



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:01 PM UTC

PDB ID : 1QO5 / pdb_00001qo5
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

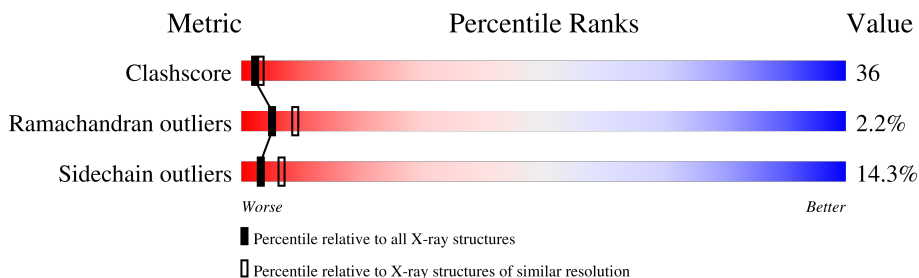
1 Overall quality at a glance

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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

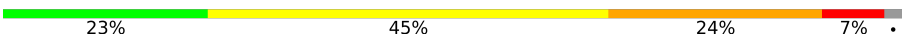
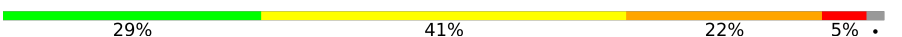
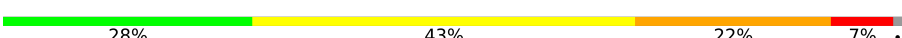
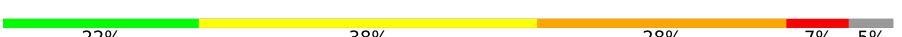
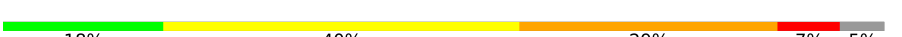
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	
1	F	363	
1	G	363	
1	H	363	

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Mol	Chain	Length	Quality of chain
1	I	363	
1	J	363	
1	K	363	
1	L	363	
1	M	363	
1	N	363	
1	O	363	
1	P	363	
1	Q	363	
1	R	363	

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	401	-	-	X	-
2	SO4	A	402	-	-	X	-
2	SO4	D	400	-	X	-	-

2 Entry composition

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 (CCD ID: SO4) (formula: O₄S).



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

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

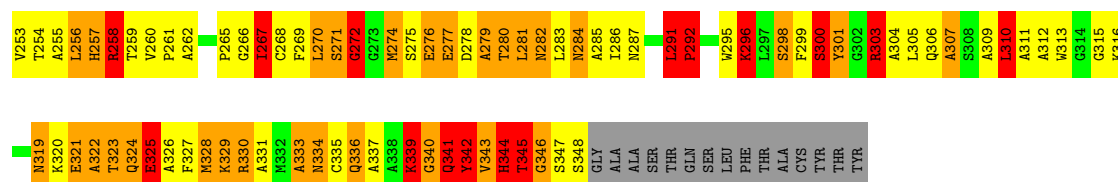
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	34	Total	O	0	0
			34	34		
3	C	44	Total	O	0	0
			44	44		
3	D	82	Total	O	0	0
			82	82		
3	E	75	Total	O	0	0
			75	75		
3	F	80	Total	O	0	0
			80	80		
3	G	75	Total	O	0	0
			75	75		
3	H	70	Total	O	0	0
			70	70		
3	I	45	Total	O	0	0
			45	45		
3	J	78	Total	O	0	0
			78	78		
3	K	71	Total	O	0	0
			71	71		
3	L	28	Total	O	0	0
			28	28		
3	M	81	Total	O	0	0
			81	81		

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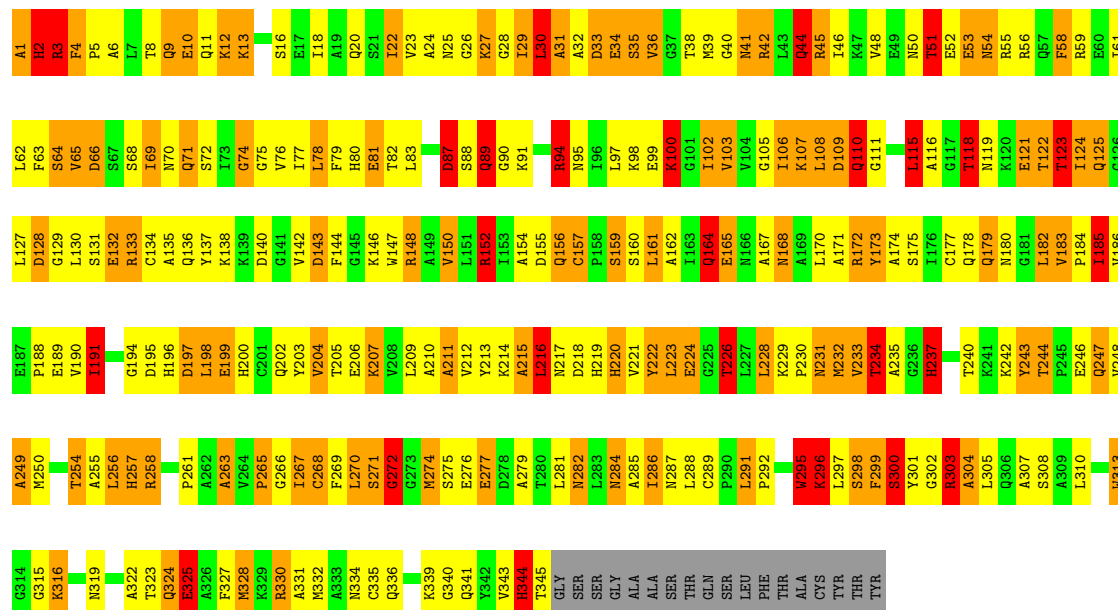
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	53	Total 53	O 53	0	0
3	O	37	Total 37	O 37	0	0
3	P	78	Total 78	O 78	0	0
3	Q	80	Total 80	O 80	0	0
3	R	72	Total 72	O 72	0	0



