



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:57 AM GMT

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 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

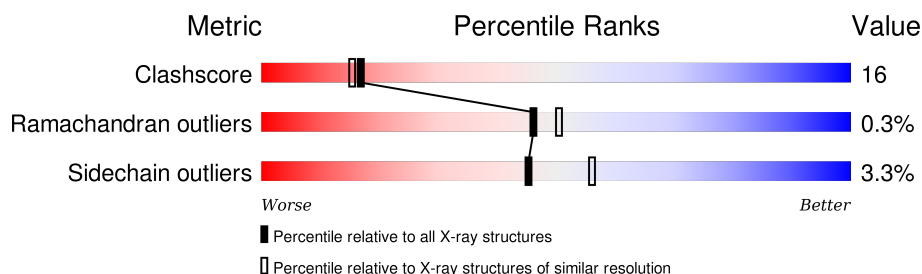
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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  $\geq 3$ , 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.

Note EDS was not executed.

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

## 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.

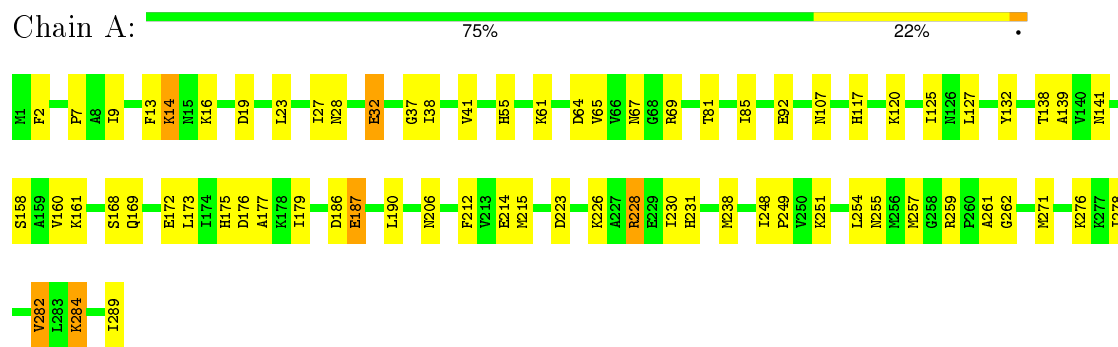
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	195	Total	O	0	0
			195	195		
2	B	193	Total	O	0	0
			193	193		
2	C	150	Total	O	0	0
			150	150		
2	D	162	Total	O	0	0
			162	162		

### 3 Residue-property plots

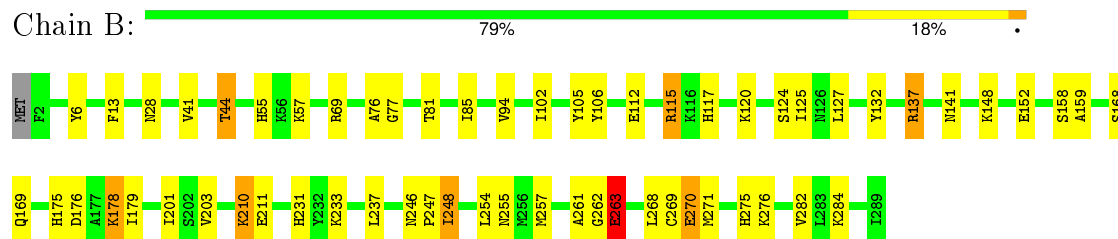
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

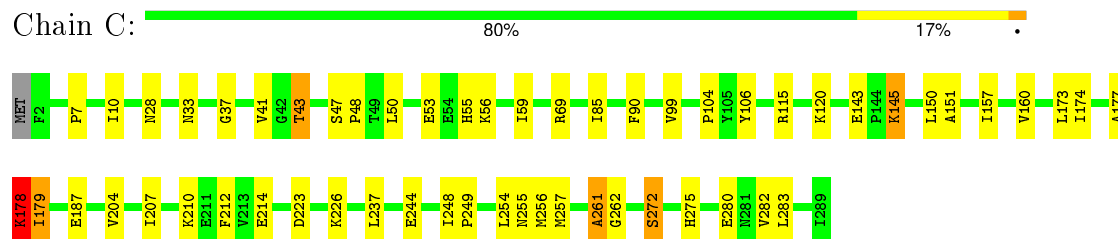
#### • Molecule 1: Dihydrodipicolinate synthase



