wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 10:07 AM EDT

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 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

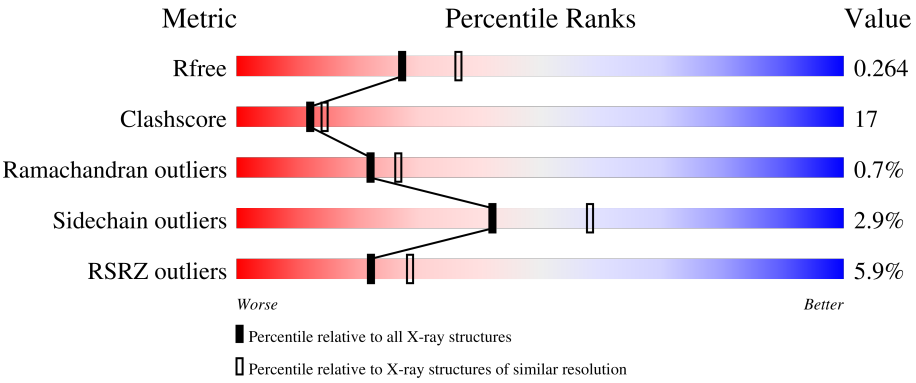
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	2% 71% 25%
1	B	263	2% 75% 22%
1	C	263	3% 63% 32%
1	D	263	6% 58% 37%
1	E	263	11% 59% 36%

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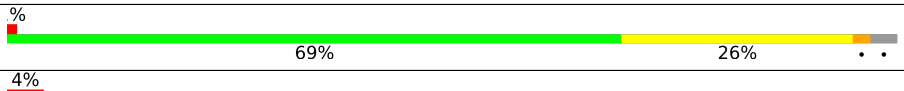
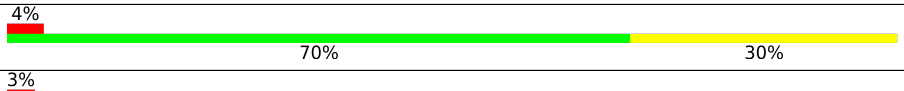
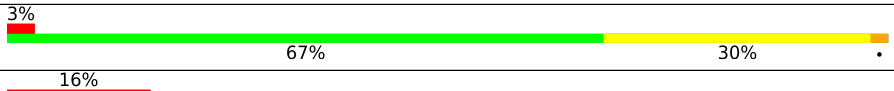
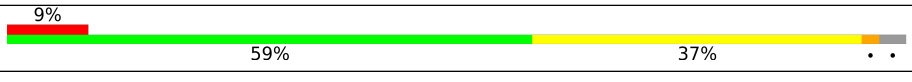
Mol	Chain	Length	Quality of chain
1	F	263	
1	G	263	
1	H	263	
1	I	263	
1	J	263	
1	K	263	
1	L	263	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25761 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 2-dehydro-3-deoxyphosphooctonate aldolase.

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 mutation	UNP O66496
A	11	ASN	CYS	engineered mutation	UNP O66496
B	10	MET	PRO	engineered mutation	UNP O66496
B	11	ASN	CYS	engineered mutation	UNP O66496
C	10	MET	PRO	engineered mutation	UNP O66496

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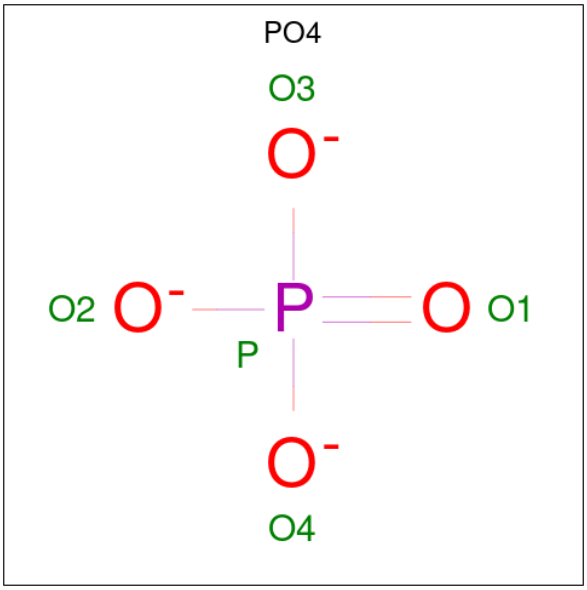
Chain	Residue	Modelled	Actual	Comment	Reference
C	11	ASN	CYS	engineered mutation	UNP O66496
D	10	MET	PRO	engineered mutation	UNP O66496
D	11	ASN	CYS	engineered mutation	UNP O66496
E	10	MET	PRO	engineered mutation	UNP O66496
E	11	ASN	CYS	engineered mutation	UNP O66496
F	10	MET	PRO	engineered mutation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

