wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:54 PM GMT

PDB ID	:	1QO5
Title	:	FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE FROM HUMAN LIVER TISSUE
Authors	:	Dalby, A.R.; Littlechild, J.A.
Deposited on	:	1999-11-03
Resolution	:	2.50 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 (i)) were used in the production of this report:

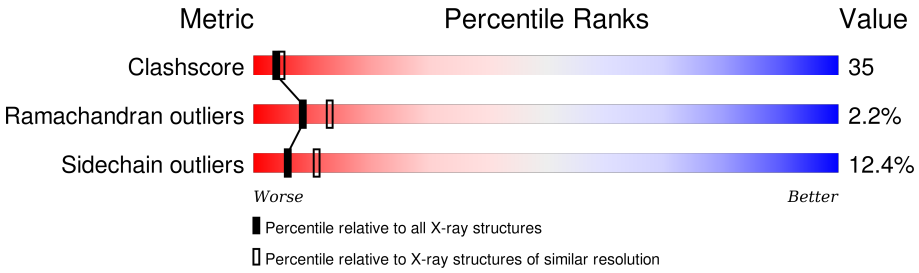
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	363	41% 36% 18% 5% •
1	B	363	29% 35% 23% 8% •
1	C	363	37% 37% 15% 6% 5%
1	D	363	36% 36% 20% 7% •
1	E	363	41% 34% 16% 6% •
1	F	363	45% 32% 14% 6% •
1	G	363	43% 33% 13% 6% 5%

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Mol	Chain	Length	Quality of chain
1	H	363	42% 36% 14% 6% •
1	I	363	31% 39% 20% 6% 5%
1	J	363	37% 40% 16% 5% •
1	K	363	48% 31% 15% • •
1	L	363	32% 40% 19% • 5%
1	M	363	43% 40% 10% 6% •
1	N	363	38% 34% 18% • 5%
1	O	363	36% 37% 16% 5% 5%
1	P	363	43% 38% 13% 5% •
1	Q	363	44% 36% 10% 5% 5%
1	R	363	44% 34% 14% • 5%

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	SO4	A	400	-	-	X	-
2	SO4	D	400	-	X	-	-
2	SO4	S	1	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 49278 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 FRUCTOSE-BISPHOSPHATE ALDOLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2730	1708	486	521	15			
1	B	348	Total	C	N	O	S	0	0	0
			2651	1660	473	504	14			
1	C	345	Total	C	N	O	S	0	0	0
			2635	1652	470	499	14			
1	D	356	Total	C	N	O	S	0	0	0
			2701	1689	482	516	14			
1	E	354	Total	C	N	O	S	0	0	0
			2687	1680	480	513	14			
1	F	353	Total	C	N	O	S	0	0	0
			2675	1674	474	513	14			
1	G	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	H	357	Total	C	N	O	S	0	0	0
			2712	1698	483	517	14			
1	I	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	J	356	Total	C	N	O	S	0	0	0
			2701	1689	482	516	14			
1	K	354	Total	C	N	O	S	0	0	0
			2686	1683	475	514	14			
1	L	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	M	360	Total	C	N	O	S	29	0	0
			2730	1708	486	521	15			
1	N	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	O	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	P	360	Total	C	N	O	S	0	0	0
			2730	1708	486	521	15			

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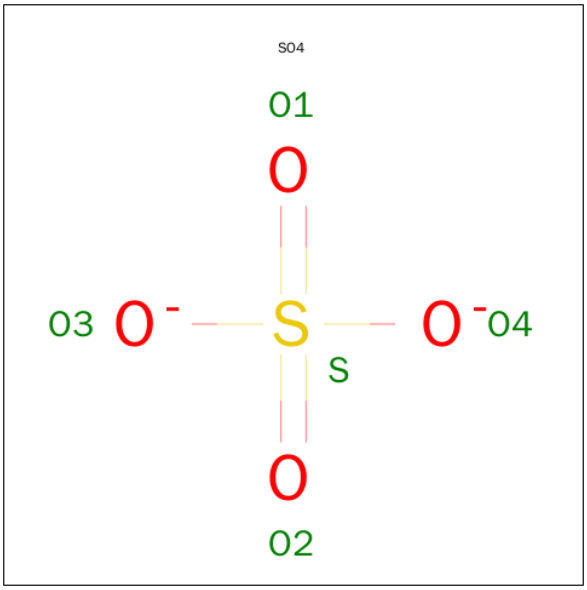
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			
1	R	344	Total	C	N	O	S	0	0	0
			2628	1648	469	497	14			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	S	1	Total O S 5 4 1	0	0
2	S	1	Total O S 5 4 1	0	0
2	S	1	Total O S 5 4 1	0	0
2	S	1	Total O S 5 4 1	0	0
2	S	1	Total O S 5 4 1	0	0
2	S	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	87	Total O 87 87	0	0
3	B	32	Total O 32 32	0	0
3	C	46	Total O 46 46	0	0
3	D	79	Total O 79 79	0	0
3	E	74	Total O 74 74	0	0
3	F	81	Total O 81 81	0	0
3	G	74	Total O 74 74	0	0
3	H	71	Total O 71 71	0	0
3	I	46	Total O 46 46	0	0
3	J	77	Total O 77 77	0	0
3	K	72	Total O 72 72	0	0
3	L	27	Total O 27 27	0	0
3	M	81	Total O 81 81	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	55	Total O 55 55	0	0
3	O	36	Total O 36 36	0	0
3	P	77	Total O 77 77	0	0
3	Q	81	Total O 81 81	0	0
3	R	71	Total O 71 71	0	0
3	S	2	Total O 2 2	0	0

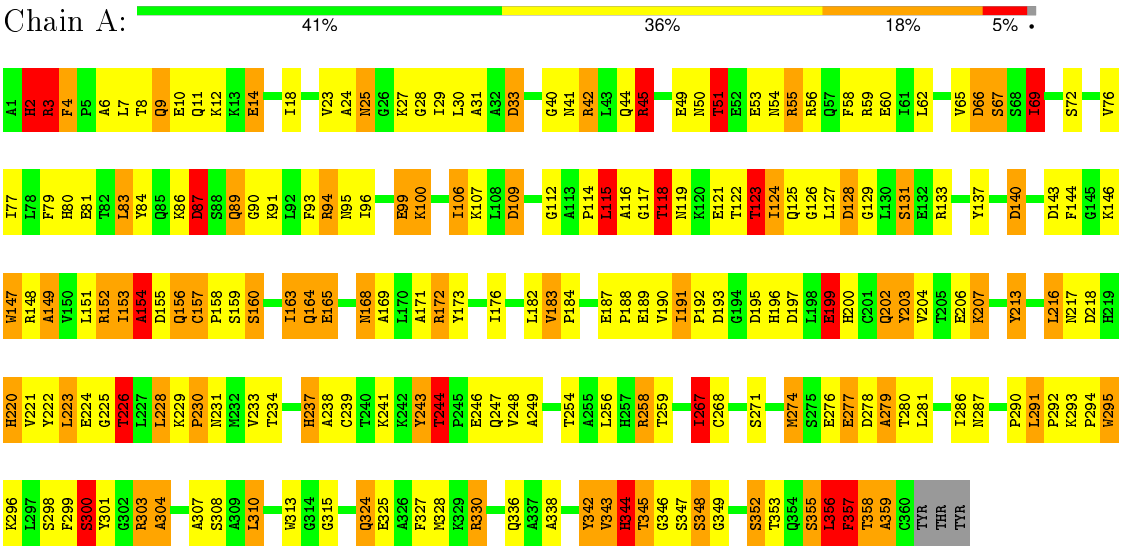
3 Residue-property plots (i)

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.

