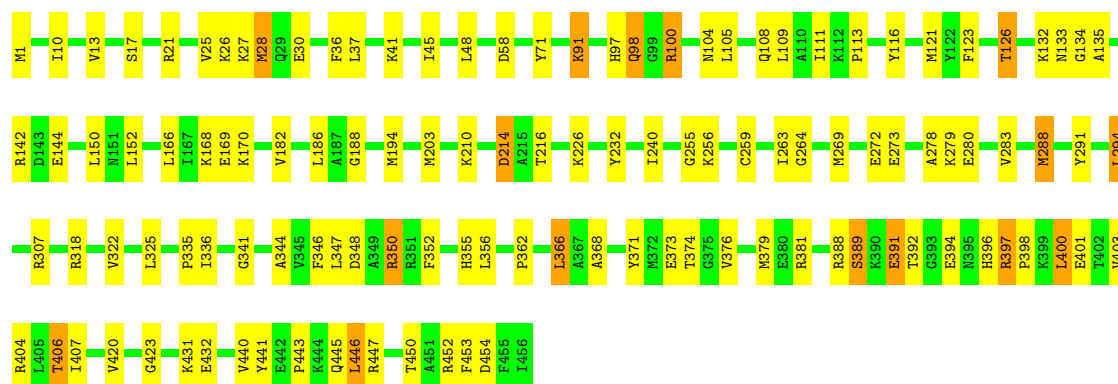
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		
3	B	77	Total	O	0	0
			77	77		
3	C	158	Total	O	0	0
			158	158		
3	D	87	Total	O	0	0
			87	87		





● Molecule 1: TYROSINE PHENOL-LYASE

Chain D:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.49Å 113.04Å 101.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	78.6 (8.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, $R_{free}$	0.186 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14905	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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: 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	0.35	0/3678	0.60	1/4955 (0.0%)
1	B	0.35	0/3678	0.59	1/4955 (0.0%)
1	C	0.36	0/3678	0.62	1/4955 (0.0%)
1	D	0.35	0/3678	0.59	1/4955 (0.0%)
All	All	0.35	0/14712	0.60	4/19820 (0.0%)

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	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ASP	N-CA-C	-7.04	91.98	111.00
1	C	214	ASP	N-CA-C	-6.72	92.86	111.00
1	D	214	ASP	N-CA-C	-6.03	94.71	111.00
1	B	214	ASP	N-CA-C	-5.65	95.75	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	223	TYR	Sidechain



## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3605	0	3548	67	0
1	B	3605	0	3548	87	1
1	C	3605	0	3548	70	0
1	D	3605	0	3548	73	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
2	C	15	0	6	2	0
2	D	15	0	6	1	0
3	A	103	0	0	2	0
3	B	77	0	0	3	0
3	C	158	0	0	3	0
3	D	87	0	0	0	0
All	All	14905	0	14216	289	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (289) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:28:MET:HE3	1:C:368:ALA:HA	1.43	1.01
1:C:97:HIS:HA	1:C:294:LEU:HD13	1.59	0.83
1:B:362:PRO:HG2	1:B:401:GLU:HG2	1.61	0.83
1:A:374:THR:OG1	1:A:376:VAL:HG13	1.79	0.82
1:B:374:THR:OG1	1:B:376:VAL:HG13	1.79	0.82
1:D:443:PRO:HG2	1:D:447:ARG:HA	1.61	0.82
1:B:389:SER:OG	1:B:392:THR:HG22	1.82	0.79
1:D:374:THR:OG1	1:D:376:VAL:HG13	1.83	0.78
1:B:123:PHE:HB3	1:B:126:THR:HG23	1.66	0.78
1:C:443:PRO:HG2	1:C:447:ARG:HA	1.66	0.77
1:D:97:HIS:HA	1:D:294:LEU:HD13	1.65	0.76
1:B:28:MET:HE3	1:B:368:ALA:HA	1.68	0.74
1:D:28:MET:HE3	1:D:368:ALA:HA	1.70	0.73
1:A:362:PRO:HG2	1:A:401:GLU:HG2	1.69	0.73
1:C:374:THR:OG1	1:C:376:VAL:HG13	1.88	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:124:THR:HG23	3:C:745:HOH:O	1.90	0.72
1:A:97:HIS:HA	1:A:294:LEU:HD13	1.72	0.72
1:B:97:HIS:HA	1:B:294:LEU:HD13	1.70	0.71
1:B:123:PHE:HB3	1:B:126:THR:CG2	2.21	0.70
1:A:443:PRO:HG2	1:A:447:ARG:HA	1.73	0.70
1:C:123:PHE:HB3	1:C:126:THR:HG23	1.74	0.70
1:B:426:LYS:HD3	3:B:826:HOH:O	1.92	0.69
1:C:389:SER:HB3	1:C:392:THR:HG22	1.74	0.69