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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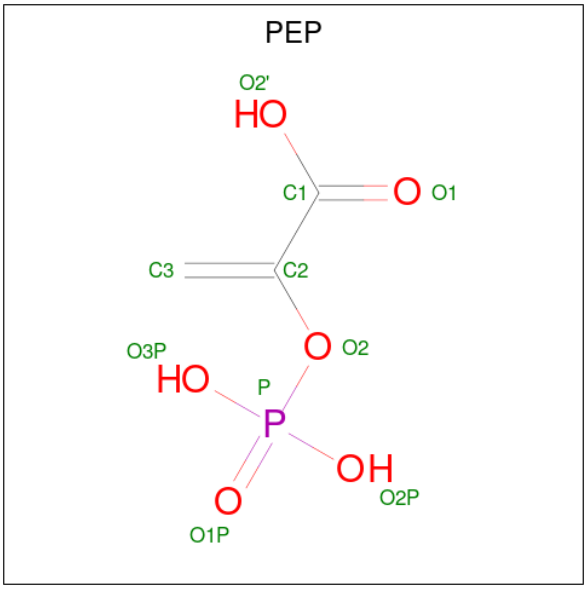
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0

- 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 10 3 6 1	0	0
3	B	1	Total C O P 10 3 6 1	0	0
3	B	1	Total C O P 10 3 6 1	0	0
3	C	1	Total C O P 10 3 6 1	0	0
3	C	1	Total C O P 10 3 6 1	0	0
3	D	1	Total C O P 10 3 6 1	0	0

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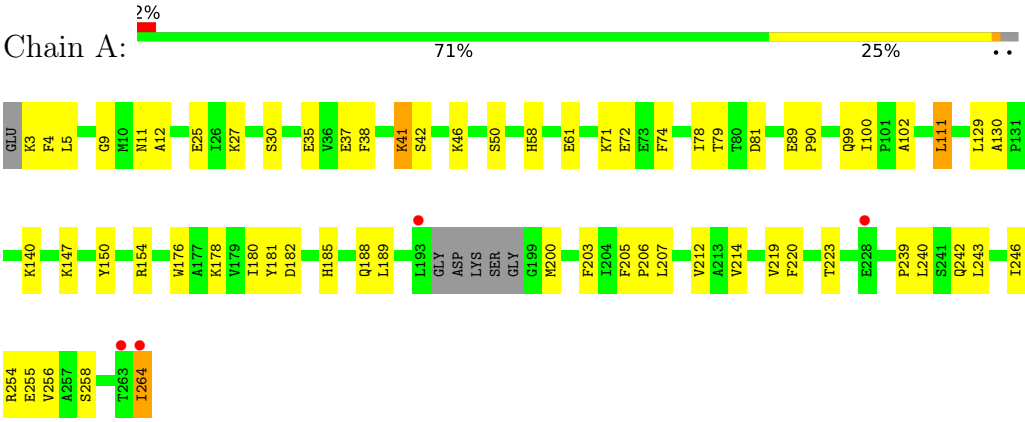
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	136	Total O 136 136	0	0
4	J	136	Total O 136 136	0	0
4	K	37	Total O 37 37	0	0
4	L	66	Total O 66 66	0	0