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#### • Molecule 1: Dihydrodipicolinate synthase



#### • Molecule 1: Dihydrodipicolinate synthase





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

All (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
1	D	263	GLU	CB-CG	6.94	1.65	1.52
1	C	178	LYS	CB-CG	6.25	1.69	1.52
1	A	187	GLU	CG-CD	5.81	1.60	1.51
1	C	53	GLU	CD-OE1	5.78	1.32	1.25
1	B	270	GLU	CG-CD	5.70	1.60	1.51
1	C	187	GLU	CG-CD	5.68	1.60	1.51
1	D	274	GLU	CG-CD	5.58	1.60	1.51
1	B	77	GLY	N-CA	5.49	1.54	1.46
1	D	187	GLU	CG-CD	5.40	1.60	1.51
1	B	263	GLU	CB-CG	5.39	1.62	1.52

All (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
1	B	137	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	64	ASP	CB-CG-OD1	5.91	123.61	118.30
1	B	115	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	115	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	272	SER	CB-CA-C	-5.34	99.96	110.10
1	A	228	ARG	NE-CZ-NH1	5.04	122.82	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.

All (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
1:A:284:LYS:HE3	1:A:289:ILE:HD12	1.42	0.99
1:D:241:MET:HE3	1:D:250:VAL:HB	1.41	0.99
1:B:141:ASN:HD21	1:B:169:GLN:HE22	1.02	0.97
1:A:271:MET:CE	1:A:276:LYS:HA	1.95	0.97
1:B:271:MET:CE	1:B:276:LYS:HA	1.95	0.96
1:D:186:ASP:HB3	1:D:238:MET:HE2	1.49	0.93
1:A:14:LYS:HE3	2:A:414:HOH:O	1.69	0.93
1:A:13:PHE:O	1:A:14:LYS:HD3	1.68	0.92
1:B:176:ASP:HB2	2:B:298:HOH:O	1.69	0.92
1:D:141:ASN:HD21	1:D:169:GLN:HE22	1.20	0.88
1:B:271:MET:HE3	1:B:276:LYS:N	1.89	0.88
1:C:223:ASP:OD2	1:C:226:LYS:HD2	1.76	0.86
1:A:141:ASN:HD21	1:A:169:GLN:HE22	1.21	0.85
1:D:241:MET:HE1	1:D:250:VAL:HG23	1.58	0.85
1:A:187:GLU:HA	1:A:238:MET:HE1	1.60	0.83
1:A:186:ASP:C	1:A:238:MET:CE	2.46	0.83
1:D:255:ASN:HD21	1:D:262:GLY:H	1.25	0.83
1:C:256:MET:CE	1:C:280:GLU:HA	2.09	0.82
1:C:41:VAL:HG12	1:C:47:SER:HB3	1.61	0.82
1:D:186:ASP:HB3	1:D:238:MET:CE	2.08	0.82
1:C:160:VAL:HG12	1:C:179:ILE:HD13	1.61	0.82
1:B:13:PHE:HB2	1:B:263:GLU:OE1	1.79	0.81
1:B:55:HIS:CD2	2:B:297:HOH:O	2.32	0.81
1:B:28:ASN:HD21	1:B:69:ARG:HH22	1.29	0.80
1:B:28:ASN:ND2	1:B:69:ARG:HH22	1.78	0.80
1:D:175:HIS:HD2	1:D:176:ASP:OD1	1.64	0.80
1:A:284:LYS:HE3	1:A:289:ILE:CD1	2.12	0.80
