Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 03:54 am BST

PDB ID	:	3TUU
Title	:	Structure of dihydrodipicolinate synthase from the common grapevine
Authors	:	Perugini, M.A.; Dobson, R.C.; Atkinson, S.C.
Deposited on	:	2011-09-19
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

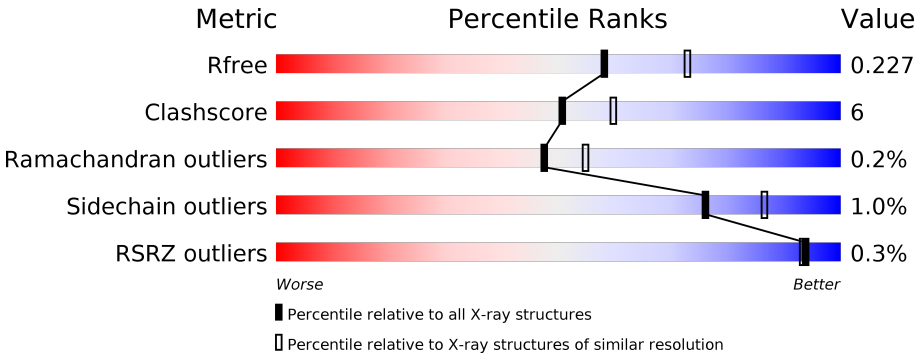
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	346	79% 9% 11%
1	B	346	% 79% 9% 11%
1	C	346	78% 10% 11%
1	D	346	79% 9% 11%
1	E	346	78% 10% 11%
1	F	346	78% 10% • 11%

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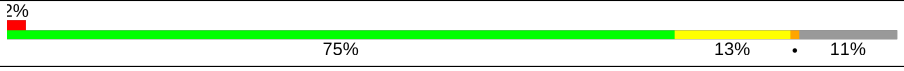
Mol	Chain	Length	Quality of chain
1	G	346	
1	H	346	