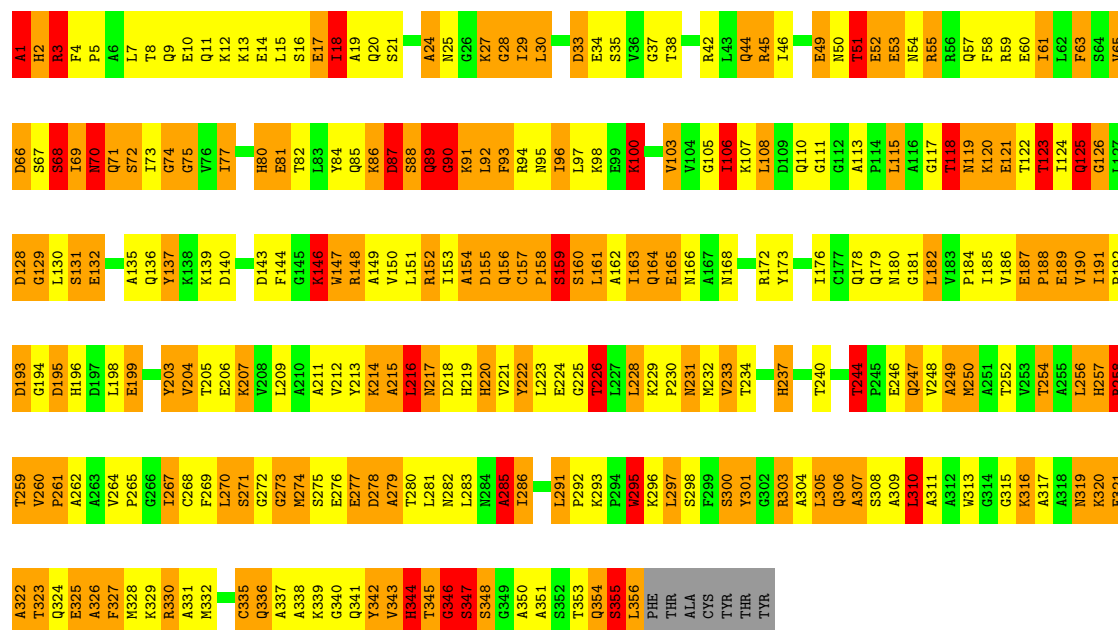
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain C: 22% 38% 27% 8% 5%

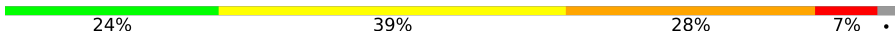


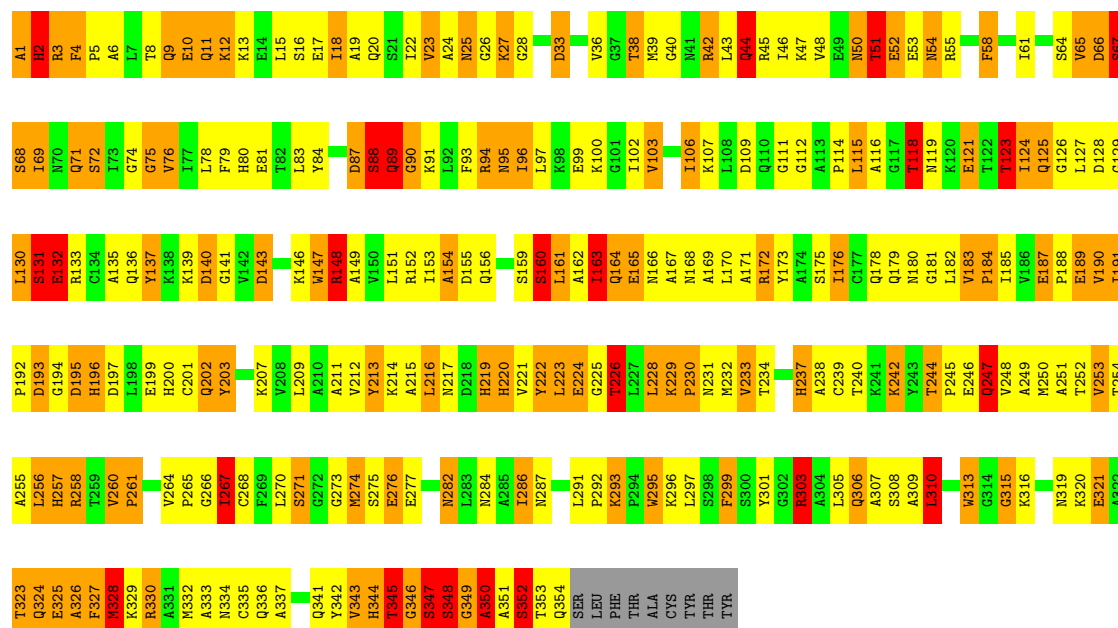
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain D: 21% 36% 34% 7%