3 Residue-property plots (i)

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

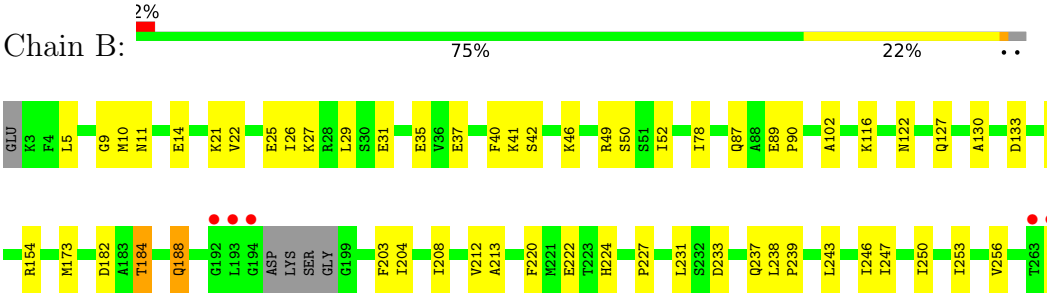
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain A:



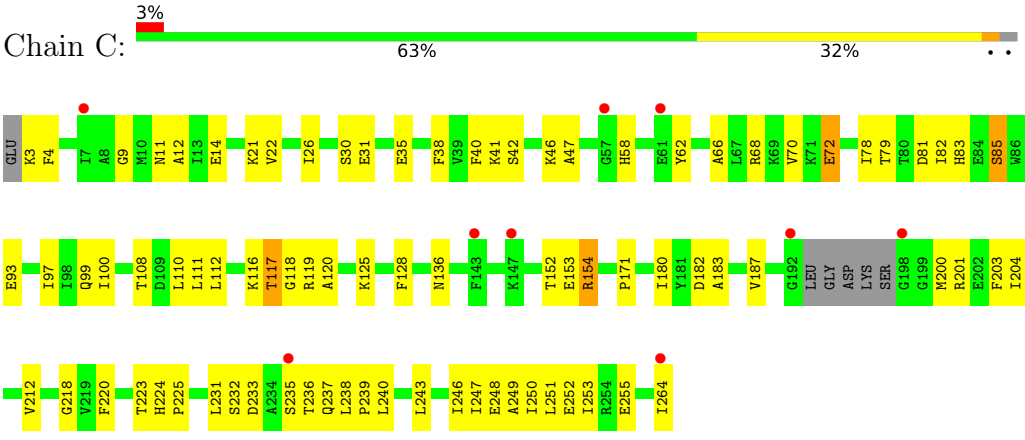
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain B:



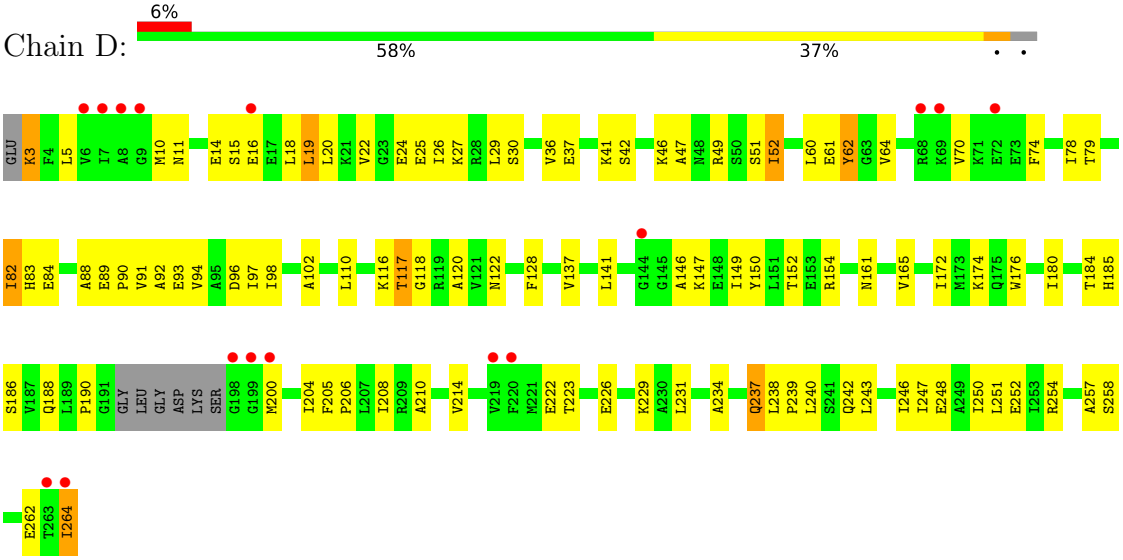
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain C:



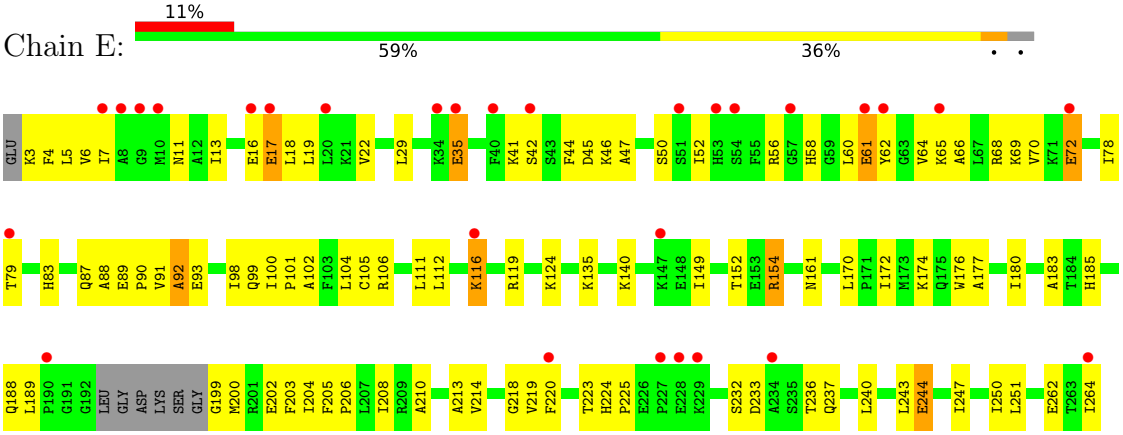
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain D:



• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain E:

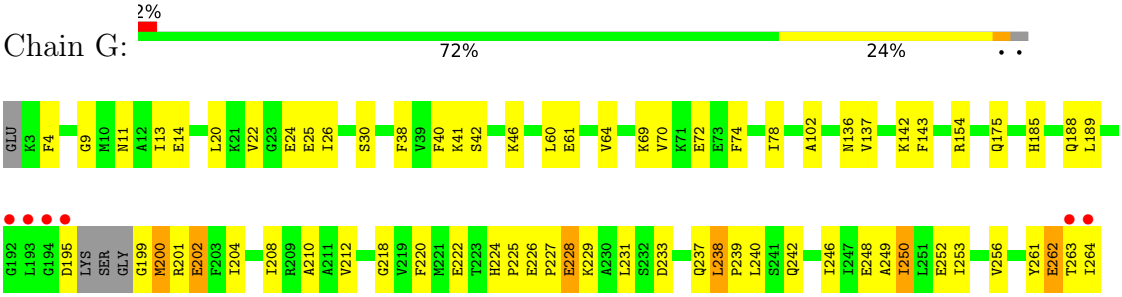


• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain F:

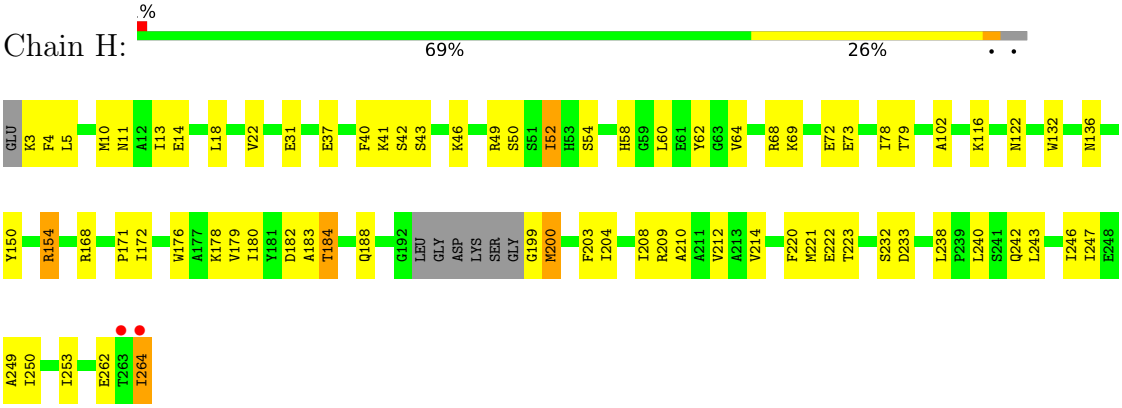
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain G:



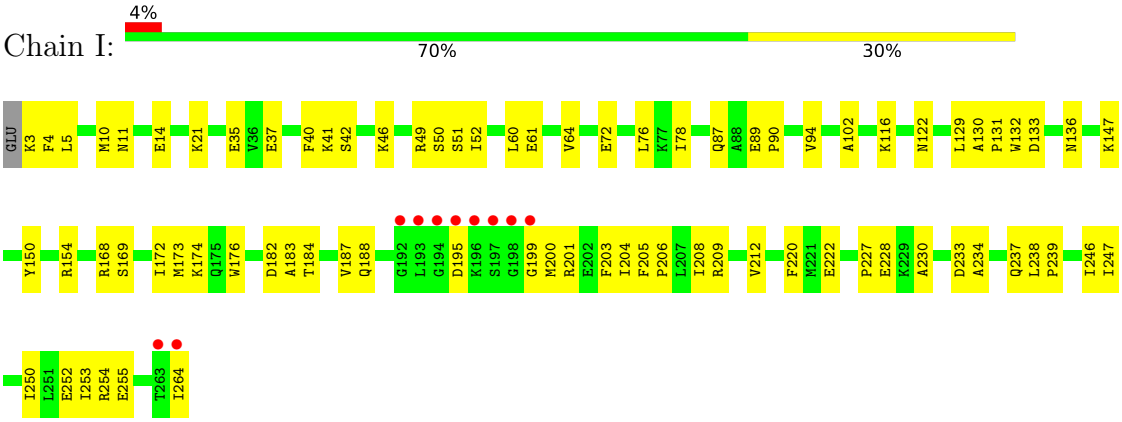
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain H:



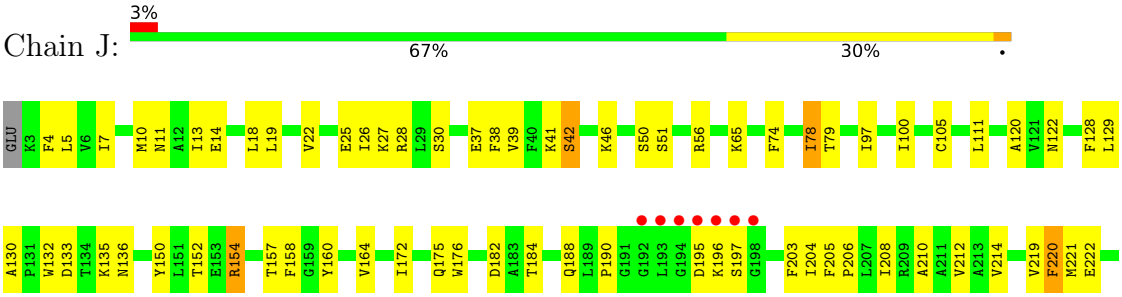
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

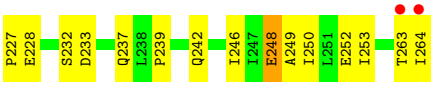
Chain I:



• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

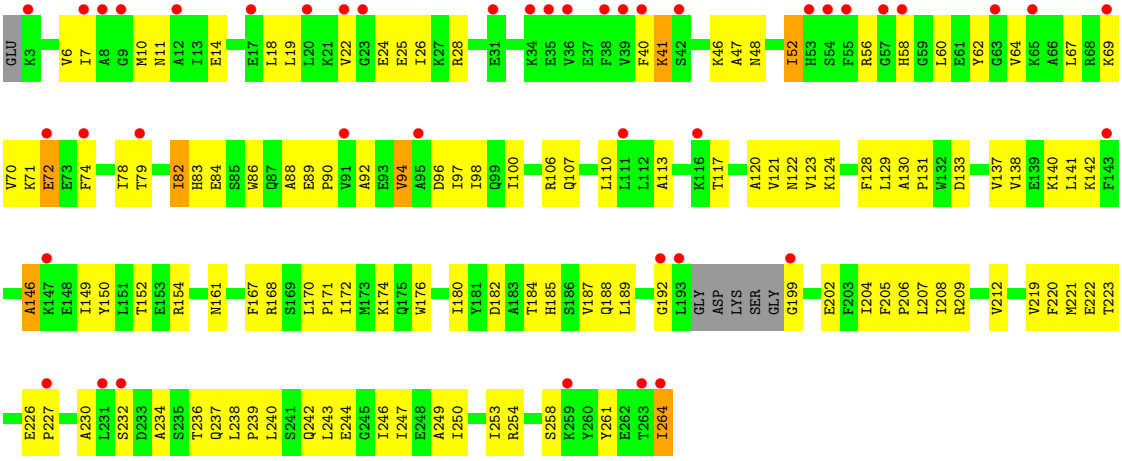
Chain J:





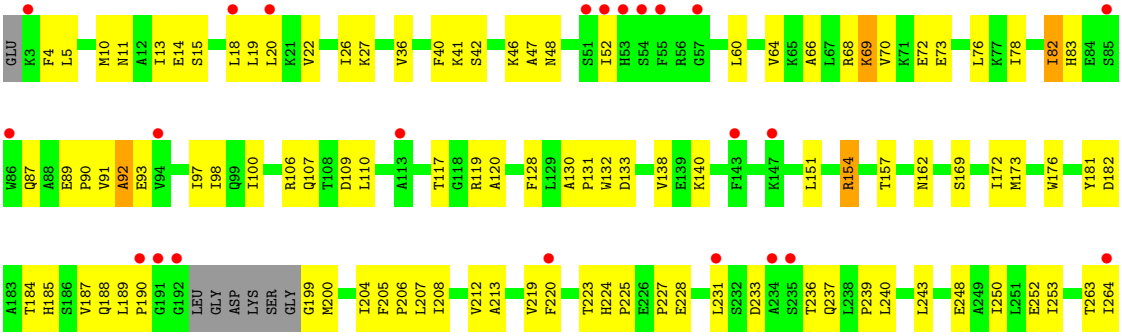
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain K:



• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain L:



4 Data and refinement statistics (i)

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) 69.6 (25.24-2.22)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.267 0.205 , 0.264	Depositor DCC
R_{free} test set	6337 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 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	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
4	E	52	0	0	3	0
4	F	49	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 17.

The worst 5 of 845 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: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 (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	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%)	9 9
1	D	252/263 (96%)	230 (91%)	17 (7%)	5 (2%)	7 6
1	E	252/263 (96%)	227 (90%)	22 (9%)	3 (1%)	13 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	251/263 (95%)	228 (91%)	23 (9%)	0	100 100
1	G	255/263 (97%)	245 (96%)	9 (4%)	1 (0%)	34 42
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%)	7 6
1	L	252/263 (96%)	226 (90%)	23 (9%)	3 (1%)	13 14
All	All	3047/3156 (96%)	2829 (93%)	197 (6%)	21 (1%)	22 26

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 (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	216/220 (98%)	212 (98%)	4 (2%)	57 73
1	B	216/220 (98%)	210 (97%)	6 (3%)	43 60
1	C	215/220 (98%)	213 (99%)	2 (1%)	78 89
1	D	215/220 (98%)	205 (95%)	10 (5%)	26 37
1	E	215/220 (98%)	207 (96%)	8 (4%)	34 48
1	F	215/220 (98%)	207 (96%)	8 (4%)	34 48
1	G	217/220 (99%)	208 (96%)	9 (4%)	30 43
1	H	215/220 (98%)	209 (97%)	6 (3%)	43 60
1	I	219/220 (100%)	215 (98%)	4 (2%)	59 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	219/220 (100%)	214 (98%)	5 (2%)	50 67
1	K	216/220 (98%)	209 (97%)	7 (3%)	39 54
1	L	215/220 (98%)	210 (98%)	5 (2%)	50 67
All	All	2593/2640 (98%)	2519 (97%)	74 (3%)	42 58

