wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:00 PM GMT

PDB ID	:	1RFU
Title	:	Crystal structure of pyridoxal kinase complexed with ADP and PLP
Authors	:	Liang, D.-C.; Jiang, T.; Li, M.-H.
Deposited on	:	2003-11-10
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

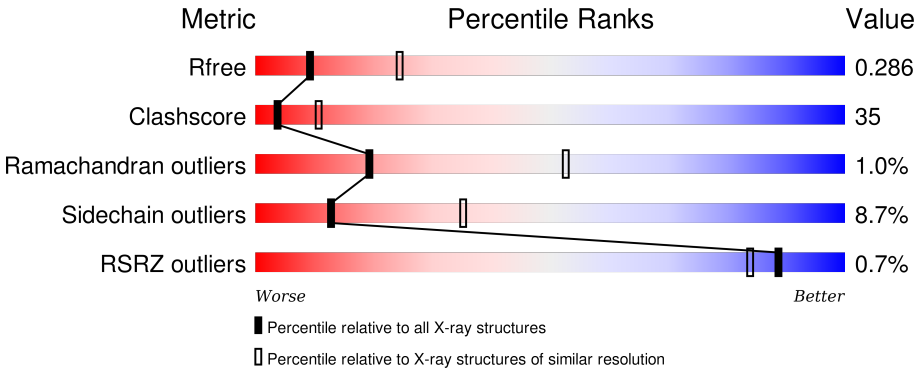
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	312	46% 49% 5%
1	B	312	39% 54% 7%
1	C	312	% 41% 52% 7%
1	D	312	2% 40% 54% 6%
1	E	312	42% 53% 5%

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Mol	Chain	Length	Quality of chain
1	F	312	44% 51%
1	G	312	42% 53% 5%
1	H	312	% 37% 58% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20123 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 pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	B	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	C	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	D	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	E	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	F	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	G	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	H	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

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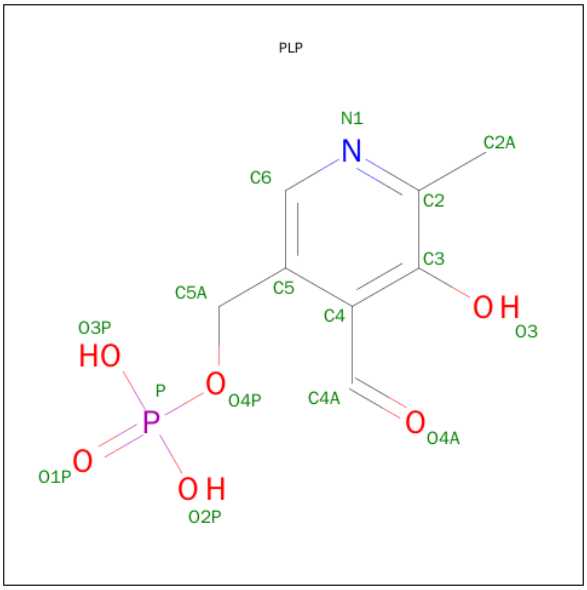
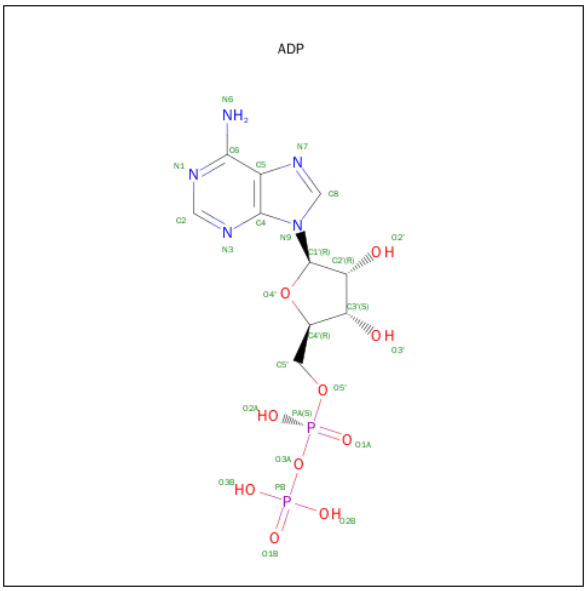
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 15 8 1 5 1	0	0
3	B	1	Total C N O P 15 8 1 5 1	0	0
3	C	1	Total C N O P 15 8 1 5 1	0	0
3	D	1	Total C N O P 15 8 1 5 1	0	0
3	E	1	Total C N O P 15 8 1 5 1	0	0
3	F	1	Total C N O P 15 8 1 5 1	0	0
3	G	1	Total C N O P 15 8 1 5 1	0	0
3	H	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total	O	0	0
			73	73		
5	B	54	Total	O	0	0
			54	54		
5	C	20	Total	O	0	0
			20	20		
5	D	9	Total	O	0	0
			9	9		