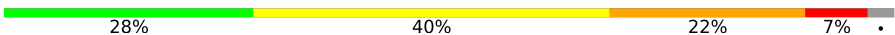


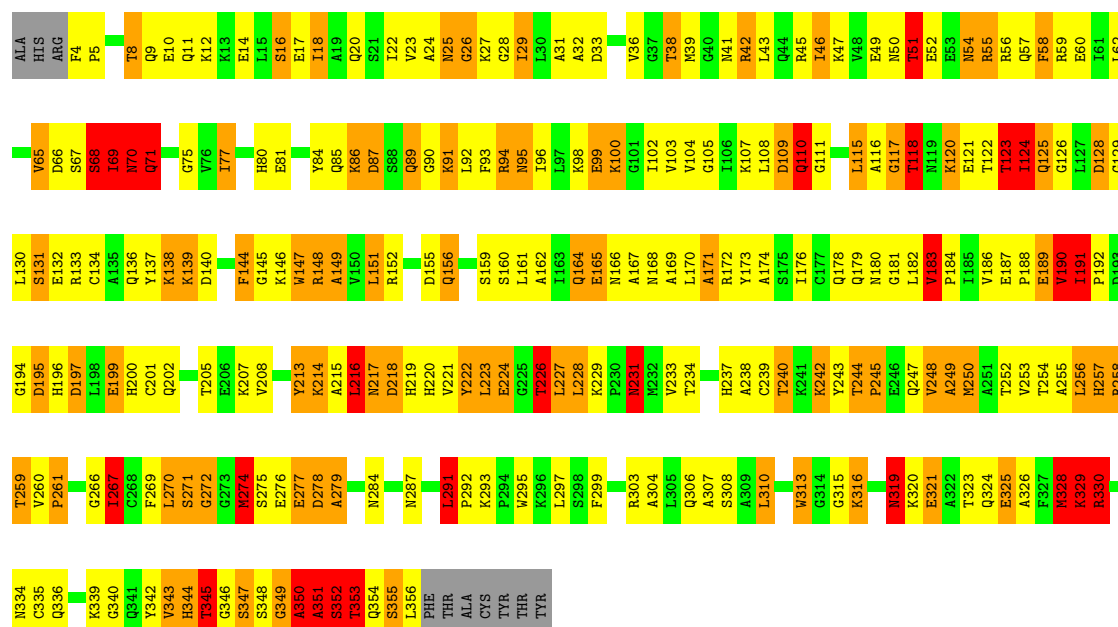
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain E:  24% 39% 28% 7%

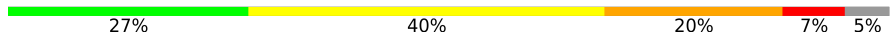


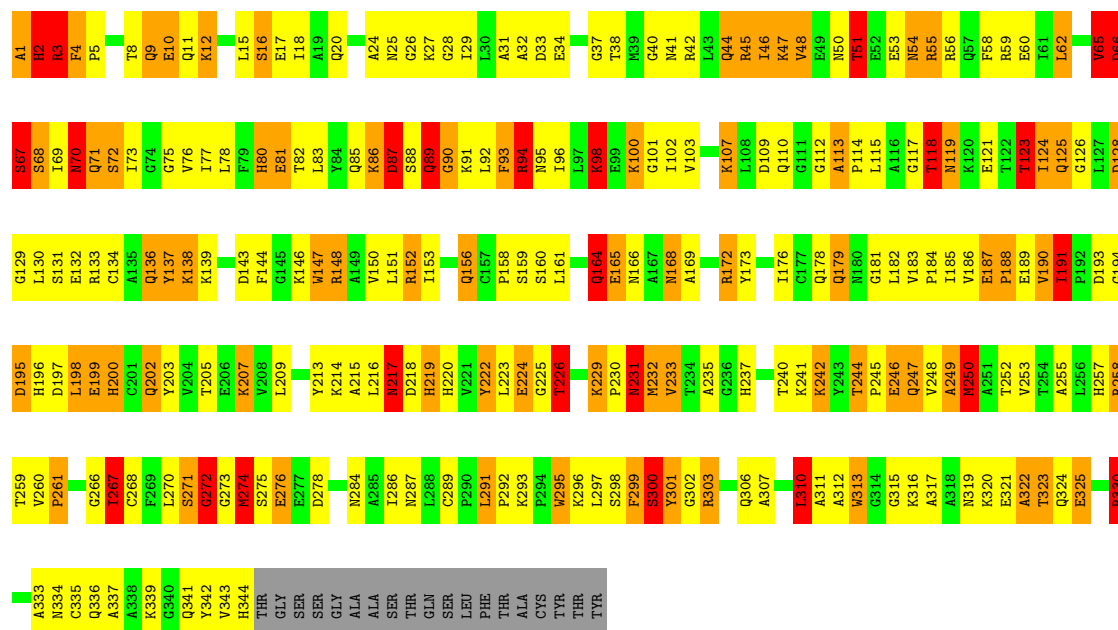
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain F:  28% 40% 22% 7%