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
2	BR	A	329	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19995 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	307	Total	C	N	O	S	0	0	0
			2354	1499	401	444	10			
1	B	307	Total	C	N	O	S	0	0	0
			2354	1499	401	444	10			
1	C	307	Total	C	N	O	S	0	0	0
			2354	1499	401	444	10			
1	D	307	Total	C	N	O	S	0	0	0
			2354	1499	401	444	10			
1	E	307	Total	C	N	O	S	0	0	0
			2354	1499	401	444	10			
1	F	307	Total	C	N	O	S	0	0	0
			2351	1498	399	444	10			
1	G	307	Total	C	N	O	S	0	0	0
			2354	1499	401	444	10			
1	H	307	Total	C	N	O	S	0	0	0
			2354	1499	401	444	10			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP D7U7T8
A	-17	GLY	-	EXPRESSION TAG	UNP D7U7T8
A	-16	SER	-	EXPRESSION TAG	UNP D7U7T8
A	-15	SER	-	EXPRESSION TAG	UNP D7U7T8
A	-14	HIS	-	EXPRESSION TAG	UNP D7U7T8
A	-13	HIS	-	EXPRESSION TAG	UNP D7U7T8
A	-12	HIS	-	EXPRESSION TAG	UNP D7U7T8
A	-11	HIS	-	EXPRESSION TAG	UNP D7U7T8
A	-10	HIS	-	EXPRESSION TAG	UNP D7U7T8
A	-9	SER	-	EXPRESSION TAG	UNP D7U7T8
A	-8	SER	-	EXPRESSION TAG	UNP D7U7T8
A	-7	GLY	-	EXPRESSION TAG	UNP D7U7T8
A	-6	LEU	-	EXPRESSION TAG	UNP D7U7T8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	EXPRESSION TAG	UNP D7U7T8
A	-4	PRO	-	EXPRESSION TAG	UNP D7U7T8
A	-3	ARG	-	EXPRESSION TAG	UNP D7U7T8
A	-2	GLY	-	EXPRESSION TAG	UNP D7U7T8
A	-1	SER	-	EXPRESSION TAG	UNP D7U7T8
A	0	HIS	-	EXPRESSION TAG	UNP D7U7T8
A	1	MET	-	EXPRESSION TAG	UNP D7U7T8
B	-18	MET	-	EXPRESSION TAG	UNP D7U7T8
B	-17	GLY	-	EXPRESSION TAG	UNP D7U7T8
B	-16	SER	-	EXPRESSION TAG	UNP D7U7T8
B	-15	SER	-	EXPRESSION TAG	UNP D7U7T8
B	-14	HIS	-	EXPRESSION TAG	UNP D7U7T8
B	-13	HIS	-	EXPRESSION TAG	UNP D7U7T8
B	-12	HIS	-	EXPRESSION TAG	UNP D7U7T8
B	-11	HIS	-	EXPRESSION TAG	UNP D7U7T8
B	-10	HIS	-	EXPRESSION TAG	UNP D7U7T8
B	-9	SER	-	EXPRESSION TAG	UNP D7U7T8
B	-8	SER	-	EXPRESSION TAG	UNP D7U7T8
B	-7	GLY	-	EXPRESSION TAG	UNP D7U7T8
B	-6	LEU	-	EXPRESSION TAG	UNP D7U7T8
B	-5	VAL	-	EXPRESSION TAG	UNP D7U7T8
B	-4	PRO	-	EXPRESSION TAG	UNP D7U7T8
B	-3	ARG	-	EXPRESSION TAG	UNP D7U7T8
B	-2	GLY	-	EXPRESSION TAG	UNP D7U7T8
B	-1	SER	-	EXPRESSION TAG	UNP D7U7T8
B	0	HIS	-	EXPRESSION TAG	UNP D7U7T8
B	1	MET	-	EXPRESSION TAG	UNP D7U7T8
C	-18	MET	-	EXPRESSION TAG	UNP D7U7T8
C	-17	GLY	-	EXPRESSION TAG	UNP D7U7T8
C	-16	SER	-	EXPRESSION TAG	UNP D7U7T8
C	-15	SER	-	EXPRESSION TAG	UNP D7U7T8
C	-14	HIS	-	EXPRESSION TAG	UNP D7U7T8
C	-13	HIS	-	EXPRESSION TAG	UNP D7U7T8
C	-12	HIS	-	EXPRESSION TAG	UNP D7U7T8
C	-11	HIS	-	EXPRESSION TAG	UNP D7U7T8
C	-10	HIS	-	EXPRESSION TAG	UNP D7U7T8
C	-9	SER	-	EXPRESSION TAG	UNP D7U7T8
C	-8	SER	-	EXPRESSION TAG	UNP D7U7T8
C	-7	GLY	-	EXPRESSION TAG	UNP D7U7T8
C	-6	LEU	-	EXPRESSION TAG	UNP D7U7T8
C	-5	VAL	-	EXPRESSION TAG	UNP D7U7T8
C	-4	PRO	-	EXPRESSION TAG	UNP D7U7T8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	EXPRESSION TAG	UNP D7U7T8
C	-2	GLY	-	EXPRESSION TAG	UNP D7U7T8
C	-1	SER	-	EXPRESSION TAG	UNP D7U7T8
C	0	HIS	-	EXPRESSION TAG	UNP D7U7T8
C	1	MET	-	EXPRESSION TAG	UNP D7U7T8
D	-18	MET	-	EXPRESSION TAG	UNP D7U7T8
D	-17	GLY	-	EXPRESSION TAG	UNP D7U7T8
D	-16	SER	-	EXPRESSION TAG	UNP D7U7T8
D	-15	SER	-	EXPRESSION TAG	UNP D7U7T8
D	-14	HIS	-	EXPRESSION TAG	UNP D7U7T8
D	-13	HIS	-	EXPRESSION TAG	UNP D7U7T8
D	-12	HIS	-	EXPRESSION TAG	UNP D7U7T8
D	-11	HIS	-	EXPRESSION TAG	UNP D7U7T8
D	-10	HIS	-	EXPRESSION TAG	UNP D7U7T8
D	-9	SER	-	EXPRESSION TAG	UNP D7U7T8
D	-8	SER	-	EXPRESSION TAG	UNP D7U7T8
D	-7	GLY	-	EXPRESSION TAG	UNP D7U7T8
D	-6	LEU	-	EXPRESSION TAG	UNP D7U7T8
D	-5	VAL	-	EXPRESSION TAG	UNP D7U7T8
D	-4	PRO	-	EXPRESSION TAG	UNP D7U7T8
D	-3	ARG	-	EXPRESSION TAG	UNP D7U7T8
D	-2	GLY	-	EXPRESSION TAG	UNP D7U7T8
D	-1	SER	-	EXPRESSION TAG	UNP D7U7T8
D	0	HIS	-	EXPRESSION TAG	UNP D7U7T8
D	1	MET	-	EXPRESSION TAG	UNP D7U7T8
E	-18	MET	-	EXPRESSION TAG	UNP D7U7T8
E	-17	GLY	-	EXPRESSION TAG	UNP D7U7T8
E	-16	SER	-	EXPRESSION TAG	UNP D7U7T8
E	-15	SER	-	EXPRESSION TAG	UNP D7U7T8
E	-14	HIS	-	EXPRESSION TAG	UNP D7U7T8
E	-13	HIS	-	EXPRESSION TAG	UNP D7U7T8
E	-12	HIS	-	EXPRESSION TAG	UNP D7U7T8
E	-11	HIS	-	EXPRESSION TAG	UNP D7U7T8
E	-10	HIS	-	EXPRESSION TAG	UNP D7U7T8
E	-9	SER	-	EXPRESSION TAG	UNP D7U7T8
E	-8	SER	-	EXPRESSION TAG	UNP D7U7T8
E	-7	GLY	-	EXPRESSION TAG	UNP D7U7T8
E	-6	LEU	-	EXPRESSION TAG	UNP D7U7T8
E	-5	VAL	-	EXPRESSION TAG	UNP D7U7T8
E	-4	PRO	-	EXPRESSION TAG	UNP D7U7T8
E	-3	ARG	-	EXPRESSION TAG	UNP D7U7T8
E	-2	GLY	-	EXPRESSION TAG	UNP D7U7T8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	EXPRESSION TAG	UNP D7U7T8
E	0	HIS	-	EXPRESSION TAG	UNP D7U7T8
E	1	MET	-	EXPRESSION TAG	UNP D7U7T8
F	-18	MET	-	EXPRESSION TAG	UNP D7U7T8
F	-17	GLY	-	EXPRESSION TAG	UNP D7U7T8
F	-16	SER	-	EXPRESSION TAG	UNP D7U7T8
F	-15	SER	-	EXPRESSION TAG	UNP D7U7T8
F	-14	HIS	-	EXPRESSION TAG	UNP D7U7T8
F	-13	HIS	-	EXPRESSION TAG	UNP D7U7T8
F	-12	HIS	-	EXPRESSION TAG	UNP D7U7T8
F	-11	HIS	-	EXPRESSION TAG	UNP D7U7T8
F	-10	HIS	-	EXPRESSION TAG	UNP D7U7T8
F	-9	SER	-	EXPRESSION TAG	UNP D7U7T8
F	-8	SER	-	EXPRESSION TAG	UNP D7U7T8
F	-7	GLY	-	EXPRESSION TAG	UNP D7U7T8
F	-6	LEU	-	EXPRESSION TAG	UNP D7U7T8
F	-5	VAL	-	EXPRESSION TAG	UNP D7U7T8
F	-4	PRO	-	EXPRESSION TAG	UNP D7U7T8
F	-3	ARG	-	EXPRESSION TAG	UNP D7U7T8
F	-2	GLY	-	EXPRESSION TAG	UNP D7U7T8
F	-1	SER	-	EXPRESSION TAG	UNP D7U7T8
F	0	HIS	-	EXPRESSION TAG	UNP D7U7T8
F	1	MET	-	EXPRESSION TAG	UNP D7U7T8
G	-18	MET	-	EXPRESSION TAG	UNP D7U7T8
G	-17	GLY	-	EXPRESSION TAG	UNP D7U7T8
G	-16	SER	-	EXPRESSION TAG	UNP D7U7T8
G	-15	SER	-	EXPRESSION TAG	UNP D7U7T8
G	-14	HIS	-	EXPRESSION TAG	UNP D7U7T8
G	-13	HIS	-	EXPRESSION TAG	UNP D7U7T8
G	-12	HIS	-	EXPRESSION TAG	UNP D7U7T8
G	-11	HIS	-	EXPRESSION TAG	UNP D7U7T8
G	-10	HIS	-	EXPRESSION TAG	UNP D7U7T8
G	-9	SER	-	EXPRESSION TAG	UNP D7U7T8
G	-8	SER	-	EXPRESSION TAG	UNP D7U7T8
G	-7	GLY	-	EXPRESSION TAG	UNP D7U7T8
G	-6	LEU	-	EXPRESSION TAG	UNP D7U7T8
G	-5	VAL	-	EXPRESSION TAG	UNP D7U7T8
G	-4	PRO	-	EXPRESSION TAG	UNP D7U7T8
G	-3	ARG	-	EXPRESSION TAG	UNP D7U7T8
G	-2	GLY	-	EXPRESSION TAG	UNP D7U7T8
G	-1	SER	-	EXPRESSION TAG	UNP D7U7T8
G	0	HIS	-	EXPRESSION TAG	UNP D7U7T8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	EXPRESSION TAG	UNP D7U7T8
H	-18	MET	-	EXPRESSION TAG	UNP D7U7T8
H	-17	GLY	-	EXPRESSION TAG	UNP D7U7T8
H	-16	SER	-	EXPRESSION TAG	UNP D7U7T8
H	-15	SER	-	EXPRESSION TAG	UNP D7U7T8
H	-14	HIS	-	EXPRESSION TAG	UNP D7U7T8
H	-13	HIS	-	EXPRESSION TAG	UNP D7U7T8
H	-12	HIS	-	EXPRESSION TAG	UNP D7U7T8
H	-11	HIS	-	EXPRESSION TAG	UNP D7U7T8
H	-10	HIS	-	EXPRESSION TAG	UNP D7U7T8
H	-9	SER	-	EXPRESSION TAG	UNP D7U7T8
H	-8	SER	-	EXPRESSION TAG	UNP D7U7T8
H	-7	GLY	-	EXPRESSION TAG	UNP D7U7T8
H	-6	LEU	-	EXPRESSION TAG	UNP D7U7T8
H	-5	VAL	-	EXPRESSION TAG	UNP D7U7T8
H	-4	PRO	-	EXPRESSION TAG	UNP D7U7T8
H	-3	ARG	-	EXPRESSION TAG	UNP D7U7T8
H	-2	GLY	-	EXPRESSION TAG	UNP D7U7T8
H	-1	SER	-	EXPRESSION TAG	UNP D7U7T8
H	0	HIS	-	EXPRESSION TAG	UNP D7U7T8
H	1	MET	-	EXPRESSION TAG	UNP D7U7T8