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

Mol	Chain	Res	Type
1	J	42	SER
1	L	82	ILE
1	J	154	ARG
1	K	124	LYS
1	E	61	GLU

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

Mol	Chain	Res	Type
1	I	188	GLN
1	K	188	GLN
1	J	11	ASN
1	K	53	HIS
1	L	11	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	E	268	-	9,9,9	1.16	1 (11%)	11,13,13	2.25	5 (45%)
3	PEP	J	268	-	9,9,9	0.96	0	11,13,13	1.75	2 (18%)
2	PO4	J	269	-	4,4,4	1.74	1 (25%)	6,6,6	0.43	0
3	PEP	G	269	-	9,9,9	1.29	1 (11%)	11,13,13	1.79	3 (27%)
2	PO4	A	269	-	4,4,4	1.57	0	6,6,6	0.45	0
3	PEP	F	268	-	9,9,9	1.13	0	11,13,13	1.85	3 (27%)
2	PO4	L	269	-	4,4,4	1.61	0	6,6,6	0.43	0
2	PO4	E	269	-	4,4,4	1.66	0	6,6,6	0.44	0
3	PEP	I	268	-	9,9,9	0.95	0	11,13,13	1.96	3 (27%)
3	PEP	I	269	-	9,9,9	1.05	0	11,13,13	2.59	2 (18%)
3	PEP	H	268	-	9,9,9	0.84	0	11,13,13	1.69	4 (36%)
3	PEP	C	269	-	9,9,9	1.15	1 (11%)	11,13,13	1.69	3 (27%)
3	PEP	K	268	-	9,9,9	1.06	0	11,13,13	1.09	1 (9%)
2	PO4	D	269	-	4,4,4	1.60	0	6,6,6	0.41	0
2	PO4	K	269	-	4,4,4	1.63	0	6,6,6	0.44	0
3	PEP	B	268	-	9,9,9	1.00	0	11,13,13	2.05	3 (27%)
3	PEP	G	268	-	9,9,9	1.21	0	11,13,13	2.12	4 (36%)
3	PEP	A	268	-	9,9,9	0.92	0	11,13,13	1.89	2 (18%)
3	PEP	C	268	-	9,9,9	1.07	0	11,13,13	1.25	1 (9%)
3	PEP	H	269	-	9,9,9	0.98	0	11,13,13	1.41	2 (18%)
3	PEP	B	269	-	9,9,9	1.53	2 (22%)	11,13,13	1.84	3 (27%)
3	PEP	L	268	-	9,9,9	1.00	0	11,13,13	1.61	3 (27%)
2	PO4	F	269	-	4,4,4	1.60	0	6,6,6	0.43	0
3	PEP	D	268	-	9,9,9	0.94	0	11,13,13	1.39	1 (9%)

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	B	268	-	-	4/9/9/9	-
3	PEP	E	268	-	-	0/9/9/9	-
3	PEP	G	268	-	-	0/9/9/9	-
3	PEP	A	268	-	-	0/9/9/9	-
3	PEP	F	268	-	-	4/9/9/9	-
3	PEP	C	268	-	-	4/9/9/9	-
3	PEP	H	269	-	-	4/9/9/9	-
3	PEP	J	268	-	-	5/9/9/9	-
3	PEP	I	268	-	-	4/9/9/9	-
3	PEP	I	269	-	-	4/9/9/9	-
3	PEP	H	268	-	-	0/9/9/9	-
3	PEP	G	269	-	-	4/9/9/9	-
3	PEP	C	269	-	-	7/9/9/9	-
3	PEP	B	269	-	-	0/9/9/9	-
3	PEP	L	268	-	-	4/9/9/9	-
3	PEP	D	268	-	-	4/9/9/9	-
3	PEP	K	268	-	-	5/9/9/9	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	269	PEP	C2-C1	3.06	1.52	1.49
3	B	269	PEP	P-O2	2.34	1.62	1.59
3	G	269	PEP	C2-C1	2.32	1.51	1.49
2	J	269	PO4	P-O4	-2.11	1.48	1.54
3	C	269	PEP	P-O2	2.11	1.62	1.59

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	269	PEP	O2'-C1-C2	6.47	124.94	113.91
3	I	268	PEP	O2'-C1-C2	4.93	122.33	113.91
3	G	268	PEP	O2'-C1-C2	4.82	122.14	113.91
3	J	268	PEP	O2'-C1-C2	4.49	121.57	113.91
3	I	269	PEP	O1-C1-C2	-4.22	115.42	121.79