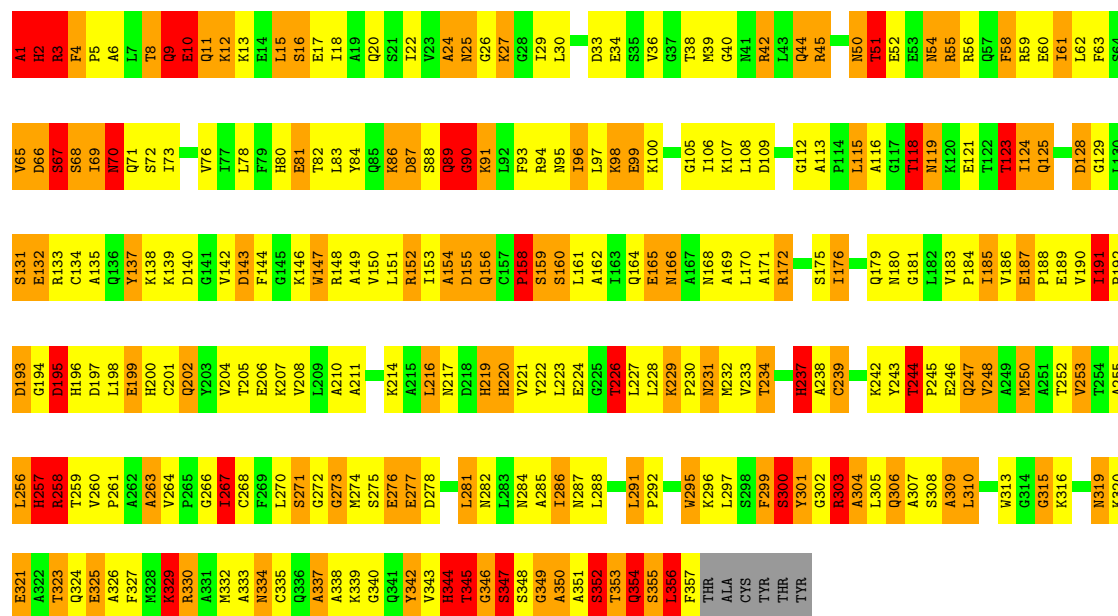
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain G:  27% 40% 20% 7% 5%



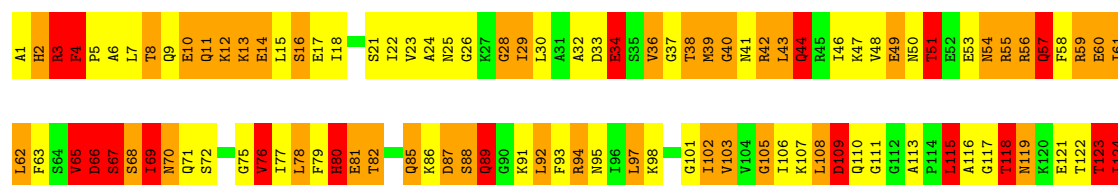
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

