Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 PM GMT

PDB ID	:	4HNN
Title	:	Dihydrodipicolinate Synthase from the common grapevine with pyruvate and lysine
Authors	:	Atkinson, S.C; Dobson, R.C.J; Perugini, M.A.
Deposited on	:	2012-10-19
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

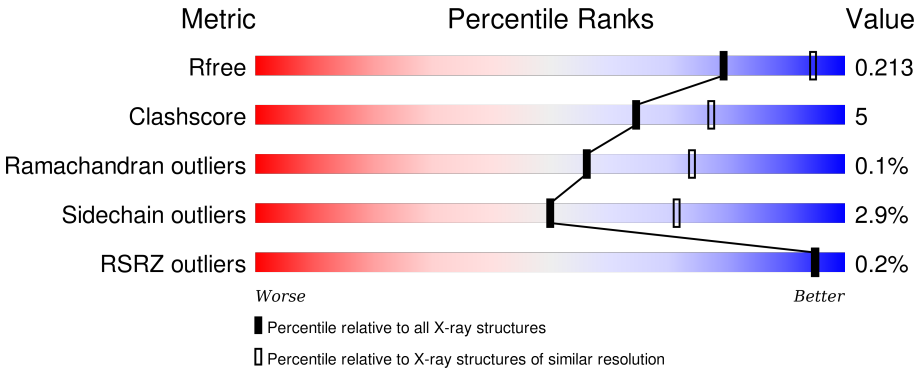
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	72% 15% • • 11%
1	B	346	70% 16% • • 11%
1	C	346	77% 11% • 11%
1	D	346	78% 11% 11%
1	E	346	77% 11% • 11%

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Mol	Chain	Length	Quality of chain
1	F	346	
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	LYS	A	401	-	-	-	X
2	LYS	B	401	-	-	-	X
2	LYS	C	401	-	-	-	X
2	LYS	F	401	-	-	-	X
2	LYS	H	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20101 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
			2362	1504	404	444	10			
1	B	307	Total	C	N	O	S	0	0	0
			2362	1504	404	444	10			
1	C	308	Total	C	N	O	S	0	0	0
			2369	1508	405	446	10			
1	D	308	Total	C	N	O	S	0	2	0
			2383	1518	409	446	10			
1	E	307	Total	C	N	O	S	0	1	0
			2363	1506	403	444	10			
1	F	320	Total	C	N	O	S	0	3	0
			2471	1573	423	464	11			
1	G	307	Total	C	N	O	S	0	3	0
			2376	1516	404	446	10			
1	H	308	Total	C	N	O	S	0	0	0
			2362	1505	402	445	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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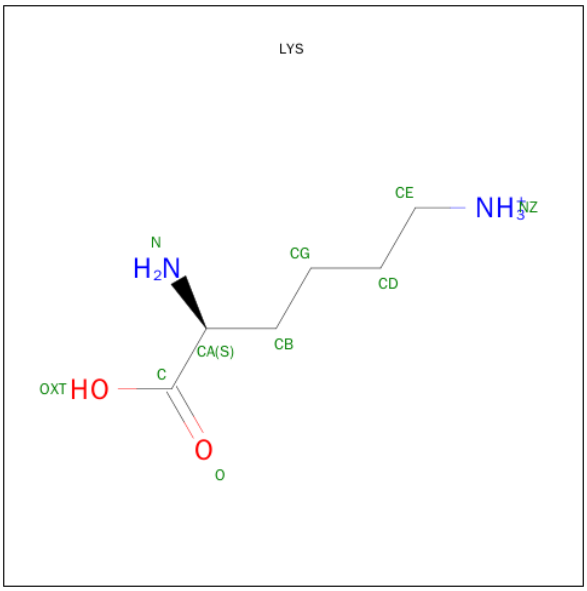
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	EXPRESSION TAG	UNP D7U7T8
H	-18	MET	-	EXPRESSION TAG	UNP D7U7T8
H	-17	GLY	-	EXPRESSION TAG	UNP D7U7T8
H	-16	SER	-	EXPRESSION TAG	UNP D7U7T8
H	-15	SER	-	EXPRESSION TAG	UNP D7U7T8
H	-14	HIS	-	EXPRESSION TAG	UNP D7U7T8
H	-13	HIS	-	EXPRESSION TAG	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 LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	6	2	2		
2	C	1	Total	C	N	O	0	0
			10	6	2	2		
2	D	1	Total	C	N	O	0	0
			10	6	2	2		
2	E	1	Total	C	N	O	0	0
			10	6	2	2		
2	F	1	Total	C	N	O	0	0
			10	6	2	2		
2	G	1	Total	C	N	O	0	0
			10	6	2	2		
2	H	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is water.

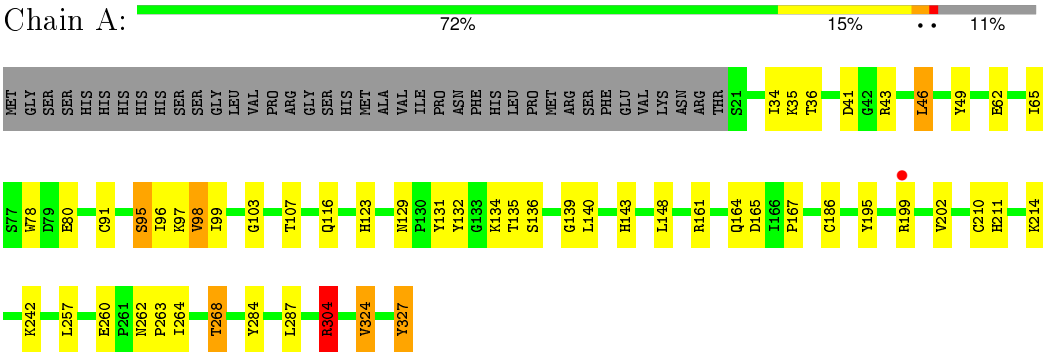
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		
3	B	142	Total	O	0	0
			142	142		
3	C	159	Total	O	0	0
			159	159		
3	D	140	Total	O	0	0
			140	140		
3	E	102	Total	O	0	0
			102	102		
3	F	119	Total	O	0	0
			119	119		
3	G	84	Total	O	0	0
			84	84		
3	H	97	Total	O	0	0
			97	97		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

