



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:20 AM UTC

PDB ID : 1MLY / pdb_00001mly
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

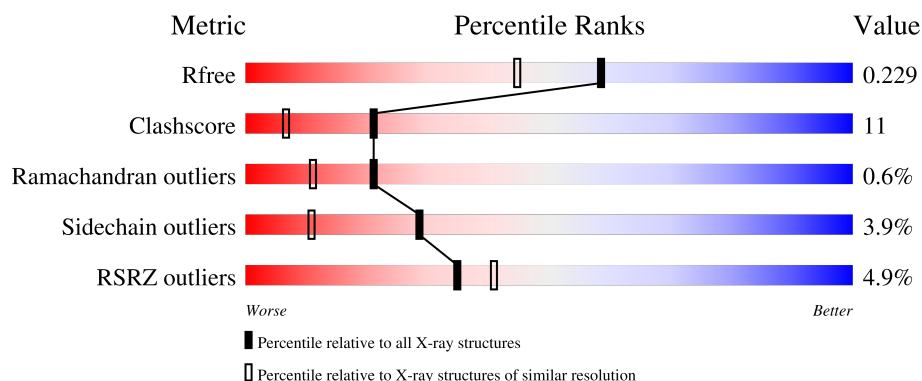
1 Overall quality at a glance

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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	429	5% 80% 17% .
1	B	429	5% 82% 16% .

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.

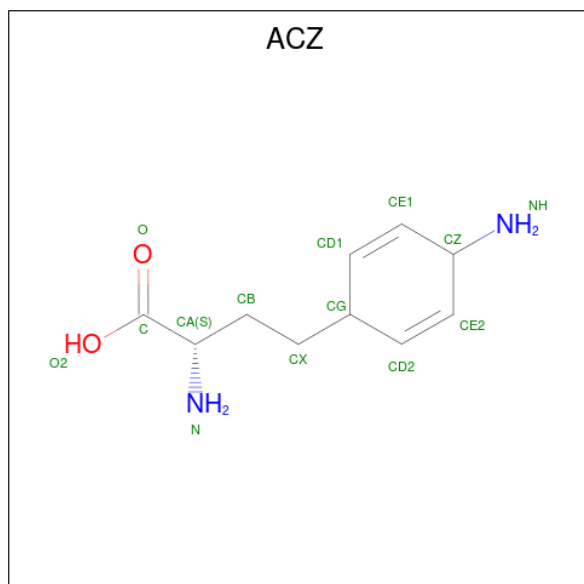
- Molecule 1 is a protein called 7,8-diamino-pelargonic acid aminotransferase.

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 (CCD ID: ACZ) (formula: C₁₀H₁₆N₂O₂).



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

Continued on next page...

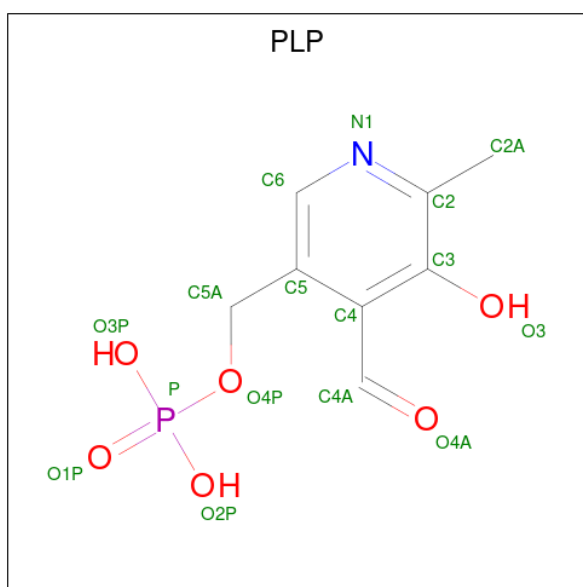
Continued from previous page...

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $\text{C}_8\text{H}_{10}\text{NO}_6\text{P}$).