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	3	Total Br 3 3	0	0
2	D	2	Total Br 2 2	0	0
2	E	2	Total Br 2 2	0	0
2	H	1	Total Br 1 1	0	0
2	B	1	Total Br 1 1	0	0
2	C	2	Total Br 2 2	0	0
2	A	2	Total Br 2 2	0	0
2	F	2	Total Br 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Cl 2 2	0	0
3	E	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is water.

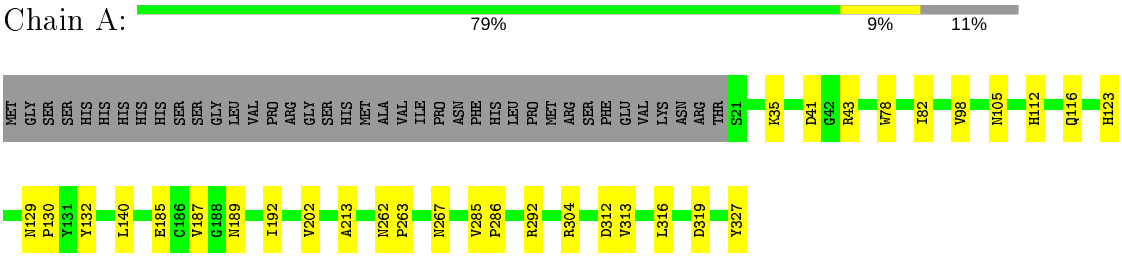
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	154	Total O 154 154	0	0
4	B	146	Total O 146 146	0	0
4	C	158	Total O 158 158	0	0
4	D	131	Total O 131 131	0	0
4	E	141	Total O 141 141	0	0
4	F	178	Total O 178 178	0	0
4	G	130	Total O 130 130	0	0
4	H	105	Total O 105 105	0	0

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 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.

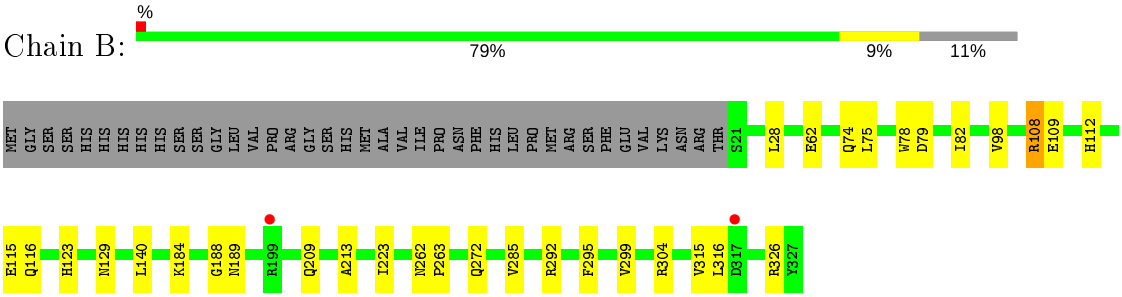
- Molecule 1: dihydrodipicolinate synthase

Chain A:



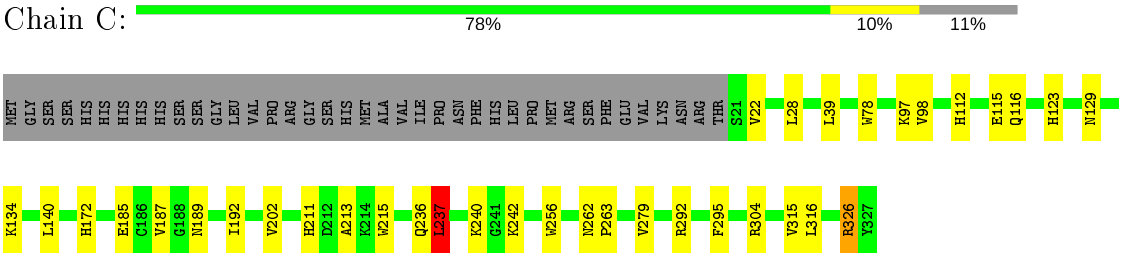
- Molecule 1: dihydrodipicolinate synthase

Chain B:



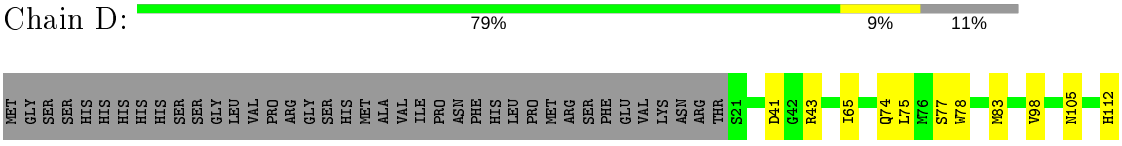
- Molecule 1: dihydrodipicolinate synthase

Chain C:



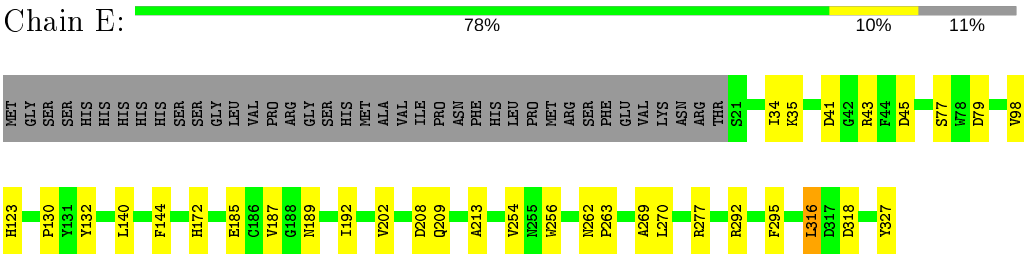
- Molecule 1: dihydrodipicolinate synthase

Chain D:



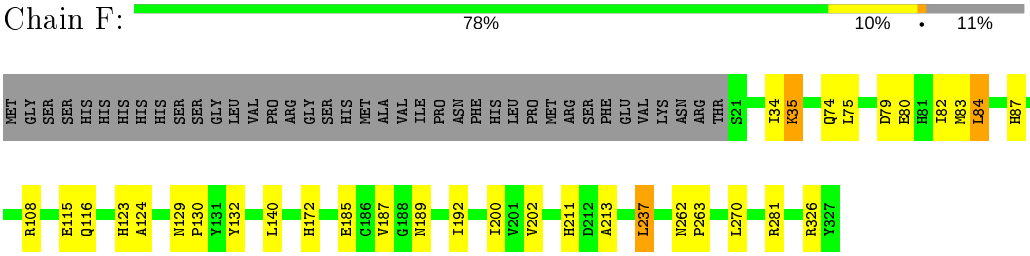
- Molecule 1: dihydrodipicolinate synthase

Chain E:



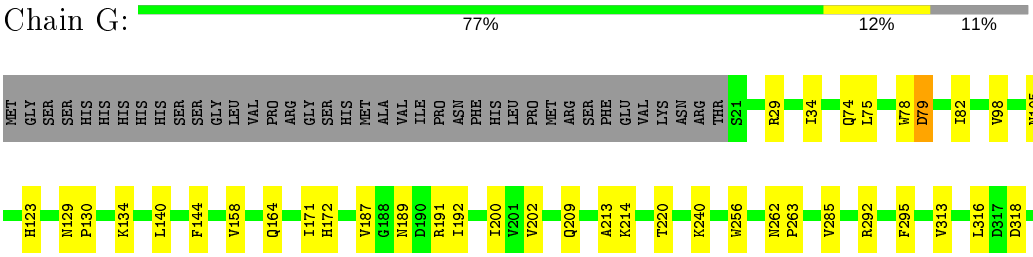
- Molecule 1: dihydrodipicolinate synthase

Chain F:



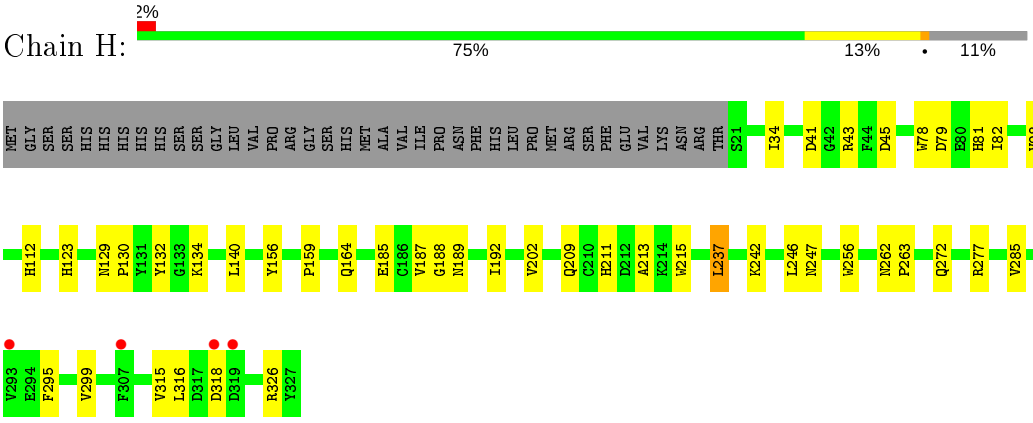
- Molecule 1: dihydrodipicolinate synthase

Chain G:



- Molecule 1: dihydrodipicolinate synthase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.55Å 78.90Å 135.35Å 93.19° 95.02° 100.61°	Depositor
Resolution (Å)	57.17 – 2.20 57.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.3 (57.17-2.20) 97.3 (57.17-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.180 , 0.227 0.181 , 0.227	Depositor DCC
R_{free} test set	7056 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19995	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: KPI, BR, CL

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	0.51	0/2390	0.64	0/3253
1	B	0.50	0/2390	0.64	0/3253
1	C	0.52	0/2390	0.66	3/3253 (0.1%)
1	D	0.52	0/2390	0.65	0/3253
1	E	0.50	0/2390	0.62	0/3253
1	F	0.57	1/2387 (0.0%)	0.67	0/3249
1	G	0.51	0/2390	0.62	1/3253 (0.0%)
1	H	0.54	1/2390 (0.0%)	0.62	0/3253
All	All	0.52	2/19117 (0.0%)	0.64	4/26020 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	132	TYR	CD1-CE1	-8.27	1.26	1.39
1	H	132	TYR	CD1-CE1	-5.65	1.30	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	237	LEU	CA-CB-CG	5.57	128.11	115.30
1	C	326	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	326	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	G	79	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2354	0	2336	23	0
1	B	2354	0	2337	29	0
1	C	2354	0	2337	27	0
1	D	2354	0	2337	28	0
1	E	2354	0	2337	29	0
1	F	2351	0	2332	28	0
1	G	2354	0	2337	36	0
1	H	2354	0	2337	39	0
2	A	2	0	0	3	0
2	B	1	0	0	0	0
2	C	2	0	0	1	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	3	0	0	2	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
4	A	154	0	0	0	0
4	B	146	0	0	0	0
4	C	158	0	0	2	0
4	D	131	0	0	0	0
4	E	141	0	0	2	0
4	F	178	0	0	0	0
4	G	130	0	0	3	0
4	H	105	0	0	0	0
All	All	19995	0	18690	215	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 6.