1:C:178:LYS:HD2	1:C:178:LYS:O	1.82	0.80
1:B:270:GLU:HG3	2:B:385:HOH:O	1.80	0.79
1:D:288:LEU:O	1:D:289:ILE:HB	1.81	0.78
1:D:263:GLU:HG3	2:D:368:HOH:O	1.82	0.78
1:C:151:ALA:HB1	1:C:178:LYS:HG3	1.66	0.78
1:B:55:HIS:HD2	2:B:297:HOH:O	1.65	0.77
2:A:337:HOH:O	1:D:187:GLU:HG3	1.83	0.77
1:C:254:LEU:HD23	1:C:257:MET:CE	2.15	0.77
1:D:241:MET:CE	1:D:250:VAL:HB	2.13	0.76
1:C:28:ASN:HD21	1:C:69:ARG:HH22	1.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:HIS:CD2	1:D:176:ASP:OD1	2.41	0.74
1:C:178:LYS:HE3	2:C:318:HOH:O	1.88	0.74
1:A:271:MET:HE2	1:A:276:LYS:CA	2.13	0.74
1:D:28:ASN:HD21	1:D:69:ARG:HH22	1.34	0.74
1:B:175:HIS:HD2	2:B:479:HOH:O	1.71	0.73
1:D:9:ILE:HA	1:D:206:ASN:HD21	1.54	0.73
1:A:186:ASP:HB3	1:A:238:MET:HE3	1.71	0.72
1:A:289:ILE:HA	2:A:293:HOH:O	1.88	0.72
1:C:143:GLU:OE1	1:C:145:LYS:HE2	1.89	0.71
1:C:55:HIS:CD2	2:C:351:HOH:O	2.43	0.71
1:C:43:THR:HG22	1:D:106:TYR:OH	1.89	0.71
1:B:271:MET:CE	1:B:276:LYS:CA	2.68	0.71
1:A:255:ASN:HD21	1:A:262:GLY:H	1.37	0.70
1:A:254:LEU:HD23	1:A:257:MET:CE	2.22	0.70
1:B:271:MET:HE2	1:B:276:LYS:HA	1.72	0.70
1:D:168:SER:HB2	2:D:350:HOH:O	1.90	0.69
1:D:221:GLU:HB2	2:D:362:HOH:O	1.90	0.69
1:A:186:ASP:O	1:A:238:MET:HE1	1.93	0.69
1:D:254:LEU:HD23	1:D:257:MET:CE	2.22	0.69
1:A:168:SER:CB	2:A:337:HOH:O	2.40	0.69
1:B:248:ILE:HD11	1:B:271:MET:HB2	1.74	0.69
1:D:28:ASN:ND2	1:D:69:ARG:HH22	1.91	0.69
1:B:13:PHE:CB	1:B:263:GLU:OE1	2.41	0.68
1:A:251:LYS:HG2	1:A:261:ALA:HB1	1.75	0.68
1:B:81:THR:OG1	1:B:117:HIS:HD2	1.75	0.68
1:C:255:ASN:HD21	1:C:262:GLY:H	1.38	0.68
1:A:284:LYS:CE	1:A:289:ILE:HD12	2.21	0.68
1:D:271:MET:CE	1:D:276:LYS:HA	2.24	0.68
1:D:186:ASP:CB	1:D:238:MET:HE2	2.22	0.68
1:C:256:MET:HE1	1:C:280:GLU:HA	1.77	0.67
1:D:288:LEU:O	1:D:289:ILE:CB	2.42	0.67
1:A:186:ASP:C	1:A:238:MET:HE1	2.14	0.67
1:D:81:THR:OG1	1:D:117:HIS:HD2	1.78	0.67
1:C:160:VAL:CG1	1:C:179:ILE:HD13	2.25	0.66
1:B:254:LEU:HD23	1:B:257:MET:CE	2.25	0.66
1:B:255:ASN:HD21	1:B:262:GLY:H	1.43	0.66
1:D:186:ASP:C	1:D:238:MET:HE2	2.16	0.66
1:C:145:LYS:HG2	2:C:293:HOH:O	1.96	0.66
1:D:239:LYS:HD2	1:D:242:PHE:CZ	2.31	0.65
1:D:148:LYS:O	1:D:152:GLU:HG2	1.96	0.65
1:A:187:GLU:HA	1:A:238:MET:CE	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:GLU:OE2	1:C:275:HIS:HD2	1.80	0.65