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

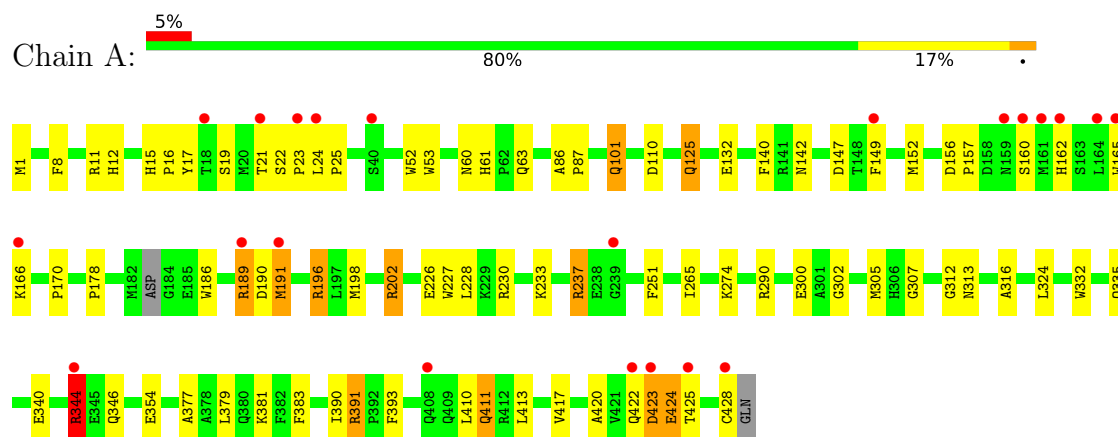
- Molecule 5 is water.

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

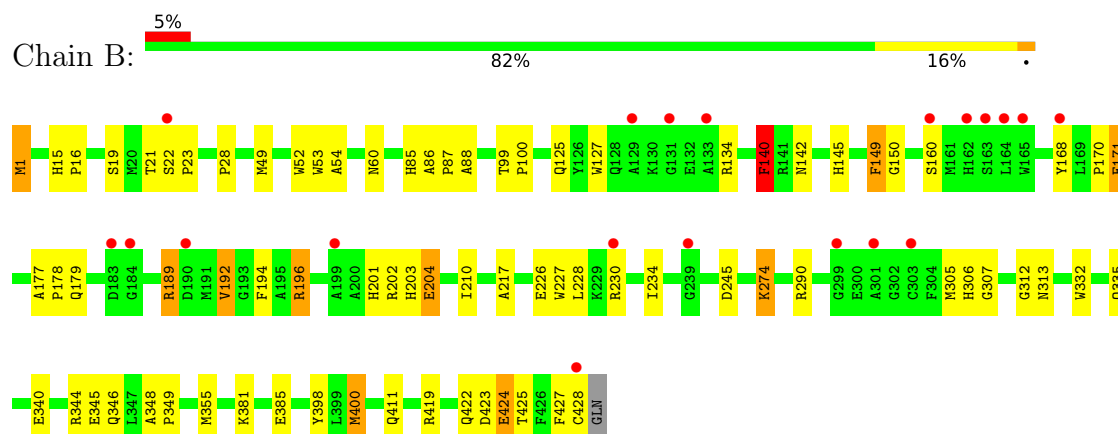
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 7,8-diamino-pelargonic acid aminotransferase



- Molecule 1: 7,8-diamino-pelargonic acid aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.66Å 56.07Å 116.17Å 90.00° 109.86° 90.00°	Depositor
Resolution (Å)	20.00 – 1.81 20.00 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.81) 99.0 (20.00-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.194 , 0.220 (Not available) , 0.229	Depositor DCC
R_{free} test set	3492 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7239	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, NA, ACZ

