



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:38 PM GMT

PDB ID : 2NXI
Title : Structural and mechanistic changes along an engineered path from metallo to non-metallo KDO8P synthase.
Authors : Kona, F.; Xu, X.; Martin, P.; Kuzmic, P.; Gatti, D.L.
Deposited on : 2006-11-17
Resolution : 2.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

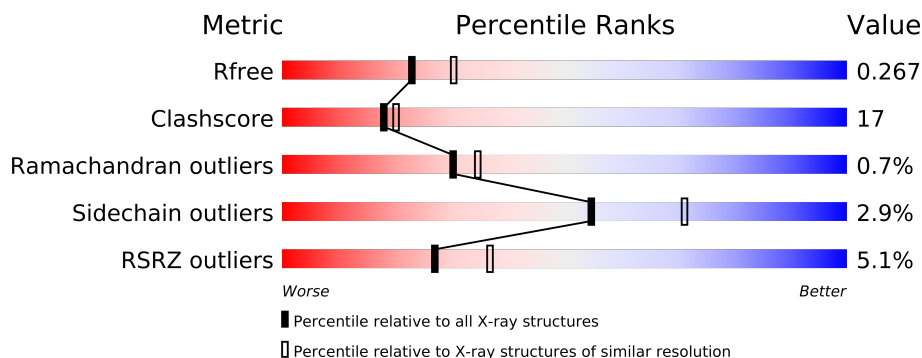
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	263	
1	B	263	
1	C	263	
1	D	263	
1	E	263	
1	F	263	
1	G	263	
1	H	263	
1	I	263	
1	J	263	
1	K	263	
1	L	263	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25761 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2-dehydro-3-deoxyphosphooctonatealdolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2029	1310	339	374	6			
1	B	258	Total	C	N	O	S	0	0	0
			2033	1312	340	375	6			
1	C	257	Total	C	N	O	S	0	0	0
			2025	1306	339	374	6			
1	D	256	Total	C	N	O	S	0	0	0
			2021	1304	338	373	6			
1	E	256	Total	C	N	O	S	0	0	0
			2021	1304	338	373	6			
1	F	255	Total	C	N	O	S	0	0	0
			2017	1302	337	372	6			
1	G	259	Total	C	N	O	S	0	0	0
			2041	1316	341	378	6			
1	H	256	Total	C	N	O	S	0	0	0
			2021	1304	338	373	6			
1	I	262	Total	C	N	O	S	0	0	0
			2060	1327	345	382	6			
1	J	262	Total	C	N	O	S	0	0	0
			2060	1327	345	382	6			
1	K	257	Total	C	N	O	S	0	0	0
			2029	1310	339	374	6			
1	L	256	Total	C	N	O	S	0	0	0
			2021	1304	338	373	6			

There are 24 discrepancies between the modelled and reference sequences:

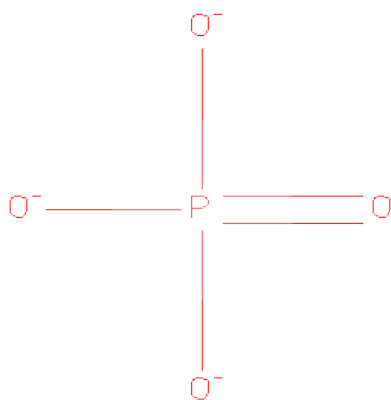
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	PRO	engineered	UNP O66496
A	11	ASN	CYS	engineered	UNP O66496
B	10	MET	PRO	engineered	UNP O66496
B	11	ASN	CYS	engineered	UNP O66496
C	10	MET	PRO	engineered	UNP O66496

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Chain	Residue	Modelled	Actual	Comment	Reference
C	11	ASN	CYS	engineered	UNP O66496
D	10	MET	PRO	engineered	UNP O66496
D	11	ASN	CYS	engineered	UNP O66496
E	10	MET	PRO	engineered	UNP O66496
E	11	ASN	CYS	engineered	UNP O66496
F	10	MET	PRO	engineered	UNP O66496
F	11	ASN	CYS	engineered	UNP O66496
G	10	MET	PRO	engineered	UNP O66496
G	11	ASN	CYS	engineered	UNP O66496
H	10	MET	PRO	engineered	UNP O66496
H	11	ASN	CYS	engineered	UNP O66496
I	10	MET	PRO	engineered	UNP O66496
I	11	ASN	CYS	engineered	UNP O66496
J	10	MET	PRO	engineered	UNP O66496
J	11	ASN	CYS	engineered	UNP O66496
K	10	MET	PRO	engineered	UNP O66496
K	11	ASN	CYS	engineered	UNP O66496
L	10	MET	PRO	engineered	UNP O66496
L	11	ASN	CYS	engineered	UNP O66496