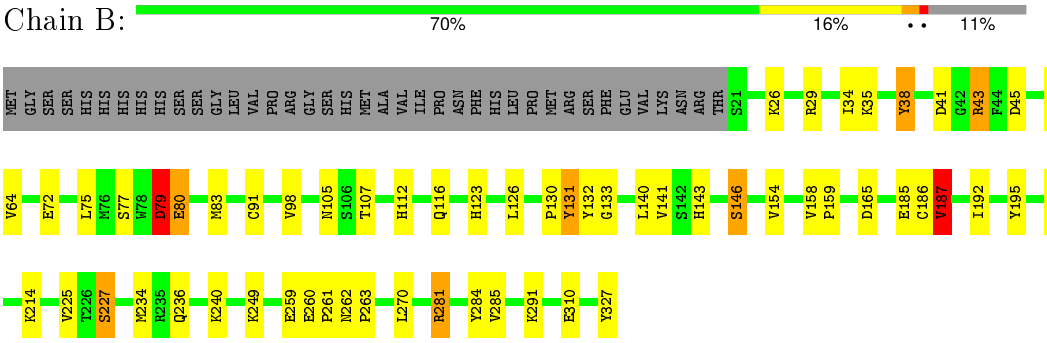
- Molecule 1: Dihydrodipicolinate synthase

Chain A:



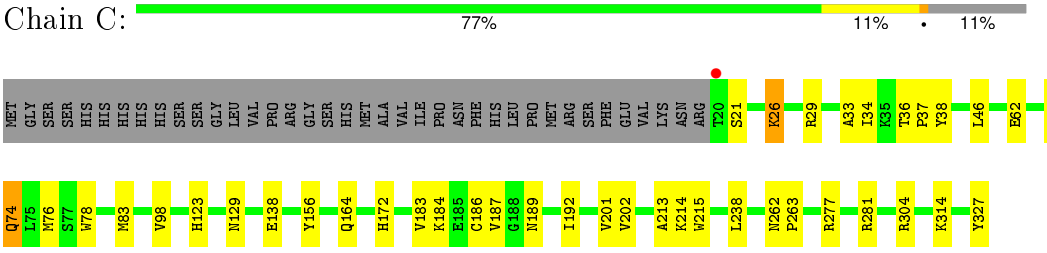
- Molecule 1: Dihydrodipicolinate synthase

Chain B:



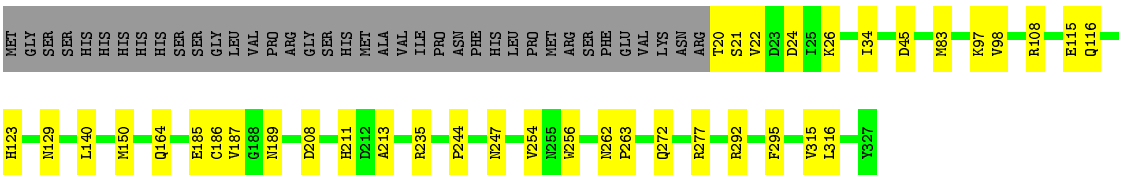
- Molecule 1: Dihydrodipicolinate synthase

Chain C:



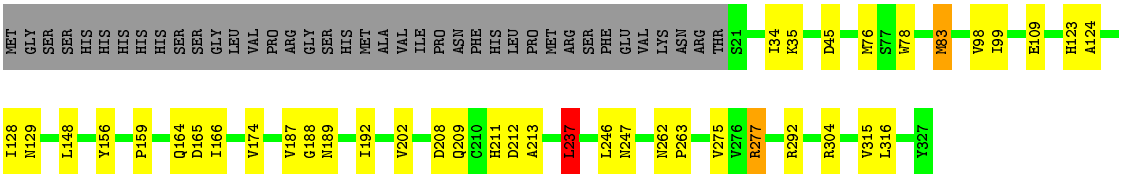
- Molecule 1: Dihydrodipicolinate synthase

Chain D:



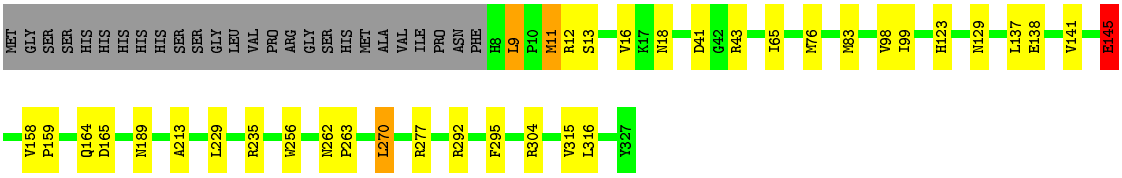
• Molecule 1: Dihydrodipicolinate synthase

Chain E:



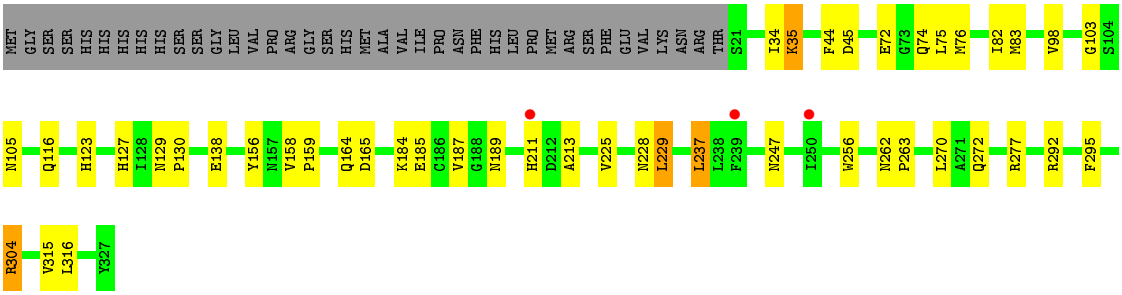
• Molecule 1: Dihydrodipicolinate synthase

Chain F:



