



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:54 PM GMT

PDB ID : 1MLY  
Title : Crystal Structure of 7,8-Diaminopelargonic Acid Synthase in complex with the cis isomer of amiclennomycin  
Authors : Sandmark, J.; Mann, S.; Marquet, A.; Schneider, G.  
Deposited on : 2002-09-02  
Resolution : 1.81 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

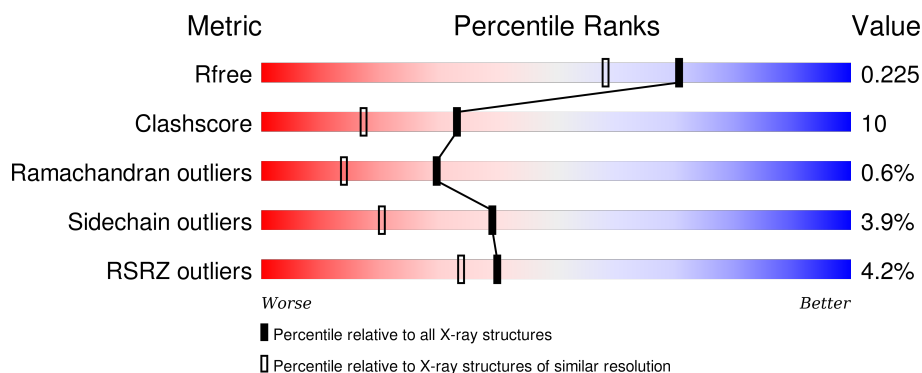
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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. 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	429	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	B	429	<div> <div>4%</div> <div>81%</div> <div>17%</div> <div>.</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
3	NA	A	702	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7239 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.

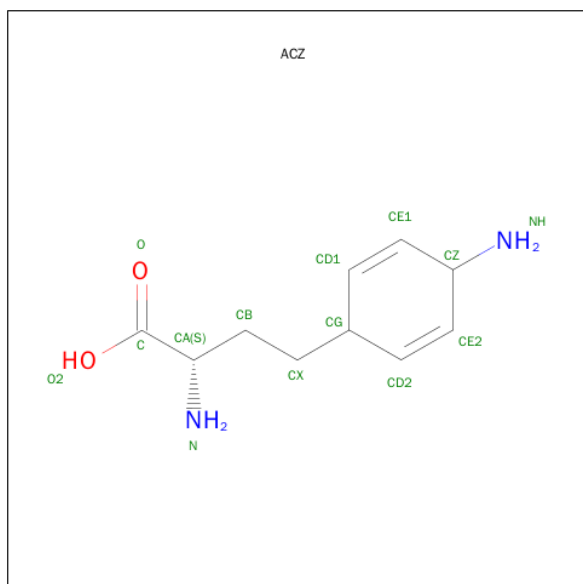
- Molecule 1 is a protein called 7,8-diamino-pelargonic acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	62	2	0
			3303	2098	574	599	32			
1	B	428	Total	C	N	O	S	53	7	0
			3339	2125	581	600	33			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	TRP	SEE REMARK 999	UNP P12995
B	14	LEU	TRP	SEE REMARK 999	UNP P12995

- Molecule 2 is CIS-AMICLENOMYCIN (three-letter code: ACZ) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	10	2	2		

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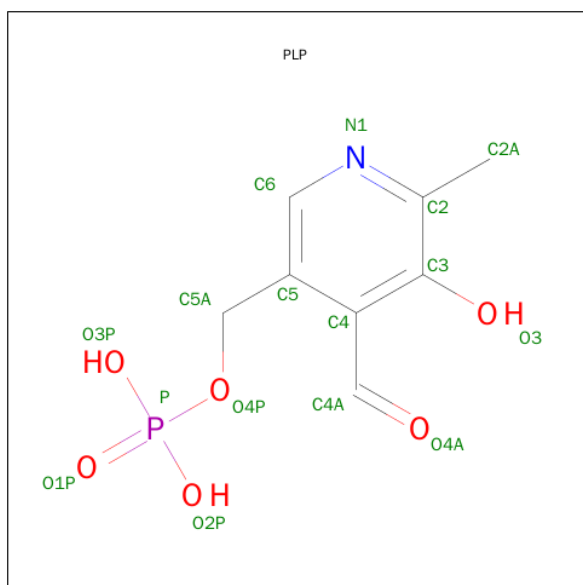
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