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	268	PEP	O1-C1-C2-C3
3	B	268	PEP	O2'-C1-C2-C3
3	B	268	PEP	O2'-C1-C2-O2
3	C	268	PEP	O1-C1-C2-C3
3	C	268	PEP	O2'-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	268	PEP	1	0
3	J	268	PEP	1	0
2	J	269	PO4	1	0
3	F	268	PEP	2	0
3	I	268	PEP	1	0
3	I	269	PEP	1	0
3	H	268	PEP	1	0
3	B	268	PEP	2	0
3	H	269	PEP	2	0
3	B	269	PEP	3	0
3	L	268	PEP	1	0
3	D	268	PEP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	257/263 (97%)	-0.33	4 (1%) 72 77	25, 38, 58, 80	0
1	B	258/263 (98%)	-0.18	5 (1%) 66 73	23, 38, 58, 94	0
1	C	257/263 (97%)	0.12	9 (3%) 44 51	31, 58, 82, 92	0
1	D	256/263 (97%)	0.36	16 (6%) 20 25	32, 65, 84, 92	0
1	E	256/263 (97%)	0.45	29 (11%) 5 7	35, 72, 100, 107	0
1	F	255/263 (96%)	0.62	27 (10%) 6 8	40, 75, 97, 102	0
1	G	259/263 (98%)	-0.20	6 (2%) 60 67	26, 41, 66, 109	0
1	H	256/263 (97%)	-0.24	2 (0%) 86 89	28, 40, 62, 84	0
1	I	262/263 (99%)	-0.12	10 (3%) 40 47	24, 40, 64, 97	0
1	J	262/263 (99%)	-0.18	9 (3%) 45 52	28, 42, 73, 101	0
1	K	257/263 (97%)	0.92	43 (16%) 1 2	40, 86, 108, 118	0
1	L	256/263 (97%)	0.47	23 (8%) 9 12	38, 65, 88, 97	0
All	All	3091/3156 (97%)	0.14	183 (5%) 22 28	23, 51, 93, 118	0

The worst 5 of 183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	264	ILE	11.0
1	B	194	GLY	10.3
1	J	264	ILE	9.6
1	H	264	ILE	8.2
1	B	264	ILE	6.9

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	K	269	5/5	0.85	0.14	122,123,123,123	0
2	PO4	L	269	5/5	0.91	0.13	103,103,104,104	0
3	PEP	G	269	10/10	0.91	0.17	67,71,76,77	0
2	PO4	F	269	5/5	0.92	0.11	90,90,90,91	0
3	PEP	H	269	10/10	0.93	0.19	62,67,73,73	0
2	PO4	E	269	5/5	0.94	0.09	97,98,98,99	0
3	PEP	C	269	10/10	0.94	0.13	88,88,89,89	0
2	PO4	A	269	5/5	0.95	0.12	53,55,55,58	0
3	PEP	F	268	10/10	0.95	0.13	72,76,77,79	0
3	PEP	I	269	10/10	0.95	0.13	55,62,70,71	0
3	PEP	C	268	10/10	0.96	0.17	53,56,59,60	0
2	PO4	D	269	5/5	0.96	0.08	80,80,80,81	0
3	PEP	B	269	10/10	0.96	0.11	52,59,65,65	0
3	PEP	K	268	10/10	0.96	0.14	76,79,81,82	0
3	PEP	L	268	10/10	0.96	0.17	69,73,74,74	0
2	PO4	J	269	5/5	0.97	0.10	61,63,64,64	0
3	PEP	D	268	10/10	0.97	0.10	50,55,60,60	0
3	PEP	E	268	10/10	0.97	0.20	66,68,71,71	0
3	PEP	G	268	10/10	0.98	0.14	33,39,44,46	0
3	PEP	I	268	10/10	0.99	0.17	30,35,38,39	0
3	PEP	B	268	10/10	0.99	0.18	31,34,36,42	0
3	PEP	J	268	10/10	0.99	0.13	32,38,44,45	0
3	PEP	H	268	10/10	0.99	0.14	28,34,38,38	0
3	PEP	A	268	10/10	0.99	0.13	32,35,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.