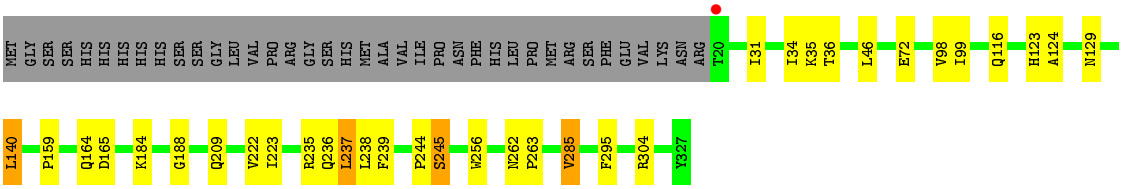
• Molecule 1: Dihydrodipicolinate synthase

Chain G:



• Molecule 1: Dihydrodipicolinate synthase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	220.61Å 137.93Å 133.94Å 90.00° 108.25° 90.00°	Depositor
Resolution (Å)	127.20 – 2.40 52.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (127.20-2.40) 98.4 (52.02-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.181 , 0.216 0.182 , 0.213	Depositor DCC
R_{free} test set	2020 reflections (1.40%)	DCC
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 146157 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20101	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: KPI

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	1.90	20/2398 (0.8%)	0.88	6/3263 (0.2%)
1	B	1.97	27/2398 (1.1%)	0.94	7/3263 (0.2%)
1	C	1.14	6/2405 (0.2%)	0.72	2/3273 (0.1%)
1	D	0.94	2/2427 (0.1%)	0.66	0/3303
1	E	0.90	3/2403 (0.1%)	0.64	3/3271 (0.1%)
1	F	0.88	3/2519 (0.1%)	0.64	1/3428 (0.0%)
1	G	0.86	2/2423 (0.1%)	0.66	4/3298 (0.1%)
1	H	0.86	3/2398 (0.1%)	0.63	1/3264 (0.0%)
All	All	1.26	66/19371 (0.3%)	0.73	24/26363 (0.1%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	186	CYS	CB-SG	-9.56	1.66	1.82
1	C	186	CYS	CB-SG	-8.60	1.67	1.82
1	G	138[A]	GLU	N-CA	-8.27	1.29	1.46
1	G	138[B]	GLU	N-CA	-8.27	1.29	1.46
1	C	72	GLU	CD-OE2	-7.91	1.17	1.25
1	A	186	CYS	CB-SG	-7.46	1.69	1.82
1	F	138[A]	GLU	N-CA	7.41	1.61	1.46
1	F	138[B]	GLU	N-CA	7.41	1.61	1.46
1	A	210	CYS	CB-SG	-7.35	1.69	1.82
1	B	64	VAL	CB-CG2	-7.09	1.38	1.52
1	B	284	TYR	CD1-CE1	-6.87	1.29	1.39
1	H	72	GLU	CD-OE2	-6.85	1.18	1.25
1	B	72	GLU	CD-OE2	-6.78	1.18	1.25
1	B	284	TYR	CD2-CE2	-6.74	1.29	1.39
1	A	131	TYR	CD2-CE2	-6.68	1.29	1.39
1	B	80	GLU	CD-OE2	-6.63	1.18	1.25
1	A	284	TYR	CD2-CE2	-6.50	1.29	1.39
1	E	187	VAL	CB-CG2	-6.35	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	145	GLU	CB-CG	-6.34	1.40	1.52
1	B	131	TYR	CD2-CE2	-6.33	1.29	1.39
1	A	284	TYR	CD1-CE1	-6.27	1.29	1.39
1	B	195	TYR	CD2-CE2	-6.27	1.29	1.39
1	B	225	VAL	CB-CG2	-6.23	1.39	1.52
1	B	146	SER	CB-OG	-6.19	1.34	1.42
1	A	132	TYR	CD1-CE1	-6.14	1.30	1.39
1	A	49	TYR	CD1-CE1	-6.12	1.30	1.39
1	C	183	VAL	CB-CG2	-6.07	1.40	1.52
1	A	80	GLU	CD-OE2	-5.92	1.19	1.25
1	D	254	VAL	CB-CG1	-5.90	1.40	1.52
1	H	285	VAL	CB-CG1	-5.90	1.40	1.52
1	B	49	TYR	CD1-CE1	-5.89	1.30	1.39
1	B	91	CYS	CB-SG	-5.88	1.72	1.81
1	A	327	TYR	CE1-CZ	-5.84	1.30	1.38
1	B	79	ASP	CB-CG	-5.78	1.39	1.51
1	B	227	SER	CB-OG	-5.74	1.34	1.42
1	A	49	TYR	CD2-CE2	-5.74	1.30	1.39
1	B	186	CYS	CB-SG	-5.74	1.72	1.81
1	A	95	SER	CB-OG	-5.71	1.34	1.42
1	C	72	GLU	CD-OE1	-5.58	1.19	1.25
1	B	132	TYR	CD1-CE1	-5.56	1.31	1.39
1	E	109	GLU	CD-OE2	-5.56	1.19	1.25
1	A	139	GLY	C-O	-5.55	1.14	1.23
1	C	62	GLU	CD-OE1	-5.55	1.19	1.25
1	B	327	TYR	CD1-CE1	-5.50	1.31	1.39
1	A	324	VAL	CB-CG1	-5.45	1.41	1.52
1	A	202	VAL	CB-CG2	-5.43	1.41	1.52
1	H	72	GLU	CD-OE1	-5.40	1.19	1.25
1	B	62	GLU	CD-OE1	-5.39	1.19	1.25
1	A	91	CYS	CB-SG	-5.34	1.73	1.81
1	A	195	TYR	CD1-CE1	-5.33	1.31	1.39
1	B	38	TYR	CD2-CE2	-5.32	1.31	1.39
1	B	49	TYR	CD2-CE2	-5.30	1.31	1.39
1	B	131	TYR	CD1-CE1	-5.29	1.31	1.39
1	B	187	VAL	CB-CG1	-5.26	1.41	1.52
1	A	72	GLU	CD-OE2	-5.25	1.19	1.25
1	A	62	GLU	CD-OE1	-5.23	1.19	1.25
1	A	98	VAL	CB-CG2	-5.15	1.42	1.52
1	E	275	VAL	CB-CG1	-5.14	1.42	1.52
1	B	154	VAL	CB-CG2	-5.12	1.42	1.52
1	B	285	VAL	CB-CG2	-5.11	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLU	CD-OE1	-5.11	1.20	1.25
1	A	131	TYR	CD1-CE1	-5.09	1.31	1.39
1	B	72	GLU	CD-OE1	-5.08	1.20	1.25
1	C	304	ARG	CG-CD	-5.03	1.39	1.51
1	B	141	VAL	CB-CG2	-5.03	1.42	1.52
1	B	210	CYS	CB-SG	-5.01	1.73	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	43	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	G	304	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	237	LEU	CA-CB-CG	6.64	130.57	115.30
1	H	237	LEU	CA-CB-CG	6.62	130.51	115.30
1	E	237	LEU	CA-CB-CG	6.58	130.43	115.30
1	G	237	LEU	CA-CB-CG	6.39	129.99	115.30
1	B	79	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	C	238	LEU	CA-CB-CG	6.13	129.41	115.30
1	E	277	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	281	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	43	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	G	304	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	126	LEU	CB-CG-CD1	5.49	120.32	111.00
1	G	229	LEU	CA-CB-CG	5.47	127.88	115.30
1	B	43	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	B	41	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	29	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	277	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	F	277	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	304	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	41	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	45	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	161	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	304	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	2362	0	2354	30	0
1	B	2362	0	2354	21	0
1	C	2369	0	2361	27	0
1	D	2383	0	2375	28	0
1	E	2363	0	2350	26	0
1	F	2471	0	2455	22	0
1	G	2376	0	2360	28	0
1	H	2362	0	2344	21	0
2	A	10	0	12	3	0
2	B	10	0	12	0	0
2	C	10	0	12	2	0
2	D	10	0	12	0	0
2	E	10	0	12	3	0
2	F	10	0	12	1	0
2	G	10	0	12	0	0
2	H	10	0	12	0	0
3	A	130	0	0	2	0
3	B	142	0	0	0	0
3	C	159	0	0	2	0
3	D	140	0	0	1	0
3	E	102	0	0	0	0
3	F	119	0	0	0	0
3	G	84	0	0	0	0
3	H	97	0	0	0	0
All	All	20101	0	19049	196	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 5.