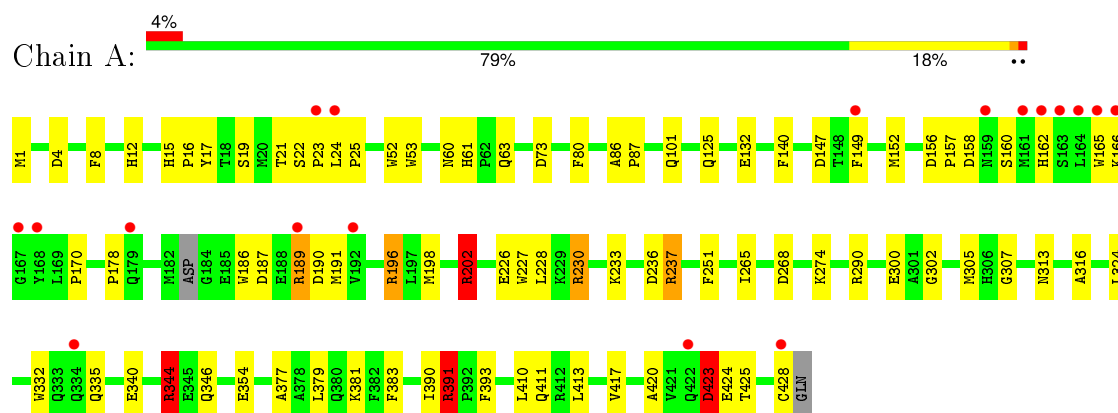
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	263	Total	O	0	0
			263	263		
5	B	274	Total	O	0	0
			274	274		

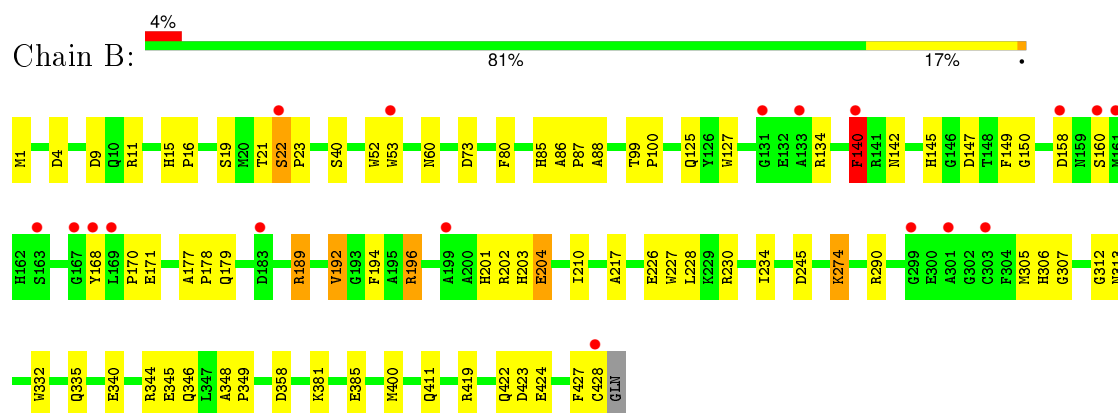
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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: 7,8-diamino-pelargonic acid aminotransferase



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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.66Å 56.07Å 116.17Å 90.00° 109.86° 90.00°	Depositor
Resolution (Å)	20.00 – 1.81 19.99 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.81) 99.0 (19.99-1.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.194 , 0.220 0.204 , 0.225	Depositor DCC
$R_{free}$ test set	3492 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 70339 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7239	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.98% 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: ACZ, NA, 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	0.62	6/3390 (0.2%)	0.87	17/4600 (0.4%)
1	B	0.63	5/3453 (0.1%)	0.95	18/4688 (0.4%)
All	All	0.62	11/6843 (0.2%)	0.91	35/9288 (0.4%)