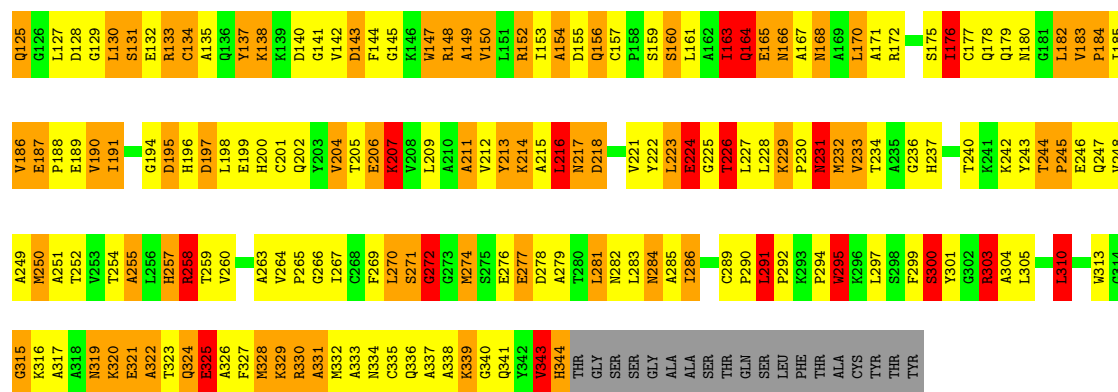
Chain H: 23% 41% 26% 8%



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

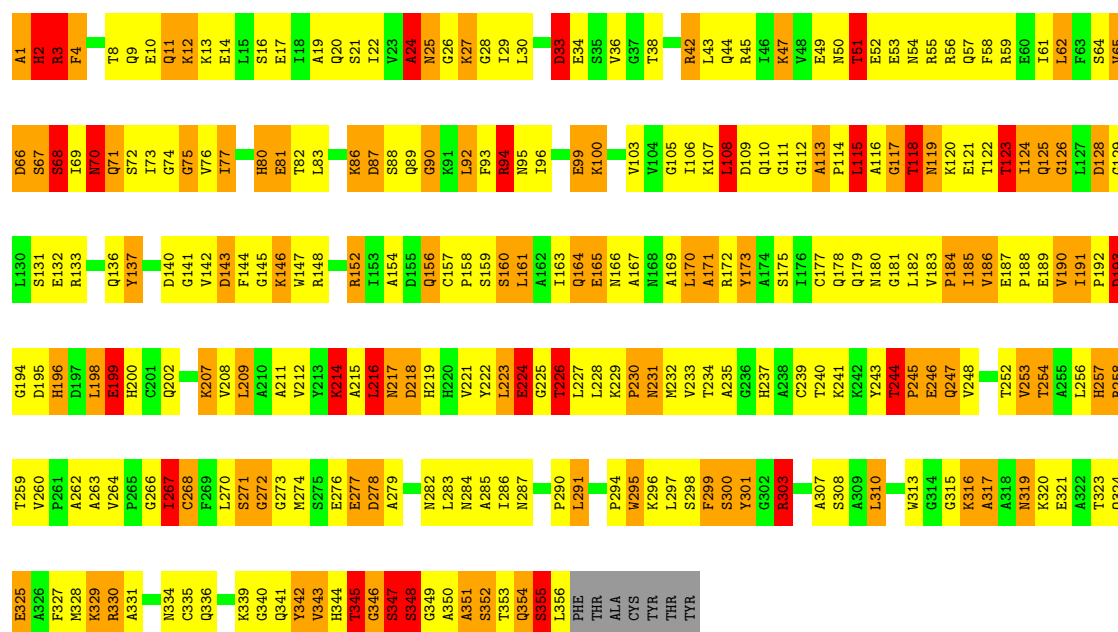
Chain I: 18% 39% 29% 10% 5%





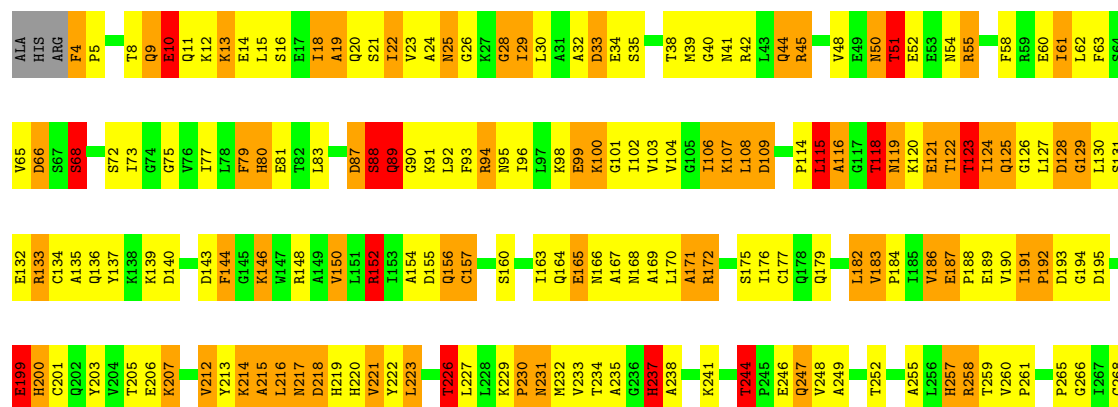
● Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