All (196) 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:A:98:VAL:H	1:A:123:HIS:HD2	1.04	1.00
1:B:98:VAL:H	1:B:123:HIS:HD2	1.09	0.99
1:C:98:VAL:H	1:C:123:HIS:HD2	1.02	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:VAL:H	1:E:123:HIS:HD2	1.03	0.98
1:G:98:VAL:H	1:G:123:HIS:HD2	1.12	0.97
1:H:98:VAL:H	1:H:123:HIS:HD2	1.11	0.96
1:C:74:GLN:HE21	1:C:74:GLN:H	1.16	0.92
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.32	0.92
1:A:116:GLN:HA	1:E:83:MET:HE2	1.50	0.92
1:E:129:ASN:HD22	1:E:164:GLN:HE21	1.18	0.90
1:C:74:GLN:NE2	1:C:74:GLN:H	1.72	0.87
1:D:211[B]:HIS:CD2	1:D:247:ASN:HD21	1.93	0.86
1:A:98:VAL:H	1:A:123:HIS:CD2	1.92	0.84
1:C:98:VAL:H	1:C:123:HIS:CD2	1.94	0.84
1:H:244:PRO:O	1:H:245:SER:HB3	1.78	0.83
1:A:304:ARG:HG3	1:A:304:ARG:O	1.78	0.82
1:H:129:ASN:HD22	1:H:164:GLN:HE21	1.24	0.82
1:F:12:ARG:HG3	1:F:12:ARG:O	1.78	0.81
1:E:98:VAL:H	1:E:123:HIS:CD2	1.96	0.80
1:H:244:PRO:O	1:H:245:SER:CB	2.29	0.79
1:B:43:ARG:NH2	1:F:9:LEU:O	2.16	0.77
1:H:98:VAL:H	1:H:123:HIS:CD2	2.01	0.75
1:C:129:ASN:HD22	1:C:164:GLN:HE21	1.32	0.74
1:C:26:LYS:HG2	1:C:201:VAL:HG21	1.69	0.74
1:D:129:ASN:HD22	1:D:164:GLN:HE21	1.32	0.74
1:C:98:VAL:N	1:C:123:HIS:HD2	1.84	0.72
1:G:129:ASN:HD22	1:G:164:GLN:HE21	1.36	0.72
1:B:112:HIS:CE1	1:B:116:GLN:OE1	2.42	0.72
1:H:304:ARG:HG3	1:H:304:ARG:O	1.92	0.70
1:A:129:ASN:HD22	1:A:164:GLN:HE21	1.38	0.69
1:A:98:VAL:N	1:A:123:HIS:HD2	1.85	0.68
1:A:107:THR:OG1	1:A:143:HIS:HD2	1.76	0.68
1:F:129:ASN:HD22	1:F:164:GLN:HE21	1.42	0.68
1:C:74:GLN:HE21	1:C:74:GLN:N	1.89	0.68
1:D:20:THR:HG22	1:D:21:SER:N	2.10	0.67
1:D:83:MET:HE3	1:G:116:GLN:HG2	1.76	0.66
1:D:211[B]:HIS:CD2	1:D:247:ASN:ND2	2.64	0.66
1:A:76:MET:O	2:A:401:LYS:HD3	1.96	0.66
1:C:72:GLU:OE1	3:C:501:HOH:O	2.14	0.65
1:D:98:VAL:H	1:D:123:HIS:CD2	2.16	0.64
1:G:262:ASN:ND2	1:G:263:PRO:HA	2.14	0.63
1:F:76:MET:O	2:F:401:LYS:HD3	1.98	0.63
1:F:98:VAL:H	1:F:123:HIS:CD2	2.18	0.62
1:C:214:LYS:O	1:C:214:LYS:HD3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:GLU:N	1:D:150:MET:HE1	2.15	0.62
1:B:98:VAL:H	1:B:123:HIS:CD2	2.02	0.61
1:E:188:GLY:HA2	1:E:209:GLN:HE22	1.64	0.61
1:G:98:VAL:H	1:G:123:HIS:CD2	2.04	0.60
1:G:185:GLU:OE1	1:G:187:VAL:HG13	2.01	0.60
1:G:304:ARG:HG3	1:G:304:ARG:O	2.02	0.59
1:C:192:ILE:HG12	1:C:202:VAL:HG11	1.85	0.58
1:H:262:ASN:ND2	1:H:263:PRO:HA	2.18	0.58
1:G:189:ASN:HD21	1:G:213:ALA:HB2	1.68	0.58
1:F:292:ARG:NH2	1:F:316:LEU:O	2.36	0.58
1:E:211[B]:HIS:CD2	1:E:212:ASP:H	2.21	0.58
1:C:262:ASN:ND2	1:C:263:PRO:HA	2.19	0.57
1:E:192:ILE:HG12	1:E:202:VAL:HG11	1.85	0.57
1:E:98:VAL:N	1:E:123:HIS:HD2	1.88	0.57
1:G:292:ARG:NH2	1:G:316:LEU:O	2.38	0.57
1:D:211[B]:HIS:CD2	1:D:211[B]:HIS:H	2.22	0.57
1:E:262:ASN:ND2	1:E:263:PRO:HA	2.20	0.57
1:A:264:ILE:O	1:A:268:THR:CG2	2.53	0.56
1:A:264:ILE:O	1:A:268:THR:HG22	2.05	0.56
1:F:189:ASN:HD21	1:F:213:ALA:HB2	1.71	0.56
1:C:214:LYS:HD3	1:C:214:LYS:C	2.27	0.56
1:F:141:VAL:O	1:F:145:GLU:HB2	2.06	0.55
1:D:129:ASN:HB2	1:D:140:LEU:HD21	1.88	0.55
1:H:98:VAL:N	1:H:123:HIS:HD2	1.94	0.55
1:C:189:ASN:HD21	1:C:213:ALA:HB2	1.73	0.54
1:H:159:PRO:HG3	1:H:165:ASP:HA	1.89	0.54
1:A:129:ASN:ND2	1:A:164:GLN:HE21	2.04	0.54
1:H:99:ILE:HG12	1:H:124:ALA:HB3	1.89	0.53
1:A:78:TRP:CZ2	2:A:401:LYS:HE2	2.43	0.53
1:D:262:ASN:ND2	1:D:263:PRO:HA	2.24	0.53
1:B:159:PRO:HG3	1:B:165:ASP:HA	1.89	0.53
1:B:77:SER:OG	1:B:79:ASP:HB3	2.09	0.52
1:F:262:ASN:ND2	1:F:263:PRO:HA	2.24	0.52
1:F:229:LEU:HD23	1:F:270:LEU:HD13	1.91	0.52
1:H:35:LYS:HG3	1:H:36:THR:N	2.20	0.52
1:E:159:PRO:HG3	1:E:165:ASP:HA	1.92	0.52
1:G:159:PRO:HG3	1:G:165:ASP:HA	1.91	0.52
1:C:83:MET:HE2	1:H:116:GLN:HA	1.92	0.52
1:C:26:LYS:CG	1:C:201:VAL:HG21	2.39	0.52
1:F:12:ARG:CG	1:F:12:ARG:O	2.54	0.51
1:D:189:ASN:HD21	1:D:213:ALA:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:ASN:HB2	1:H:140:LEU:HD11	1.92	0.51
1:B:38:TYR:CZ	1:B:281:ARG:HD2	2.45	0.51
1:E:237:LEU:HD23	1:E:246:LEU:HD23	1.93	0.51
1:A:324:VAL:HG12	1:A:327:TYR:HD2	1.75	0.51
1:E:292:ARG:NH2	1:E:316:LEU:O	2.43	0.51
1:D:189:ASN:ND2	1:D:213:ALA:HB2	2.26	0.51
1:D:292:ARG:HD2	1:D:315:VAL:O	2.11	0.51
1:C:38:TYR:CZ	1:C:281:ARG:HD2	2.46	0.50
1:B:131:TYR:O	1:B:133:GLY:N	2.42	0.50
1:E:208:ASP:C	1:E:211[B]:HIS:CE1	2.85	0.50
1:D:272:GLN:OE1	1:D:292:ARG:HG2	2.11	0.50
1:G:256:TRP:CZ2	1:G:295:PHE:HB2	2.47	0.50
1:A:165:ASP:O	1:A:167:PRO:HD3	2.11	0.50
1:A:327:TYR:OH	3:A:578:HOH:O	2.08	0.49
1:D:20:THR:HG22	1:D:21:SER:H	1.75	0.49
1:A:129:ASN:HD22	1:A:164:GLN:NE2	2.09	0.49
1:B:107:THR:OG1	1:B:143:HIS:HD2	1.95	0.49