1:B:443:PRO:HG2	1:B:447:ARG:HA	1.74	0.68
1:D:362:PRO:HG2	1:D:401:GLU:HG2	1.75	0.67
1:D:123:PHE:HB3	1:D:126:THR:CG2	2.24	0.67
1:C:389:SER:CB	1:C:392:THR:HG22	2.25	0.67
1:B:127:ARG:HD3	1:B:131:GLU:OE2	1.94	0.67
1:A:28:MET:HE3	1:A:368:ALA:HA	1.77	0.66
1:A:123:PHE:HB3	1:A:126:THR:HG23	1.77	0.65
1:D:108:GLN:HG2	1:D:133:ASN:HD21	1.62	0.64
1:B:26:LYS:O	1:B:30:GLU:HG3	1.98	0.64
1:D:28:MET:CE	1:D:368:ALA:HA	2.28	0.63
1:A:379:MET:HE2	1:A:404:ARG:CZ	2.29	0.63
1:A:111:ILE:HG21	1:A:135:ALA:HB2	1.81	0.63
1:D:214:ASP:OD1	1:D:216:THR:HG23	1.98	0.62
1:B:355:HIS:CD2	1:B:356:LEU:HD13	2.34	0.62
1:D:113:PRO:HA	1:D:134:GLY:O	1.98	0.62
1:C:123:PHE:HB3	1:C:126:THR:CG2	2.29	0.62
1:D:389:SER:OG	1:D:392:THR:HG22	2.00	0.62
1:D:30:GLU:O	1:D:452:ARG:NH2	2.33	0.62
1:C:98:GLN:HE21	1:C:100:ARG:HD2	1.65	0.62
1:A:392:THR:O	1:A:394:GLU:HG3	1.99	0.61
1:B:201:HIS:O	1:B:205:SER:HB3	2.00	0.61
1:A:389:SER:OG	1:A:392:THR:HG22	2.01	0.61
1:C:362:PRO:HG2	1:C:401:GLU:HG2	1.83	0.61
1:D:389:SER:CB	1:D:392:THR:HG22	2.31	0.59
1:D:123:PHE:HB3	1:D:126:THR:HG23	1.83	0.59
1:D:37:LEU:HD11	1:D:450:THR:HA	1.83	0.59
1:B:111:ILE:HG21	1:B:135:ALA:HB2	1.84	0.59
1:A:182:VAL:HG23	1:A:182:VAL:O	2.03	0.59
1:A:123:PHE:HB3	1:A:126:THR:CG2	2.32	0.59
1:A:441:TYR:HD2	1:A:452:ARG:HG3	1.67	0.59
1:B:440:VAL:HG11	1:B:454:ASP:HB2	1.85	0.58
1:C:170:LYS:O	1:C:174:ASN:ND2	2.36	0.58
1:D:379:MET:HE2	1:D:404:ARG:CZ	2.33	0.58
1:A:389:SER:CB	1:A:392:THR:HG22	2.33	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:389:SER:OG	1:C:392:THR:HG22	2.03	0.58
1:A:28:MET:CE	1:A:368:ALA:HA	2.33	0.58
1:D:350:ARG:NH2	1:D:398:PRO:O	2.37	0.57
1:B:440:VAL:CG1	1:B:454:ASP:HB2	2.35	0.57
1:B:113:PRO:HA	1:B:134:GLY:O	2.05	0.57
1:B:392:THR:HG23	1:B:394:GLU:HB2	1.87	0.56
1:C:28:MET:CE	1:C:371:TYR:HB3	2.35	0.56
1:B:389:SER:O	1:B:393:GLY:HA2	2.05	0.56
1:D:389:SER:HB3	1:D:392:THR:HG22	1.87	0.56
1:D:21:ARG:O	1:D:25:VAL:HG23	2.06	0.56
1:D:344:ALA:HB2	1:D:406:THR:HG23	1.87	0.56
1:B:159:ASP:CG	1:B:162:LYS:HG3	2.27	0.56
1:B:389:SER:CB	1:B:392:THR:HG22	2.36	0.56
1:A:100:ARG:HG2	1:A:125:THR:HG21	1.88	0.55
1:C:144:GLU:HB3	1:C:150:LEU:HD23	1.87	0.55
1:D:441:TYR:HD2	1:D:452:ARG:HG3	1.71	0.55
1:C:440:VAL:HG22	1:C:452:ARG:O	2.06	0.55
1:A:188:GLY:HA2	1:A:346:PHE:CE1	2.42	0.55
1:B:144:GLU:HB3	1:B:150:LEU:HD23	1.87	0.55
1:C:275:PHE:CZ	1:C:279:LYS:HD2	2.42	0.55
1:D:188:GLY:HA2	1:D:346:PHE:CE1	2.42	0.55
1:D:71:TYR:CE2	1:D:288:MET:HG2	2.42	0.55
1:B:441:TYR:CE2	1:B:443:PRO:HD3	2.42	0.55
1:C:30:GLU:O	1:C:452:ARG:NH2	2.39	0.55
1:A:214:ASP:OD1	1:A:216:THR:HG23	2.07	0.55
1:B:203:MET:O	1:B:206:THR:HB	2.07	0.54
1:B:441:TYR:HD2	1:B:452:ARG:HG3	1.71	0.54