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	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	GLU	CB-CG	18.39	1.87	1.52
1	A	381	LYS	CD-CE	11.44	1.79	1.51
1	A	196	ARG	CD-NE	-10.68	1.28	1.46
1	A	423	ASP	CB-CG	-9.92	1.30	1.51
1	B	424	GLU	CB-CG	-9.78	1.33	1.52
1	A	300	GLU	CB-CG	-9.76	1.33	1.52
1	A	202	ARG	CD-NE	-8.25	1.32	1.46
1	B	196	ARG	NE-CZ	-8.01	1.22	1.33
1	A	189	ARG	CD-NE	6.15	1.56	1.46
1	B	140[A]	PHE	CB-CG	5.40	1.60	1.51
1	B	140[B]	PHE	CB-CG	5.40	1.60	1.51

All (35) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140[A]	PHE	CB-CG-CD1	17.32	132.92	120.80
1	B	140[B]	PHE	CB-CG-CD1	17.32	132.92	120.80
1	A	423	ASP	CA-CB-CG	16.59	149.90	113.40
1	B	140[A]	PHE	CB-CG-CD2	-14.77	110.46	120.80
1	B	140[B]	PHE	CB-CG-CD2	-14.77	110.46	120.80
1	A	423	ASP	CB-CG-OD1	10.54	127.79	118.30
1	A	423	ASP	CB-CG-OD2	-9.35	109.89	118.30
1	A	196	ARG	CG-CD-NE	-9.05	92.80	111.80
1	A	196	ARG	CB-CG-CD	8.77	134.40	111.60
1	B	140[A]	PHE	CB-CA-C	7.61	125.61	110.40
1	B	140[B]	PHE	CB-CA-C	7.61	125.61	110.40
1	B	196	ARG	CD-NE-CZ	7.49	134.08	123.60
1	B	423	ASP	CB-CG-OD1	7.27	124.85	118.30
1	B	171	GLU	CA-CB-CG	-6.96	98.10	113.40
1	A	156	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	196	ARG	CA-CB-CG	6.38	127.44	113.40
1	A	158	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	358	ASP	CB-CG-OD2	6.01	123.70	118.30
1	B	158	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	4	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	345	GLU	CA-CB-CG	5.72	125.99	113.40
1	B	73	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	187	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	423	ASP	N-CA-C	5.56	126.01	111.00
1	B	202	ARG	N-CA-CB	-5.55	100.60	110.60
1	A	344	ARG	CD-NE-CZ	5.48	131.28	123.60
1	A	391	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	147	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	179	GLN	CA-CB-CG	5.39	125.26	113.40
1	A	236	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	73	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	268	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	4	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	190	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	9	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ARG	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	3303	0	3263	62	1
1	B	3339	0	3287	78	1
2	A	14	0	12	2	0
2	B	14	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	6	1	0
4	B	15	0	6	0	0
5	A	263	0	0	8	1
5	B	274	0	0	6	1
All	All	7239	0	6586	134	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (134) 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:B:53[B]:TRP:CD1	1:B:400[B]:MET:HE1	1.22	1.71
1:B:53[B]:TRP:CD1	1:B:400[B]:MET:CE	1.79	1.59
1:B:53[B]:TRP:NE1	1:B:400[B]:MET:HE1	1.05	1.32
