



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:32 am BST

PDB ID : 2YXG
Title : Crystal structure of Dihyrodipicolinate Synthase (dapA)
Authors : Padmanabhan, B.; Bessho, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-04-26
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

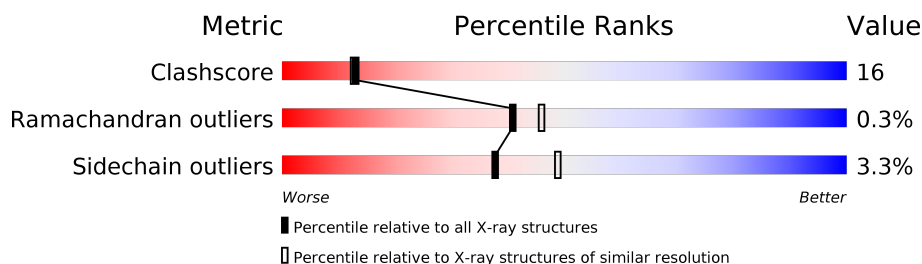
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	289	<div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	B	289	<div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	C	289	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	D	289	<div> <div>70%</div> <div>27%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9549 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 Dihydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2216	1419	363	426	8			
1	B	288	Total	C	N	O	S	0	0	0
			2211	1416	362	425	8			
1	C	288	Total	C	N	O	S	0	0	0
			2211	1416	362	425	8			
1	D	288	Total	C	N	O	S	0	0	0
			2211	1416	362	425	8			

- Molecule 2 is water.

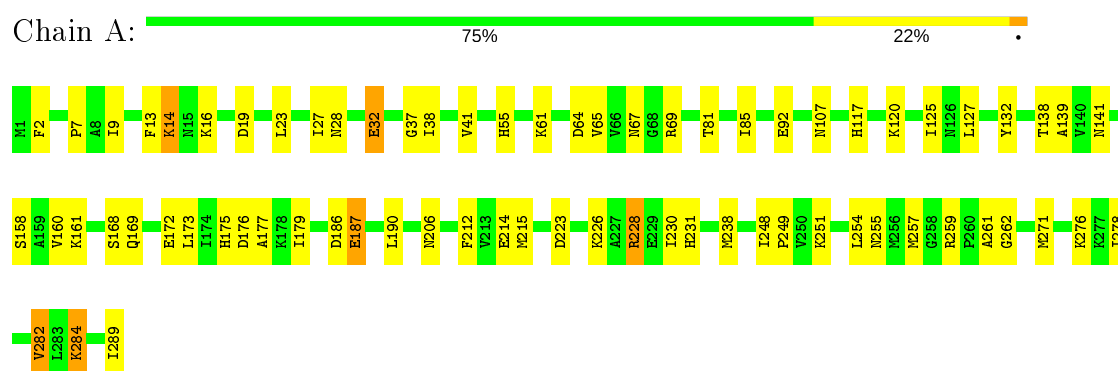
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	195	Total	O	0	0
			195	195		
2	B	193	Total	O	0	0
			193	193		
2	C	150	Total	O	0	0
			150	150		
2	D	162	Total	O	0	0
			162	162		

3 Residue-property plots

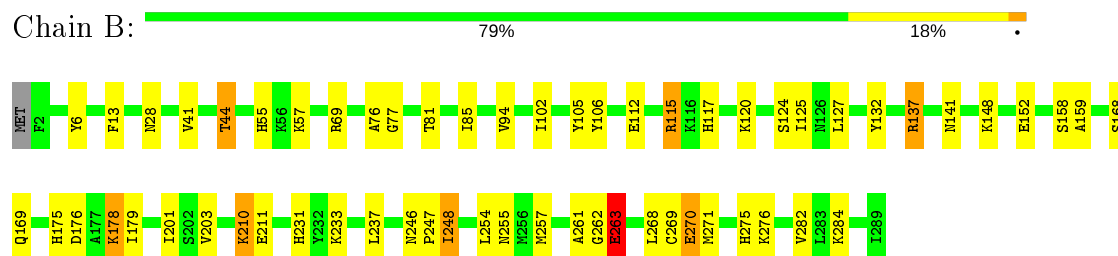
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