1:B:362:PRO:HG2	1:B:401:GLU:CG	2.37	0.54
1:A:144:GLU:HB3	1:A:150:LEU:HD23	1.90	0.54
1:C:28:MET:CE	1:C:368:ALA:HA	2.29	0.54
1:A:51:SER:HB2	1:A:257:LYS:HE3	1.89	0.54
1:A:389:SER:HB3	1:A:392:THR:HG22	1.89	0.54
1:C:165:THR:O	1:C:169:GLU:HG2	2.07	0.54
1:C:198:ARG:NH1	3:C:710:HOH:O	2.40	0.54
1:C:420:VAL:HG23	1:C:424:ILE:HD12	1.89	0.54
1:A:275:PHE:CZ	1:A:279:LYS:HD2	2.42	0.54
1:A:440:VAL:HG11	1:A:454:ASP:HB2	1.90	0.53
1:B:279:LYS:O	1:B:282:VAL:HG12	2.09	0.53
1:A:98:GLN:HE21	1:A:100:ARG:HD2	1.74	0.53
1:D:111:ILE:HG21	1:D:135:ALA:HB2	1.90	0.53
1:B:152:LEU:HD23	1:B:155:LYS:HG2	1.91	0.53
1:A:350:ARG:NH2	1:A:398:PRO:O	2.41	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:28:MET:CE	1:B:371:TYR:HB3	2.39	0.53
1:A:108:GLN:HG2	1:A:133:ASN:HD21	1.74	0.52
1:C:98:GLN:NE2	1:C:100:ARG:HD2	2.24	0.52
1:B:275:PHE:CZ	1:B:279:LYS:HD2	2.44	0.52
1:C:91:LYS:HB3	1:C:91:LYS:HZ2	1.75	0.52
1:C:108:GLN:HG2	1:C:133:ASN:HD21	1.74	0.52
1:B:353:CYS:HB3	1:B:355:HIS:CE1	2.44	0.51
1:A:22:ASP:O	1:A:26:LYS:HG3	2.09	0.51
1:A:350:ARG:HH21	1:A:399:LYS:C	2.13	0.51
1:C:379:MET:HE2	1:C:404:ARG:CZ	2.40	0.51
1:B:104:ASN:O	1:B:108:GLN:HG3	2.11	0.51
1:D:98:GLN:HE21	1:D:100:ARG:HD2	1.75	0.51
1:B:430:HIS:HB2	3:B:886:HOH:O	2.10	0.51
1:B:108:GLN:HG2	1:B:133:ASN:HD21	1.76	0.51
1:D:400:LEU:HD12	1:D:400:LEU:H	1.76	0.51
1:B:86:GLU:CD	1:B:307:ARG:HH22	2.14	0.51
1:C:355:HIS:CD2	1:C:356:LEU:HD13	2.46	0.51
1:D:26:LYS:O	1:D:30:GLU:HG3	2.10	0.51
1:C:45:ILE:O	1:C:376:VAL:HA	2.11	0.51
1:A:255:GLY:HA2	1:A:259:CYS:HB2	1.93	0.51
1:B:111:ILE:CG2	1:B:135:ALA:HB2	2.41	0.50
1:A:18:MET:HG3	1:B:313:GLU:HG2	1.91	0.50
1:B:446:LEU:HD11	1:D:283:VAL:HG21	1.94	0.50
1:D:264:GLY:HA2	1:D:294:LEU:HD11	1.94	0.50
1:D:116:TYR:CE2	1:D:170:LYS:HD2	2.47	0.50
1:C:111:ILE:HG21	1:C:135:ALA:HB2	1.94	0.50
1:D:182:VAL:O	1:D:182:VAL:HG23	2.12	0.49
1:C:290:SER:HB2	3:C:716:HOH:O	2.12	0.49
1:B:392:THR:O	1:B:394:GLU:HG3	2.12	0.49
1:C:100:ARG:HG2	1:C:125:THR:HG21	1.93	0.49
1:C:91:LYS:HB3	1:C:91:LYS:NZ	2.27	0.49
1:D:355:HIS:CD2	1:D:356:LEU:HD13	2.48	0.49
1:A:111:ILE:CG2	1:A:135:ALA:HB2	2.42	0.49
1:D:194:MET:HG2	1:D:232:TYR:OH	2.13	0.49
1:D:28:MET:CE	1:D:371:TYR:HB3	2.43	0.49
1:B:98:GLN:HG3	1:B:256:LYS:HD2	1.95	0.49
1:B:255:GLY:HA2	1:B:259:CYS:HB2	1.95	0.49
1:B:37:LEU:HD11	1:B:450:THR:HA	1.94	0.49
1:C:316:GLU:HG2	1:C:320:LYS:HD2	1.95	0.48
1:C:100:ARG:HG3	2:C:1000:PLP:O3P	2.13	0.48
1:A:255:GLY:CA	1:A:259:CYS:HB2	2.44	0.48
1:C:98:GLN:HG3	1:C:256:LYS:HD2	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:98:GLN:HE21	1:B:100:ARG:HD2	1.78	0.48
1:A:75:GLU:OE2	1:C:41:LYS:HD3	2.13	0.48
1:A:26:LYS:O	1:A:30:GLU:HG3	2.13	0.48