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	0.71	9/3390 (0.3%)	1.11	7/4600 (0.2%)
1	B	0.69	7/3453 (0.2%)	0.98	8/4688 (0.2%)
All	All	0.70	16/6843 (0.2%)	1.05	15/9288 (0.2%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	ARG	CD-NE	-12.82	1.28	1.46
1	B	171	GLU	CB-CG	11.55	1.87	1.52
1	A	202	ARG	CD-NE	-9.87	1.32	1.46
1	B	196	ARG	NE-CZ	-9.47	1.22	1.33
1	A	381	LYS	CD-CE	9.13	1.79	1.52
1	A	423	ASP	CB-CG	-8.45	1.30	1.52
1	B	400[A]	MET	CA-C	7.82	1.62	1.52
1	B	400[B]	MET	CA-C	7.82	1.62	1.52
1	A	189	ARG	CD-NE	7.61	1.56	1.46
1	B	424	GLU	CB-CG	-6.29	1.33	1.52
1	A	300	GLU	CB-CG	-6.28	1.33	1.52
1	A	344	ARG	NE-CZ	5.67	1.39	1.33
1	A	196	ARG	N-CA	-5.58	1.39	1.46
1	A	101	GLN	CA-CB	5.52	1.62	1.53
1	B	140[A]	PHE	CA-C	5.09	1.59	1.52
1	B	140[B]	PHE	CA-C	5.09	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ASP	CA-CB-CG	37.30	149.90	112.60
1	A	190	ASP	CA-CB-CG	10.13	122.73	112.60
1	A	423	ASP	N-CA-C	10.11	126.01	108.02
1	A	196	ARG	CB-CG-CD	10.04	134.40	111.30
1	A	196	ARG	CG-CD-NE	-8.73	92.80	112.00
1	B	171	GLU	CA-CB-CG	-8.00	98.10	114.10
1	B	196	ARG	CD-NE-CZ	6.92	134.08	124.40
1	A	196	ARG	CA-CB-CG	6.67	127.44	114.10
1	B	54	ALA	N-CA-C	6.08	119.16	111.69
1	B	345	GLU	CA-CB-CG	5.94	125.99	114.10
1	B	149[A]	PHE	N-CA-C	5.84	117.65	111.28
1	B	149[B]	PHE	N-CA-C	5.84	117.65	111.28
1	B	179	GLN	CA-CB-CG	5.58	125.26	114.10
1	B	202	ARG	N-CA-CB	-5.32	100.60	110.18
1	A	422	GLN	N-CA-C	-5.23	106.41	112.89

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	68	1
1	B	3339	0	3287	82	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7239	0	6586	144	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 11.

All (144) 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:CE	1.79	1.61
1:B:53[B]:TRP:CD1	1:B:400[B]:MET:HE1	1.34	1.51
1:B:53[B]:TRP:NE1	1:B:400[B]:MET:HE1	0.99	1.29
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	1.66	1.06
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	1.99	0.98
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:53[B]:TRP:HE1	1:B:400[B]:MET:HE1	1.30	0.94
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
1:B:53[B]:TRP:CE3	1:B:274:LYS:NZ	2.48	0.80
1:A:428:CYS:C	5:A:851:HOH:O	2.25	0.79
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:B:53[A]:TRP:CD1	1:B:274:LYS:HZ3	2.05	0.74
1:A:423:ASP:HB2	1:A:425:THR:OG1	1.87	0.73
1:A:21:THR:C	1:A:23:PRO:HD2	2.13	0.73
4:A:730:PLP:O3P	5:A:797:HOH:O	2.07	0.72
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: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:B:52:TRP:C	1:B:53[B]:TRP:CD1	2.73	0.67
1:A:17:TYR:OH	1:A:147:ASP:OD1	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:52:TRP:C	1:B:53[B]:TRP:CG	2.73	0.65
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:53[B]:TRP:CG	1:B:400[B]:MET:HE3	2.32	0.63
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:53[A]:TRP:CE2	1:B:400[A]:MET:HE1	2.35	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:1:MET:HE3	1:B:28:PRO:HB2	1.84	0.59
1:B:125:GLN:HE22	1:B:305:MET:H	1.50	0.59
1:A:152:MET:HE1	1:A:165:TRP:CE2	2.38	0.59
1:B:53[A]:TRP:HB2	1:B:274:LYS:HD3	1.84	0.59
1:A:17:TYR:OH	1:A:147:ASP:CG	2.46	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:423:ASP:C	1:A:425:THR:N	2.62	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
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:B:140[B]:PHE:CE1	5:B:884:HOH:O	2.61	0.53
1:B:49:MET:HE1	1:B:398:TYR:CE2	2.44	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:21:THR:C	1:B:23:PRO:HD3	2.36	0.50
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:152:MET:HE1	1:A:165:TRP:NE1	2.27	0.50
1:A:393:PHE:CG	2:A:731:ACZ:HCA	2.47	0.50
1:B:140[B]:PHE:HE1	1:B:194:PHE:CE2	2.30	0.50
1:A:21:THR:C	1:A:23:PRO:CD	2.83	0.49
1:A:52:TRP:C	1:A:53:TRP:CG	2.89	0.49
1:B:53[B]:TRP:HB2	1:B:274:LYS:HD3	1.93	0.49
1:B:53[B]:TRP:HD1	1:B:400[B]:MET:HE3	1.56	0.48
1:B:203[B]:HIS:CD2	1:B:204:GLU:HG2	2.48	0.48
1:A:15:HIS:HB3	1:A:16:PRO:HD2	1.94	0.48
1:B:140[B]:PHE:CE2	1:B:178:PRO:HG3	2.48	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:B:423:ASP:OD1	1:B:425:THR:OG1	2.29	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:17:TYR:HH	1:A:147:ASP:CG	2.23	0.46
1:A:142:ASN:H	1:A:156:ASP:CG	2.22	0.46
1:B:312:GLY:O	1:B:313:ASN:C	2.58	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:A:423:ASP:C	1:A:425:THR:H	2.25	0.45
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:413:LEU:O	1:A:417:VAL:HG23	2.17	0.44
1:B:355:MET:HE2	1:B:427:PHE:CG	2.53	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:52:TRP:C	1:A:53:TRP:CD1	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:MET:HE2	1:A:191:MET:HB3	1.88	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:423:ASP:O	1:A:424:GLU:C	2.60	0.43
1:A:86:ALA:HB3	1:A:87:PRO:HD3	2.01	0.42
1:A:391:ARG:HH11	1:A:391:ARG:CG	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:A:140:PHE:CE2	1:A:178:PRO:HG3	2.56	0.41
1:A:312:GLY:O	1:A:313:ASN:C	2.62	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:A:61:HIS:CE1	1:A:63:GLN:HB2	2.56	0.41
1:A:302:GLY:O	1:B:19:SER:HB2	2.21	0.41
1:A:313:ASN:ND2	1:A:316:ALA:H	2.19	0.41
1:A:346:GLN:NE2	1:A:411[A]:GLN:HG3	2.36	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 ⓘ