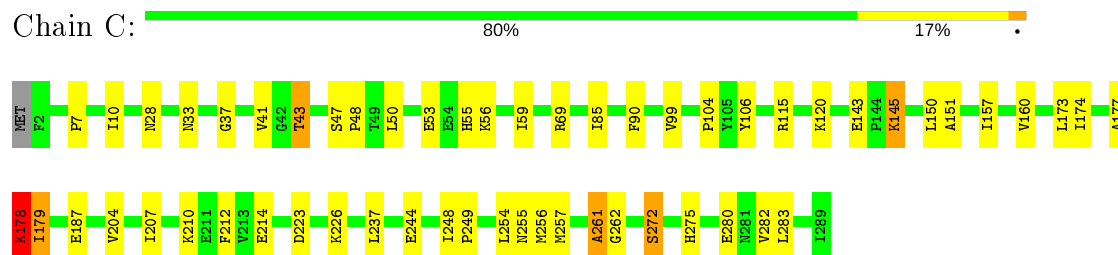
• Molecule 1: Dihydrodipicolinate synthase



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V250	K251	T252	A253	L254	K255	M256	M257	A261	G262	E263	L266	P267	L268	K271	E274	K275	K276	K277	M281	V282	L288	L289	N141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181	D186	E187	L190	G197	V203	V204	A205	N206	K210	E211	F212	V213	E214	E221	L237	M238	K239	A240	M241	F242	N246	P247	L248	P249	M2141	L142	E143	P144	K145	K148	E152	I157	V160	K161	S168	Q169	E172	L173	H174	H175	D176	I179	T180	V181
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.47 Å 76.53 Å 101.86 Å 90.00° 106.87° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	97.5 (20.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.158 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9549	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.03	2/2254 (0.1%)	0.88	3/3058 (0.1%)
1	B	1.04	3/2249 (0.1%)	0.90	4/3051 (0.1%)
1	C	1.02	3/2249 (0.1%)	0.86	2/3051 (0.1%)
1	D	1.13	7/2249 (0.3%)	0.89	2/3051 (0.1%)
All	All	1.06	15/9001 (0.2%)	0.88	11/12211 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	86	GLU	CD-OE2	14.81	1.42	1.25
1	D	86	GLU	CB-CG	11.85	1.74	1.52
1	D	263	GLU	CG-CD	8.15	1.64	1.51
1	D	86	GLU	CG-CD	7.75	1.63	1.51
1	A	32	GLU	CG-CD	7.38	1.63	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	ARG	NE-CZ-NH2	-12.55	114.03	120.30
1	D	137	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	D	137	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	B	76	ALA	C-N-CA	-8.95	103.50	122.30
1	A	228	ARG	NE-CZ-NH2	-7.81	116.39	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	157	ILE	Peptide

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	2216	0	2270	77	0
1	B	2211	0	2265	63	0
1	C	2211	0	2265	62	0
1	D	2211	0	2265	96	0
2	A	195	0	0	15	0
2	B	193	0	0	15	0
2	C	150	0	0	9	0
2	D	162	0	0	10	0
All	All	9549	0	9065	294	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 16.

The worst 5 of 294 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:D:86:GLU:CG	1:D:86:GLU:CB	1.74	1.65
1:A:187:GLU:HG3	2:D:350:HOH:O	1.53	1.09
1:A:271:MET:HE2	1:A:276:LYS:HA	1.33	1.08
1:A:172:GLU:HG2	2:A:480:HOH:O	1.55	1.04
1:A:177:ALA:HB1	1:A:179:ILE:HG13	1.40	1.03

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	287/289 (99%)	281 (98%)	6 (2%)	0	100	100
1	B	286/289 (99%)	279 (98%)	6 (2%)	1 (0%)	41	46
1	C	286/289 (99%)	277 (97%)	7 (2%)	2 (1%)	22	22
1	D	286/289 (99%)	282 (99%)	3 (1%)	1 (0%)	41	46
All	All	1145/1156 (99%)	1119 (98%)	22 (2%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	272	SER
1	D	261	ALA
1	B	261	ALA
1	C	261	ALA

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	247/248 (100%)	240 (97%)	7 (3%)	43	56
1	B	247/248 (100%)	237 (96%)	10 (4%)	31	40
1	C	247/248 (100%)	238 (96%)	9 (4%)	35	45
1	D	247/248 (100%)	240 (97%)	7 (3%)	43	56
All	All	988/992 (100%)	955 (97%)	33 (3%)	38	49

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	248	ILE
1	C	99	VAL
1	D	221	GLU
1	B	263	GLU
1	B	284	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	231	HIS
1	C	33	ASN
1	D	246	ASN
1	B	246	ASN
1	B	255	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.