All (215) 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:C:98:VAL:H	1:C:123:HIS:CD2	1.81	0.99
1:E:98:VAL:H	1:E:123:HIS:HD2	1.01	0.98
1:A:98:VAL:H	1:A:123:HIS:HD2	1.11	0.96
1:G:98:VAL:H	1:G:123:HIS:HD2	1.07	0.96
1:D:98:VAL:H	1:D:123:HIS:HD2	1.05	0.93
1:H:98:VAL:H	1:H:123:HIS:HD2	1.12	0.93
1:D:129:ASN:HD22	1:D:164:GLN:HE21	1.11	0.92
1:E:98:VAL:H	1:E:123:HIS:CD2	1.88	0.91
1:C:98:VAL:H	1:C:123:HIS:HD2	0.91	0.90
1:H:134:LYS:HD2	1:H:164:GLN:HB2	1.51	0.90
1:B:98:VAL:H	1:B:123:HIS:HD2	1.20	0.90
1:D:78:TRP:HE1	1:D:116:GLN:NE2	1.68	0.90
1:F:98:VAL:H	1:F:123:HIS:HD2	1.13	0.89
1:C:98:VAL:N	1:C:123:HIS:HD2	1.74	0.85
1:C:78:TRP:HE1	1:C:116:GLN:NE2	1.77	0.81
1:G:78:TRP:HE1	1:G:116:GLN:NE2	1.78	0.81
1:G:98:VAL:H	1:G:123:HIS:CD2	1.98	0.81
1:A:98:VAL:H	1:A:123:HIS:CD2	2.01	0.78
1:F:185:GLU:OE1	1:F:187:VAL:HG22	1.85	0.77
1:F:98:VAL:H	1:F:123:HIS:CD2	2.02	0.76
1:E:185:GLU:OE1	1:E:187:VAL:HG13	1.86	0.75
1:G:134:LYS:HD3	1:G:164:GLN:HB2	1.67	0.75
1:F:83:MET:O	1:F:84:LEU:CB	2.33	0.75
1:D:98:VAL:H	1:D:123:HIS:CD2	1.97	0.75
1:G:79:ASP:OD1	1:H:112:HIS:HE1	1.70	0.74
1:D:78:TRP:HE1	1:D:116:GLN:HE21	1.34	0.73
1:H:262:ASN:ND2	1:H:263:PRO:HA	2.04	0.72
1:C:172:HIS:HE1	4:C:998:HOH:O	1.72	0.72
1:A:78:TRP:HE1	1:A:116:GLN:NE2	1.87	0.72
1:G:292:ARG:NH2	1:G:316:LEU:O	2.23	0.72
1:H:98:VAL:H	1:H:123:HIS:CD2	2.04	0.71
1:E:98:VAL:N	1:E:123:HIS:HD2	1.83	0.70
1:B:292:ARG:HD2	1:B:315:VAL:O	1.91	0.70
1:B:108:ARG:HH11	1:B:108:ARG:HG2	1.57	0.69
1:A:262:ASN:ND2	1:A:263:PRO:HA	2.08	0.69
1:H:192:ILE:HG12	1:H:202:VAL:HG11	1.74	0.69
1:A:129:ASN:HB2	1:A:140:LEU:HD21	1.73	0.69
1:E:262:ASN:ND2	1:E:263:PRO:HA	2.08	0.69
1:H:189:ASN:HD21	1:H:213:ALA:HB2	1.57	0.68
1:H:185:GLU:OE1	1:H:187:VAL:HG22	1.93	0.68
1:E:77:SER:HB3	1:H:108:ARG:NH2	2.08	0.67
1:H:45:ASP:OD2	1:H:277:ARG:HD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:OE1	1:A:187:VAL:HG22	1.94	0.67
1:D:74:GLN:HG2	1:D:75:LEU:HD13	1.76	0.67
1:C:292:ARG:NH2	1:C:316:LEU:O	2.28	0.67
1:F:189:ASN:HD21	1:F:213:ALA:HB2	1.59	0.67
1:B:74:GLN:HG2	1:B:75:LEU:HD13	1.77	0.66
1:B:108:ARG:CG	1:B:108:ARG:HH11	2.09	0.65
1:D:41:ASP:OD1	1:D:43:ARG:HD3	1.96	0.65
1:G:78:TRP:HE1	1:G:116:GLN:HE21	1.44	0.65
1:D:98:VAL:N	1:D:123:HIS:HD2	1.88	0.65
1:A:35:LYS:HE3	1:A:267:ASN:OD1	1.98	0.63
1:A:78:TRP:HE1	1:A:116:GLN:HE21	1.45	0.63
1:D:292:ARG:HD2	1:D:315:VAL:O	1.99	0.63
1:F:83:MET:O	1:F:84:LEU:HB3	1.99	0.62
1:B:292:ARG:NH2	1:B:316:LEU:O	2.32	0.62
1:H:159:PRO:HG2	1:H:187:VAL:CG1	2.31	0.61
1:B:116:GLN:HG2	1:D:83:MET:HE3	1.80	0.61
1:E:292:ARG:NH2	1:E:316:LEU:O	2.34	0.61
1:B:108:ARG:NH1	1:B:108:ARG:HG2	2.14	0.61
1:D:77:SER:HB3	1:F:108:ARG:HH22	1.66	0.60
1:H:188:GLY:HA2	1:H:209:GLN:HE22	1.67	0.60
1:H:292:ARG:NH2	1:H:316:LEU:O	2.35	0.60
1:H:129:ASN:HB2	1:H:140:LEU:HD21	1.83	0.60
1:C:129:ASN:HB2	1:C:140:LEU:HD21	1.84	0.59
1:E:41:ASP:OD1	1:E:43:ARG:HD3	2.02	0.59
1:F:262:ASN:ND2	1:F:263:PRO:HA	2.17	0.59
1:G:189:ASN:HD21	1:G:213:ALA:HB2	1.66	0.59
1:G:74:GLN:HG2	1:G:75:LEU:HD13	1.83	0.59
1:G:79:ASP:OD1	1:H:112:HIS:CE1	2.52	0.58
1:F:74:GLN:HG2	1:F:75:LEU:HD13	1.85	0.58
1:H:189:ASN:ND2	1:H:213:ALA:HB2	2.19	0.57
1:B:129:ASN:HB2	1:B:140:LEU:HD21	1.84	0.57
1:C:262:ASN:ND2	1:C:263:PRO:HA	2.18	0.57
1:H:237:LEU:HD23	1:H:246:LEU:HG	1.86	0.57
1:B:116:GLN:HG2	1:D:83:MET:CE	2.34	0.57
1:H:292:ARG:HD2	1:H:315:VAL:O	2.06	0.56
1:E:172:HIS:HE1	4:E:388:HOH:O	1.88	0.56
1:H:134:LYS:CD	1:H:164:GLN:HB2	2.31	0.56
1:A:189:ASN:HD21	1:A:213:ALA:HB2	1.71	0.56
1:B:98:VAL:H	1:B:123:HIS:CD2	2.11	0.55
1:D:129:ASN:HB2	1:D:140:LEU:HD21	1.86	0.55
1:D:272:GLN:OE1	1:D:292:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:ASN:HD22	1:H:192:ILE:HD12	1.72	0.55
1:E:115:GLU:OE1	1:H:326:ARG:NH2	2.39	0.55
1:E:292:ARG:NH1	1:E:318:ASP:OD1	2.36	0.54
1:D:292:ARG:NH2	1:D:316:LEU:O	2.41	0.53
1:E:140:LEU:HD22	1:E:144:PHE:CE2	2.43	0.53
1:F:98:VAL:N	1:F:123:HIS:HD2	1.95	0.53
1:H:292:ARG:NH1	1:H:318:ASP:OD1	2.31	0.53
1:D:129:ASN:HD22	1:D:164:GLN:NE2	1.93	0.52
1:G:292:ARG:NH1	1:G:318:ASP:OD1	2.43	0.52
1:B:262:ASN:ND2	1:B:263:PRO:HA	2.24	0.52
1:G:98:VAL:N	1:G:123:HIS:HD2	1.90	0.52
1:B:326:ARG:NH2	1:C:115:GLU:OE1	2.43	0.51
1:E:256:TRP:CZ2	1:E:295:PHE:HB2	2.45	0.51
1:D:262:ASN:ND2	1:D:263:PRO:HA	2.25	0.51
1:E:189:ASN:HD21	1:E:213:ALA:HB2	1.75	0.51
1:E:327:TYR:CE2	1:H:108:ARG:NH1	2.78	0.51
1:G:187:VAL:CG2	1:G:191:ARG:CB	2.89	0.51
1:E:262:ASN:HD22	1:E:263:PRO:HA	1.75	0.50
1:A:98:VAL:N	1:A:123:HIS:HD2	1.94	0.50
1:C:78:TRP:HE1	1:C:116:GLN:HE21	1.52	0.50
1:D:326:ARG:NH2	1:F:115:GLU:OE2	2.44	0.50
1:E:192:ILE:HG12	1:E:202:VAL:HG11	1.94	0.49
1:H:262:ASN:HD22	1:H:263:PRO:HA	1.77	0.49
1:B:82:ILE:CD1	1:B:116:GLN:HB3	2.42	0.49
1:A:116:GLN:HE22	1:E:79:ASP:HB2	1.78	0.49
1:G:129:ASN:HB2	1:G:140:LEU:HD21	1.94	0.49
1:G:189:ASN:ND2	1:G:213:ALA:HB2	2.28	0.49
1:G:140:LEU:HD22	1:G:144:PHE:CE2	2.47	0.49
1:F:82:ILE:HD12	1:F:116:GLN:HB3	1.94	0.48
1:H:211:HIS:HB2	1:H:237:LEU:HD11	1.94	0.48
1:G:262:ASN:ND2	1:G:263:PRO:HA	2.29	0.48