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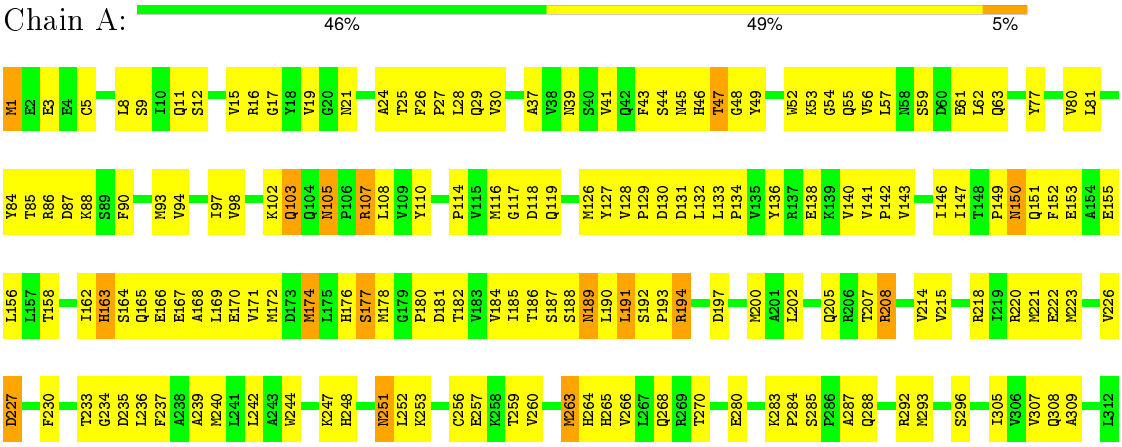
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	41	Total O 41 41	0	0
5	F	37	Total O 37 37	0	0
5	G	21	Total O 21 21	0	0
5	H	12	Total O 12 12	0	0

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 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.

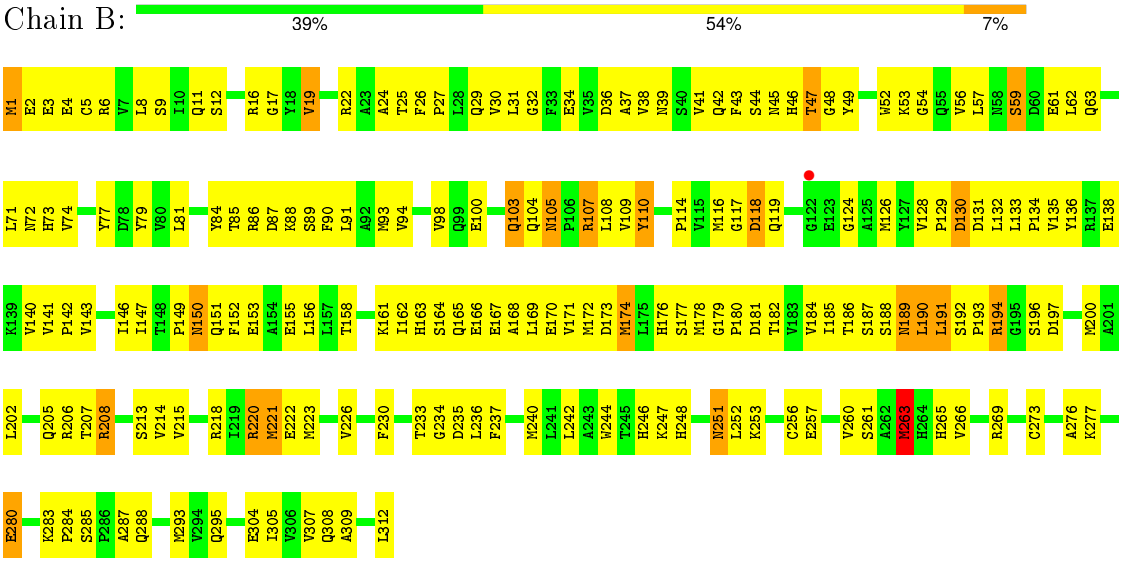
- Molecule 1: pyridoxal kinase

Chain A:



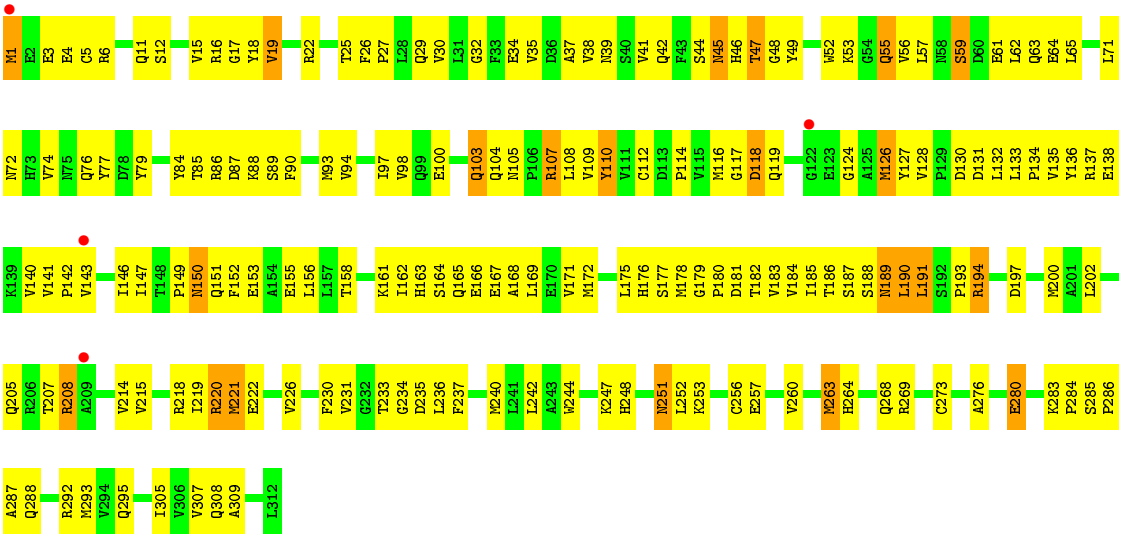
- Molecule 1: pyridoxal kinase

Chain B:



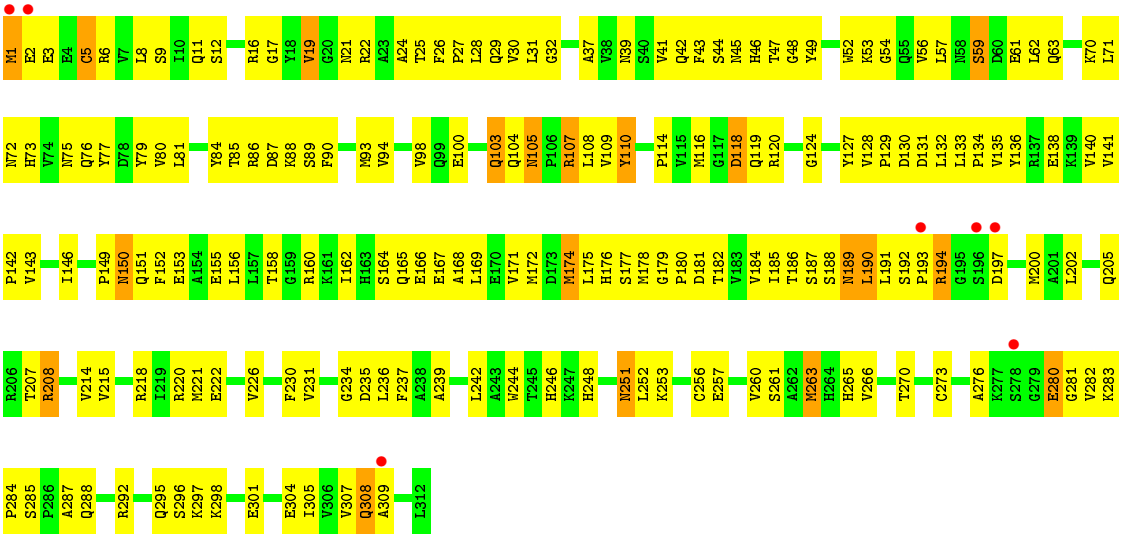
- Molecule 1: pyridoxal kinase

Chain C:



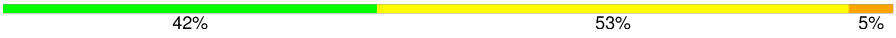
- Molecule 1: pyridoxal kinase

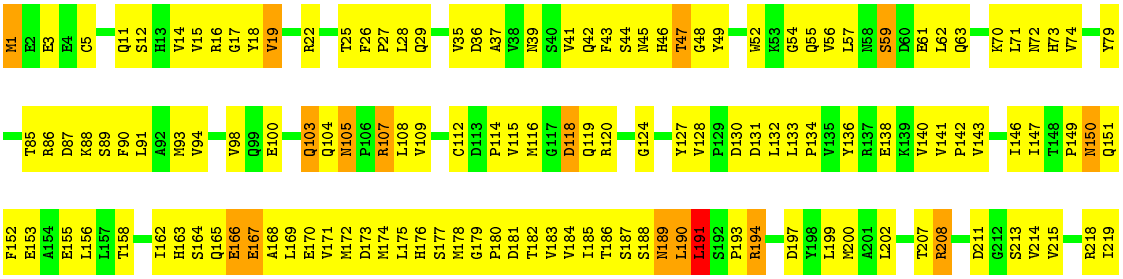
Chain D:

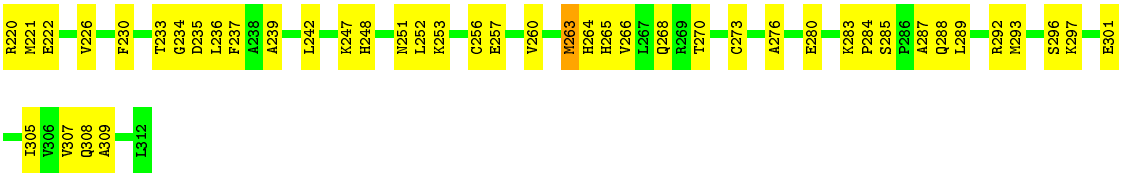


- Molecule 1: pyridoxal kinase

Chain E:

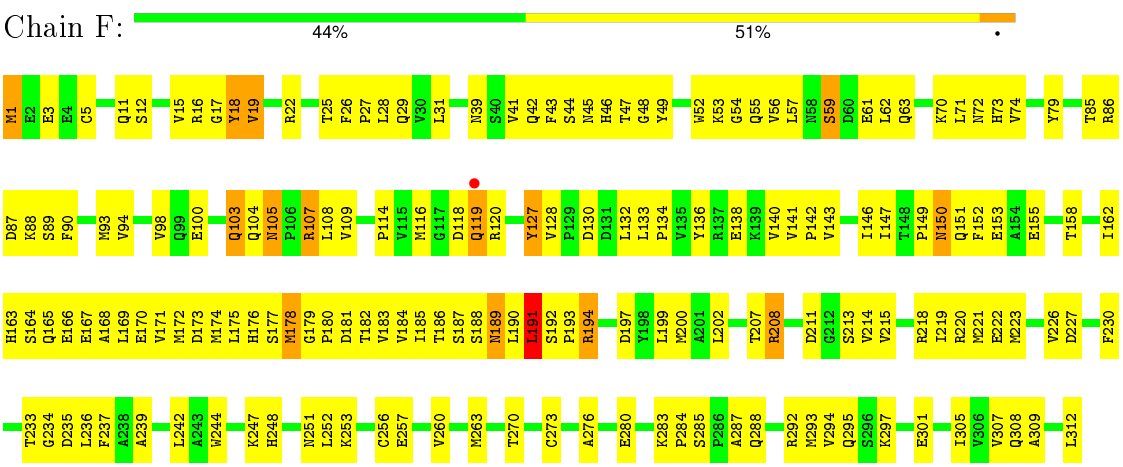






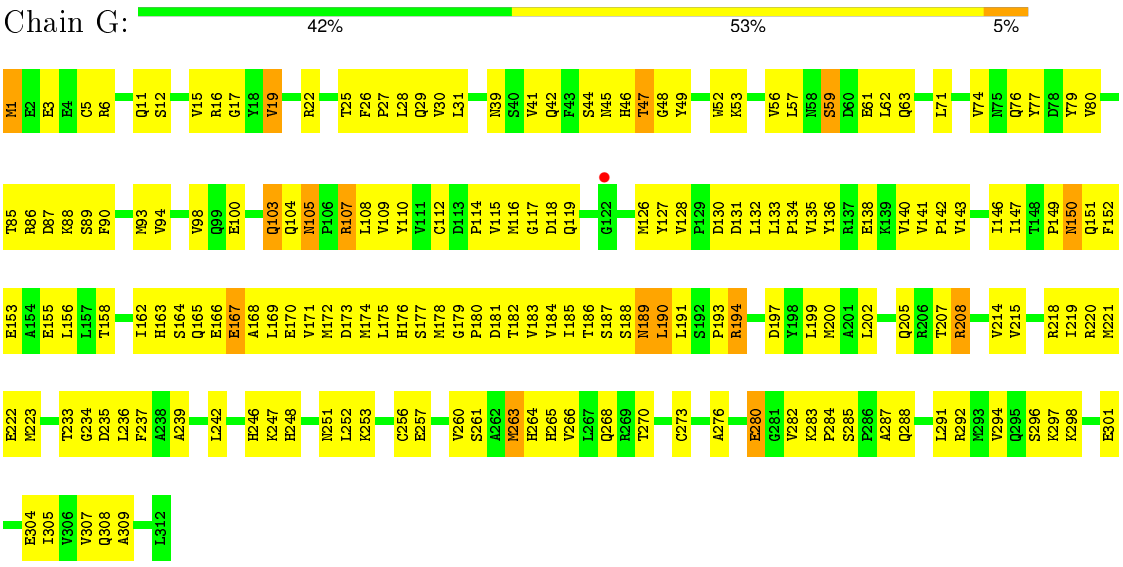
- Molecule 1: pyridoxal kinase

Chain F:



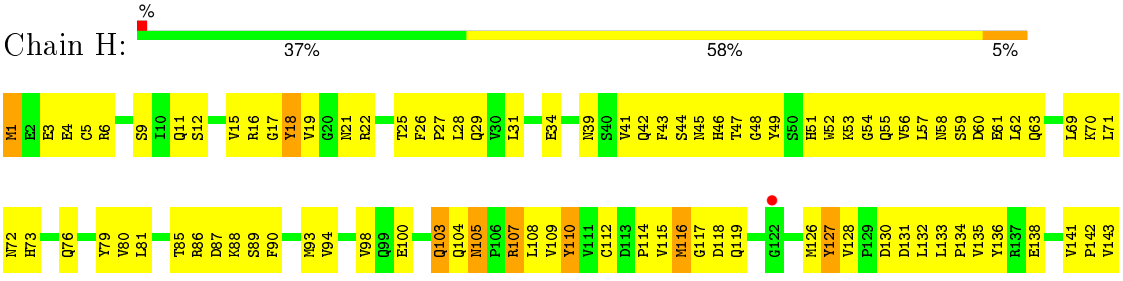
- Molecule 1: pyridoxal kinase

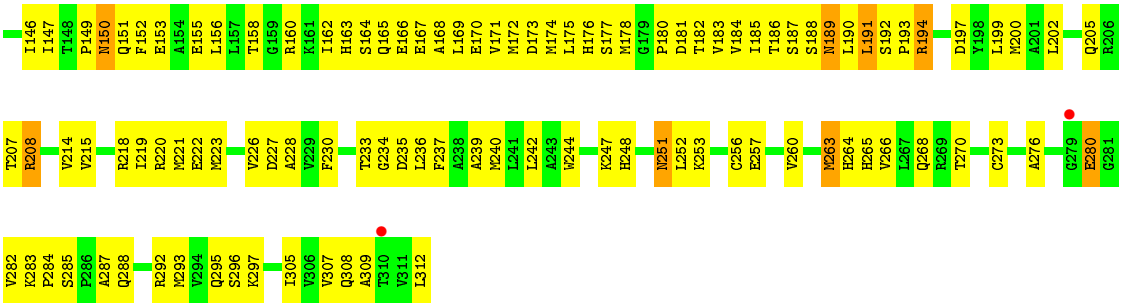
Chain G:



- Molecule 1: pyridoxal kinase

Chain H:




I146
I147
T148
P149
N150
Q151
F152
E153
A154
E155
L156
L157
T158
G159
R160
K161
I162
H163
S164
Q165
E166
E167
A168
L169
E170
V171
M172
D173
M174
L175
H176
S177
M178
G179
P180
D181
T182
V183
V184
I185
T186
S187
S188
N189
L190
L191
S192
P193
R194
D197
Y198
L199
M200
A201
L202
Q205
R206
T207
R208
V214
V215
R218
I219
R220
M221
E222
M223
V226
D227
A228
V229
F230
T233
G234
D235
L236
F237
A238
A239
M240
I241
L242
A243
W244
K247
H248
N251
L252
K253
C256
E257
V260
M263
H264
H265
V266
L267
Q268
R269
T270
C273
A276
G279
E280
G281
V282
K283
P284
S285
P286
A287
Q288
R292
M293
V294
Q295
S296
K297
I305
V306
V307
Q308
A309
T310
V311
L312

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	109.09Å 109.09Å 284.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.5 (20.00-2.80) 56.7 (19.94-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.281 0.238 , 0.286	Depositor DCC
R_{free} test set	2258 reflections (5.17%)	DCC
Wilson B-factor (Å^2)	56.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 28.8	EDS
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Outliers	4 of 75513 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20123	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.15 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.5074e-08.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, PLP

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	0/2484	0.74	1/3367 (0.0%)
1	B	0.54	0/2484	0.79	5/3367 (0.1%)
1	C	0.47	0/2484	0.74	3/3367 (0.1%)
1	D	0.45	0/2484	0.71	1/3367 (0.0%)
1	E	0.54	0/2484	0.76	1/3367 (0.0%)
1	F	0.55	0/2484	0.76	1/3367 (0.0%)
1	G	0.45	0/2484	0.71	1/3367 (0.0%)
1	H	0.44	0/2484	0.71	1/3367 (0.0%)
All	All	0.50	0/19872	0.74	14/26936 (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	E	0	1
1	F	0	2
1	H	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	220	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	C	220	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	F	178	MET	CG-SD-CE	6.12	110.00	100.20
1	B	221	MET	CG-SD-CE	6.12	109.99	100.20
1	C	126	MET	CG-SD-CE	6.12	109.99	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	18	TYR	Sidechain
1	F	127	TYR	Sidechain
1	F	18	TYR	Sidechain
1	H	127	TYR	Sidechain
1	H	18	TYR	Sidechain

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	2439	0	2442	176	0
1	B	2439	0	2442	200	0
1	C	2439	0	2442	198	0
1	D	2439	0	2442	182	0
1	E	2439	0	2442	172	0
1	F	2439	0	2442	180	0
1	G	2439	0	2442	163	0
1	H	2439	0	2442	209	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	15	0	7	2	0
3	B	15	0	6	1	0
3	C	15	0	6	1	0
3	D	15	0	7	1	0
3	E	15	0	6	1	0
3	F	15	0	7	2	0
3	G	15	0	6	1	0
3	H	15	0	7	1	0
4	A	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	12	2	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	2	0
4	G	27	0	12	1	0
4	H	27	0	12	2	0
5	A	73	0	0	4	0
5	B	54	0	0	5	0
5	C	20	0	0	2	0
5	D	9	0	0	2	0
5	E	41	0	0	3	0
5	F	37	0	0	5	0
5	G	21	0	0	2	0
5	H	12	0	0	3	0
All	All	20123	0	19684	1390	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 35.

The worst 5 of 1390 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:129:PRO:HG3	1:B:191:LEU:HB2	1.22	1.19
1:B:39:ASN:H	1:F:42:GLN:HE22	1.07	0.95
1:A:191:LEU:HB2	1:D:129:PRO:HG3	1.50	0.93
1:H:208:ARG:HH11	1:H:208:ARG:HG3	1.31	0.93
1:A:39:ASN:H	1:E:42:GLN:HE22	1.05	0.92

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	310/312 (99%)	279 (90%)	29 (9%)	2 (1%)	30	65
1	B	310/312 (99%)	276 (89%)	30 (10%)	4 (1%)	15	44
1	C	310/312 (99%)	272 (88%)	34 (11%)	4 (1%)	15	44
1	D	310/312 (99%)	274 (88%)	34 (11%)	2 (1%)	30	65
1	E	310/312 (99%)	274 (88%)	31 (10%)	5 (2%)	12	38
1	F	310/312 (99%)	274 (88%)	34 (11%)	2 (1%)	30	65
1	G	310/312 (99%)	275 (89%)	32 (10%)	3 (1%)	19	52
1	H	310/312 (99%)	271 (87%)	36 (12%)	3 (1%)	19	52
All	All	2480/2496 (99%)	2195 (88%)	260 (10%)	25 (1%)	19	52