1:D:336:ILE:HG22	1:D:347:LEU:HD23	1.96	0.48
1:B:389:SER:N	1:B:394:GLU:O	2.44	0.47
1:A:37:LEU:HD11	1:A:450:THR:HA	1.96	0.47
1:C:182:VAL:O	1:C:182:VAL:HG23	2.15	0.47
1:B:445:GLN:HG2	1:D:280:GLU:OE1	2.14	0.47
1:D:144:GLU:HB3	1:D:150:LEU:HD23	1.95	0.47
1:D:391:GLU:H	1:D:391:GLU:HG2	1.47	0.47
1:A:103:GLU:OE2	2:A:1000:PLP:H6	2.13	0.47
1:D:440:VAL:HG11	1:D:454:ASP:HB2	1.95	0.47
1:B:264:GLY:HA2	1:B:294:LEU:HD11	1.96	0.47
1:B:288:MET:HB2	1:B:291:TYR:CE2	2.49	0.47
1:A:410:ARG:HA	3:A:612:HOH:O	2.14	0.47
1:B:188:GLY:HA2	1:B:346:PHE:CE1	2.50	0.47
1:B:392:THR:CG2	1:B:394:GLU:HB2	2.45	0.47
1:B:387:GLY:HA2	1:B:447:ARG:NE	2.30	0.47
1:A:58:ASP:N	1:A:58:ASP:OD1	2.48	0.47
1:A:98:GLN:OE1	1:C:293:GLY:HA2	2.15	0.46
1:A:389:SER:N	1:A:394:GLU:O	2.45	0.46
1:C:28:MET:HE1	1:C:371:TYR:HB3	1.97	0.46
1:B:280:GLU:OE1	1:D:445:GLN:HG2	2.14	0.46
1:D:397:ARG:CG	1:D:397:ARG:HH11	2.29	0.46
1:B:453:PHE:CD1	1:B:453:PHE:N	2.84	0.46
1:D:381:ARG:HA	1:D:381:ARG:HE	1.81	0.46
1:A:355:HIS:CD2	1:A:356:LEU:HD13	2.50	0.46
1:B:392:THR:HG23	1:B:394:GLU:CB	2.44	0.46
1:C:389:SER:N	1:C:394:GLU:O	2.44	0.46
1:B:271:ASP:HB3	1:B:274:MET:HB2	1.98	0.46
1:B:335:PRO:HB2	1:B:348:ASP:HB3	1.97	0.46
1:B:182:VAL:O	1:B:182:VAL:HG23	2.16	0.46
1:D:111:ILE:CG2	1:D:135:ALA:HB2	2.46	0.46
1:C:392:THR:HG23	1:C:394:GLU:HG3	1.98	0.46
1:C:253:MET:HG2	1:C:266:PHE:CZ	2.51	0.46
1:B:170:LYS:O	1:B:174:ASN:ND2	2.48	0.46
1:B:389:SER:HA	1:B:396:HIS:NE2	2.31	0.45
1:A:142:ARG:HD3	1:A:144:GLU:OE1	2.17	0.45
1:B:204:ALA:HB3	1:B:211:ILE:HD11	1.98	0.45
1:A:19:ILE:HD11	1:A:24:ARG:HG2	1.97	0.45
1:D:263:ILE:HG13	1:D:264:GLY:N	2.31	0.45
1:B:443:PRO:HD2	1:B:451:ALA:HA	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:127:ARG:O	1:B:130:GLN:HB2	2.17	0.45
1:C:188:GLY:HA2	1:C:346:PHE:CE1	2.50	0.45
1:A:152:LEU:HD23	1:A:155:LYS:HG2	1.98	0.45
1:A:45:ILE:O	1:A:376:VAL:HA	2.17	0.45
1:A:188:GLY:O	1:A:341:GLY:HA3	2.16	0.45
1:D:381:ARG:NE	1:D:381:ARG:HA	2.31	0.45
1:B:283:VAL:HG21	1:D:446:LEU:HD11	1.98	0.45
1:C:21:ARG:O	1:C:25:VAL:HG23	2.17	0.45
1:A:374:THR:HG21	1:A:423:GLY:HA3	1.98	0.45
1:C:440:VAL:HG11	1:C:454:ASP:HB2	1.98	0.45
1:C:364:GLN:OE1	1:C:380:GLU:HG2	2.17	0.45
1:D:45:ILE:O	1:D:376:VAL:HA	2.16	0.45
1:B:364:GLN:OE1	1:B:384:VAL:HG11	2.16	0.45
1:A:104:ASN:O	1:A:108:GLN:HG3	2.17	0.44
1:C:360:GLN:HG2	1:C:456:ILE:CD1	2.47	0.44
1:A:364:GLN:OE1	1:A:380:GLU:HG2	2.17	0.44
1:C:348:ASP:OD2	1:C:351:ARG:HG3	2.17	0.44
1:A:379:MET:HE3	1:A:381:ARG:CD	2.48	0.44
1:A:152:LEU:HD23	1:A:155:LYS:CG	2.47	0.44
1:B:45:ILE:O	1:B:376:VAL:HA	2.17	0.44
1:D:188:GLY:O	1:D:341:GLY:HA3	2.17	0.44
1:A:443:PRO:HG3	1:A:450:THR:OG1	2.17	0.44