1:B:158:VAL:HG13	1:B:158:VAL:O	2.13	0.49
1:G:44:PHE:HZ	1:G:76:MET:HG2	1.77	0.49
1:A:211:HIS:HD2	1:A:237:LEU:HD22	1.78	0.49
1:B:35:LYS:HG2	1:B:270:LEU:CD1	2.43	0.48
1:G:211[B]:HIS:H	1:G:211[B]:HIS:CD2	2.31	0.48
1:E:76:MET:O	2:E:401:LYS:HD3	2.13	0.48
1:F:158:VAL:HG22	1:F:158:VAL:O	2.13	0.48
1:A:304:ARG:CG	1:A:304:ARG:O	2.54	0.48
1:A:268:THR:HG21	1:A:287:LEU:H	1.79	0.47
1:E:189:ASN:HD21	1:E:213:ALA:HB2	1.79	0.47
1:F:256:TRP:CZ2	1:F:295:PHE:HB2	2.49	0.47
1:E:128:ILE:HA	1:E:156:TYR:HB3	1.96	0.47
1:H:222:VAL:HG12	1:H:238:LEU:HD21	1.95	0.47
1:E:99:ILE:HG12	1:E:124:ALA:HB3	1.97	0.47
1:D:20:THR:O	1:F:16:VAL:HG11	2.15	0.47
1:B:26:LYS:HG2	1:B:201:VAL:HG21	1.97	0.46
1:B:79:ASP:HB3	1:B:80:GLU:H	1.39	0.46
1:D:256:TRP:CZ2	1:D:295:PHE:HB2	2.51	0.46
1:F:159:PRO:HG3	1:F:165:ASP:HA	1.97	0.46
1:C:76:MET:O	2:C:401:LYS:HD3	2.15	0.46
1:C:156:TYR:CD1	1:C:184:KPI:HD	2.51	0.46
1:G:35:LYS:HD2	1:G:270:LEU:HD12	1.98	0.46
1:D:45:ASP:OD2	1:D:277:ARG:HD2	2.15	0.45
1:E:208:ASP:C	1:E:211[B]:HIS:HE1	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:LEU:CD2	1:F:270:LEU:HD13	2.46	0.45
1:A:46:LEU:HA	1:A:46:LEU:HD12	1.63	0.45
1:C:189:ASN:ND2	1:C:213:ALA:HB2	2.31	0.45
1:A:324:VAL:HG11	1:A:327:TYR:HB3	1.97	0.45
1:B:192:ILE:HG12	1:B:202:VAL:HG11	1.97	0.45
1:B:185:GLU:OE2	1:B:187:VAL:HB	2.17	0.45
1:A:78:TRP:CE2	2:A:401:LYS:HE2	2.52	0.44
1:G:211[B]:HIS:CD2	1:G:247:ASN:HD21	2.36	0.44
1:G:158:VAL:O	1:G:158:VAL:HG13	2.17	0.44
1:A:35:LYS:HG3	1:A:36:THR:N	2.26	0.44
1:G:103:GLY:HA2	1:G:127:HIS:CD2	2.52	0.44
1:F:292:ARG:HD2	1:F:315:VAL:O	2.18	0.44
1:H:236:GLN:HB2	1:H:236:GLN:HE21	1.56	0.44
1:H:129:ASN:ND2	1:H:164:GLN:HE21	2.04	0.44
1:D:24:ASP:HB3	1:D:97:LYS:HE2	2.00	0.44
1:G:292:ARG:HD2	1:G:315:VAL:O	2.18	0.43
1:E:148:LEU:HD11	1:E:174:VAL:HB	1.99	0.43
1:E:292:ARG:HD2	1:E:315:VAL:O	2.18	0.43
1:C:138:GLU:H	1:C:138:GLU:CD	2.20	0.43
1:D:22:VAL:HB	1:D:26:LYS:HD2	2.00	0.43
1:F:11:MET:HG2	1:F:11:MET:O	2.19	0.43
1:A:262:ASN:HA	1:A:263:PRO:HA	1.72	0.43
1:D:20:THR:CG2	1:D:21:SER:N	2.80	0.43
1:G:272:GLN:OE1	1:G:292:ARG:HG2	2.19	0.42
1:A:260:GLU:HA	1:A:260:GLU:OE1	2.20	0.42
1:B:291:LYS:HD3	1:B:291:LYS:HA	1.75	0.42
1:D:185:GLU:OE2	1:D:187:VAL:HB	2.19	0.42
1:E:211[B]:HIS:ND1	1:E:247:ASN:ND2	2.63	0.42
1:E:78:TRP:CE2	2:E:401:LYS:HE2	2.53	0.42
1:E:78:TRP:CZ2	2:E:401:LYS:HE2	2.55	0.42
1:A:103:GLY:HA3	3:A:591:HOH:O	2.20	0.42
1:B:29:ARG:HD3	1:B:214:LYS:HE2	2.01	0.42
1:B:262:ASN:HA	1:B:263:PRO:HA	1.77	0.42
1:H:184:KPI:HG	1:H:223:ILE:HD12	2.02	0.42
1:H:188:GLY:HA2	1:H:209:GLN:HE22	1.84	0.42
1:F:65:ILE:HD13	1:F:99:ILE:HB	2.02	0.42
1:C:214:LYS:HG3	1:C:215:TRP:CE2	2.55	0.42
1:C:78:TRP:CE2	2:C:401:LYS:HE2	2.55	0.41
1:A:97:LYS:HD3	1:A:97:LYS:HA	1.69	0.41
1:G:225:VAL:O	1:G:228:ASN:HB2	2.20	0.41
1:D:244:PRO:HD2	3:D:604:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:256:TRP:CZ2	1:H:295:PHE:HB2	2.55	0.41
1:E:129:ASN:HB3	1:E:166:ILE:HD11	2.03	0.41
1:G:156:TYR:CD1	1:G:184:KPI:HD	2.54	0.41
1:C:172:HIS:HE1	3:C:502:HOH:O	2.03	0.41
1:H:31:ILE:HB	1:H:223:ILE:HG12	2.02	0.41
1:D:116:GLN:HG2	1:G:83:MET:CE	2.50	0.41
1:A:135:THR:OG1	1:A:136:SER:N	2.53	0.41
1:B:260:GLU:HB3	1:B:261:PRO:HD2	2.02	0.41
1:F:13:SER:HB3	1:F:18:ASN:HD22	1.84	0.41
1:F:41:ASP:OD1	1:F:43:ARG:NH1	2.49	0.41
1:C:327:TYR:CE2	1:D:108:ARG:CZ	3.04	0.41
1:C:33:ALA:HA	1:C:65:ILE:HB	2.02	0.41
1:G:45:ASP:OD2	1:G:277:ARG:HD2	2.21	0.41
1:G:72:GLU:HA	1:G:74:GLN:NE2	2.36	0.41
1:E:304:ARG:HG3	1:E:304:ARG:O	2.21	0.41
1:D:208:ASP:O	1:D:211[B]:HIS:NE2	2.54	0.41
1:G:82:ILE:HG13	1:G:116:GLN:HE21	1.86	0.41
1:C:36:THR:HA	1:C:37:PRO:HD3	1.92	0.41
1:D:292:ARG:NH2	1:D:316:LEU:O	2.53	0.40
1:E:45:ASP:OD2	1:E:277:ARG:HD2	2.21	0.40
1:H:235:ARG:HG3	1:H:239:PHE:CD2	2.55	0.40
1:D:211[B]:HIS:CG	1:D:247:ASN:ND2	2.89	0.40
1:F:229:LEU:HD23	1:F:270:LEU:CD1	2.51	0.40
1:B:35:LYS:HG2	1:B:270:LEU:HD12	2.04	0.40
1:G:105:ASN:HA	1:G:130:PRO:HA	2.03	0.40
1:A:65:ILE:HD13	1:A:99:ILE:HB	2.03	0.40
1:G:262:ASN:HD22	1:G:263:PRO:HA	1.85	0.40
1:B:105:ASN:HA	1:B:130:PRO:HA	2.02	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%)	298 (98%)	6 (2%)	0	100	100
1	B	304/346 (88%)	300 (99%)	3 (1%)	1 (0%)	46	63
1	C	305/346 (88%)	302 (99%)	3 (1%)	0	100	100
1	D	307/346 (89%)	301 (98%)	6 (2%)	0	100	100
1	E	305/346 (88%)	300 (98%)	5 (2%)	0	100	100
1	F	320/346 (92%)	315 (98%)	5 (2%)	0	100	100
1	G	307/346 (89%)	303 (99%)	4 (1%)	0	100	100
1	H	305/346 (88%)	298 (98%)	6 (2%)	1 (0%)	46	63
All	All	2457/2768 (89%)	2417 (98%)	38 (2%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	SER
1	B	79	ASP