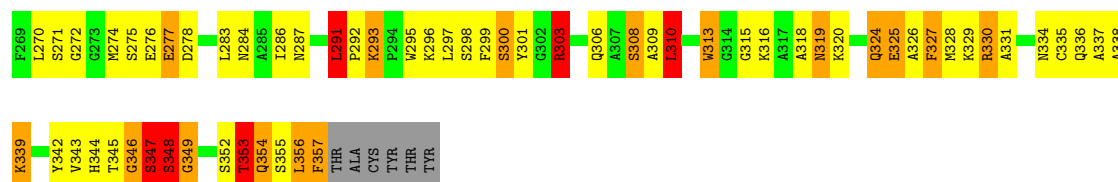
Chain J: 23% 45% 24% 7%



● Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

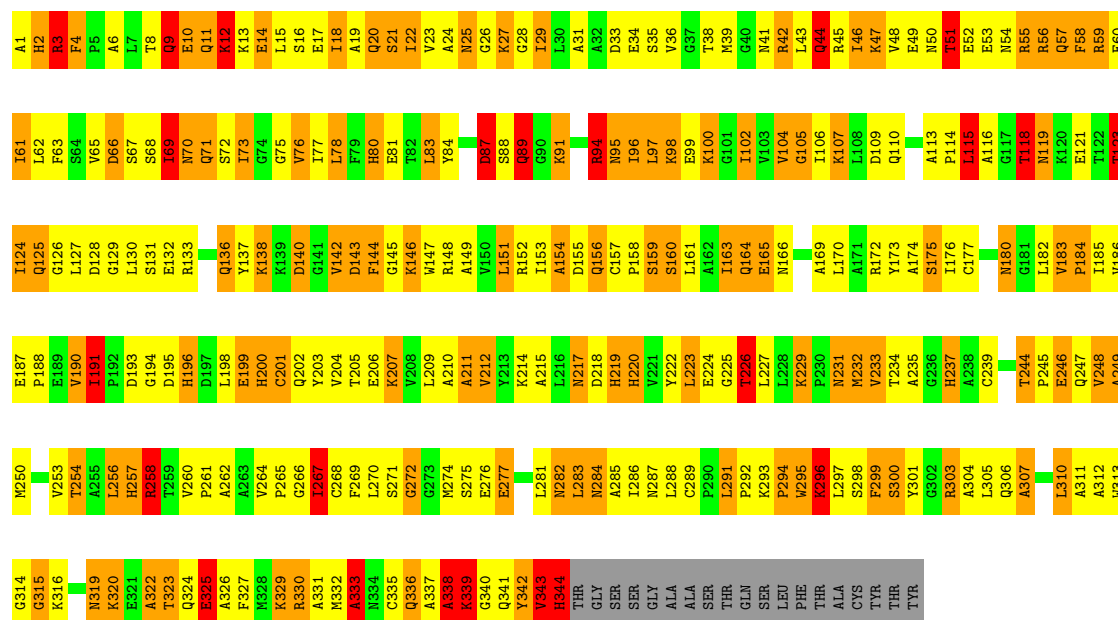
Chain K: 29% 41% 22% 5%





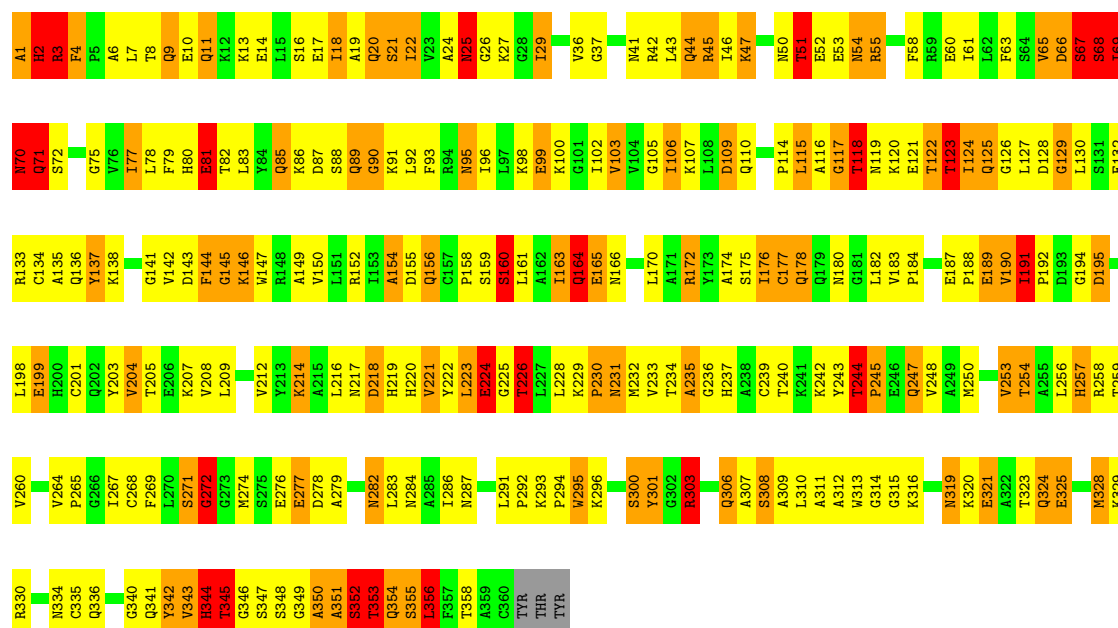
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain L: 19% 40% 29% 6% 5%



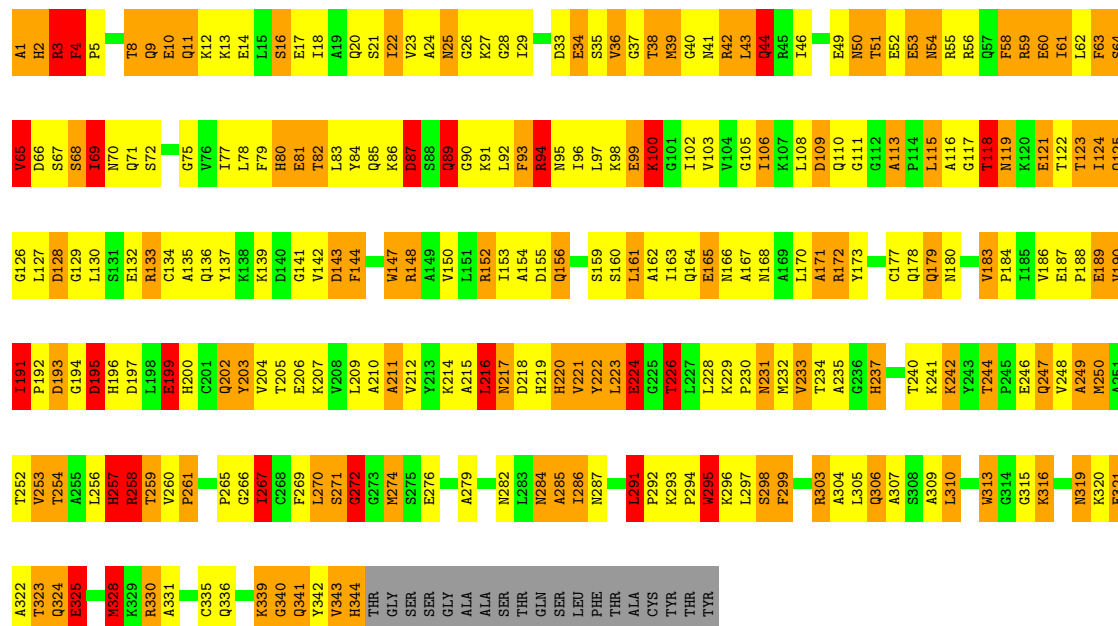
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain M: 28% 43% 22% 7%