1:A:379:MET:HE3	1:A:381:ARG:HG2	1.99	0.44
1:D:100:ARG:HD2	2:D:1000:PLP:O3P	2.18	0.44
1:C:350:ARG:NH1	1:C:399:LYS:O	2.50	0.44
1:A:453:PHE:CD1	1:A:453:PHE:N	2.85	0.44
1:D:374:THR:CG2	1:D:423:GLY:HA3	2.48	0.44
1:C:349:ALA:HB3	1:C:401:GLU:HG3	2.00	0.44
1:A:28:MET:CE	1:A:371:TYR:HB3	2.48	0.44
1:C:214:ASP:OD1	1:C:216:THR:HG23	2.18	0.44
1:A:440:VAL:HG22	1:A:452:ARG:O	2.18	0.44
1:A:350:ARG:NH2	1:A:399:LYS:O	2.39	0.43
1:C:389:SER:O	1:C:393:GLY:HA2	2.18	0.43
1:B:440:VAL:HG22	1:B:452:ARG:C	2.39	0.43
1:A:379:MET:CE	1:A:404:ARG:CZ	2.96	0.43
1:B:374:THR:CG2	1:B:423:GLY:HA3	2.48	0.43
1:C:336:ILE:HG22	1:C:347:LEU:HD23	2.00	0.43
1:B:388:ARG:HB2	1:B:394:GLU:C	2.38	0.43
1:C:111:ILE:CG2	1:C:135:ALA:HB2	2.49	0.43
1:B:391:GLU:HG2	1:B:391:GLU:H	1.56	0.43
1:C:120:ASN:OD1	1:C:120:ASN:N	2.51	0.43
1:B:322:VAL:HG22	1:B:407:ILE:HG13	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:21:ARG:O	1:B:25:VAL:HG23	2.19	0.43
1:D:104:ASN:O	1:D:108:GLN:HG3	2.18	0.43
1:A:441:TYR:CD2	1:A:452:ARG:HG3	2.50	0.43
1:B:379:MET:HE2	1:B:404:ARG:CZ	2.49	0.43
1:D:335:PRO:HB2	1:D:348:ASP:HB3	2.01	0.43
1:D:453:PHE:N	1:D:453:PHE:CD1	2.87	0.43
1:D:366:LEU:HB3	1:D:403:VAL:HG21	2.01	0.43
1:B:166:LEU:CD2	1:B:170:LYS:HG3	2.49	0.42
1:A:98:GLN:HG3	1:A:256:LYS:HD2	2.01	0.42
1:D:109:LEU:HD11	1:D:278:ALA:HA	2.00	0.42
1:A:26:LYS:O	1:A:29:GLN:HB2	2.19	0.42
1:C:381:ARG:HE	1:C:381:ARG:HA	1.84	0.42
1:C:392:THR:O	1:C:394:GLU:HG3	2.20	0.42
1:B:254:SER:HB2	2:B:1000:PLP:H5A2	2.00	0.42
1:D:441:TYR:CE2	1:D:443:PRO:HD3	2.55	0.42
1:D:397:ARG:HG2	1:D:397:ARG:HH11	1.85	0.42
1:B:440:VAL:HG22	1:B:452:ARG:O	2.19	0.42
1:D:288:MET:HB2	1:D:291:TYR:CE2	2.55	0.42
1:B:348:ASP:CG	1:B:351:ARG:HG3	2.39	0.42
1:D:322:VAL:HG22	1:D:407:ILE:HG13	2.02	0.42
1:D:255:GLY:HA2	1:D:259:CYS:HB2	2.02	0.42
1:A:16:VAL:HG22	1:B:7:PRO:O	2.19	0.42
1:D:58:ASP:OD1	1:D:58:ASP:N	2.52	0.42
1:C:71:TYR:CE2	1:C:288:MET:HG2	2.55	0.42
1:B:4:PRO:HD3	1:B:320:LYS:HD3	2.02	0.42
1:B:226:LYS:HB2	1:B:240:ILE:CD1	2.50	0.42
1:B:18:MET:HG2	3:B:925:HOH:O	2.20	0.42
1:B:370:ILE:HG22	1:B:376:VAL:HG22	2.02	0.42
1:A:98:GLN:CG	1:A:256:LYS:HD2	2.50	0.42
1:D:389:SER:N	1:D:394:GLU:O	2.47	0.41
1:C:152:LEU:HD23	1:C:155:LYS:CG	2.49	0.41
1:D:374:THR:HG21	1:D:423:GLY:HA3	2.02	0.41
1:D:98:GLN:HG3	1:D:256:LYS:HD2	2.02	0.41
3:A:657:HOH:O	1:C:41:LYS:HG2	2.20	0.41
1:C:318:ARG:HD3	1:C:318:ARG:C	2.41	0.41
1:B:128:PHE:CD2	1:B:129:HIS:N	2.89	0.41
1:D:352:PHE:O	1:D:431:LYS:HD2	2.21	0.41
1:D:203:MET:HB2	1:D:203:MET:HE3	1.97	0.41
1:A:379:MET:HE1	1:A:381:ARG:HD2	2.02	0.41
1:D:226:LYS:HB2	1:D:240:ILE:CD1	2.51	0.41
1:C:441:TYR:HD2	1:C:452:ARG:HG3	1.86	0.41