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



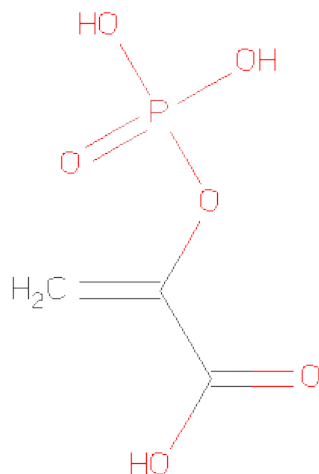
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	O	P	0	0
			10	3	6	1		
3	F	1	Total	C	O	P	0	0
			10	3	6	1		
3	G	1	Total	C	O	P	0	0
			10	3	6	1		
3	G	1	Total	C	O	P	0	0
			10	3	6	1		
3	H	1	Total	C	O	P	0	0
			10	3	6	1		
3	H	1	Total	C	O	P	0	0
			10	3	6	1		
3	I	1	Total	C	O	P	0	0
			10	3	6	1		
3	I	1	Total	C	O	P	0	0
			10	3	6	1		
3	J	1	Total	C	O	P	0	0
			10	3	6	1		
3	K	1	Total	C	O	P	0	0
			10	3	6	1		
3	L	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total	O	0	0
			147	147		
4	B	145	Total	O	0	0
			145	145		
4	C	93	Total	O	0	0
			93	93		
4	D	60	Total	O	0	0
			60	60		
4	E	52	Total	O	0	0
			52	52		
4	F	49	Total	O	0	0
			49	49		
4	G	125	Total	O	0	0
			125	125		
4	H	132	Total	O	0	0
			132	132		

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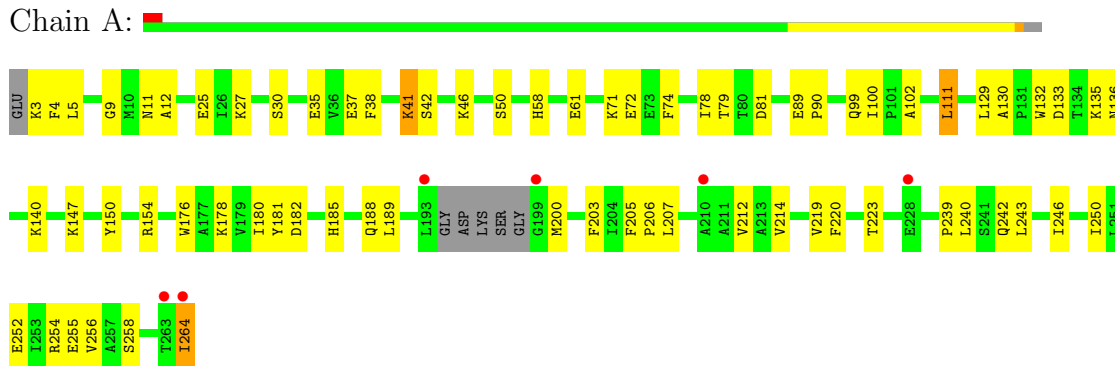
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	136	Total 136	O 136	0	0
4	J	136	Total 136	O 136	0	0
4	K	37	Total 37	O 37	0	0
4	L	66	Total 66	O 66	0	0

3 Residue-property plots

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

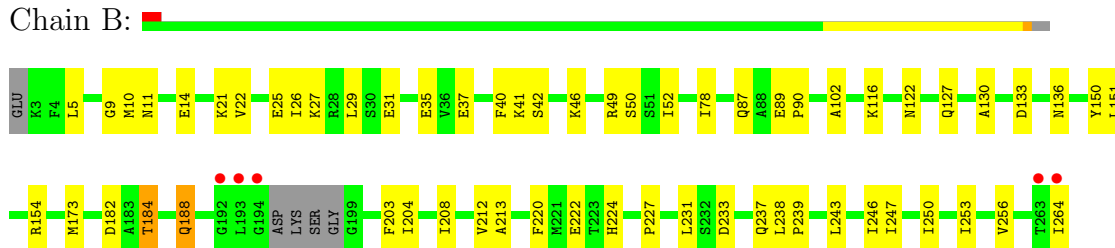
- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