1:B:53[B]:TRP:NE1	1:B:400[B]:MET:CE	1.94	1.13
1:B:53[B]:TRP:CD1	1:B:400[B]:MET:HE3	1.80	1.10
1:A:237:ARG:NH2	5:A:883:HOH:O	1.85	1.05
1:B:149[B]:PHE:CE1	1:B:168:TYR:HD2	1.75	1.04
1:B:53[B]:TRP:CE2	1:B:400[B]:MET:HE1	1.95	1.00
1:B:149[B]:PHE:HE1	1:B:168:TYR:CD2	1.81	0.98
1:A:340:GLU:HG2	1:A:344:ARG:HD3	1.45	0.97
1:B:422[B]:GLN:HG2	5:B:949:HOH:O	1.70	0.88
1:B:53[B]:TRP:HD1	1:B:400[B]:MET:CE	1.85	0.87
1:A:125:GLN:HE22	1:A:305:MET:H	1.20	0.85
1:B:226:GLU:OE2	1:B:230[A]:ARG:NH1	2.11	0.84
1:B:419:ARG:O	1:B:422[A]:GLN:HG2	1.78	0.82
1:B:149[B]:PHE:CE1	1:B:168:TYR:CD2	2.61	0.81
1:B:149[B]:PHE:HE1	1:B:168:TYR:HD2	0.91	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53[B]:TRP:CE3	1:B:274:LYS:NZ	2.48	0.80
1:B:53[B]:TRP:CG	1:B:400[B]:MET:HE1	2.12	0.78
1:A:149[B]:PHE:HD1	1:B:150:GLY:HA2	1.49	0.78
1:B:140[B]:PHE:HD2	1:B:178:PRO:HD3	1.50	0.75
1:A:428:CYS:C	5:A:851:HOH:O	2.25	0.74
1:A:423:ASP:HB2	1:A:425:THR:OG1	1.87	0.73
4:A:730:PLP:O3P	5:A:797:HOH:O	2.07	0.72
1:B:53[B]:TRP:HE1	1:B:400[B]:MET:HE1	1.48	0.70
1:A:428:CYS:O	5:A:851:HOH:O	2.09	0.69
1:A:340:GLU:HG2	1:A:344:ARG:CD	2.21	0.69
1:A:149[B]:PHE:CD1	1:B:150:GLY:HA2	2.28	0.68
1:A:21:THR:C	1:A:23:PRO:HD2	2.13	0.68
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.59	0.67
1:A:149[B]:PHE:HD1	1:B:150:GLY:CA	2.08	0.67
1:A:17:TYR:OH	1:A:147:ASP:OD1	2.13	0.66
1:A:1:MET:HG2	5:A:986:HOH:O	1.94	0.66
1:B:53[B]:TRP:HE3	1:B:274:LYS:HZ3	1.38	0.66
1:B:189:ARG:O	1:B:192:VAL:HG13	1.96	0.65
1:A:19:SER:O	1:A:23:PRO:HD3	1.98	0.63
1:B:52:TRP:C	1:B:53[B]:TRP:CD1	2.73	0.62
1:A:393:PHE:CD1	2:A:731:ACZ:HCA	2.35	0.62
1:A:391:ARG:NH2	5:A:827:HOH:O	2.34	0.60
1:B:52:TRP:C	1:B:53[B]:TRP:CG	2.73	0.60
1:A:226:GLU:OE2	1:A:230:ARG:NH1	2.34	0.60
1:B:140[B]:PHE:HE1	1:B:194:PHE:CD2	2.20	0.60
1:B:340:GLU:O	1:B:344:ARG:HG3	2.00	0.60
1:B:125:GLN:HE22	1:B:305:MET:H	1.50	0.59
1:B:53[A]:TRP:HB2	1:B:274:LYS:HD3	1.84	0.59
1:B:53[B]:TRP:HE1	1:B:400[B]:MET:CE	2.09	0.59
1:A:423:ASP:CB	1:A:425:THR:OG1	2.51	0.58
1:A:251:PHE:CE1	1:A:324:LEU:HD21	2.39	0.57
1:A:53:TRP:N	1:A:53:TRP:CD1	2.73	0.57
1:A:22:SER:N	1:A:23:PRO:CD	2.68	0.57
1:B:142:ASN:HD22	1:B:177:ALA:HB2	1.70	0.56
1:B:140[B]:PHE:HZ	1:B:227:TRP:CZ3	2.24	0.56
1:B:422[B]:GLN:HG2	5:B:1005:HOH:O	2.05	0.56
1:B:427:PHE:O	1:B:428:CYS:HB2	2.05	0.56
1:B:53[B]:TRP:CG	1:B:400[B]:MET:CE	2.73	0.56
1:A:423:ASP:O	1:A:425:THR:N	2.39	0.56
1:B:140[B]:PHE:CE1	1:B:194:PHE:CD2	2.94	0.55
1:B:381:LYS:NZ	1:B:385:GLU:OE2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140[A]:PHE:CE1	1:B:210:ILE:HB	2.42	0.55
1:A:198:MET:O	1:A:202:ARG:HB3	2.07	0.55
1:B:140[A]:PHE:CE2	1:B:178:PRO:HG3	2.42	0.55
1:B:140[B]:PHE:HD2	1:B:178:PRO:CD	2.20	0.54
1:A:17:TYR:OH	1:A:147:ASP:CG	2.46	0.54
1:B:140[B]:PHE:CE1	5:B:884:HOH:O	2.61	0.53
1:A:152:MET:HE1	1:A:165:TRP:CE2	2.43	0.53