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	425/429 (99%)	407 (96%)	15 (4%)	3 (1%)	18	8
1	B	433/429 (101%)	417 (96%)	14 (3%)	2 (0%)	24	14
All	All	858/858 (100%)	824 (96%)	29 (3%)	5 (1%)	21	11

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 ⓘ

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%)	328 (95%)	17 (5%)	22	6
1	B	350/345 (101%)	338 (97%)	12 (3%)	32	14
All	All	695/690 (101%)	666 (96%)	29 (4%)	28	10

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	60	ASN
1	A	101	GLN
1	A	110	ASP
1	A	125	GLN
1	A	132	GLU
1	A	166	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	191	MET
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	411[A]	GLN
1	A	411[B]	GLN
1	B	1	MET
1	B	60	ASN
1	B	140[A]	PHE
1	B	140[B]	PHE
1	B	160	SER
1	B	171	GLU
1	B	189	ARG
1	B	192	VAL
1	B	196	ARG
1	B	204	GLU
1	B	290	ARG
1	B	424	GLU

Sometimes 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	65	ASN
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	A	418	ASN
1	B	125	GLN
1	B	142	ASN
1	B	145	HIS
1	B	262	HIS
1	B	335	GLN
1	B	342	GLN
1	B	346	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	411	GLN
1	B	418	ASN

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 oligosaccharides 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	$\# Z > 2$
2	ACZ	A	731	4	12,14,14	5.66	7 (58%)	9,18,18	1.33	2 (22%)
4	PLP	A	730	2	15,15,16	3.42	4 (26%)	21,22,23	1.30	2 (9%)
2	ACZ	B	831	4	12,14,14	5.67	7 (58%)	9,18,18	1.39	2 (22%)
4	PLP	B	830	2	15,15,16	3.29	4 (26%)	21,22,23	1.43	6 (28%)