1:A:177:ALA:HB2	2:A:329:HOH:O	1.97	0.64
1:B:271:MET:HE3	1:B:276:LYS:CA	2.27	0.64
1:C:256:MET:HE3	1:C:280:GLU:HA	1.78	0.64
1:C:256:MET:HE3	1:C:280:GLU:HG3	1.80	0.64
1:D:289:ILE:O	1:D:289:ILE:HG22	1.97	0.64
1:B:178:LYS:HB2	2:B:298:HOH:O	1.97	0.63
1:A:254:LEU:HA	1:A:257:MET:HE2	1.80	0.63
1:D:288:LEU:O	1:D:289:ILE:HD12	1.99	0.63
1:A:14:LYS:HE2	1:A:19:ASP:OD2	1.99	0.62
1:C:207:ILE:HD13	1:C:254:LEU:HD21	1.81	0.62
1:D:241:MET:HE1	1:D:250:VAL:CG2	2.29	0.62
1:B:211:GLU:HG2	2:B:433:HOH:O	1.99	0.62
1:A:175:HIS:HD2	1:A:176:ASP:OD1	1.82	0.62
1:D:181:VAL:CG2	1:D:197:GLY:HA2	2.29	0.62
1:A:168:SER:HB2	2:A:337:HOH:O	2.00	0.62
1:D:44:THR:HG21	1:D:203:VAL:HG22	1.80	0.61
1:D:58:VAL:O	1:D:62:VAL:HG23	2.01	0.61
1:D:241:MET:CE	1:D:250:VAL:CB	2.79	0.61
1:B:248:ILE:HD11	1:B:271:MET:CA	2.30	0.60
1:A:187:GLU:CA	1:A:238:MET:HE1	2.31	0.60
1:D:256:MET:O	1:D:289:ILE:HG21	2.00	0.60
1:C:28:ASN:ND2	1:C:69:ARG:HH22	2.00	0.60
1:D:44:THR:CG2	1:D:246:ASN:HD21	2.15	0.59
1:B:41:VAL:HG12	1:B:41:VAL:O	2.02	0.59
1:D:289:ILE:HG12	2:D:402:HOH:O	2.01	0.59
1:B:248:ILE:HD11	1:B:271:MET:CB	2.33	0.59
1:C:160:VAL:HG12	1:C:179:ILE:CD1	2.29	0.59
1:C:256:MET:HE3	1:C:280:GLU:CA	2.31	0.59
1:A:175:HIS:CD2	1:A:176:ASP:OD1	2.56	0.59
1:D:212:PHE:CE1	1:D:238:MET:HE3	2.38	0.58
1:B:271:MET:CE	1:B:276:LYS:N	2.65	0.58
1:C:7:PRO:HD2	1:C:37:GLY:O	2.03	0.58
1:A:187:GLU:N	1:A:238:MET:CE	2.67	0.58
1:B:275:HIS:NE2	2:B:380:HOH:O	2.32	0.58
1:D:44:THR:HB	1:D:246:ASN:HD21	1.69	0.58
1:A:173:LEU:O	1:A:177:ALA:HB3	2.04	0.58
1:A:177:ALA:HB1	1:A:179:ILE:CG1	2.23	0.58
1:B:141:ASN:HD21	1:B:169:GLN:NE2	1.87	0.58
1:B:41:VAL:HG11	1:B:55:HIS:CD2	2.39	0.58
1:D:239:LYS:HD2	1:D:242:PHE:HZ	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:HG22	1:B:246:ASN:HD21	1.69	0.58
1:D:181:VAL:HG23	1:D:197:GLY:HA2	1.86	0.57
1:C:173:LEU:HD22	1:C:179:ILE:HD11	1.85	0.57
1:B:117:HIS:HE1	2:B:301:HOH:O	1.87	0.57
1:D:255:ASN:HD21	1:D:262:GLY:N	1.99	0.57
1:D:289:ILE:O	1:D:289:ILE:CG2	2.53	0.57
1:D:277:LYS:HE2	1:D:281:ASN:HD21	1.69	0.57
1:A:7:PRO:HD2	1:A:37:GLY:O	2.05	0.57
1:D:44:THR:HG22	1:D:246:ASN:HD21	1.70	0.57
1:C:151:ALA:CB	1:C:178:LYS:HG3	2.33	0.56
1:B:44:THR:CG2	1:B:246:ASN:HD21	2.17	0.56
1:D:168:SER:CB	2:D:350:HOH:O	2.51	0.56
1:C:178:LYS:NZ	2:C:427:HOH:O	2.37	0.56