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	257/292 (88%)	241 (94%)	16 (6%)	23	35
1	B	257/292 (88%)	244 (95%)	13 (5%)	29	46
1	C	258/292 (88%)	250 (97%)	8 (3%)	47	69
1	D	260/292 (89%)	258 (99%)	2 (1%)	86	94
1	E	257/292 (88%)	253 (98%)	4 (2%)	70	86
1	F	269/292 (92%)	261 (97%)	8 (3%)	48	70
1	G	258/292 (88%)	253 (98%)	5 (2%)	65	83
1	H	255/292 (87%)	250 (98%)	5 (2%)	63	81
All	All	2071/2336 (89%)	2010 (97%)	61 (3%)	50	71

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	46	LEU
1	A	95	SER
1	A	96	ILE
1	A	134	LYS
1	A	140	LEU
1	A	148	LEU
1	A	199	ARG
1	A	214	LYS
1	A	236	GLN
1	A	237	LEU
1	A	238	LEU
1	A	242	LYS
1	A	257	LEU
1	A	268	THR
1	A	304	ARG
1	B	34	ILE
1	B	75	LEU
1	B	83	MET
1	B	140	LEU
1	B	146	SER
1	B	187	VAL
1	B	227	SER
1	B	234	MET
1	B	236	GLN
1	B	240	LYS
1	B	249	LYS
1	B	259	GLU
1	B	310	GLU
1	C	21	SER
1	C	26	LYS
1	C	34	ILE
1	C	46	LEU
1	C	74	GLN
1	C	187	VAL
1	C	277	ARG
1	C	314	LYS
1	D	34	ILE
1	D	235	ARG
1	E	34	ILE
1	E	35	LYS
1	E	83	MET
1	E	237	LEU