Chain A:



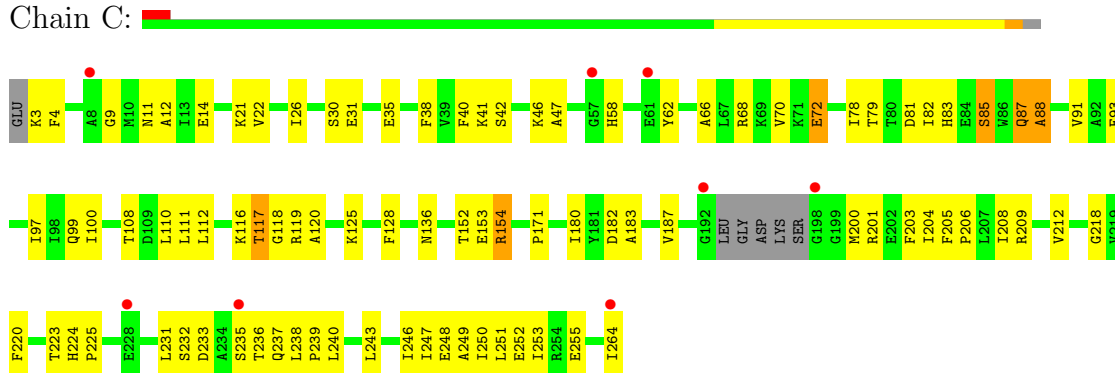
- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

Chain B:



- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

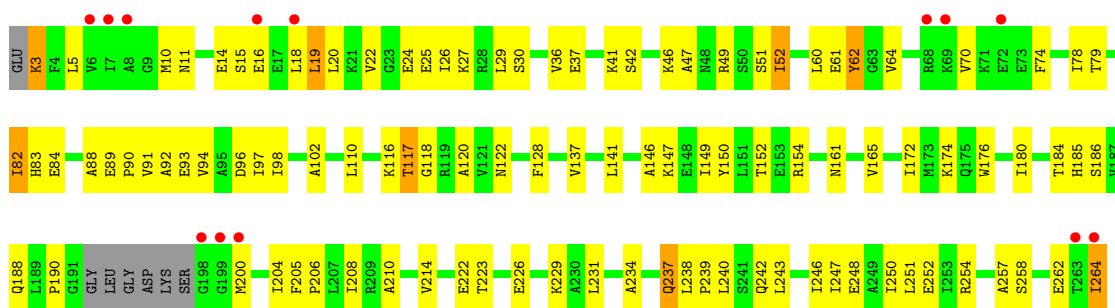
Chain C:



- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

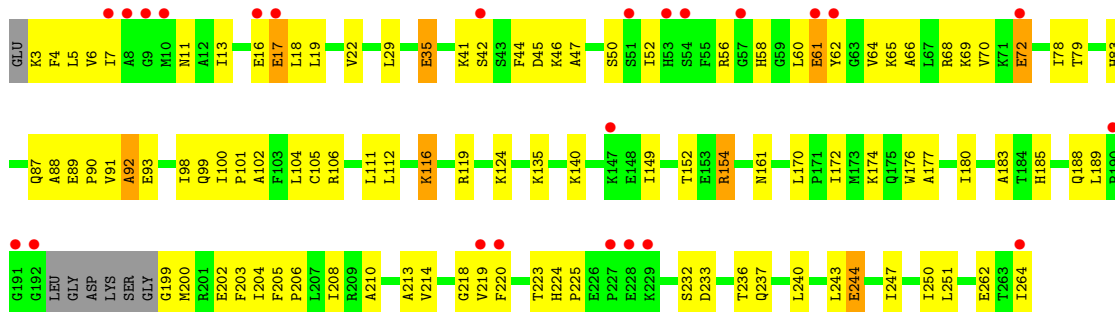
Chain D:





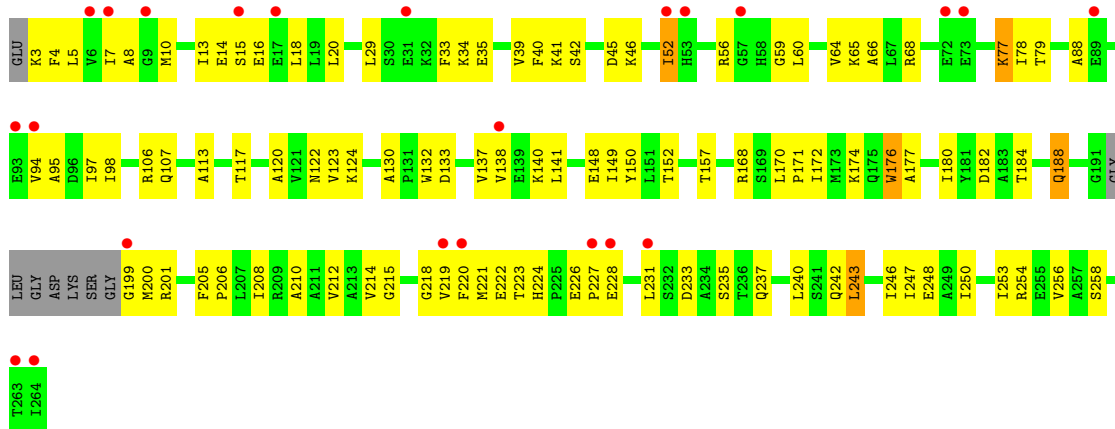
- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

Chain E:



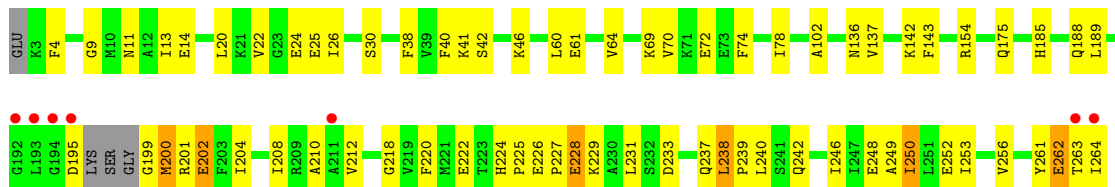
- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

Chain F:



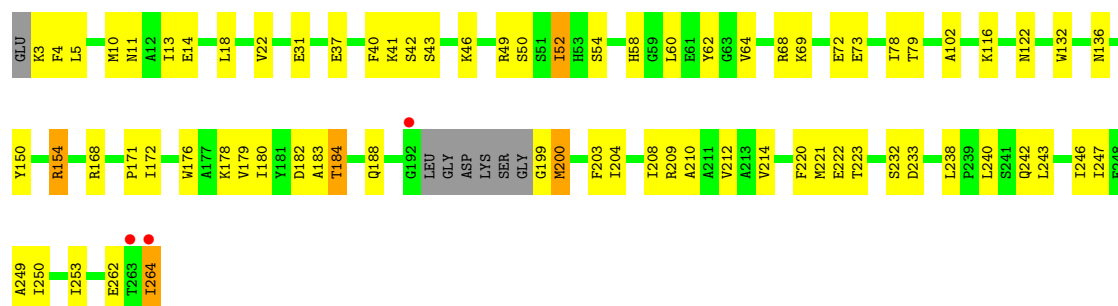
- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

Chain G:



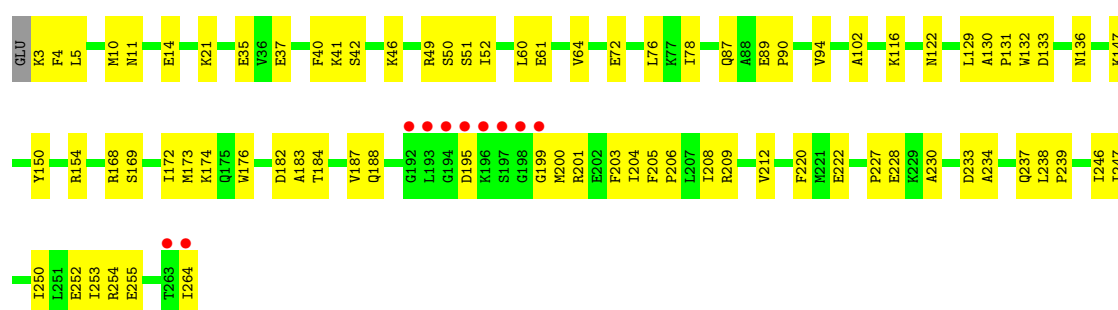
- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

Chain H:



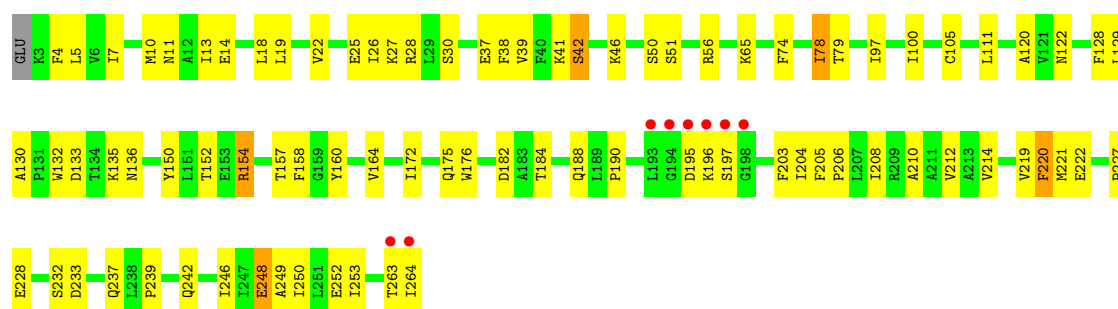
- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

Chain I:



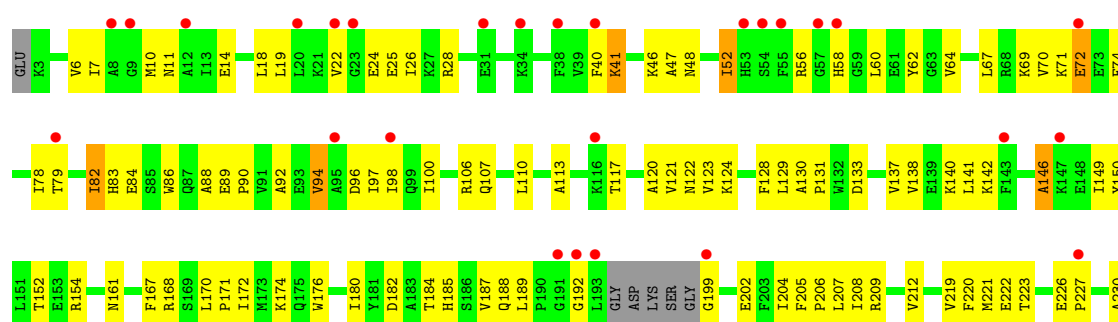
- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

Chain J:



- Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

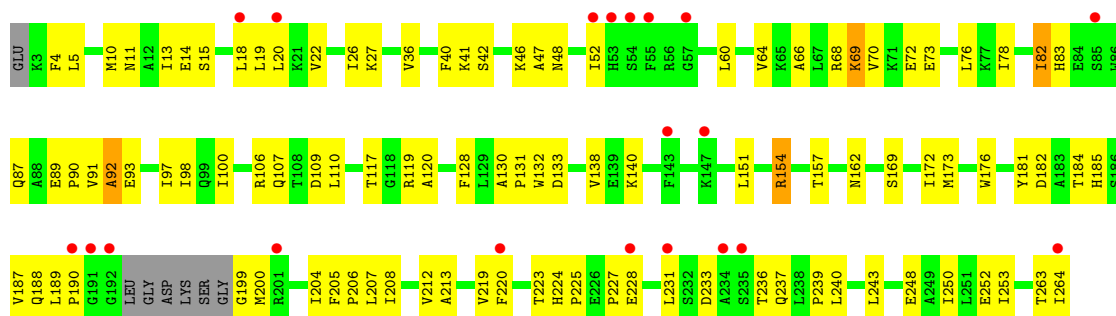
Chain K:





● Molecule 1: 2-dehydro-3-deoxyphosphooctonatealdolase

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.88Å 197.47Å 124.87Å 90.00° 93.84° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 25.24 – 2.22	Depositor EDS
% Data completeness (in resolution range)	76.3 (25.00-2.30) 69.7 (25.24-2.22)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.22Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.207 , 0.267 0.207 , 0.267	Depositor DCC
R_{free} test set	6233 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	6 of 125801 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25761	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 21.62 % 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 6.7524e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PEP

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	0.45	1/2068 (0.0%)	0.65	0/2786
1	B	0.41	0/2072	0.62	0/2791
1	C	0.39	1/2064 (0.0%)	0.58	0/2780
1	D	0.34	0/2060	0.59	0/2775
1	E	0.37	1/2060 (0.0%)	0.53	0/2775
1	F	0.33	0/2056	0.55	0/2770
1	G	0.43	1/2080 (0.0%)	0.62	0/2802
1	H	0.40	0/2060	0.64	0/2775
1	I	0.42	1/2100 (0.0%)	0.62	0/2829
1	J	0.40	0/2100	0.62	0/2829
1	K	0.35	1/2068 (0.0%)	0.53	0/2786
1	L	0.34	0/2060	0.56	0/2775
All	All	0.39	6/24848 (0.0%)	0.59	0/33473