Note EDS was not executed.

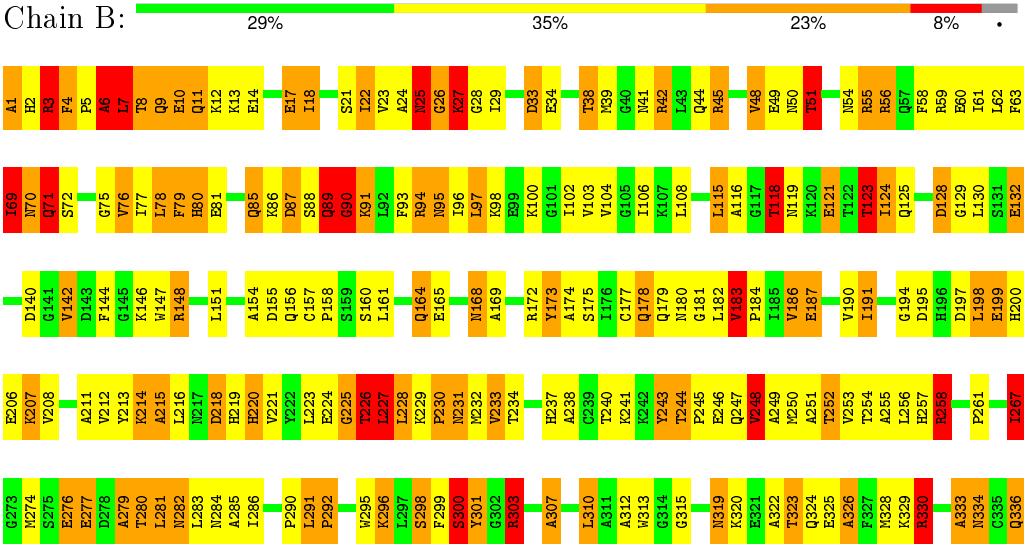
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain A:



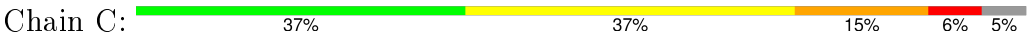
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

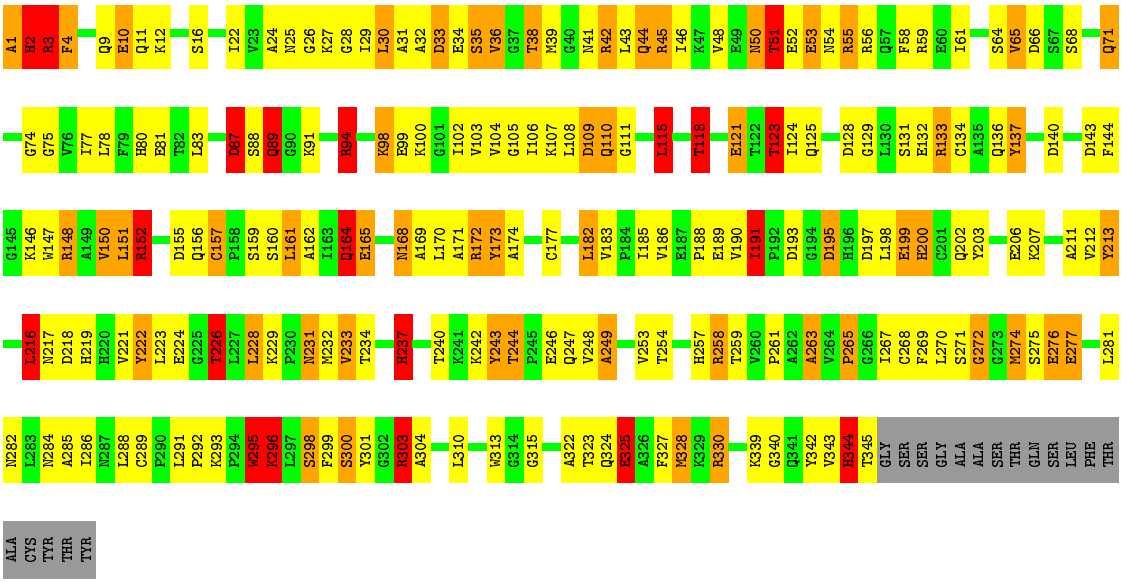
Chain B:



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

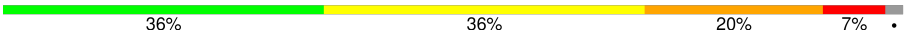
Chain C:

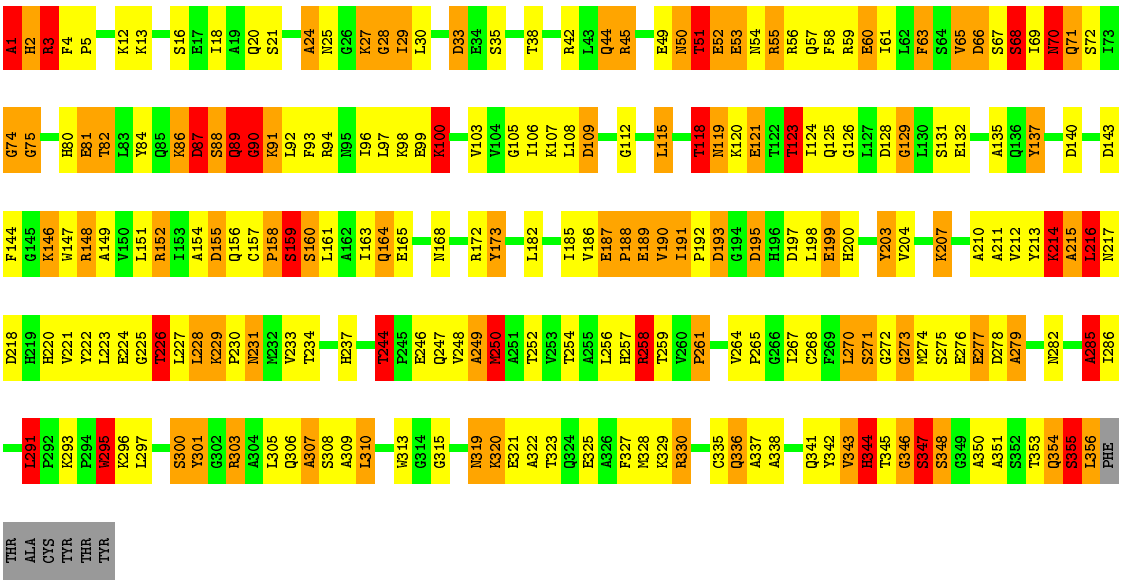




• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

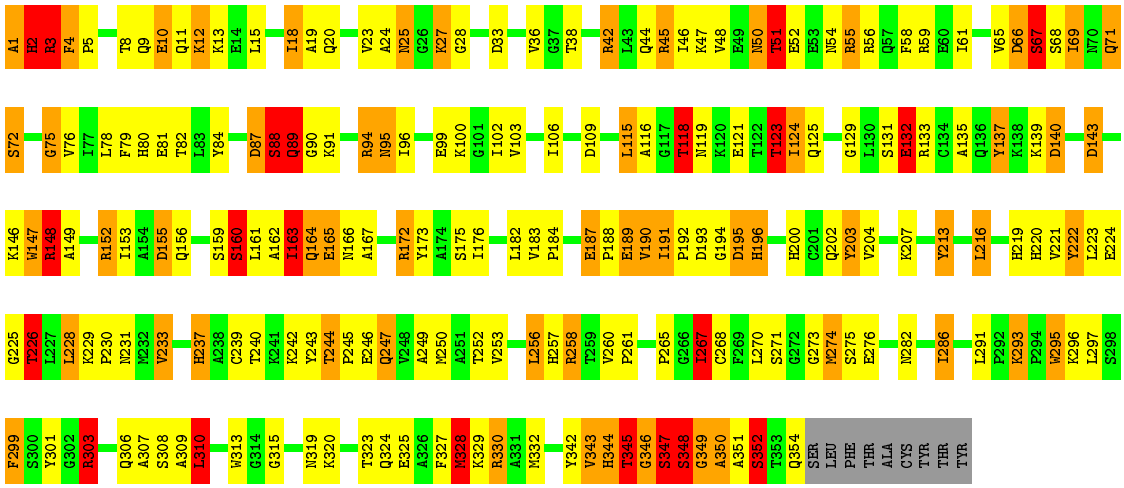
Chain D:





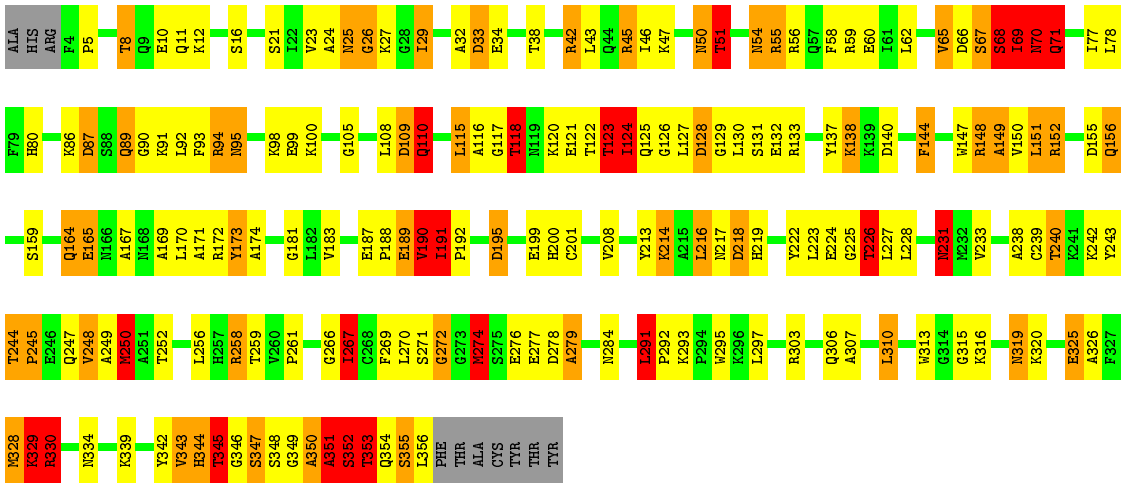
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain E:



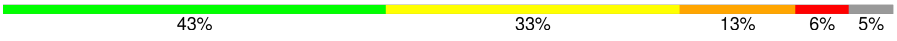
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

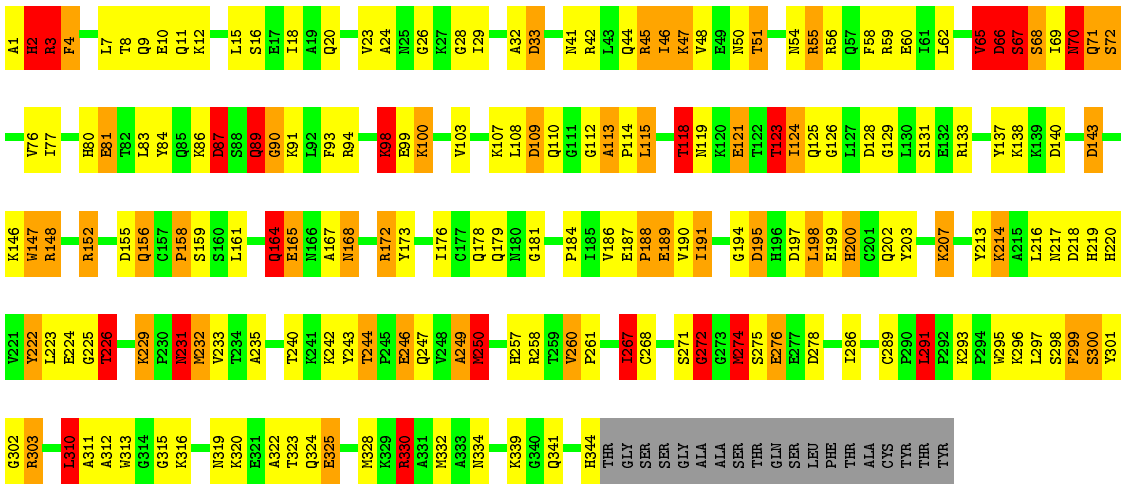
Chain F:



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

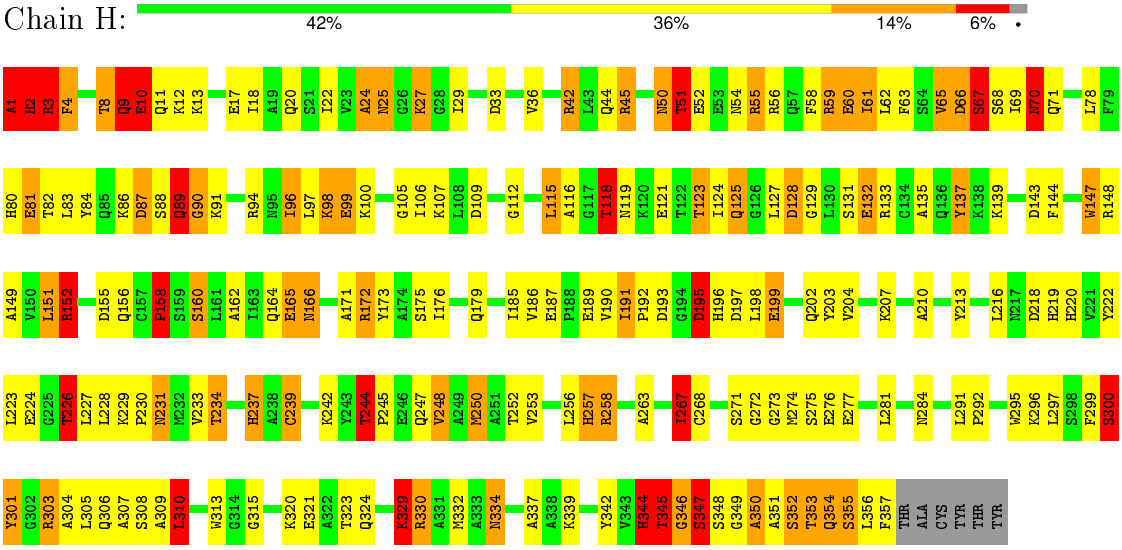
Chain G:





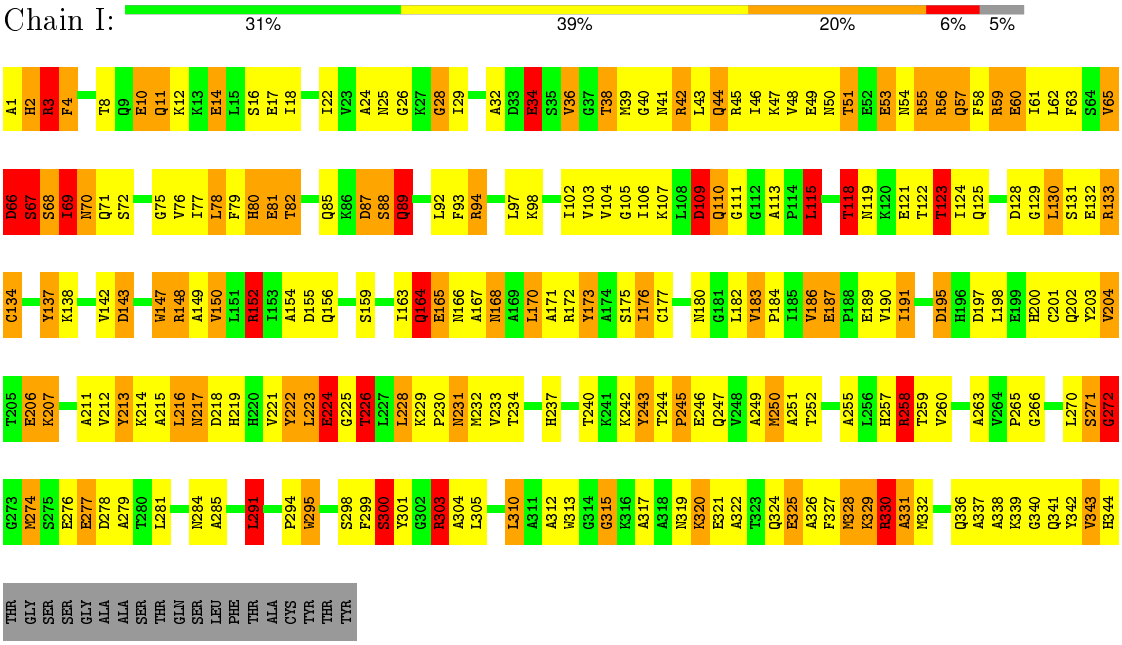
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain H:



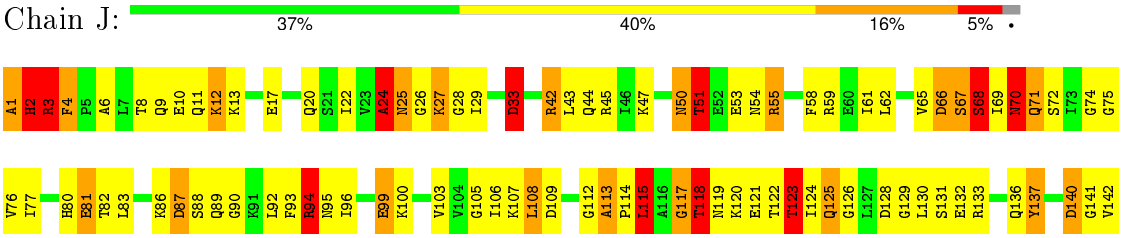
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

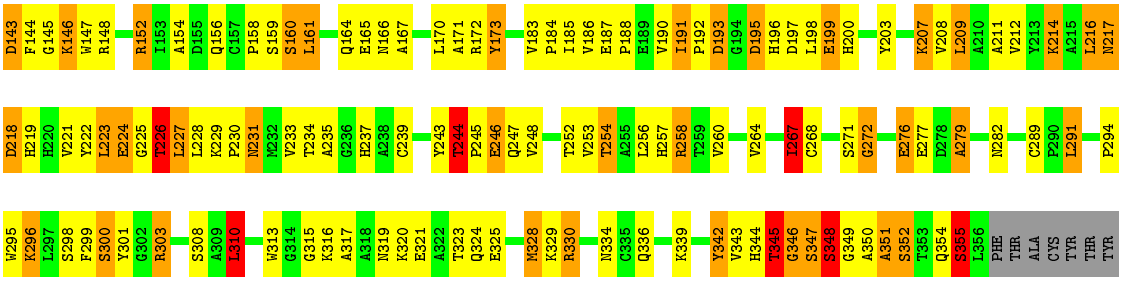
Chain I:



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

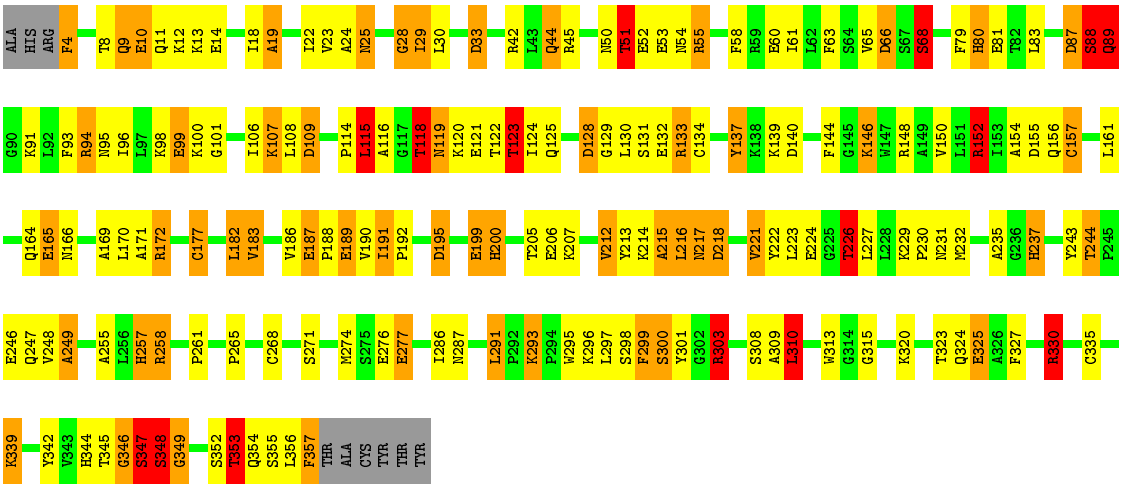
Chain J:





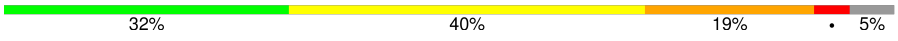
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

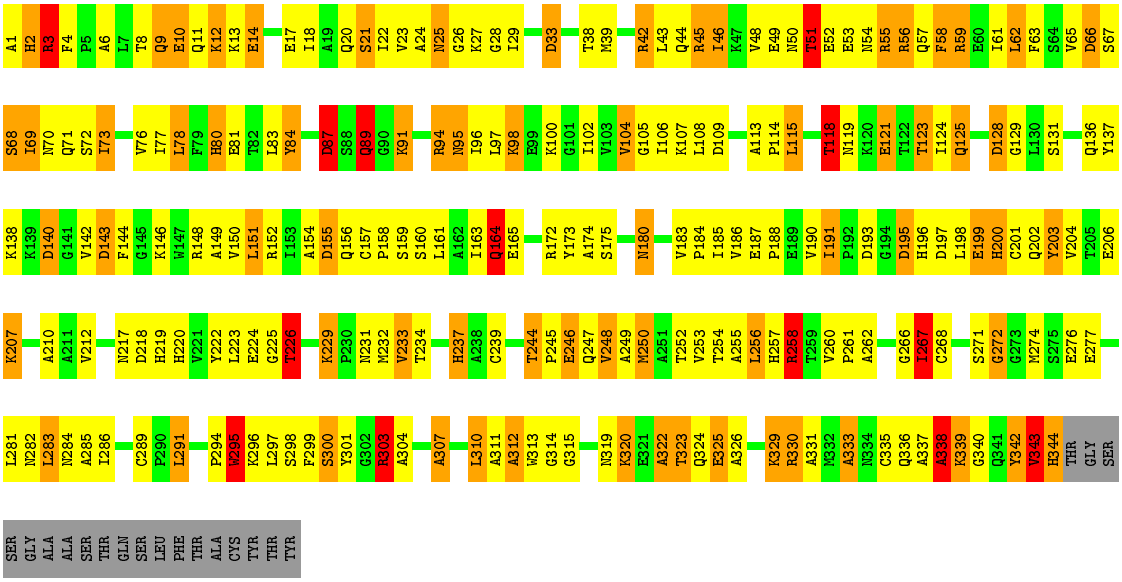
Chain K:



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

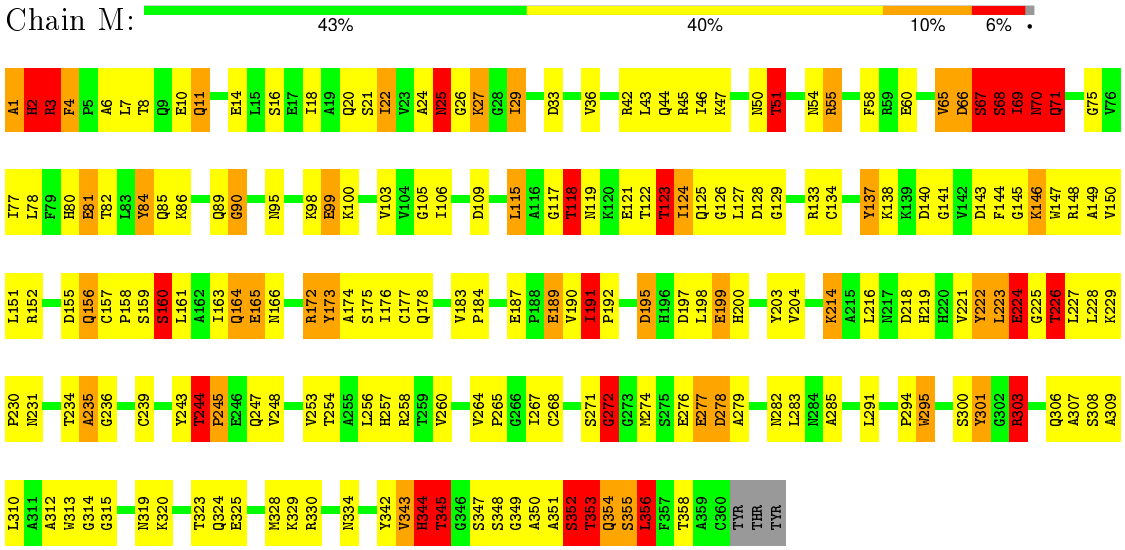
Chain L:





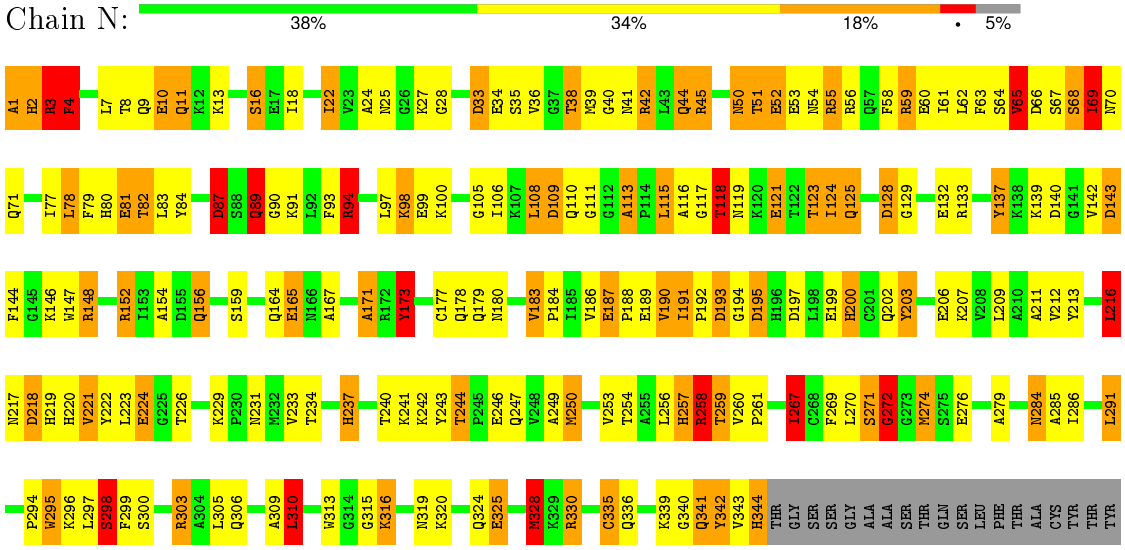
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain M:



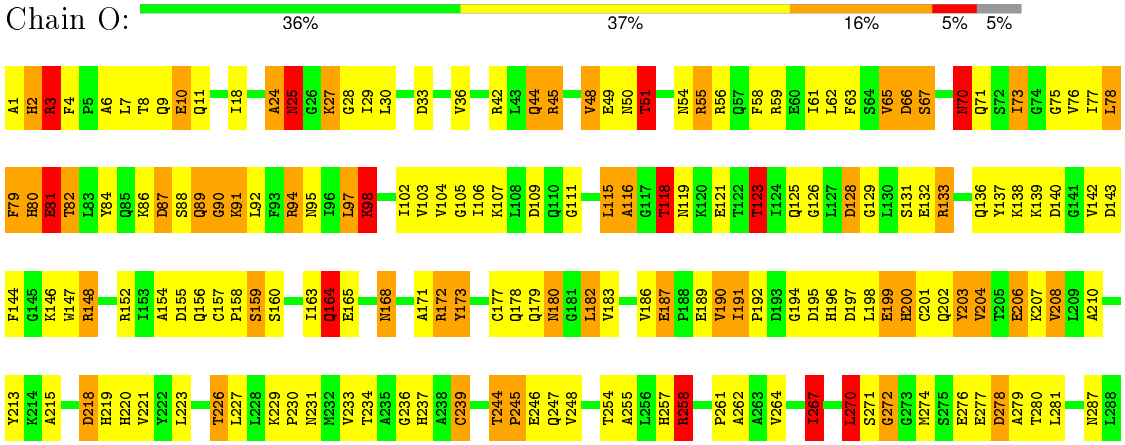
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

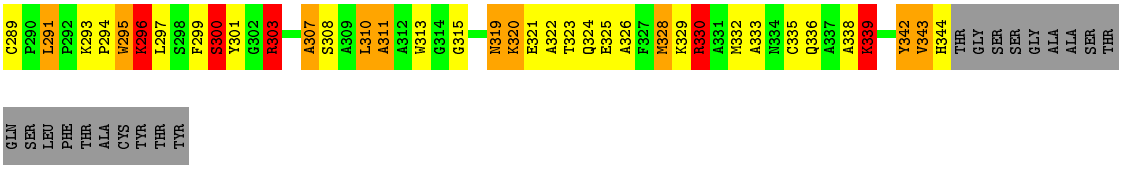
Chain N:



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

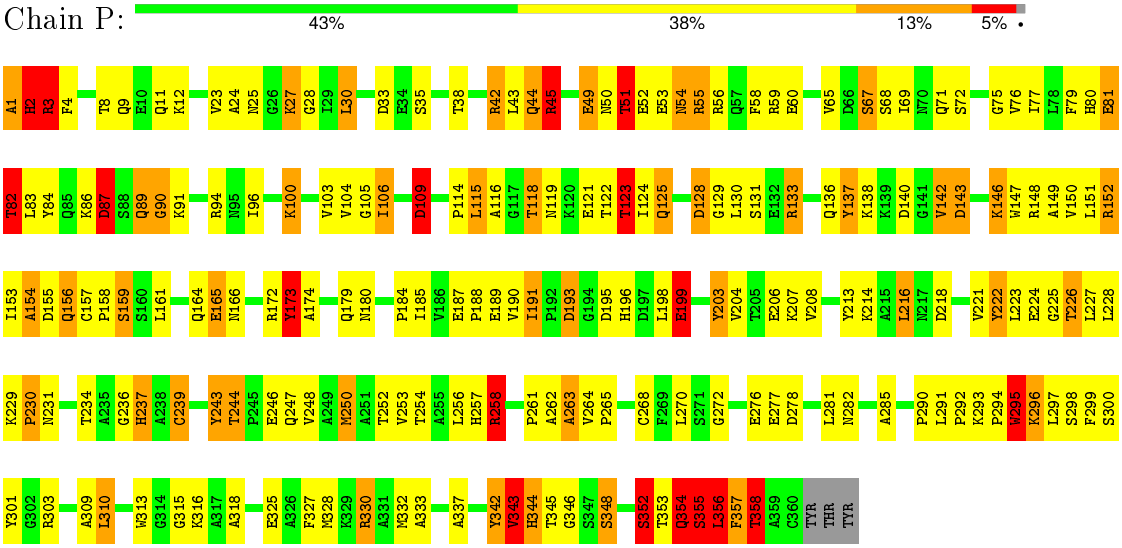
Chain O:





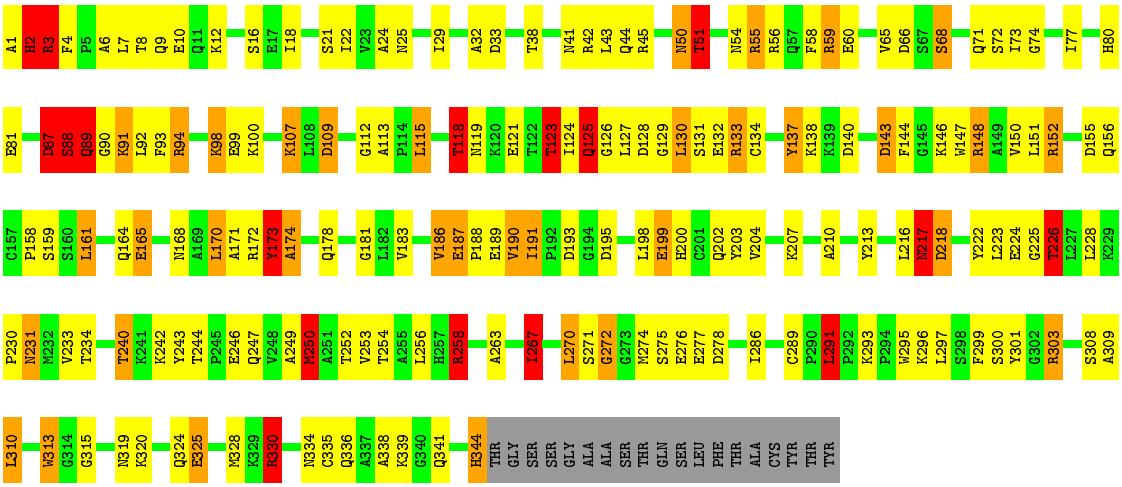
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain P:



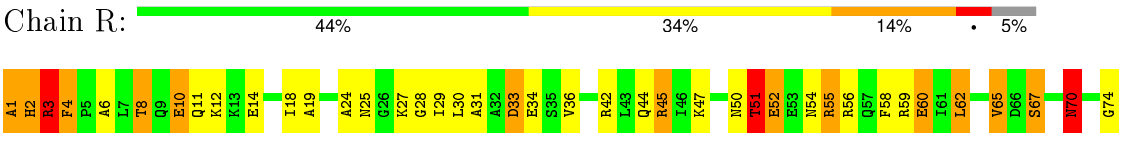
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

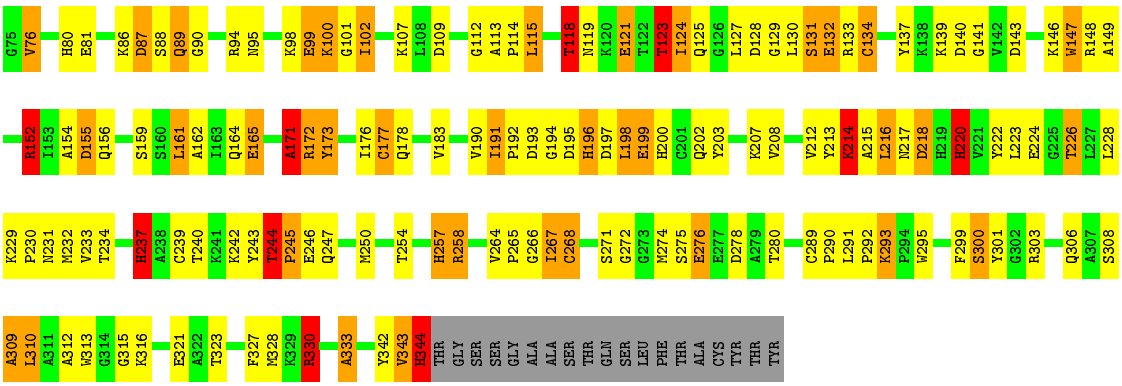
Chain Q:



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain R:




G75 V76 H80 E81 K86 D87 S88 Q89 G90 R94 N95 K98 E99 K100 G101 I102 K107 L108 D109 G112 A113 P114 L115 T118 N119 K120 E121 T122 T123 I124 Q125 G126 L127 D128 G129 L130 S131 E132 R133 C134 Y137 K138 K139 D140 G141 V142 D143 K146 W147 R148 A149
R152 I153 A154 D155 Q156 S159 S160 L161 A162 I163 Q164 E165 A171 R172 Y173 I176 C177 Q178 V183 V190 I191 P192 D193 G194 D195 H196 D197 L198 E199 H200 C201 Q202 Y203 K207 V208 V212 Y213 K214 A215 L216 N217 D218 H219 H220 V221 Y222 L223 E224 G225 T226 L227 L228
K229 P230 N231 M232 V233 T234 H237 A238 C239 T240 K241 K242 Y243 T244 P245 E246 Q247 M250 T254 H257 R258 V264 P265 G266 I267 C268 S271 G272 G273 M274 S275 E276 E277 D278 A279 T280 C289 P290 L291 P292 K293 P294 W295 F299 S300 Y301 G302 R303 Q306 A307 S308
A309 L310 A311 A312 W313 G314 G315 K316 E321 A322 T323 F327 M328 K329 R330 A333 Y342 V343 H344 THR GLY SER SER GLY ALA ALA SER THR GLN SER LEU PHE THR ALA CYS TYR THR TYR

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	291.10Å 489.84Å 103.36Å 90.00° 103.68° 90.00°	Depositor
Resolution (Å)	29.00 – 2.50	Depositor
% Data completeness (in resolution range)	71.0 (29.00-2.50)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	0.12	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	49278	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.13	2/2776 (0.1%)	2.86	194/3754 (5.2%)
1	B	1.31	11/2696 (0.4%)	2.80	253/3645 (6.9%)
1	C	1.01	0/2680	2.67	155/3624 (4.3%)
1	D	1.28	13/2746 (0.5%)	2.90	248/3713 (6.7%)
1	E	1.08	7/2732 (0.3%)	2.93	189/3694 (5.1%)
1	F	1.03	4/2719 (0.1%)	2.80	183/3677 (5.0%)
1	G	1.03	1/2673 (0.0%)	2.64	169/3614 (4.7%)
1	H	1.01	4/2758 (0.1%)	2.67	175/3729 (4.7%)
1	I	1.08	3/2673 (0.1%)	2.70	210/3614 (5.8%)
1	J	1.06	2/2746 (0.1%)	2.93	184/3713 (5.0%)
1	K	1.06	2/2731 (0.1%)	2.68	163/3693 (4.4%)
1	L	1.06	1/2673 (0.0%)	2.54	160/3614 (4.4%)
1	M	1.06	5/2776 (0.2%)	2.62	170/3754 (4.5%)
1	N	1.06	2/2673 (0.1%)	2.86	180/3614 (5.0%)
1	O	1.07	0/2673	2.49	155/3614 (4.3%)
1	P	1.04	1/2776 (0.0%)	2.69	168/3754 (4.5%)
1	Q	1.02	2/2673 (0.1%)	2.80	158/3614 (4.4%)
1	R	1.04	1/2673 (0.0%)	2.66	156/3614 (4.3%)
All	All	1.08	61/48847 (0.1%)	2.74	3270/66048 (5.0%)

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	A	0	7
1	B	0	13
1	C	0	6
1	D	0	13
1	E	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	4
1	G	0	8
1	H	0	7
1	I	0	11
1	J	0	4
1	K	0	6
1	L	0	6
1	M	0	8
1	N	0	6
1	O	0	5
1	P	0	6
1	Q	0	6
1	R	0	10
All	All	0	133

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	187	GLU	CD-OE1	-12.36	1.12	1.25
1	I	67	SER	CA-CB	9.89	1.67	1.52
1	D	187	GLU	CD-OE2	9.61	1.36	1.25
1	J	25	ASN	N-CA	8.98	1.64	1.46
1	E	25	ASN	N-CA	8.96	1.64	1.46

The worst 5 of 3270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	42	ARG	NE-CZ-NH2	58.27	149.44	120.30
1	A	258	ARG	NE-CZ-NH1	54.61	147.61	120.30
1	Q	258	ARG	NE-CZ-NH1	48.20	144.40	120.30
1	D	258	ARG	NE-CZ-NH1	42.36	141.48	120.30
1	L	258	ARG	NE-CZ-NH2	-41.78	99.41	120.30

There are no chirality outliers.

5 of 133 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	THR	Mainchain
1	A	153	ILE	Mainchain
1	A	159	SER	Mainchain
1	A	220	HIS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	4	PHE	Mainchain

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	2730	0	2736	243	0
1	B	2651	0	2662	264	0
1	C	2635	0	2651	219	0
1	D	2701	0	2711	217	0
1	E	2687	0	2693	194	0
1	F	2675	0	2683	168	0
1	G	2628	0	2644	153	0
1	H	2712	0	2720	209	0
1	I	2628	0	2644	256	0
1	J	2701	0	2714	195	0
1	K	2686	0	2694	151	0
1	L	2628	0	2645	191	0
1	M	2730	0	2739	251	0
1	N	2628	0	2644	234	0
1	O	2628	0	2645	209	0
1	P	2730	0	2739	177	0
1	Q	2628	0	2645	147	0
1	R	2628	0	2644	155	0
2	A	5	0	0	2	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	G	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	N	5	0	0	0	0
2	R	5	0	0	0	0
2	S	35	0	0	3	0
3	A	87	0	0	17	0
3	B	32	0	0	4	0
3	C	46	0	0	3	0
3	D	79	0	0	6	0
3	E	74	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	81	0	0	14	0
3	G	74	0	0	5	0
3	H	71	0	0	9	0
3	I	46	0	0	7	0
3	J	77	0	0	18	0
3	K	72	0	0	6	0
3	L	27	0	0	2	0
3	M	81	0	0	9	0
3	N	55	0	0	5	0
3	O	36	0	0	8	0
3	P	77	0	0	12	0
3	Q	81	0	0	10	0
3	R	71	0	0	10	0
3	S	2	0	0	0	0
All	All	49278	0	48253	3328	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 3328 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:D:70:ASN:CB	1:D:70:ASN:CA	1.74	1.64
1:D:70:ASN:HD22	1:D:70:ASN:CA	1.30	1.41
1:E:89:GLN:OE1	1:E:89:GLN:CB	1.72	1.36
1:D:70:ASN:ND2	1:D:70:ASN:CA	1.87	1.35
1:A:356:LEU:HD13	1:A:357:PHE:CE1	1.65	1.32