1:A:175:HIS:HE1	2:D:397:HOH:O	1.89	0.56
1:C:33:ASN:HD22	1:C:210:LYS:HB2	1.70	0.55
1:A:248:ILE:HB	1:A:249:PRO:HD3	1.88	0.55
1:B:271:MET:HE3	1:B:275:HIS:C	2.27	0.55
1:D:237:LEU:HA	1:D:282:VAL:HG11	1.88	0.55
1:D:254:LEU:HD23	1:D:257:MET:HE3	1.89	0.55
1:C:56:LYS:HE3	1:C:90:PHE:CE1	2.43	0.54
1:D:212:PHE:CE1	1:D:238:MET:CE	2.90	0.54
1:C:256:MET:HE3	1:C:280:GLU:CB	2.38	0.54
1:D:271:MET:HE1	1:D:276:LYS:HA	1.89	0.54
1:A:28:ASN:HD21	1:A:69:ARG:HH22	1.55	0.54
1:C:207:ILE:CD1	1:C:254:LEU:CD2	2.85	0.54
1:B:44:THR:HG23	2:B:294:HOH:O	2.08	0.54
1:A:28:ASN:O	1:A:32:GLU:HG3	2.07	0.54
1:D:143:GLU:OE1	1:D:145:LYS:HE2	2.07	0.54
1:D:254:LEU:HD23	1:D:257:MET:HE1	1.90	0.54
1:C:254:LEU:HD23	1:C:257:MET:HE1	1.89	0.53
1:A:186:ASP:O	1:A:238:MET:CE	2.54	0.53
1:B:112:GLU:OE2	1:B:115:ARG:NH2	2.42	0.53
1:A:190:LEU:HD23	1:A:190:LEU:C	2.29	0.53
1:B:254:LEU:HD23	1:B:257:MET:HE3	1.90	0.53
1:D:271:MET:HE3	1:D:276:LYS:HA	1.90	0.53
1:D:122:ALA:HA	1:D:129:ILE:HD11	1.90	0.53
1:A:168:SER:HB3	2:A:337:HOH:O	2.05	0.52
1:A:254:LEU:HD23	1:A:257:MET:HE1	1.91	0.52
1:B:44:THR:CG2	2:B:294:HOH:O	2.58	0.52
1:B:148:LYS:HG3	1:B:178:LYS:HG2	1.91	0.52
1:C:207:ILE:CD1	1:C:254:LEU:HD21	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:HIS:HD2	2:A:296:HOH:O	1.91	0.52
1:A:160:VAL:HG23	1:A:179:ILE:HD13	1.92	0.52
1:B:248:ILE:HD13	1:B:269:CYS:O	2.10	0.52
1:A:13:PHE:C	1:A:14:LYS:HD3	2.28	0.52
1:A:81:THR:OG1	1:A:117:HIS:HD2	1.94	0.51
1:D:254:LEU:HA	1:D:257:MET:CE	2.40	0.51
1:D:254:LEU:HA	1:D:257:MET:HE3	1.93	0.51
1:B:159:ALA:HA	1:B:179:ILE:HG12	1.92	0.51
1:A:187:GLU:N	1:A:238:MET:HE2	2.25	0.51
1:C:256:MET:HE3	1:C:280:GLU:CG	2.40	0.51
1:D:132:TYR:CD1	1:D:161:LYS:HD3	2.46	0.51
1:D:7:PRO:HD2	1:D:37:GLY:O	2.10	0.51
1:A:177:ALA:CA	2:A:329:HOH:O	2.58	0.50
1:B:271:MET:CE	1:B:275:HIS:C	2.80	0.50
1:D:41:VAL:HG13	1:D:50:LEU:HD12	1.93	0.50
1:B:125:ILE:HD12	1:B:127:LEU:HB2	1.94	0.50
1:D:247:PRO:HD2	1:D:268:LEU:CD1	2.42	0.50
1:A:187:GLU:CA	1:A:238:MET:CE	2.88	0.49
1:C:255:ASN:ND2	1:C:261:ALA:HB3	2.27	0.49
1:D:41:VAL:HG12	1:D:47:SER:HB3	1.93	0.49
1:D:252:THR:HG21	1:D:271:MET:HE2	1.94	0.49
1:C:160:VAL:CG1	1:C:179:ILE:CD1	2.88	0.49
1:A:117:HIS:HE1	2:A:292:HOH:O	1.96	0.49
1:A:223:ASP:OD2	1:A:226:LYS:HD3	2.13	0.49