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	ACZ	A	731	4	-	3/9/19/19	0/1/1/1
4	PLP	A	730	2	-	0/6/6/8	0/1/1/1
2	ACZ	B	831	4	-	1/9/19/19	0/1/1/1
4	PLP	B	830	2	-	0/6/6/8	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	731	ACZ	CZ-CE2	-12.74	1.39	1.50
2	B	831	ACZ	CZ-CE1	-12.67	1.39	1.50
2	B	831	ACZ	CZ-CE2	-11.80	1.40	1.50
2	A	731	ACZ	CZ-CE1	-11.62	1.40	1.50
4	A	730	PLP	C3-C2	8.07	1.49	1.41
4	B	830	PLP	C5-C4	7.75	1.49	1.40
4	A	730	PLP	C5-C4	7.35	1.48	1.40
4	B	830	PLP	C3-C2	7.11	1.48	1.41
2	A	731	ACZ	CG-CD2	-6.22	1.38	1.50
2	B	831	ACZ	CG-CD1	-6.02	1.39	1.50
2	B	831	ACZ	CG-CD2	-5.68	1.39	1.50
2	A	731	ACZ	CG-CD1	-5.46	1.40	1.50
4	A	730	PLP	O3-C3	-5.30	1.24	1.36
4	B	830	PLP	O3-C3	-5.05	1.25	1.36
4	A	730	PLP	C3-C4	4.76	1.49	1.40
4	B	830	PLP	C3-C4	4.14	1.48	1.40
2	A	731	ACZ	O2-C	-2.68	1.22	1.30
2	B	831	ACZ	O2-C	-2.52	1.22	1.30
2	A	731	ACZ	CE1-CD1	2.27	1.40	1.33
2	B	831	ACZ	CD2-CE2	2.19	1.40	1.33
2	A	731	ACZ	CD2-CE2	2.12	1.39	1.33
2	B	831	ACZ	CE1-CD1	2.02	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	830	PLP	C4A-C4-C5	2.66	123.68	120.94
4	B	830	PLP	O2P-P-O4P	2.39	112.91	106.67
4	A	730	PLP	C3-C4-C5	-2.30	115.83	118.59
2	B	831	ACZ	CX-CG-CD2	2.24	121.20	111.58
4	B	830	PLP	C6-N1-C2	2.19	123.16	119.20
4	B	830	PLP	C2A-C2-C3	-2.17	118.25	120.80
4	A	730	PLP	C6-N1-C2	2.17	123.14	119.20
2	A	731	ACZ	CX-CG-CD1	2.15	120.84	111.58
4	B	830	PLP	C3-C4-C5	-2.12	116.05	118.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	831	ACZ	O2-C-O	-2.11	119.28	124.08
2	A	731	ACZ	CX-CG-CD2	2.04	120.36	111.58
4	B	830	PLP	C2A-C2-N1	2.01	121.44	117.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	731	ACZ	CD1-CG-CX-CB
2	B	831	ACZ	CD1-CG-CX-CB
2	A	731	ACZ	CD2-CG-CX-CB
2	A	731	ACZ	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	731	ACZ	2	0
4	A	730	PLP	1	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, 95th 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 ²)	Q<0.9
1	A	427/429 (99%)	0.31	22 (5%) 33 37	11, 24, 39, 52	24 (5%)
1	B	428/429 (99%)	0.32	20 (4%) 36 43	11, 24, 39, 46	22 (5%)
All	All	855/858 (99%)	0.31	42 (4%) 35 41	11, 24, 39, 52	46 (5%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	HIS	5.7
1	B	133	ALA	5.4
1	A	23	PRO	4.9
1	A	344	ARG	4.5
1	A	161	MET	3.5
1	A	425	THR	3.4
1	B	428	CYS	3.4
1	B	160	SER	3.3
1	B	183	ASP	3.0
1	A	166	LYS	3.0
1	A	24	LEU	3.0
1	B	163	SER	3.0
1	A	165	TRP	2.9
1	B	131	GLY	2.9
1	A	18	THR	2.8
1	A	160	SER	2.8
1	B	199	ALA	2.8
1	A	428	CYS	2.7
1	B	168	TYR	2.7
1	B	162	HIS	2.7
1	A	408	GLN	2.6
1	B	303	CYS	2.6
1	A	189	ARG	2.5
1	B	301	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	422	GLN	2.5
1	A	159	ASN	2.5
1	A	40	SER	2.4
1	B	299	GLY	2.4
1	B	190	ASP	2.4
1	A	21	THR	2.4
1	B	239	GLY	2.3
1	A	164	LEU	2.3
1	B	165	TRP	2.3
1	B	184	GLY	2.3
1	B	164	LEU	2.2
1	B	22	SER	2.2
1	A	423	ASP	2.1
1	A	239	GLY	2.1
1	A	149[A]	PHE	2.1
1	A	191	MET	2.1
1	B	129	ALA	2.1
1	B	230[A]	ARG	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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
2	ACZ	B	831	14/14	0.75	0.12	26,32,34,35	0
2	ACZ	A	731	14/14	0.86	0.10	23,30,34,35	0
3	NA	B	701	1/1	0.95	0.17	15,15,15,15	0
3	NA	A	702	1/1	0.96	0.21	12,12,12,12	0
4	PLP	B	830	15/16	0.96	0.07	16,19,21,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PLP	A	730	15/16	0.97	0.06	15,18,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.