1:G:29:ARG:HG3	1:G:220:THR:O	2.13	0.48
1:F:129:ASN:HB2	1:F:140:LEU:HD21	1.94	0.48
1:H:98:VAL:N	1:H:123:HIS:HD2	1.95	0.48
1:A:82:ILE:HD12	1:A:116:GLN:HB3	1.95	0.48
1:B:115:GLU:OE2	1:C:326:ARG:NH2	2.47	0.48
1:F:80:GLU:O	1:F:83:MET:O	2.31	0.48
1:B:272:GLN:OE1	1:B:292:ARG:HG2	2.13	0.47
1:G:187:VAL:HG23	1:G:191:ARG:CB	2.44	0.47
1:B:188:GLY:HA2	1:B:209:GLN:HE22	1.79	0.47
1:E:189:ASN:ND2	1:E:213:ALA:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:TRP:CZ2	1:G:295:PHE:HB2	2.49	0.47
1:H:105:ASN:HA	1:H:130:PRO:HA	1.96	0.47
1:G:116:GLN:HE22	1:H:79:ASP:HB2	1.79	0.47
1:A:304:ARG:HD3	2:A:329:BR:BR	2.69	0.47
1:C:112:HIS:HE1	1:F:79:ASP:OD1	1.98	0.47
1:B:108:ARG:HG3	1:B:109:GLU:N	2.30	0.47
1:C:192:ILE:HG12	1:C:202:VAL:HG11	1.96	0.46
1:D:327:TYR:HE2	1:F:108:ARG:HH11	1.59	0.46
1:G:78:TRP:CZ2	1:G:82:ILE:HB	2.50	0.46
1:C:185:GLU:OE1	1:C:187:VAL:HG22	2.15	0.46
1:C:304:ARG:HD3	2:C:329:BR:BR	2.71	0.46
1:H:295:PHE:O	1:H:299:VAL:HG23	2.16	0.46
1:H:79:ASP:HA	1:H:82:ILE:HG22	1.97	0.46
1:B:326:ARG:HH22	1:C:115:GLU:CD	2.18	0.46
1:G:313:VAL:HG12	2:G:330:BR:BR	2.70	0.46
1:C:256:TRP:CZ2	1:C:295:PHE:HB2	2.50	0.46
1:A:313:VAL:HG12	2:A:329:BR:BR	2.71	0.46
1:C:97:LYS:HA	1:C:123:HIS:CD2	2.51	0.46
1:D:327:TYR:CE2	1:F:108:ARG:HD3	2.50	0.46
1:H:272:GLN:OE1	1:H:292:ARG:HG2	2.16	0.46
1:B:184:KPI:HBA	1:B:223:ILE:HD12	1.98	0.46
1:E:209:GLN:NE2	4:E:508:HOH:O	2.29	0.46
1:B:189:ASN:HD21	1:B:213:ALA:HB2	1.80	0.46
1:G:82:ILE:HD12	1:G:116:GLN:HB3	1.98	0.46
1:G:187:VAL:HG23	1:G:191:ARG:HB3	1.97	0.45
1:F:129:ASN:CB	1:F:140:LEU:HD21	2.47	0.45
1:C:22:VAL:HG12	4:C:1142:HOH:O	2.17	0.45
1:F:192:ILE:HG12	1:F:202:VAL:HG11	1.98	0.45
1:G:189:ASN:HD22	1:G:192:ILE:HD12	1.82	0.45
1:C:236:GLN:HG2	1:C:240:LYS:HE2	1.99	0.45
1:F:211:HIS:HB2	1:F:237:LEU:HD11	1.98	0.45
1:A:105:ASN:HA	1:A:130:PRO:HA	1.98	0.45
1:G:29:ARG:NH1	4:G:481:HOH:O	2.49	0.45
1:B:112:HIS:O	1:B:116:GLN:HG3	2.17	0.44
1:E:256:TRP:CZ3	1:E:269:ALA:HB2	2.52	0.44
1:D:129:ASN:CB	1:D:140:LEU:HD21	2.47	0.44
1:G:240:LYS:HG3	2:G:329:BR:BR	2.72	0.44
1:G:158:VAL:O	1:G:158:VAL:HG13	2.16	0.44
1:C:129:ASN:CB	1:C:140:LEU:HD21	2.47	0.44
1:B:189:ASN:ND2	1:B:213:ALA:HB2	2.32	0.44
1:C:189:ASN:HD21	1:C:213:ALA:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:TRP:CZ2	1:D:295:PHE:HB2	2.52	0.44
1:D:326:ARG:HH22	1:F:115:GLU:CD	2.20	0.44
1:H:215:TRP:HB3	1:H:242:LYS:HG2	1.99	0.44
1:A:192:ILE:HG12	1:A:202:VAL:HG11	2.00	0.44
1:A:285:VAL:HG13	1:A:286:PRO:HD2	2.00	0.43
1:G:172:HIS:HE1	4:G:352:HOH:O	2.01	0.43
1:C:211:HIS:HB2	1:C:237:LEU:HD11	1.99	0.43
1:B:79:ASP:OD1	1:D:112:HIS:HE1	2.01	0.43
1:F:105:ASN:HA	1:F:130:PRO:HA	2.01	0.43
1:A:327:TYR:CE2	1:G:108:ARG:HD3	2.52	0.43
1:D:115:GLU:CD	1:F:326:ARG:HH22	2.22	0.43
1:H:78:TRP:CE3	1:H:81:HIS:HB3	2.53	0.43
1:C:215:TRP:HB3	1:C:242:LYS:HG2	2.01	0.43
1:D:129:ASN:ND2	1:D:164:GLN:HE21	1.95	0.43
1:G:192:ILE:HG12	1:G:202:VAL:HG11	2.01	0.43
1:B:295:PHE:O	1:B:299:VAL:HG23	2.19	0.42
1:H:41:ASP:OD1	1:H:43:ARG:HD3	2.19	0.42
1:E:45:ASP:OD2	1:E:277:ARG:HD2	2.20	0.42
1:A:129:ASN:CB	1:A:140:LEU:HD21	2.47	0.42
1:B:78:TRP:CZ2	1:B:82:ILE:HB	2.54	0.42
1:E:105:ASN:HA	1:E:130:PRO:HA	2.01	0.42
1:E:140:LEU:HD23	1:E:140:LEU:HA	1.81	0.42
1:H:159:PRO:HG2	1:H:187:VAL:HG12	2.01	0.42
1:F:172:HIS:CD2	1:F:200:ILE:HD11	2.54	0.42
1:B:140:LEU:HD23	1:B:140:LEU:HA	1.91	0.42
1:B:28:LEU:HD22	1:B:62:GLU:HB3	2.02	0.42
1:C:39:LEU:O	1:C:279:VAL:HG11	2.19	0.42
1:F:35:LYS:HG2	1:F:270:LEU:CD1	2.49	0.42
1:B:304:ARG:HG3	1:B:304:ARG:O	2.19	0.42
1:C:28:LEU:HD21	1:C:97:LYS:HG3	2.02	0.42
1:C:292:ARG:HD2	1:C:315:VAL:O	2.20	0.42
1:E:208:ASP:HB3	1:E:254:VAL:HG11	2.02	0.41
1:A:312:ASP:HA	2:A:329:BR:BR	2.75	0.41
1:A:292:ARG:NH2	1:A:316:LEU:O	2.51	0.41
1:D:105:ASN:HA	1:D:130:PRO:HA	2.02	0.41
1:G:171:ILE:HG22	1:G:200:ILE:HD13	2.02	0.41
1:F:99:ILE:HG12	1:F:124:ALA:HB3	2.03	0.41
1:F:75:LEU:HD23	1:F:281:ARG:HB2	2.03	0.41
1:E:77:SER:HB3	1:H:108:ARG:HH22	1.81	0.41
1:G:129:ASN:CB	1:G:140:LEU:HD21	2.50	0.41
1:G:209:GLN:NE2	4:G:635:HOH:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:211:HIS:HB2	1:H:237:LEU:CD1	2.50	0.40
1:A:112:HIS:HE1	1:E:79:ASP:OD1	2.04	0.40
1:E:115:GLU:CD	1:H:326:ARG:HH22	2.25	0.40
1:A:41:ASP:OD1	1:A:43:ARG:HD3	2.22	0.40
1:F:84:LEU:HA	1:F:87:HIS:HB3	2.03	0.40
1:G:105:ASN:HA	1:G:130:PRO:HA	2.03	0.40
1:D:65:ILE:HD12	1:D:126:LEU:HD22	2.03	0.40
1:E:35:LYS:HG2	1:E:270:LEU:CD1	2.50	0.40
1:H:256:TRP:CZ2	1:H:295:PHE:HB2	2.57	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	304/346 (88%)	300 (99%)	3 (1%)	1 (0%)	41 46
1	B	304/346 (88%)	298 (98%)	6 (2%)	0	100 100
1	C	304/346 (88%)	302 (99%)	2 (1%)	0	100 100
1	D	304/346 (88%)	302 (99%)	1 (0%)	1 (0%)	41 46
1	E	304/346 (88%)	302 (99%)	0	2 (1%)	22 22
1	F	304/346 (88%)	300 (99%)	3 (1%)	1 (0%)	41 46
1	G	304/346 (88%)	302 (99%)	2 (1%)	0	100 100
1	H	304/346 (88%)	298 (98%)	6 (2%)	0	100 100
All	All	2432/2768 (88%)	2404 (99%)	23 (1%)	5 (0%)	47 55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	84	LEU