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	D	191	LEU
1	H	191	LEU
1	B	191	LEU
1	C	191	LEU

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	273/273 (100%)	249 (91%)	24 (9%)	12	35
1	B	273/273 (100%)	249 (91%)	24 (9%)	12	35
1	C	273/273 (100%)	249 (91%)	24 (9%)	12	35
1	D	273/273 (100%)	249 (91%)	24 (9%)	12	35
1	E	273/273 (100%)	249 (91%)	24 (9%)	12	35
1	F	273/273 (100%)	251 (92%)	22 (8%)	15	39
1	G	273/273 (100%)	250 (92%)	23 (8%)	14	37
1	H	273/273 (100%)	248 (91%)	25 (9%)	11	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2184/2184 (100%)	1994 (91%)	190 (9%)	13 35

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	130	ASP
1	E	127	TYR
1	H	127	TYR
1	D	189	ASN
1	E	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	105	ASN
1	E	103	GLN
1	H	103	GLN
1	D	119	GLN
1	E	13	HIS

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)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PLP	A	401	2	15,15,16	2.02	4 (26%)	21,22,23	2.58	7 (33%)
4	ADP	A	402	2	22,29,29	1.21	2 (9%)	27,45,45	2.80	5 (18%)
3	PLP	B	1401	2	15,15,16	1.61	2 (13%)	21,22,23	2.38	7 (33%)
4	ADP	B	1402	2	22,29,29	1.80	7 (31%)	27,45,45	2.72	4 (14%)
3	PLP	C	2401	2	15,15,16	1.67	3 (20%)	21,22,23	2.27	7 (33%)
4	ADP	C	2402	2	22,29,29	1.80	6 (27%)	27,45,45	2.73	3 (11%)
3	PLP	D	3401	2	15,15,16	1.56	2 (13%)	21,22,23	2.46	5 (23%)
4	ADP	D	3402	2	22,29,29	1.73	6 (27%)	27,45,45	2.77	4 (14%)
3	PLP	E	4401	2	15,15,16	1.67	2 (13%)	21,22,23	2.44	6 (28%)
4	ADP	E	4402	2	22,29,29	1.72	6 (27%)	27,45,45	2.63	4 (14%)
3	PLP	F	5401	2	15,15,16	1.67	2 (13%)	21,22,23	2.38	5 (23%)
4	ADP	F	5402	2	22,29,29	1.80	7 (31%)	27,45,45	2.72	4 (14%)
3	PLP	G	6401	2	15,15,16	1.78	2 (13%)	21,22,23	2.34	7 (33%)
4	ADP	G	6402	2	22,29,29	1.75	6 (27%)	27,45,45	2.65	4 (14%)
3	PLP	H	7401	2	15,15,16	1.47	3 (20%)	21,22,23	2.27	6 (28%)
4	ADP	H	7402	2	22,29,29	1.74	6 (27%)	27,45,45	2.72	4 (14%)

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
3	PLP	A	401	2	-	0/6/6/8	0/1/1/1
4	ADP	A	402	2	-	0/12/32/32	0/3/3/3
3	PLP	B	1401	2	-	0/6/6/8	0/1/1/1
4	ADP	B	1402	2	-	0/12/32/32	0/3/3/3
3	PLP	C	2401	2	-	0/6/6/8	0/1/1/1
4	ADP	C	2402	2	-	0/12/32/32	0/3/3/3
3	PLP	D	3401	2	-	0/6/6/8	0/1/1/1
4	ADP	D	3402	2	-	0/12/32/32	0/3/3/3
3	PLP	E	4401	2	-	0/6/6/8	0/1/1/1
4	ADP	E	4402	2	-	0/12/32/32	0/3/3/3
3	PLP	F	5401	2	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	F	5402	2	-	0/12/32/32	0/3/3/3
3	PLP	G	6401	2	-	0/6/6/8	0/1/1/1
4	ADP	G	6402	2	-	0/12/32/32	0/3/3/3
3	PLP	H	7401	2	-	0/6/6/8	0/1/1/1
4	ADP	H	7402	2	-	0/12/32/32	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4401	PLP	C3-C2	-4.37	1.37	1.40
3	G	6401	PLP	C3-C2	-3.69	1.38	1.40
4	G	6402	ADP	PB-O3B	-3.49	1.42	1.54
4	B	1402	ADP	PB-O3B	-3.46	1.42	1.54
4	H	7402	ADP	PB-O3B	-3.41	1.42	1.54