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	358/363 (99%)	324 (90%)	27 (8%)	7 (2%)	9 15
1	B	346/363 (95%)	300 (87%)	35 (10%)	11 (3%)	5 6
1	C	343/363 (94%)	317 (92%)	22 (6%)	4 (1%)	16 29
1	D	354/363 (98%)	319 (90%)	24 (7%)	11 (3%)	5 7
1	E	352/363 (97%)	316 (90%)	25 (7%)	11 (3%)	5 7
1	F	351/363 (97%)	315 (90%)	25 (7%)	11 (3%)	5 7
1	G	342/363 (94%)	311 (91%)	25 (7%)	6 (2%)	11 18
1	H	355/363 (98%)	319 (90%)	22 (6%)	14 (4%)	4 5
1	I	342/363 (94%)	300 (88%)	34 (10%)	8 (2%)	8 12
1	J	354/363 (98%)	320 (90%)	24 (7%)	10 (3%)	6 9
1	K	352/363 (97%)	325 (92%)	22 (6%)	5 (1%)	14 24
1	L	342/363 (94%)	307 (90%)	30 (9%)	5 (2%)	13 22
1	M	358/363 (99%)	318 (89%)	29 (8%)	11 (3%)	5 7
1	N	342/363 (94%)	307 (90%)	29 (8%)	6 (2%)	11 18
1	O	342/363 (94%)	305 (89%)	33 (10%)	4 (1%)	16 29
1	P	358/363 (99%)	328 (92%)	23 (6%)	7 (2%)	9 15
1	Q	342/363 (94%)	319 (93%)	18 (5%)	5 (2%)	13 22
1	R	342/363 (94%)	316 (92%)	23 (7%)	3 (1%)	21 37
All	All	6275/6534 (96%)	5666 (90%)	470 (8%)	139 (2%)	8 13

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	3	ARG
1	A	87	ASP
1	A	357	PHE
1	B	69	ILE

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	287/290 (99%)	250 (87%)	37 (13%)	5 10
1	B	279/290 (96%)	244 (88%)	35 (12%)	6 10
1	C	277/290 (96%)	240 (87%)	37 (13%)	5 9
1	D	284/290 (98%)	250 (88%)	34 (12%)	6 12
1	E	282/290 (97%)	247 (88%)	35 (12%)	6 11
1	F	282/290 (97%)	241 (86%)	41 (14%)	4 7
1	G	276/290 (95%)	238 (86%)	38 (14%)	4 8
1	H	285/290 (98%)	252 (88%)	33 (12%)	7 13
1	I	276/290 (95%)	236 (86%)	40 (14%)	4 7
1	J	284/290 (98%)	249 (88%)	35 (12%)	6 11
1	K	283/290 (98%)	249 (88%)	34 (12%)	6 12
1	L	276/290 (95%)	240 (87%)	36 (13%)	5 9
1	M	287/290 (99%)	256 (89%)	31 (11%)	8 15
1	N	276/290 (95%)	242 (88%)	34 (12%)	6 11
1	O	276/290 (95%)	243 (88%)	33 (12%)	6 12
1	P	287/290 (99%)	255 (89%)	32 (11%)	8 14
1	Q	276/290 (95%)	245 (89%)	31 (11%)	7 14
1	R	276/290 (95%)	244 (88%)	32 (12%)	7 13
All	All	5049/5220 (97%)	4421 (88%)	628 (12%)	6 11

5 of 628 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	267	ILE
1	J	231	ASN
1	Q	173	TYR
1	I	16	SER
1	I	245	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	70	ASN
1	J	287	ASN
1	Q	125	GLN
1	I	89	GLN

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Mol	Chain	Res	Type
1	J	50	ASN

5.3.3 RNA

There are no RNA molecules 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

15 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	SO4	A	400	-	4,4,4	1.03	0	6,6,6	1.20	0
2	SO4	D	400	-	4,4,4	2.17	2 (50%)	6,6,6	2.19	2 (33%)
2	SO4	E	400	-	4,4,4	1.48	0	6,6,6	0.38	0
2	SO4	G	400	-	4,4,4	1.88	1 (25%)	6,6,6	0.36	0
2	SO4	J	400	-	4,4,4	1.40	0	6,6,6	0.45	0
2	SO4	K	400	-	4,4,4	1.67	1 (25%)	6,6,6	1.23	1 (16%)
2	SO4	N	400	-	4,4,4	1.46	1 (25%)	6,6,6	1.12	1 (16%)
2	SO4	R	400	-	4,4,4	1.62	0	6,6,6	1.67	1 (16%)
2	SO4	S	1	-	4,4,4	1.68	1 (25%)	6,6,6	0.78	0
2	SO4	S	2	-	4,4,4	1.10	0	6,6,6	1.04	1 (16%)
2	SO4	S	3	-	4,4,4	1.16	0	6,6,6	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	S	4	-	4,4,4	0.91	0	6,6,6	0.79	0
2	SO4	S	5	-	4,4,4	1.50	1 (25%)	6,6,6	1.10	1 (16%)
2	SO4	S	6	-	4,4,4	1.00	0	6,6,6	1.49	2 (33%)
2	SO4	S	7	-	4,4,4	0.77	0	6,6,6	0.83	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	SO4	A	400	-	-	0/0/0/0	0/0/0/0
2	SO4	D	400	-	-	0/0/0/0	0/0/0/0
2	SO4	E	400	-	-	0/0/0/0	0/0/0/0
2	SO4	G	400	-	-	0/0/0/0	0/0/0/0
2	SO4	J	400	-	-	0/0/0/0	0/0/0/0
2	SO4	K	400	-	-	0/0/0/0	0/0/0/0
2	SO4	N	400	-	-	0/0/0/0	0/0/0/0
2	SO4	R	400	-	-	0/0/0/0	0/0/0/0
2	SO4	S	1	-	-	0/0/0/0	0/0/0/0
2	SO4	S	2	-	-	0/0/0/0	0/0/0/0
2	SO4	S	3	-	-	0/0/0/0	0/0/0/0
2	SO4	S	4	-	-	0/0/0/0	0/0/0/0
2	SO4	S	5	-	-	0/0/0/0	0/0/0/0
2	SO4	S	6	-	-	0/0/0/0	0/0/0/0
2	SO4	S	7	-	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1	SO4	O1-S	2.22	1.54	1.47
2	N	400	SO4	O1-S	2.36	1.55	1.47
2	D	400	SO4	O2-S	2.73	1.56	1.47
2	S	5	SO4	O4-S	2.76	1.57	1.47
2	K	400	SO4	O2-S	3.11	1.57	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	400	SO4	O4-S-O3	-3.57	94.46	108.98
2	S	6	SO4	O2-S-O1	-2.74	100.82	109.50
2	N	400	SO4	O4-S-O3	-2.39	99.27	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	400	SO4	O2-S-O1	-2.31	102.17	109.50
2	S	2	SO4	O4-S-O3	2.01	117.14	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	SO4	2	0
2	S	1	SO4	2	0
2	S	6	SO4	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.