1:D:125:ILE:HD12	1:D:127:LEU:HB2	1.94	0.49
1:C:106:TYR:OH	1:D:43:THR:OG1	2.17	0.49
1:A:214:GLU:HG3	1:A:230:ILE:CD1	2.43	0.49
1:D:241:MET:CE	1:D:250:VAL:HG23	2.38	0.48
1:A:255:ASN:HD21	1:A:262:GLY:N	2.10	0.48
1:B:237:LEU:HA	1:B:282:VAL:HG11	1.94	0.48
1:D:112:GLU:OE2	1:D:115:ARG:NH2	2.45	0.48
1:A:168:SER:O	1:A:172:GLU:HG3	2.13	0.48
1:A:2:PHE:HE2	1:A:158:SER:HG	1.60	0.48
1:D:241:MET:CE	1:D:250:VAL:CG2	2.92	0.48
1:D:117:HIS:HE1	2:D:326:HOH:O	1.97	0.48
1:D:277:LYS:CE	1:D:281:ASN:HD21	2.27	0.48
1:D:174:ILE:HD11	1:D:181:VAL:HG21	1.94	0.48
1:C:178:LYS:NZ	2:C:423:HOH:O	2.47	0.48
1:A:125:ILE:HD12	1:A:127:LEU:HB2	1.95	0.48
1:B:254:LEU:HA	1:B:257:MET:HE2	1.95	0.47
1:C:248:ILE:HB	1:C:249:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:HG21	1:B:203:VAL:HG22	1.96	0.47
1:A:107:ASN:HA	1:B:137:ARG:HH21	1.80	0.47
1:A:27:ILE:HG23	1:A:38:ILE:HD12	1.97	0.47
1:A:289:ILE:H	1:A:289:ILE:HD13	1.79	0.47
1:D:44:THR:CB	1:D:246:ASN:HD21	2.28	0.47
1:C:178:LYS:HE2	2:C:319:HOH:O	2.14	0.47
1:D:210:LYS:O	1:D:214:GLU:HG3	2.15	0.47
1:A:177:ALA:CB	2:A:329:HOH:O	2.60	0.46
1:C:41:VAL:HG11	1:C:55:HIS:CD2	2.50	0.46
1:B:85:ILE:HD11	1:B:120:LYS:HB3	1.97	0.46
1:D:210:LYS:NZ	1:D:214:GLU:OE2	2.47	0.46
1:D:271:MET:HE3	1:D:276:LYS:CA	2.44	0.46
1:C:178:LYS:CD	1:C:178:LYS:O	2.60	0.46
1:C:143:GLU:OE1	1:C:145:LYS:CE	2.62	0.46
1:C:43:THR:CG2	1:D:106:TYR:OH	2.60	0.46
1:B:85:ILE:HG23	1:B:124:SER:CB	2.46	0.46
1:B:6:TYR:HB2	1:B:201:ILE:HD12	1.98	0.46
1:B:210:LYS:HA	1:B:210:LYS:HE2	1.97	0.46
1:D:41:VAL:HG12	1:D:41:VAL:O	2.16	0.46
1:A:9:ILE:HA	1:A:206:ASN:HD21	1.80	0.46
1:C:207:ILE:HD12	1:C:257:MET:CE	2.46	0.45
1:C:254:LEU:HD23	1:C:257:MET:HE2	1.96	0.45
1:D:190:LEU:HD23	1:D:190:LEU:C	2.37	0.45
1:C:85:ILE:HD11	1:C:120:LYS:HB3	1.97	0.45
1:C:237:LEU:HA	1:C:282:VAL:HG11	1.99	0.45
1:C:55:HIS:CE1	1:C:59:ILE:HD11	2.52	0.45
1:D:160:VAL:HG23	1:D:179:ILE:HD13	1.98	0.45
1:A:41:VAL:HG21	1:A:55:HIS:CE1	2.52	0.45
1:D:271:MET:HE3	1:D:276:LYS:N	2.32	0.45
1:B:44:THR:HB	1:B:246:ASN:HD21	1.81	0.45
1:A:85:ILE:HD11	1:A:120:LYS:HB3	1.98	0.45
1:C:47:SER:N	1:C:48:PRO:CD	2.79	0.45
1:C:41:VAL:HG13	1:C:50:LEU:HD12	1.98	0.45
1:C:10:ILE:HD13	1:C:254:LEU:HD12	1.99	0.44
1:D:288:LEU:O	1:D:289:ILE:CD1	2.65	0.44
1:D:203:VAL:HG12	1:D:241:MET:HE2	1.99	0.44