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3402	ADP	N3-C2-N1	-13.17	118.81	128.89
4	A	402	ADP	N3-C2-N1	-13.04	118.91	128.89
4	C	2402	ADP	N3-C2-N1	-12.89	119.02	128.89
4	H	7402	ADP	N3-C2-N1	-12.86	119.05	128.89
4	B	1402	ADP	N3-C2-N1	-12.85	119.06	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	PLP	2	0
4	A	402	ADP	3	0
3	B	1401	PLP	1	0
4	B	1402	ADP	2	0
3	C	2401	PLP	1	0
4	C	2402	ADP	1	0
3	D	3401	PLP	1	0
4	D	3402	ADP	1	0
3	E	4401	PLP	1	0
4	E	4402	ADP	1	0
3	F	5401	PLP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	5402	ADP	2	0
3	G	6401	PLP	1	0
4	G	6402	ADP	1	0
3	H	7401	PLP	1	0
4	H	7402	ADP	2	0

5.7 Other polymers

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	312/312 (100%)	-0.14	0 100 100	13, 35, 55, 69	0
1	B	312/312 (100%)	-0.21	1 (0%) 94 92	15, 32, 49, 66	0
1	C	312/312 (100%)	-0.18	4 (1%) 79 71	19, 36, 50, 65	0
1	D	312/312 (100%)	-0.12	7 (2%) 65 54	23, 40, 54, 65	0
1	E	312/312 (100%)	-0.25	0 100 100	9, 31, 47, 61	0
1	F	312/312 (100%)	-0.19	1 (0%) 94 92	7, 32, 49, 65	0
1	G	312/312 (100%)	-0.23	1 (0%) 94 92	20, 37, 53, 63	0
1	H	312/312 (100%)	-0.15	3 (0%) 84 77	24, 39, 52, 61	0
All	All	2496/2496 (100%)	-0.18	17 (0%) 89 84	7, 35, 52, 69	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	SER	4.6
1	C	209	ALA	4.2
1	H	310	THR	3.6
1	D	1	MET	3.2
1	D	309	ALA	2.9

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
3	PLP	C	2401	15/16	0.96	0.20	1.11	44,45,55,55	0
3	PLP	G	6401	15/16	0.97	0.17	0.12	29,32,41,42	0
3	PLP	E	4401	15/16	0.98	0.17	0.06	11,13,25,26	0
4	ADP	E	4402	27/27	0.96	0.18	-0.06	17,27,32,35	0
4	ADP	D	3402	27/27	0.96	0.17	-0.13	32,42,50,51	0
3	PLP	F	5401	15/16	0.97	0.17	-0.20	14,17,29,31	0
2	ZN	B	1403	1/1	0.96	0.17	-0.24	54,54,54,54	0
4	ADP	B	1402	27/27	0.98	0.17	-0.29	17,25,32,32	0
2	ZN	F	5403	1/1	0.96	0.15	-0.39	52,52,52,52	0
3	PLP	B	1401	15/16	0.97	0.17	-0.42	19,24,39,40	0
3	PLP	D	3401	15/16	0.95	0.16	-0.45	40,42,55,56	0
3	PLP	H	7401	15/16	0.97	0.16	-0.45	25,26,32,33	0
4	ADP	F	5402	27/27	0.97	0.16	-0.47	26,31,36,37	0
4	ADP	A	402	27/27	0.96	0.17	-0.63	19,26,32,33	0
4	ADP	C	2402	27/27	0.97	0.16	-0.66	30,33,37,39	0
4	ADP	G	6402	27/27	0.98	0.15	-0.75	30,34,38,39	0
3	PLP	A	401	15/16	0.95	0.16	-0.85	17,21,44,44	0
4	ADP	H	7402	27/27	0.96	0.15	-0.93	41,43,53,54	0
2	ZN	E	4403	1/1	0.94	0.14	-1.02	59,59,59,59	0
2	ZN	A	403	1/1	0.97	0.14	-1.57	48,48,48,48	0
2	ZN	H	7403	1/1	0.97	0.12	-1.60	59,59,59,59	0
2	ZN	G	6403	1/1	0.96	0.12	-1.96	85,85,85,85	0
2	ZN	D	3403	1/1	0.97	0.09	-2.12	45,45,45,45	0
2	ZN	C	2403	1/1	0.97	0.10	-2.74	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.