1:C:182:VAL:HA	1:C:183:THR:HA	1.90	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:400:LEU:HB2	1:A:402:THR:HG23	2.03	0.41
1:C:216:THR:HG21	2:C:1000:PLP:C5	2.51	0.41
1:B:155:LYS:HD2	1:B:339:PRO:HD2	2.02	0.41
1:A:180:LEU:O	1:A:213:TYR:HA	2.21	0.41
1:D:28:MET:HE1	1:D:371:TYR:HB3	2.03	0.41
1:D:389:SER:HA	1:D:396:HIS:NE2	2.36	0.41
1:C:438:THR:HG22	1:C:454:ASP:O	2.21	0.41
1:C:440:VAL:HG22	1:C:452:ARG:C	2.41	0.40
1:B:86:GLU:CD	1:B:307:ARG:NH2	2.74	0.40
1:D:397:ARG:CG	1:D:397:ARG:NH1	2.84	0.40
1:C:430:HIS:O	1:C:433:ASP:HB2	2.21	0.40
1:B:182:VAL:HA	1:B:183:THR:HA	1.87	0.40
1:D:10:ILE:HG21	1:D:13:VAL:HG12	2.03	0.40
1:C:391:GLU:HG2	1:C:391:GLU:H	1.61	0.40
1:C:264:GLY:HA2	1:C:294:LEU:HD11	2.03	0.40
1:B:348:ASP:OD2	1:B:351:ARG:HG3	2.21	0.40
1:B:159:ASP:OD2	1:B:162:LYS:HG3	2.22	0.40
1:C:104:ASN:O	1:C:108:GLN:HG3	2.22	0.40
1:D:91:LYS:HB3	1:D:91:LYS:HZ2	1.86	0.40
1:A:389:SER:HA	1:A:396:HIS:NE2	2.36	0.40
1:D:440:VAL:CG1	1:D:454:ASP:HB2	2.51	0.40
1:B:58:ASP:OD1	1:B:58:ASP:N	2.54	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	Distance(Å)	Clash(Å)
1:B:22:ASP:OD1	1:B:22:ASP:OD1[2.575]	1.80	0.40

## 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	454/456 (100%)	437 (96%)	17 (4%)	0	100	100
1	B	454/456 (100%)	433 (95%)	20 (4%)	1 (0%)	56	57

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	454/456 (100%)	438 (96%)	16 (4%)	0	100	100
1	D	454/456 (100%)	433 (95%)	21 (5%)	0	100	100
All	All	1816/1824 (100%)	1741 (96%)	74 (4%)	1 (0%)	59	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	391	GLU

### 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	380/380 (100%)	334 (88%)	46 (12%)	7	4
1	B	380/380 (100%)	333 (88%)	47 (12%)	7	3
1	C	380/380 (100%)	339 (89%)	41 (11%)	9	5
1	D	380/380 (100%)	338 (89%)	42 (11%)	9	5
All	All	1520/1520 (100%)	1344 (88%)	176 (12%)	8	4

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	17	SER
1	A	21	ARG
1	A	27	LYS
1	A	28	MET
1	A	36	PHE
1	A	37	LEU
1	A	41	LYS
1	A	48	LEU
1	A	91	LYS
1	A	98	GLN
1	A	100	ARG
1	A	105	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	121	MET
1	A	126	THR
1	A	132	LYS
1	A	142	ARG
1	A	152	LEU
1	A	166	LEU
1	A	168	LYS
1	A	169	GLU
1	A	173	GLU
1	A	186	LEU
1	A	210	LYS
1	A	257	LYS
1	A	269	MET
1	A	272	GLU
1	A	273	GLU
1	A	279	LYS
1	A	294	LEU
1	A	307	ARG
1	A	318	ARG
1	A	325	LEU
1	A	366	LEU
1	A	373	GLU
1	A	380	GLU
1	A	388	ARG
1	A	389	SER
1	A	391	GLU
1	A	397	ARG
1	A	400	LEU
1	A	406	THR
1	A	420	VAL
1	A	432	GLU
1	A	446	LEU
1	A	452	ARG
1	B	1	MET
1	B	27	LYS
1	B	36	PHE
1	B	37	LEU
1	B	41	LYS
1	B	48	LEU
1	B	91	LYS
1	B	100	ARG
1	B	105	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	121	MET
1	B	126	THR