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Mol	Chain	Res	Type
1	A	132	TYR
1	D	132	TYR
1	E	316	LEU
1	E	132	TYR

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	255/292 (87%)	254 (100%)	1 (0%)	91	96
1	B	255/292 (87%)	253 (99%)	2 (1%)	81	90
1	C	255/292 (87%)	253 (99%)	2 (1%)	81	90
1	D	255/292 (87%)	253 (99%)	2 (1%)	81	90
1	E	255/292 (87%)	254 (100%)	1 (0%)	91	96
1	F	254/292 (87%)	251 (99%)	3 (1%)	71	83
1	G	255/292 (87%)	252 (99%)	3 (1%)	71	83
1	H	255/292 (87%)	249 (98%)	6 (2%)	49	62
All	All	2039/2336 (87%)	2019 (99%)	20 (1%)	76	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	ASP
1	B	108	ARG
1	B	285	VAL
1	C	134	LYS
1	C	237	LEU
1	D	235	ARG
1	D	237	LEU
1	E	34	ILE
1	F	34	ILE
1	F	35	LYS
1	F	237	LEU

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Mol	Chain	Res	Type
1	G	34	ILE
1	G	214	LYS
1	G	285	VAL
1	H	34	ILE
1	H	108	ARG
1	H	156	TYR
1	H	237	LEU
1	H	247	ASN
1	H	285	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	116	GLN
1	A	123	HIS
1	A	189	ASN
1	A	206	ASN
1	A	209	GLN
1	A	247	ASN
1	A	262	ASN
1	B	123	HIS
1	B	127	HIS
1	B	189	ASN
1	B	206	ASN
1	B	209	GLN
1	B	247	ASN
1	B	262	ASN
1	C	90	ASN
1	C	112	HIS
1	C	116	GLN
1	C	123	HIS
1	C	172	HIS
1	C	189	ASN
1	C	206	ASN
1	C	209	GLN
1	C	262	ASN
1	D	112	HIS
1	D	116	GLN
1	D	123	HIS
1	D	127	HIS
1	D	164	GLN

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Mol	Chain	Res	Type
1	D	189	ASN
1	D	206	ASN
1	D	209	GLN
1	D	247	ASN
1	D	262	ASN
1	E	123	HIS
1	E	172	HIS
1	E	176	GLN
1	E	189	ASN
1	E	206	ASN
1	E	209	GLN
1	E	247	ASN
1	E	262	ASN
1	F	112	HIS
1	F	123	HIS
1	F	189	ASN
1	F	194	GLN
1	F	206	ASN
1	F	247	ASN
1	F	262	ASN
1	G	116	GLN
1	G	123	HIS
1	G	172	HIS
1	G	189	ASN
1	G	206	ASN
1	G	209	GLN
1	G	247	ASN
1	G	262	ASN
1	H	112	HIS
1	H	123	HIS
1	H	189	ASN
1	H	206	ASN
1	H	209	GLN
1	H	247	ASN
1	H	262	ASN
1	H	306	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KPI	H	184	1	10,13,14	2.90	1 (10%)	6,15,17	1.45	1 (16%)
1	KPI	E	184	1	10,13,14	2.93	2 (20%)	6,15,17	1.23	1 (16%)
1	KPI	G	184	1	10,13,14	2.83	2 (20%)	6,15,17	1.76	2 (33%)
1	KPI	A	184	1	10,13,14	2.91	1 (10%)	6,15,17	1.55	2 (33%)
1	KPI	C	184	1	10,13,14	2.98	2 (20%)	6,15,17	1.59	2 (33%)
1	KPI	B	184	1	10,13,14	2.85	2 (20%)	6,15,17	1.51	2 (33%)
1	KPI	D	184	1	10,13,14	2.87	2 (20%)	6,15,17	1.65	2 (33%)
1	KPI	F	184	1	10,13,14	2.92	2 (20%)	6,15,17	1.47	2 (33%)