1:D:102:ILE:HA	1:D:132:TYR:HB3	2.00	0.44
1:D:248:ILE:HB	1:D:249:PRO:HD3	2.00	0.44
1:A:138:THR:O	1:A:139:ALA:HB3	2.18	0.44
1:A:186:ASP:HB3	1:A:238:MET:CE	2.42	0.44
1:B:148:LYS:HE2	1:B:152:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:PHE:HE1	1:D:238:MET:CE	2.31	0.43
1:A:215:MET:HB2	1:A:230:ILE:HG21	1.98	0.43
1:D:115:ARG:HG2	1:D:115:ARG:HH11	1.83	0.43
1:D:241:MET:HE1	1:D:250:VAL:CB	2.47	0.43
1:C:257:MET:HB2	1:C:257:MET:HE3	1.74	0.43
1:B:233:LYS:HE2	2:B:433:HOH:O	2.17	0.43
1:B:271:MET:HE1	1:B:275:HIS:O	2.18	0.43
1:A:61:LYS:HE3	1:A:65:VAL:CG2	2.49	0.43
1:A:92:GLU:HA	1:A:127:LEU:HD11	2.01	0.43
1:A:23:LEU:HD23	1:A:61:LYS:HG2	2.01	0.43
1:B:6:TYR:HB2	1:B:201:ILE:CD1	2.49	0.42
1:B:247:PRO:HD2	1:B:268:LEU:CD1	2.49	0.42
1:B:102:ILE:HA	1:B:132:TYR:HB3	2.01	0.42
1:A:132:TYR:CD1	1:A:161:LYS:HD3	2.54	0.42
1:D:203:VAL:HG12	1:D:241:MET:CE	2.49	0.42
1:C:43:THR:HG23	2:C:308:HOH:O	2.19	0.42
1:D:39:VAL:HG11	1:D:100:LEU:HD22	2.01	0.42
1:D:288:LEU:O	1:D:289:ILE:CG1	2.68	0.42
1:B:247:PRO:HD2	1:B:268:LEU:HD13	2.01	0.42
1:A:278:ILE:O	1:A:282:VAL:HG13	2.19	0.42
1:C:256:MET:CE	1:C:280:GLU:HG3	2.49	0.42
1:A:177:ALA:HA	2:A:329:HOH:O	2.18	0.41
1:B:105:TYR:O	1:B:106:TYR:HB3	2.20	0.41
1:B:233:LYS:NZ	2:B:433:HOH:O	2.53	0.41
1:D:181:VAL:HG22	1:D:197:GLY:HA2	2.02	0.41
1:C:33:ASN:ND2	2:C:387:HOH:O	2.53	0.41
1:D:44:THR:CG2	2:D:308:HOH:O	2.67	0.41
1:C:207:ILE:HD12	1:C:257:MET:HE2	2.01	0.41
1:D:143:GLU:OE1	1:D:145:LYS:CE	2.69	0.41
1:B:231:HIS:HD2	2:B:296:HOH:O	2.03	0.41
1:A:284:LYS:HA	1:A:289:ILE:CD1	2.50	0.41
1:C:223:ASP:CG	1:C:226:LYS:HD2	2.40	0.41
1:D:44:THR:HG23	2:D:308:HOH:O	2.21	0.41
1:D:212:PHE:CZ	1:D:238:MET:CE	3.04	0.41
1:C:210:LYS:O	1:C:214:GLU:HG3	2.21	0.41
1:C:150:LEU:HB3	1:C:157:ILE:HD13	2.02	0.41
1:C:174:ILE:O	1:C:177:ALA:HB2	2.21	0.41
1:A:28:ASN:ND2	1:A:69:ARG:HH22	2.18	0.41
1:B:28:ASN:HD21	1:B:69:ARG:NH2	2.09	0.40
1:D:105:TYR:O	1:D:106:TYR:HB3	2.21	0.40
1:D:92:GLU:HA	1:D:127:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:HD2	2:A:351:HOH:O	2.21	0.40
1:A:14:LYS:CE	2:A:414:HOH:O	2.47	0.40
1:A:254:LEU:HA	1:A:257:MET:CE	2.47	0.40
1:C:55:HIS:HD2	2:C:351:HOH:O	1.95	0.40
1:B:254:LEU:HD22	2:B:377:HOH:O	2.22	0.40
1:B:270:GLU:CD	1:B:270:GLU:H	2.24	0.40