1:A:423:ASP:C	1:A:425:THR:N	2.62	0.53
1:B:140[B]:PHE:CD2	1:B:178:PRO:HD3	2.39	0.52
1:B:140[B]:PHE:CD2	1:B:178:PRO:HG3	2.44	0.52
1:B:203[B]:HIS:NE2	1:B:204:GLU:HG2	2.25	0.51
1:A:24:LEU:HB3	1:A:25:PRO:HD2	1.91	0.51
1:A:147:ASP:HB3	1:B:306:HIS:CE1	2.45	0.51
1:B:145:HIS:HD2	1:B:245:ASP:OD2	1.92	0.51
1:A:346:GLN:HE22	1:A:411[A]:GLN:HG3	1.75	0.51
1:B:332:TRP:HA	1:B:335:GLN:HE21	1.76	0.51
1:B:201:HIS:ND1	1:B:204:GLU:OE2	2.38	0.51
1:A:160:SER:N	5:A:817:HOH:O	2.43	0.50
1:A:149[B]:PHE:HE2	1:A:170:PRO:HD3	1.77	0.50
1:A:393:PHE:CG	2:A:731:ACZ:HCA	2.47	0.50
1:B:53[B]:TRP:CD1	1:B:400[B]:MET:HE2	2.24	0.50
1:B:140[B]:PHE:HE1	1:B:194:PHE:CE2	2.30	0.50
1:B:53[B]:TRP:HB2	1:B:274:LYS:HD3	1.93	0.49
1:B:203[B]:HIS:CD2	1:B:204:GLU:HG2	2.48	0.48
1:B:140[B]:PHE:CE2	1:B:178:PRO:HG3	2.48	0.48
1:A:15:HIS:HB3	1:A:16:PRO:HD2	1.94	0.48
1:A:162:HIS:ND1	5:A:902:HOH:O	2.35	0.48
1:A:149[B]:PHE:CD1	1:B:150:GLY:CA	2.91	0.48
1:A:379:LEU:HD11	1:A:420:ALA:HB1	1.95	0.48
1:A:379:LEU:HG	1:A:383:PHE:CE2	2.49	0.47
1:B:99:THR:HB	1:B:100:PRO:HD2	1.95	0.47
1:A:8:PHE:CD1	1:A:12:HIS:CD2	3.03	0.47
1:A:230:ARG:HG2	1:A:230:ARG:HH11	1.80	0.47
1:B:15:HIS:HB3	1:B:16:PRO:HD2	1.98	0.46
1:A:52:TRP:C	1:A:53:TRP:CG	2.89	0.46
1:B:85:HIS:CE1	1:B:88:ALA:HB2	2.50	0.46
1:B:140[B]:PHE:CD1	5:B:884:HOH:O	2.56	0.46
1:B:21:THR:C	1:B:23:PRO:HD3	2.36	0.46
1:B:86:ALA:HB3	1:B:87:PRO:HD3	1.98	0.45
1:A:24:LEU:HB3	1:A:377:ALA:HB2	1.99	0.45
1:A:21:THR:C	1:A:23:PRO:CD	2.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:O	1:A:417:VAL:HG23	2.17	0.44
1:B:52:TRP:O	1:B:53[A]:TRP:HB2	2.18	0.43
1:B:140[B]:PHE:CZ	1:B:227:TRP:CZ3	3.04	0.43
1:A:230:ARG:HH11	1:A:230:ARG:CG	2.31	0.43
1:B:348:ALA:N	1:B:349:PRO:CD	2.81	0.43
1:A:152:MET:CE	1:A:165:TRP:NE1	2.81	0.43
1:A:157:PRO:HA	1:A:162:HIS:CG	2.54	0.43
1:A:152:MET:HE1	1:A:165:TRP:NE1	2.33	0.43
1:A:383:PHE:CD2	1:A:390:ILE:HB	2.52	0.43
1:B:192:VAL:HG22	5:B:944:HOH:O	2.17	0.43
1:B:346:GLN:HE22	1:B:411:GLN:HA	1.84	0.43
1:A:332:TRP:HA	1:A:335:GLN:HE21	1.84	0.43
1:A:86:ALA:HB3	1:A:87:PRO:HD3	2.01	0.42
1:A:391:ARG:CG	1:A:391:ARG:HH11	2.28	0.42
1:B:210:ILE:HD11	1:B:228:LEU:CD2	2.50	0.42
1:B:145:HIS:HE1	5:B:855:HOH:O	2.02	0.42
1:B:217:ALA:HB2	2:B:831:ACZ:HD22	2.02	0.42
1:B:230[B]:ARG:HH22	1:B:234:ILE:HG13	1.85	0.41
1:B:312:GLY:O	1:B:313:ASN:C	2.58	0.41
1:A:140:PHE:CE2	1:A:178:PRO:HG3	2.56	0.41
1:B:127:TRP:CD2	1:B:134:ARG:HD2	2.55	0.41
1:B:22:SER:N	1:B:23:PRO:HD3	2.35	0.41
1:A:228:LEU:HB3	1:A:265:ILE:HD13	2.02	0.41
1:B:1:MET:HE3	1:B:40:SER:OG	2.21	0.41
1:A:302:GLY:O	1:B:19:SER:HB2	2.21	0.41
1:A:61:HIS:CE1	1:A:63:GLN:HB2	2.56	0.41
1:A:423:ASP:C	1:A:425:THR:H	2.25	0.41
1:A:346:GLN:NE2	1:A:411[A]:GLN:HG3	2.36	0.41
1:A:313:ASN:ND2	1:A:316:ALA:H	2.19	0.41
1:A:186:TRP:HZ3	1:A:227:TRP:CD1	2.39	0.40
1:A:149[B]:PHE:HZ	1:B:170:PRO:CD	2.34	0.40