1	B	127	ARG
1	B	132	LYS
1	B	142	ARG
1	B	149	SER
1	B	152	LEU
1	B	166	LEU
1	B	168	LYS
1	B	169	GLU
1	B	186	LEU
1	B	205	SER
1	B	210	LYS
1	B	269	MET
1	B	272	GLU
1	B	273	GLU
1	B	279	LYS
1	B	288	MET
1	B	294	LEU
1	B	307	ARG
1	B	318	ARG
1	B	325	LEU
1	B	366	LEU
1	B	380	GLU
1	B	388	ARG
1	B	389	SER
1	B	391	GLU
1	B	392	THR
1	B	397	ARG
1	B	400	LEU
1	B	406	THR
1	B	420	VAL
1	B	426	LYS
1	B	432	GLU
1	B	446	LEU
1	B	450	THR
1	B	452	ARG
1	B	453	PHE
1	C	1	MET
1	C	21	ARG
1	C	27	LYS
1	C	36	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	37	LEU
1	C	48	LEU
1	C	91	LYS
1	C	98	GLN
1	C	100	ARG
1	C	105	LEU
1	C	121	MET
1	C	126	THR
1	C	132	LYS
1	C	152	LEU
1	C	166	LEU
1	C	168	LYS
1	C	169	GLU
1	C	186	LEU
1	C	205	SER
1	C	210	LYS
1	C	257	LYS
1	C	269	MET
1	C	272	GLU
1	C	273	GLU
1	C	279	LYS
1	C	294	LEU
1	C	318	ARG
1	C	325	LEU
1	C	366	LEU
1	C	373	GLU
1	C	380	GLU
1	C	388	ARG
1	C	389	SER
1	C	391	GLU
1	C	392	THR
1	C	397	ARG
1	C	400	LEU
1	C	406	THR
1	C	420	VAL
1	C	432	GLU
1	C	446	LEU
1	D	1	MET
1	D	17	SER
1	D	27	LYS
1	D	28	MET
1	D	36	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	41	LYS
1	D	48	LEU
1	D	91	LYS
1	D	98	GLN
1	D	100	ARG
1	D	105	LEU
1	D	121	MET
1	D	126	THR
1	D	132	LYS
1	D	142	ARG
1	D	152	LEU
1	D	166	LEU
1	D	168	LYS
1	D	169	GLU
1	D	186	LEU
1	D	210	LYS
1	D	269	MET
1	D	272	GLU
1	D	273	GLU
1	D	279	LYS
1	D	288	MET
1	D	294	LEU
1	D	307	ARG
1	D	318	ARG
1	D	325	LEU
1	D	350	ARG
1	D	366	LEU
1	D	373	GLU
1	D	388	ARG
1	D	389	SER
1	D	391	GLU
1	D	397	ARG
1	D	400	LEU
1	D	406	THR
1	D	420	VAL
1	D	432	GLU
1	D	446	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	130	GLN
1	C	130	GLN
1	D	130	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	$\# Z  > 2$
2	PLP	A	1000	1	14,15,16	3.06	5 (35%)	20,22,23	3.91	13 (65%)
2	PLP	B	1000	1	14,15,16	3.15	5 (35%)	20,22,23	3.93	13 (65%)
2	PLP	C	1000	1	14,15,16	3.06	4 (28%)	20,22,23	3.88	13 (65%)
2	PLP	D	1000	1	14,15,16	3.01	4 (28%)	20,22,23	3.91	13 (65%)

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	1000	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1000	1	-	0/6/6/8	0/1/1/1
2	PLP	C	1000	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1000	1	-	0/6/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	PLP	C4-C5	8.60	1.54	1.39
2	C	1000	PLP	C4-C5	8.37	1.53	1.39
2	B	1000	PLP	C4-C5	8.31	1.53	1.39
2	D	1000	PLP	C4-C5	7.69	1.52	1.39
2	B	1000	PLP	C3-C2	6.40	1.45	1.40
2	D	1000	PLP	C3-C2	6.09	1.45	1.40
2	C	1000	PLP	C3-C2	5.70	1.44	1.40
2	A	1000	PLP	C3-C2	5.19	1.44	1.40
2	A	1000	PLP	C2-N1	3.14	1.39	1.33
2	B	1000	PLP	C2-N1	2.96	1.39	1.33
2	D	1000	PLP	C2-N1	2.91	1.39	1.33
2	C	1000	PLP	C2-N1	2.74	1.38	1.33