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	72	GLU	CD-OE2	7.77	1.34	1.25
1	A	72	GLU	CD-OE2	7.76	1.34	1.25
1	E	72	GLU	CD-OE2	7.32	1.33	1.25
1	K	72	GLU	CD-OE2	7.22	1.33	1.25
1	I	72	GLU	CD-OE2	7.22	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2029	0	2069	62	0
1	B	2033	0	2072	52	0
1	C	2025	0	2061	75	0
1	D	2021	0	2058	86	0
1	E	2021	0	2058	80	0
1	F	2017	0	2055	89	0
1	G	2041	0	2076	55	0
1	H	2021	0	2058	68	0
1	I	2060	0	2098	64	0
1	J	2060	0	2098	64	0
1	K	2029	0	2069	112	0
1	L	2021	0	2058	82	0
2	A	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	J	5	0	0	1	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	10	0	2	0	0
3	B	20	0	4	5	0
3	C	20	0	4	0	0
3	D	10	0	2	1	0
3	E	10	0	2	1	0
3	F	10	0	2	2	0
3	G	20	0	4	0	0
3	H	20	0	4	3	0
3	I	20	0	4	2	0
3	J	10	0	2	1	0
3	K	10	0	2	0	0
3	L	10	0	2	1	0
4	A	147	0	0	5	0
4	B	145	0	0	3	0
4	C	93	0	0	9	0
4	D	60	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	52	0	0	3	0
4	F	49	0	0	4	0
4	G	125	0	0	7	0
4	H	132	0	0	3	0
4	I	136	0	0	6	0
4	J	136	0	0	3	0
4	K	37	0	0	5	0
4	L	66	0	0	7	0
All	All	25761	0	24864	845	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

The worst 5 of 845 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:184:THR:HG21	1:B:222:GLU:H	1.21	1.06
1:H:184:THR:HG21	1:H:222:GLU:H	1.20	1.04
1:D:146:ALA:HB1	1:D:149:ILE:HD11	1.37	1.00
1:K:188:GLN:HA	1:K:199:GLY:HA3	1.44	0.99
1:C:238:LEU:HD12	1:C:239:PRO:HD2	1.50	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/263 (96%)	241 (95%)	12 (5%)	0	100	100
1	B	254/263 (97%)	245 (96%)	9 (4%)	0	100	100
1	C	253/263 (96%)	234 (92%)	15 (6%)	4 (2%)	14	12
1	D	252/263 (96%)	230 (91%)	17 (7%)	5 (2%)	11	8
1	E	252/263 (96%)	227 (90%)	22 (9%)	3 (1%)	19	19
1	F	251/263 (95%)	228 (91%)	23 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	255/263 (97%)	245 (96%)	9 (4%)	1 (0%)	43	52
1	H	252/263 (96%)	242 (96%)	10 (4%)	0	100	100
1	I	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
1	J	260/263 (99%)	245 (94%)	15 (6%)	0	100	100
1	K	253/263 (96%)	217 (86%)	31 (12%)	5 (2%)	11	8
1	L	252/263 (96%)	226 (90%)	23 (9%)	3 (1%)	19	19
All	All	3047/3156 (96%)	2829 (93%)	197 (6%)	21 (1%)	30	34

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	262	GLU
1	K	94	VAL
1	C	85	SER
1	K	146	ALA
1	C	88	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/220 (98%)	212 (98%)	4 (2%)	69	85
1	B	216/220 (98%)	210 (97%)	6 (3%)	56	73
1	C	215/220 (98%)	213 (99%)	2 (1%)	87	95
1	D	215/220 (98%)	205 (95%)	10 (5%)	36	47
1	E	215/220 (98%)	207 (96%)	8 (4%)	45	60
1	F	215/220 (98%)	207 (96%)	8 (4%)	45	60
1	G	217/220 (99%)	208 (96%)	9 (4%)	41	55
1	H	215/220 (98%)	209 (97%)	6 (3%)	56	73
1	I	219/220 (100%)	215 (98%)	4 (2%)	71	86
1	J	219/220 (100%)	214 (98%)	5 (2%)	63	80
1	K	216/220 (98%)	209 (97%)	7 (3%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	215/220 (98%)	210 (98%)	5 (2%)	63	80
All	All	2593/2640 (98%)	2519 (97%)	74 (3%)	55	71