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
1	KPI	H	184	1	-	0/9/14/16	-
1	KPI	E	184	1	-	1/9/14/16	-
1	KPI	G	184	1	-	1/9/14/16	-
1	KPI	A	184	1	-	0/9/14/16	-
1	KPI	C	184	1	-	0/9/14/16	-
1	KPI	B	184	1	-	1/9/14/16	-
1	KPI	D	184	1	-	1/9/14/16	-
1	KPI	F	184	1	-	0/9/14/16	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	184	KPI	C1-CX1	-8.83	1.33	1.50
1	A	184	KPI	C1-CX1	-8.73	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	184	KPI	C1-CX1	-8.71	1.33	1.50
1	H	184	KPI	C1-CX1	-8.62	1.33	1.50
1	E	184	KPI	C1-CX1	-8.56	1.33	1.50
1	B	184	KPI	C1-CX1	-8.39	1.34	1.50
1	D	184	KPI	C1-CX1	-8.38	1.34	1.50
1	G	184	KPI	C1-CX1	-8.34	1.34	1.50
1	E	184	KPI	CX2-CX1	-2.77	1.47	1.52
1	B	184	KPI	CX2-CX1	-2.39	1.48	1.52
1	C	184	KPI	CX2-CX1	-2.38	1.48	1.52
1	G	184	KPI	CX2-CX1	-2.37	1.48	1.52
1	D	184	KPI	CX2-CX1	-2.24	1.48	1.52
1	F	184	KPI	CX2-CX1	-2.17	1.48	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	184	KPI	CE-NZ-CX1	2.63	128.85	121.77
1	F	184	KPI	C1-CX1-CX2	2.49	120.68	117.92
1	G	184	KPI	C1-CX1-CX2	2.45	120.64	117.92
1	D	184	KPI	C1-CX1-CX2	2.39	120.57	117.92
1	H	184	KPI	C1-CX1-CX2	2.34	120.52	117.92
1	A	184	KPI	CE-NZ-CX1	2.33	128.04	121.77
1	D	184	KPI	CE-NZ-CX1	2.25	127.82	121.77
1	C	184	KPI	C1-CX1-CX2	2.24	120.40	117.92
1	B	184	KPI	CE-NZ-CX1	2.18	127.63	121.77
1	A	184	KPI	C1-CX1-CX2	2.16	120.32	117.92
1	C	184	KPI	CE-NZ-CX1	2.13	127.49	121.77
1	B	184	KPI	CD-CE-NZ	-2.02	106.98	110.66
1	E	184	KPI	C1-CX1-CX2	2.02	120.16	117.92
1	F	184	KPI	CE-NZ-CX1	2.01	127.18	121.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	184	KPI	O-C-CA-CB
1	G	184	KPI	O-C-CA-CB
1	B	184	KPI	O-C-CA-CB
1	D	184	KPI	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	184	KPI	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 23 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	306/346 (88%)	-0.58	0 100 100	15, 22, 33, 39	0
1	B	306/346 (88%)	-0.48	2 (0%) 87 86	14, 22, 33, 40	0
1	C	306/346 (88%)	-0.51	0 100 100	14, 21, 32, 41	0
1	D	306/346 (88%)	-0.45	0 100 100	15, 23, 33, 41	0
1	E	306/346 (88%)	-0.48	0 100 100	15, 22, 33, 42	0
1	F	306/346 (88%)	-0.58	0 100 100	14, 21, 33, 41	0
1	G	306/346 (88%)	-0.45	0 100 100	14, 22, 34, 41	0
1	H	306/346 (88%)	-0.18	6 (1%) 65 63	15, 23, 36, 42	0
All	All	2448/2768 (88%)	-0.46	8 (0%) 94 93	14, 22, 34, 42	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	307	PHE	2.8
1	H	293	VAL	2.8
1	B	317	ASP	2.4
1	H	319	ASP	2.3
1	H	290	ALA	2.3
1	H	289	LEU	2.2
1	H	318	ASP	2.0
1	B	199	ARG	2.0

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

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, 95^{th} 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
1	KPI	B	184	14/15	0.90	0.14	18,20,26,27	0
1	KPI	D	184	14/15	0.91	0.14	20,21,26,27	0
1	KPI	G	184	14/15	0.92	0.16	19,20,26,27	0
1	KPI	H	184	14/15	0.93	0.10	21,22,27,27	0
1	KPI	E	184	14/15	0.94	0.13	20,21,27,28	0
1	KPI	C	184	14/15	0.94	0.15	19,20,25,26	0
1	KPI	F	184	14/15	0.94	0.12	19,20,25,27	0
1	KPI	A	184	14/15	0.95	0.10	19,20,26,27	0

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. 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	BR	E	329	1/1	0.94	0.05	90,90,90,90	0
2	BR	G	329	1/1	0.96	0.05	54,54,54,54	0
2	BR	B	328	1/1	0.97	0.06	43,43,43,43	1
2	BR	C	328	1/1	0.97	0.08	51,51,51,51	0
2	BR	G	330	1/1	0.97	0.16	59,59,59,59	0
2	BR	G	328	1/1	0.97	0.09	51,51,51,51	0
2	BR	H	328	1/1	0.97	0.11	57,57,57,57	0
2	BR	D	329	1/1	0.98	0.12	59,59,59,59	0
2	BR	A	328	1/1	0.98	0.05	36,36,36,36	1
3	CL	G	332	1/1	0.98	0.17	39,39,39,39	0
2	BR	D	328	1/1	0.98	0.10	58,58,58,58	0
2	BR	F	328	1/1	0.98	0.06	49,49,49,49	0
3	CL	G	331	1/1	0.99	0.13	24,24,24,24	1
3	CL	C	330	1/1	0.99	0.16	17,17,17,17	0
2	BR	A	329	1/1	0.99	0.14	59,59,59,59	0
3	CL	H	329	1/1	0.99	0.12	21,21,21,21	0
3	CL	A	330	1/1	0.99	0.14	21,21,21,21	0
3	CL	B	329	1/1	0.99	0.17	11,11,11,11	0
2	BR	E	328	1/1	0.99	0.09	50,50,50,50	0
3	CL	E	330	1/1	0.99	0.12	17,17,17,17	1
2	BR	C	329	1/1	0.99	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	F	330	1/1	1.00	0.09	21,21,21,21	0
2	BR	F	329	1/1	1.00	0.03	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.