All (3) 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:B:21:THR:O	1:B:21:THR:O[2_556]	1.39	0.81
1:A:189:ARG:NH1	5:A:809:HOH:O[4_445]	1.77	0.43
5:B:943:HOH:O	5:B:1099:HOH:O[2_556]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/429 (99%)	407 (96%)	15 (4%)	3 (1%)	26	11
1	B	433/429 (101%)	417 (96%)	14 (3%)	2 (0%)	34	17
All	All	858/858 (100%)	824 (96%)	29 (3%)	5 (1%)	30	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	GLU
1	B	274	LYS
1	A	274	LYS
1	A	307	GLY
1	B	307	GLY

### 5.3.2 Protein sidechains [i](#)

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	345/345 (100%)	329 (95%)	16 (5%)	33	15
1	B	350/345 (101%)	338 (97%)	12 (3%)	44	26
All	All	695/690 (101%)	667 (96%)	28 (4%)	39	19

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASN

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Mol	Chain	Res	Type
1	A	80	PHE
1	A	101	GLN
1	A	132	GLU
1	A	166	LYS
1	A	191	MET
1	A	202	ARG
1	A	230	ARG
1	A	233	LYS
1	A	237	ARG
1	A	290	ARG
1	A	344	ARG
1	A	354	GLU
1	A	391	ARG
1	A	410	LEU
1	A	423	ASP
1	B	11	ARG
1	B	22	SER
1	B	60	ASN
1	B	80	PHE
1	B	140[A]	PHE
1	B	140[B]	PHE
1	B	160	SER
1	B	189	ARG
1	B	192	VAL
1	B	196	ARG
1	B	204	GLU
1	B	290	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	85	HIS
1	A	125	GLN
1	A	135	GLN
1	A	142	ASN
1	A	313	ASN
1	A	335	GLN
1	A	342	GLN
1	B	125	GLN
1	B	142	ASN
1	B	145	HIS