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	176	TRP
1	G	220	PHE
1	K	264	ILE
1	F	188	GLN
1	F	248	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	161	ASN
1	G	237	GLN
1	K	242	GLN
1	F	175	GLN
1	H	11	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 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	$\# Z > 2$
3	PEP	A	268	-	9,9,9	0.79	0	13,13,13	2.23	4 (30%)
2	PO4	A	269	-	4,4,4	0.81	0	6,6,6	0.31	0
3	PEP	B	268	-	9,9,9	0.82	0	13,13,13	2.16	4 (30%)
3	PEP	B	269	-	9,9,9	1.38	1 (11%)	13,13,13	2.41	5 (38%)
3	PEP	C	268	-	9,9,9	0.89	0	13,13,13	1.58	2 (15%)
3	PEP	C	269	-	9,9,9	0.96	0	13,13,13	2.29	4 (30%)
3	PEP	D	268	-	9,9,9	0.77	0	13,13,13	1.64	2 (15%)
2	PO4	D	269	-	4,4,4	0.83	0	6,6,6	0.31	0
3	PEP	E	268	-	9,9,9	0.99	0	13,13,13	2.32	7 (53%)
2	PO4	E	269	-	4,4,4	0.88	0	6,6,6	0.31	0
3	PEP	F	268	-	9,9,9	0.96	0	13,13,13	1.85	4 (30%)
2	PO4	F	269	-	4,4,4	0.83	0	6,6,6	0.31	0
3	PEP	G	268	-	9,9,9	1.05	1 (11%)	13,13,13	2.38	6 (46%)
3	PEP	G	269	-	9,9,9	1.13	1 (11%)	13,13,13	1.93	4 (30%)
3	PEP	H	268	-	9,9,9	0.69	0	13,13,13	1.76	5 (38%)
3	PEP	H	269	-	9,9,9	0.82	0	13,13,13	1.52	3 (23%)
3	PEP	I	268	-	9,9,9	0.78	0	13,13,13	2.01	4 (30%)
3	PEP	I	269	-	9,9,9	0.87	0	13,13,13	2.98	3 (23%)
3	PEP	J	268	-	9,9,9	0.80	0	13,13,13	1.92	3 (23%)
2	PO4	J	269	-	4,4,4	0.93	0	6,6,6	0.31	0
3	PEP	K	268	-	9,9,9	0.87	0	13,13,13	1.44	2 (15%)
2	PO4	K	269	-	4,4,4	0.85	0	6,6,6	0.31	0
3	PEP	L	268	-	9,9,9	0.82	0	13,13,13	1.77	3 (23%)
2	PO4	L	269	-	4,4,4	0.84	0	6,6,6	0.31	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
3	PEP	A	268	-	-	0/9/9/9	0/0/0/0
2	PO4	A	269	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEP	B	268	-	-	0/9/9/9	0/0/0/0
3	PEP	B	269	-	-	0/9/9/9	0/0/0/0
3	PEP	C	268	-	-	0/9/9/9	0/0/0/0
3	PEP	C	269	-	-	0/9/9/9	0/0/0/0
3	PEP	D	268	-	-	0/9/9/9	0/0/0/0
2	PO4	D	269	-	-	0/0/0/0	0/0/0/0
3	PEP	E	268	-	-	0/9/9/9	0/0/0/0
2	PO4	E	269	-	-	0/0/0/0	0/0/0/0
3	PEP	F	268	-	-	0/9/9/9	0/0/0/0
2	PO4	F	269	-	-	0/0/0/0	0/0/0/0
3	PEP	G	268	-	-	0/9/9/9	0/0/0/0
3	PEP	G	269	-	-	0/9/9/9	0/0/0/0
3	PEP	H	268	-	-	0/9/9/9	0/0/0/0
3	PEP	H	269	-	-	0/9/9/9	0/0/0/0
3	PEP	I	268	-	-	0/9/9/9	0/0/0/0
3	PEP	I	269	-	-	2/9/9/9	0/0/0/0
3	PEP	J	268	-	-	0/9/9/9	0/0/0/0
2	PO4	J	269	-	-	0/0/0/0	0/0/0/0
3	PEP	K	268	-	-	0/9/9/9	0/0/0/0
2	PO4	K	269	-	-	0/0/0/0	0/0/0/0
3	PEP	L	268	-	-	0/9/9/9	0/0/0/0
2	PO4	L	269	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	269	PEP	C2-C1	3.07	1.52	1.49
3	G	269	PEP	C2-C1	2.34	1.51	1.49
3	G	268	PEP	C2-C1	2.01	1.51	1.49