2	C	1000	PLP	P-O3P	-2.36	1.46	1.54
2	D	1000	PLP	P-O3P	-2.24	1.46	1.54
2	A	1000	PLP	P-O3P	-2.17	1.46	1.54
2	B	1000	PLP	P-O3P	-2.13	1.46	1.54
2	B	1000	PLP	C2A-C2	2.11	1.54	1.50
2	A	1000	PLP	P-O1P	-2.05	1.44	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	PLP	O3P-P-O4P	-9.17	81.34	106.65
2	B	1000	PLP	O3P-P-O4P	-9.13	81.45	106.65
2	C	1000	PLP	O3P-P-O4P	-8.95	81.96	106.65
2	D	1000	PLP	O3P-P-O4P	-8.87	82.16	106.65
2	C	1000	PLP	O3P-P-O1P	-6.56	88.98	110.44
2	D	1000	PLP	O3P-P-O1P	-6.46	89.32	110.44
2	B	1000	PLP	O3P-P-O1P	-6.46	89.33	110.44
2	D	1000	PLP	O3P-P-O2P	-6.45	82.49	107.61
2	C	1000	PLP	O3P-P-O2P	-6.43	82.58	107.61
2	B	1000	PLP	O3P-P-O2P	-6.41	82.66	107.61
2	A	1000	PLP	O3P-P-O2P	-6.35	82.88	107.61
2	A	1000	PLP	O3P-P-O1P	-6.26	89.98	110.44
2	C	1000	PLP	C2A-C2-C3	6.15	128.49	121.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	PLP	C2A-C2-C3	6.12	128.46	121.02
2	D	1000	PLP	C2A-C2-C3	6.02	128.34	121.02
2	A	1000	PLP	C2A-C2-C3	5.69	127.94	121.02
2	A	1000	PLP	O2P-P-O4P	4.83	119.98	106.65
2	C	1000	PLP	O2P-P-O4P	4.51	119.09	106.65
2	D	1000	PLP	O2P-P-O4P	4.42	118.85	106.65
2	B	1000	PLP	O2P-P-O4P	4.34	118.63	106.65
2	A	1000	PLP	O4P-C5A-C5	4.03	117.46	109.26
2	B	1000	PLP	O4P-P-O1P	3.89	118.12	106.71
2	D	1000	PLP	O4P-P-O1P	3.84	117.96	106.71
2	D	1000	PLP	O4P-C5A-C5	3.67	116.73	109.26
2	A	1000	PLP	O4P-P-O1P	3.62	117.31	106.71
2	C	1000	PLP	C6-N1-C2	3.58	126.95	119.28
2	C	1000	PLP	O4P-P-O1P	3.58	117.19	106.71
2	B	1000	PLP	C6-N1-C2	3.55	126.89	119.28
2	B	1000	PLP	O4P-C5A-C5	3.48	116.33	109.26
2	A	1000	PLP	C6-N1-C2	3.43	126.63	119.28
2	D	1000	PLP	C6-N1-C2	3.42	126.60	119.28
2	C	1000	PLP	C3-C2-N1	-3.23	116.22	120.66
2	C	1000	PLP	O2P-P-O1P	3.23	121.00	110.44
2	D	1000	PLP	O3-C3-C2	-3.20	111.92	117.61
2	B	1000	PLP	C3-C2-N1	-3.19	116.29	120.66
2	D	1000	PLP	C3-C2-N1	-3.14	116.35	120.66
2	D	1000	PLP	O2P-P-O1P	3.11	120.61	110.44
2	B	1000	PLP	O3-C3-C2	-3.10	112.10	117.61
2	B	1000	PLP	O2P-P-O1P	3.08	120.51	110.44
2	A	1000	PLP	O3-C3-C2	-3.05	112.18	117.61
2	C	1000	PLP	O3-C3-C2	-2.99	112.29	117.61
2	A	1000	PLP	C3-C2-N1	-2.99	116.56	120.66
2	A	1000	PLP	O2P-P-O1P	2.98	120.19	110.44
2	A	1000	PLP	C5-C6-N1	-2.58	119.20	123.86
2	C	1000	PLP	O4P-C5A-C5	2.53	114.41	109.26
2	D	1000	PLP	C5-C6-N1	-2.53	119.30	123.86
2	B	1000	PLP	C5-C6-N1	-2.53	119.30	123.86
2	C	1000	PLP	C5-C6-N1	-2.50	119.35	123.86
2	B	1000	PLP	C3-C4-C5	-2.14	117.23	121.29
2	C	1000	PLP	C3-C4-C5	-2.13	117.26	121.29
2	A	1000	PLP	C3-C4-C5	-2.12	117.27	121.29
2	D	1000	PLP	C3-C4-C5	-2.07	117.37	121.29

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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