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Mol	Chain	Res	Type
1	B	159	ASN
1	B	262	HIS
1	B	313	ASN
1	B	335	GLN
1	B	342	GLN
1	B	346	GLN
1	B	411	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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PLP	A	730	2	15,15,16	4.09	4 (26%)	21,22,23	1.28	1 (4%)
2	ACZ	A	731	4	6,14,14	1.25	1 (16%)	6,18,18	2.20	2 (33%)
4	PLP	B	830	2	15,15,16	3.84	4 (26%)	21,22,23	1.40	4 (19%)
2	ACZ	B	831	4	6,14,14	1.23	1 (16%)	6,18,18	2.15	1 (16%)

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



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	A	730	2	-	0/6/6/8	0/1/1/1
2	ACZ	A	731	4	-	0/5/19/19	0/1/1/1
4	PLP	B	830	2	-	0/6/6/8	0/1/1/1
2	ACZ	B	831	4	-	0/5/19/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	730	PLP	O3-C3	-5.23	1.24	1.37
4	B	830	PLP	O3-C3	-4.99	1.25	1.37
2	B	831	ACZ	CD2-CE2	2.06	1.40	1.33
2	A	731	ACZ	CE1-CD1	2.14	1.40	1.33
4	B	830	PLP	C3-C4	3.19	1.48	1.40
4	A	730	PLP	C3-C4	3.66	1.49	1.40
4	A	730	PLP	C5-C4	7.16	1.48	1.40
4	B	830	PLP	C5-C4	7.54	1.49	1.40
4	B	830	PLP	C3-C2	10.96	1.48	1.40
4	A	730	PLP	C3-C2	12.40	1.49	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	730	PLP	C3-C4-C5	-2.70	115.83	118.78
4	B	830	PLP	C3-C4-C5	-2.50	116.05	118.78
4	B	830	PLP	C2A-C2-C3	-2.31	118.25	121.04
2	A	731	ACZ	CE2-CZ-NH	2.08	117.14	111.04
4	B	830	PLP	O2P-P-O4P	2.20	112.91	106.56
4	B	830	PLP	C4A-C4-C5	2.69	123.68	120.88
2	B	831	ACZ	CE2-CZ-NH	4.62	124.59	111.04
2	A	731	ACZ	CE1-CZ-NH	4.70	124.82	111.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	730	PLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	731	ACZ	2	0
2	B	831	ACZ	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	427/429 (99%)	0.09	18 (4%)	40 34	15, 24, 40, 52	22 (5%)
1	B	428/429 (99%)	0.09	18 (4%)	40 34	14, 24, 40, 46	15 (3%)
All	All	855/858 (99%)	0.09	36 (4%)	40 34	14, 24, 40, 52	37 (4%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	ALA	8.3
1	A	162	HIS	5.0
1	A	23	PRO	4.6
1	B	428	CYS	4.1
1	A	149[A]	PHE	3.9
1	B	163	SER	3.9
1	B	301	ALA	3.8
1	B	140[A]	PHE	3.7
1	B	167	GLY	3.7
1	A	166	LYS	3.6
1	A	165	TRP	3.4
1	A	164	LEU	3.2
1	B	168	TYR	3.2
1	A	189	ARG	2.9
1	A	167	GLY	2.9
1	A	24	LEU	2.8
1	B	160	SER	2.8
1	B	183	ASP	2.7
1	A	334	GLN	2.6
1	A	161	MET	2.5
1	A	168	TYR	2.5
1	B	299	GLY	2.4
1	B	169	LEU	2.4
1	A	422	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	53[A]	TRP	2.3
1	A	159	ASN	2.3
1	A	163	SER	2.3
1	A	192	VAL	2.2
1	B	303	CYS	2.2
1	B	161	MET	2.2
1	B	22	SER	2.2
1	B	131	GLY	2.2
1	B	158	ASP	2.1
1	A	428	CYS	2.1
1	A	179	GLN	2.1
1	B	199	ALA	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
3	NA	A	702	1/1	0.97	0.24	6.96	12,12,12,12	0
3	NA	B	701	1/1	0.97	0.21	1.98	15,15,15,15	0
2	ACZ	B	831	14/14	0.80	0.14	1.20	26,32,34,35	0
2	ACZ	A	731	14/14	0.88	0.11	0.72	23,30,34,35	0
4	PLP	B	830	15/16	0.96	0.08	-0.41	16,19,21,23	0
4	PLP	A	730	15/16	0.97	0.07	-1.00	15,18,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.