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	269	PEP	P-O2-C2	6.61	138.63	123.31
3	I	269	PEP	O2'-C1-C2	6.31	124.94	113.90
3	B	269	PEP	P-O2-C2	5.52	136.11	123.31
3	A	268	PEP	P-O2-C2	5.14	135.22	123.31
3	C	269	PEP	P-O2-C2	5.08	135.09	123.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	269	PEP	O2'-C1-C2-C3
3	I	269	PEP	O1-C1-C2-C3

There are no ring outliers.

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, 95th 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	257/263 (97%)	-0.30	6 (2%) 57 67	25, 38, 58, 80	0
1	B	258/263 (98%)	-0.16	5 (1%) 64 73	23, 38, 58, 94	0
1	C	257/263 (97%)	0.16	8 (3%) 47 56	31, 58, 82, 92	0
1	D	256/263 (97%)	0.35	13 (5%) 27 37	32, 65, 84, 92	0
1	E	256/263 (97%)	0.45	24 (9%) 9 14	35, 72, 100, 107	0
1	F	255/263 (96%)	0.59	23 (9%) 10 16	40, 75, 97, 102	0
1	G	259/263 (98%)	-0.16	7 (2%) 52 62	26, 41, 66, 109	0
1	H	256/263 (97%)	-0.21	3 (1%) 75 83	28, 40, 62, 84	0
1	I	262/263 (99%)	-0.10	10 (3%) 38 49	24, 40, 64, 97	0
1	J	262/263 (99%)	-0.15	8 (3%) 47 56	28, 42, 73, 101	0
1	K	257/263 (97%)	0.84	31 (12%) 5 8	40, 86, 108, 118	0
1	L	256/263 (97%)	0.49	20 (7%) 13 19	38, 65, 88, 97	0
All	All	3091/3156 (97%)	0.15	158 (5%) 27 37	23, 51, 93, 118	0

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	264	ILE	11.3
1	B	194	GLY	9.5
1	J	264	ILE	9.5
1	H	264	ILE	7.7
1	B	264	ILE	7.4

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PEP	H	269	10/10	0.17	1.43	62,67,73,73	0
2	PO4	A	269	5/5	0.12	0.39	53,55,55,58	0
3	PEP	G	269	10/10	0.18	0.28	67,71,76,77	0
3	PEP	E	268	10/10	0.20	0.27	66,68,71,71	0
3	PEP	I	268	10/10	0.16	0.27	30,35,38,39	0
3	PEP	B	268	10/10	0.15	0.13	31,34,36,42	0
3	PEP	C	268	10/10	0.17	0.11	53,56,59,60	0
3	PEP	G	268	10/10	0.14	0.10	33,39,44,46	0
3	PEP	B	269	10/10	0.11	-0.17	52,59,65,65	0
3	PEP	A	268	10/10	0.12	-0.21	32,35,38,39	0
3	PEP	I	269	10/10	0.14	-0.33	55,62,70,71	0
3	PEP	L	268	10/10	0.16	-0.34	69,73,74,74	0
3	PEP	H	268	10/10	0.13	-0.36	28,34,38,38	0
3	PEP	J	268	10/10	0.12	-0.38	32,38,44,45	0
3	PEP	C	269	10/10	0.14	-0.46	88,88,89,89	0
2	PO4	J	269	5/5	0.11	-0.64	61,63,64,64	0
3	PEP	F	268	10/10	0.14	-0.76	72,76,77,79	0
3	PEP	K	268	10/10	0.13	-0.87	76,79,81,82	0
3	PEP	D	268	10/10	0.11	-0.93	50,55,60,60	0
2	PO4	F	269	5/5	0.12	-0.95	90,90,90,91	0
2	PO4	L	269	5/5	0.11	-1.18	103,103,104,104	0
2	PO4	K	269	5/5	0.15	-1.50	122,123,123,123	0
2	PO4	E	269	5/5	0.09	-1.82	97,98,98,99	0
2	PO4	D	269	5/5	0.07	-2.14	80,80,80,81	0

6.5 Other polymers ⓘ

There are no such residues in this entry.