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Mol	Chain	Res	Type
1	F	9	LEU
1	F	11	MET
1	F	83	MET
1	F	137	LEU
1	F	145	GLU
1	F	235	ARG
1	F	270	LEU
1	F	304	ARG
1	G	34	ILE
1	G	35	LYS
1	G	75	LEU
1	G	229	LEU
1	G	237	LEU
1	H	34	ILE
1	H	46	LEU
1	H	140	LEU
1	H	237	LEU
1	H	285	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	116	GLN
1	A	123	HIS
1	A	143	HIS
1	A	164	GLN
1	B	90	ASN
1	B	112	HIS
1	B	123	HIS
1	B	143	HIS
1	C	74	GLN
1	C	116	GLN
1	C	123	HIS
1	C	127	HIS
1	C	164	GLN
1	C	172	HIS
1	C	176	GLN
1	C	189	ASN
1	C	198	ASN
1	C	206	ASN
1	C	209	GLN

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Mol	Chain	Res	Type
1	C	247	ASN
1	C	262	ASN
1	D	116	GLN
1	D	123	HIS
1	D	127	HIS
1	D	164	GLN
1	D	189	ASN
1	D	194	GLN
1	D	206	ASN
1	D	209	GLN
1	D	236	GLN
1	D	262	ASN
1	E	116	GLN
1	E	123	HIS
1	E	164	GLN
1	E	189	ASN
1	E	206	ASN
1	E	209	GLN
1	E	236	GLN
1	E	262	ASN
1	F	18	ASN
1	F	54	ASN
1	F	123	HIS
1	F	127	HIS
1	F	164	GLN
1	F	189	ASN
1	F	206	ASN
1	F	209	GLN
1	F	236	GLN
1	F	247	ASN
1	F	262	ASN
1	G	116	GLN
1	G	123	HIS
1	G	127	HIS
1	G	164	GLN
1	G	189	ASN
1	G	206	ASN
1	G	209	GLN
1	G	262	ASN
1	H	116	GLN
1	H	123	HIS
1	H	127	HIS

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Mol	Chain	Res	Type
1	H	164	GLN
1	H	176	GLN
1	H	189	ASN
1	H	194	GLN
1	H	206	ASN
1	H	209	GLN
1	H	236	GLN
1	H	247	ASN
1	H	262	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	A	184	1	10,13,14	2.15	3 (30%)	9,15,17	1.29	2 (22%)
1	KPI	B	184	1	10,13,14	2.26	3 (30%)	9,15,17	0.87	0
1	KPI	C	184	1	10,13,14	2.36	4 (40%)	9,15,17	0.96	0
1	KPI	D	184	1	10,13,14	1.58	2 (20%)	9,15,17	1.35	1 (11%)
1	KPI	E	184	1	10,13,14	1.87	2 (20%)	9,15,17	1.08	1 (11%)
1	KPI	F	184	1	10,13,14	2.28	3 (30%)	9,15,17	1.49	2 (22%)
1	KPI	G	184	1	10,13,14	1.82	3 (30%)	9,15,17	1.23	2 (22%)
1	KPI	H	184	1	10,13,14	2.10	3 (30%)	9,15,17	1.33	2 (22%)