There are no symmetry-related clashes.

## 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	287/289 (99%)	281 (98%)	6 (2%)	0	100	100
1	B	286/289 (99%)	279 (98%)	6 (2%)	1 (0%)	46	50
1	C	286/289 (99%)	277 (97%)	7 (2%)	2 (1%)	26	25
1	D	286/289 (99%)	282 (99%)	3 (1%)	1 (0%)	46	50
All	All	1145/1156 (99%)	1119 (98%)	22 (2%)	4 (0%)	46	50

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 [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	247/248 (100%)	240 (97%)	7 (3%)	51	63
1	B	247/248 (100%)	237 (96%)	10 (4%)	38	47
1	C	247/248 (100%)	238 (96%)	9 (4%)	42	52
1	D	247/248 (100%)	240 (97%)	7 (3%)	51	63
All	All	988/992 (100%)	955 (97%)	33 (3%)	45	56

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	16	LYS
1	A	67	ASN
1	A	212	PHE
1	A	259	ARG
1	A	282	VAL
1	A	284	LYS
1	B	44	THR
1	B	57	LYS
1	B	94	VAL
1	B	158	SER
1	B	168	SER
1	B	178	LYS
1	B	210	LYS
1	B	248	ILE
1	B	263	GLU
1	B	284	LYS
1	C	43	THR
1	C	99	VAL
1	C	104	PRO
1	C	145	LYS
1	C	178	LYS
1	C	179	ILE
1	C	204	VAL
1	C	212	PHE
1	C	283	LEU
1	D	18	VAL
1	D	44	THR

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Mol	Chain	Res	Type
1	D	172	GLU
1	D	204	VAL
1	D	221	GLU
1	D	266	LEU
1	D	271	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	33	ASN
1	A	55	HIS
1	A	67	ASN
1	A	117	HIS
1	A	169	GLN
1	A	175	HIS
1	A	206	ASN
1	A	231	HIS
1	A	255	ASN
1	B	28	ASN
1	B	55	HIS
1	B	117	HIS
1	B	169	GLN
1	B	206	ASN
1	B	231	HIS
1	B	246	ASN
1	B	255	ASN
1	C	28	ASN
1	C	33	ASN
1	C	55	HIS
1	C	71	GLN
1	C	126	ASN
1	C	175	HIS
1	C	231	HIS
1	C	255	ASN
1	C	275	HIS
1	D	28	ASN
1	D	117	HIS
1	D	169	GLN
1	D	175	HIS
1	D	206	ASN
1	D	246	ASN

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Mol	Chain	Res	Type
1	D	255	ASN
1	D	281	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 [i](#)

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.