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	A	184	1	-	0/8/14/16	0/0/0/0
1	KPI	B	184	1	-	0/8/14/16	0/0/0/0
1	KPI	C	184	1	-	0/8/14/16	0/0/0/0
1	KPI	D	184	1	-	0/8/14/16	0/0/0/0
1	KPI	E	184	1	-	0/8/14/16	0/0/0/0
1	KPI	F	184	1	-	0/8/14/16	0/0/0/0
1	KPI	G	184	1	-	0/8/14/16	0/0/0/0
1	KPI	H	184	1	-	0/8/14/16	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	184	KPI	CX2-CX1	-5.42	1.42	1.52
1	A	184	KPI	CX2-CX1	-4.94	1.43	1.52
1	E	184	KPI	CX2-CX1	-4.77	1.44	1.52
1	B	184	KPI	CX2-CX1	-4.67	1.44	1.52
1	F	184	KPI	CX2-CX1	-4.44	1.44	1.52
1	G	184	KPI	CX2-CX1	-4.35	1.44	1.52
1	H	184	KPI	CX1-NZ	-4.10	1.22	1.29
1	F	184	KPI	CB-CA	-3.84	1.50	1.53
1	H	184	KPI	CX2-CX1	-3.82	1.45	1.52
1	D	184	KPI	CX2-CX1	-3.68	1.45	1.52
1	C	184	KPI	CX1-NZ	-3.25	1.23	1.29
1	B	184	KPI	CB-CA	-3.16	1.50	1.53
1	A	184	KPI	CB-CA	-3.07	1.50	1.53
1	B	184	KPI	CX1-NZ	-2.99	1.24	1.29
1	F	184	KPI	CX1-NZ	-2.97	1.24	1.29
1	C	184	KPI	CE-NZ	-2.64	1.40	1.47
1	H	184	KPI	CE-NZ	-2.33	1.41	1.47
1	C	184	KPI	CB-CA	-2.28	1.51	1.53
1	A	184	KPI	CX1-NZ	-2.26	1.25	1.29
1	E	184	KPI	CX1-NZ	-2.20	1.25	1.29
1	G	184	KPI	CB-CA	-2.15	1.51	1.53
1	G	184	KPI	CX1-NZ	-2.14	1.25	1.29
1	D	184	KPI	CE-NZ	-2.06	1.42	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	184	KPI	CD-CE-NZ	-2.78	106.20	110.73
1	A	184	KPI	O-C-CA	-2.49	119.01	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	184	KPI	O-C-CA	-2.35	119.36	125.49
1	F	184	KPI	O-C-CA	-2.33	119.41	125.49
1	H	184	KPI	CD-CE-NZ	-2.32	106.95	110.73
1	G	184	KPI	O-C-CA	-2.04	120.19	125.49
1	E	184	KPI	CE-NZ-CX1	2.23	128.51	122.10
1	A	184	KPI	CE-NZ-CX1	2.23	128.52	122.10
1	G	184	KPI	CE-NZ-CX1	2.82	130.21	122.10
1	D	184	KPI	CE-NZ-CX1	3.14	131.14	122.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	184	KPI	1	0
1	G	184	KPI	1	0
1	H	184	KPI	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands 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	$\#\|Z\| > 2$
2	LYS	A	401	-	6,9,9	0.31	0	4,10,10	0.82	0
2	LYS	B	401	-	6,9,9	0.33	0	4,10,10	0.58	0
2	LYS	C	401	-	6,9,9	0.24	0	4,10,10	0.93	0
2	LYS	D	401	-	6,9,9	0.41	0	4,10,10	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LYS	E	401	-	6,9,9	0.43	0	4,10,10	0.73	0
2	LYS	F	401	-	6,9,9	0.30	0	4,10,10	0.63	0
2	LYS	G	401	-	6,9,9	0.29	0	4,10,10	0.53	0
2	LYS	H	401	-	6,9,9	0.39	0	4,10,10	0.53	0

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	LYS	A	401	-	-	0/5/9/9	0/0/0/0
2	LYS	B	401	-	-	0/5/9/9	0/0/0/0
2	LYS	C	401	-	-	0/5/9/9	0/0/0/0
2	LYS	D	401	-	-	0/5/9/9	0/0/0/0
2	LYS	E	401	-	-	0/5/9/9	0/0/0/0
2	LYS	F	401	-	-	0/5/9/9	0/0/0/0
2	LYS	G	401	-	-	0/5/9/9	0/0/0/0
2	LYS	H	401	-	-	0/5/9/9	0/0/0/0

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.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	LYS	3	0
2	C	401	LYS	2	0
2	E	401	LYS	3	0
2	F	401	LYS	1	0

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

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%)	-0.45	1 (0%) 94 94	13, 23, 35, 44	0
1	B	306/346 (88%)	-0.51	0 100 100	13, 20, 30, 41	0
1	C	307/346 (88%)	-0.55	1 (0%) 94 94	11, 17, 28, 38	0
1	D	307/346 (88%)	-0.53	0 100 100	12, 19, 29, 39	0
1	E	306/346 (88%)	-0.36	0 100 100	16, 25, 38, 43	0
1	F	319/346 (92%)	-0.29	0 100 100	15, 23, 41, 55	0
1	G	306/346 (88%)	-0.18	3 (0%) 84 83	15, 27, 43, 50	0
1	H	307/346 (88%)	-0.32	1 (0%) 94 94	14, 26, 41, 47	0
All	All	2464/2768 (89%)	-0.40	6 (0%) 95 95	11, 22, 39, 55	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	ARG	3.1
1	C	20	THR	3.0
1	H	20	THR	2.3
1	G	250	ILE	2.1
1	G	211[A]	HIS	2.0
1	G	239	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
1	KPI	F	184	14/15	0.97	0.11	-	16,20,26,26	0
1	KPI	D	184	14/15	0.95	0.13	-	16,18,23,23	0
1	KPI	E	184	14/15	0.97	0.10	-	19,21,25,27	0
1	KPI	C	184	14/15	0.98	0.11	-	10,11,17,20	0
1	KPI	A	184	14/15	0.96	0.14	-	20,21,22,23	0
1	KPI	G	184	14/15	0.96	0.13	-	21,23,26,28	0
1	KPI	H	184	14/15	0.96	0.13	-	24,24,29,30	0
1	KPI	B	184	14/15	0.97	0.12	-	18,19,21,22	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
2	LYS	B	401	10/10	0.96	0.21	3.91	17,20,21,21	0
2	LYS	H	401	10/10	0.94	0.17	3.59	16,19,20,20	0
2	LYS	A	401	10/10	0.96	0.19	3.29	16,17,17,17	0
2	LYS	F	401	10/10	0.93	0.18	2.53	19,21,21,21	0
2	LYS	C	401	10/10	0.97	0.17	2.28	11,15,15,16	0
2	LYS	G	401	10/10	0.97	0.16	1.93	17,18,18,19	0
2	LYS	D	401	10/10	0.97	0.15	1.77	17,19,19,19	0
2	LYS	E	401	10/10	0.96	0.17	1.61	21,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.