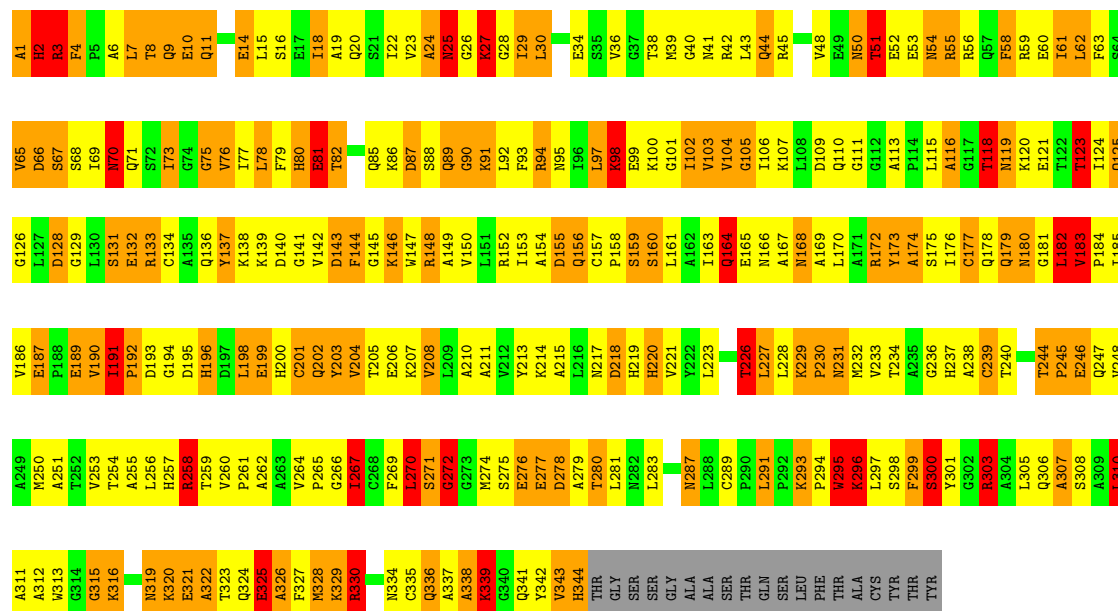
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain N:



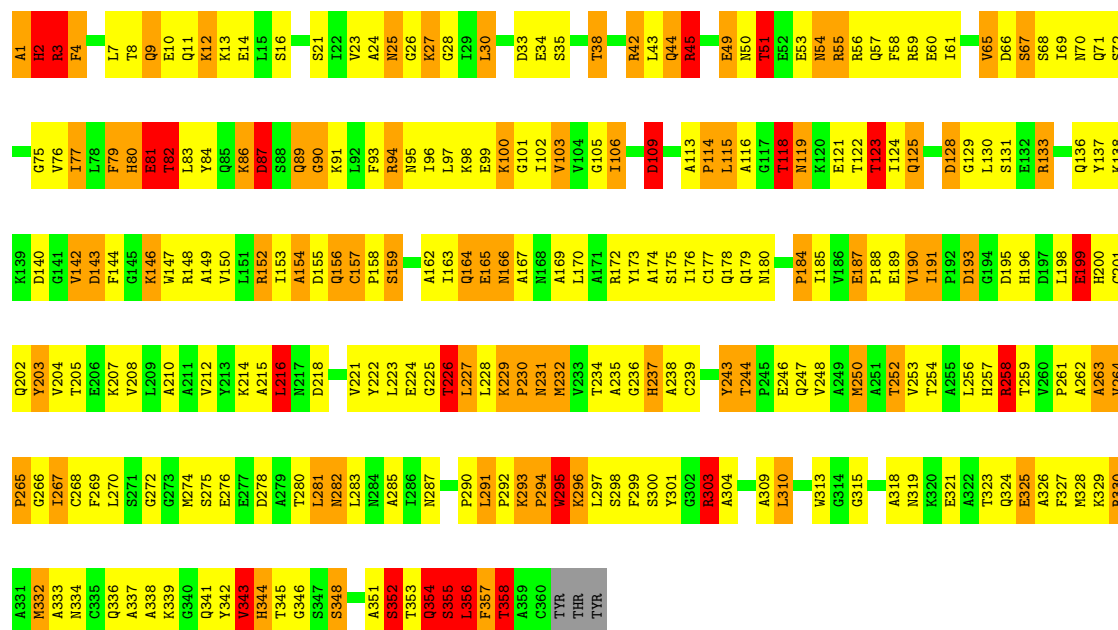
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain O:



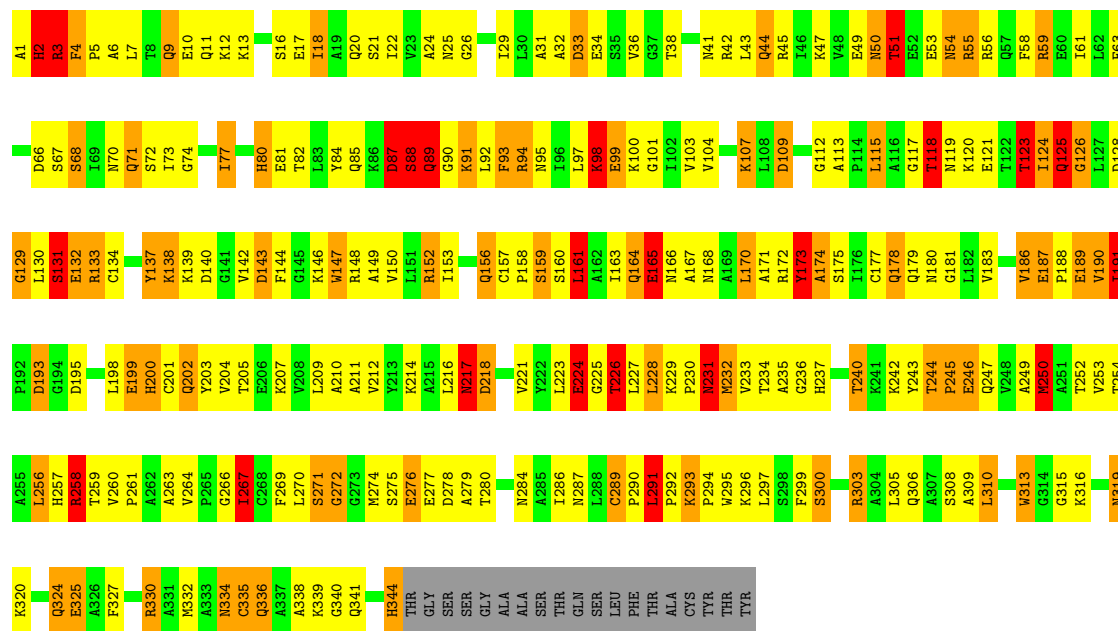
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain P:



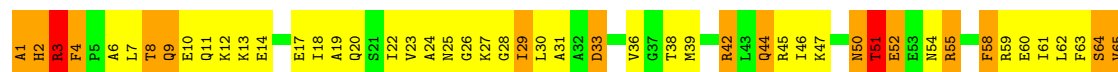
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain Q: 27% 42% 19% 6% 5%



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Chain R: 27% 40% 22% 5% 5%





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	1.51	22/2776 (0.8%)	3.29	395/3754 (10.5%)
1	B	1.79	56/2696 (2.1%)	3.58	525/3645 (14.4%)
1	C	1.34	5/2680 (0.2%)	3.27	404/3624 (11.1%)
1	D	1.69	34/2746 (1.2%)	3.59	488/3713 (13.1%)
1	E	1.44	16/2732 (0.6%)	3.57	434/3694 (11.7%)
1	F	1.36	9/2719 (0.3%)	3.25	380/3677 (10.3%)
1	G	1.40	15/2673 (0.6%)	3.21	380/3614 (10.5%)
1	H	1.36	13/2758 (0.5%)	3.34	405/3729 (10.9%)
1	I	1.45	13/2673 (0.5%)	3.42	449/3614 (12.4%)
1	J	1.43	13/2746 (0.5%)	3.29	384/3713 (10.3%)
1	K	1.42	13/2731 (0.5%)	3.19	377/3693 (10.2%)
1	L	1.39	7/2673 (0.3%)	3.13	368/3614 (10.2%)
1	M	1.43	14/2776 (0.5%)	3.27	380/3754 (10.1%)
1	N	1.41	11/2673 (0.4%)	3.39	431/3614 (11.9%)
1	O	1.41	15/2673 (0.6%)	3.22	431/3614 (11.9%)
1	P	1.37	8/2776 (0.3%)	3.13	347/3754 (9.2%)
1	Q	1.34	7/2673 (0.3%)	3.17	364/3614 (10.1%)
1	R	1.38	9/2673 (0.3%)	3.28	369/3614 (10.2%)
All	All	1.45	280/48847 (0.6%)	3.31	7311/66048 (11.1%)

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	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 280 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	TYR	C-O	-15.14	1.06	1.24
1	B	214	LYS	N-CA	-13.19	1.30	1.46
1	D	70	ASN	CA-CB	12.44	1.74	1.53
1	E	89	GLN	CA-C	11.65	1.68	1.52
1	G	4	PHE	CA-CB	10.55	1.61	1.52

The worst 5 of 7311 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	89	GLN	OE1-CD-NE2	46.95	169.55	122.60
1	J	94	ARG	CD-NE-CZ	38.79	178.70	124.40
1	C	3	ARG	CD-NE-CZ	37.00	176.21	124.40
1	E	94	ARG	CD-NE-CZ	36.10	174.94	124.40
1	D	1	ALA	CA-C-N	35.59	177.08	121.56

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

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	2739	252	0
1	B	2651	0	2665	279	0
1	C	2635	0	2651	227	0
1	D	2701	0	2713	235	0
1	E	2687	0	2696	205	0
1	F	2675	0	2685	174	0
1	G	2628	0	2645	163	0
1	H	2712	0	2721	224	0
1	I	2628	0	2644	260	0
1	J	2701	0	2714	199	0
1	K	2686	0	2694	154	0
1	L	2628	0	2645	202	0
1	M	2730	0	2739	255	0
1	N	2628	0	2644	243	0
1	O	2628	0	2645	218	0
1	P	2730	0	2740	186	0
1	Q	2628	0	2645	153	0
1	R	2628	0	2645	164	0
2	A	10	0	0	4	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	G	15	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	M	5	0	0	0	0
2	O	5	0	0	0	0
2	P	10	0	0	0	0
2	R	10	0	0	1	0
3	A	86	0	0	17	0
3	B	34	0	0	4	0
3	C	44	0	0	2	0
3	D	82	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	75	0	0	7	0
3	F	80	0	0	14	0
3	G	75	0	0	5	0
3	H	70	0	0	9	0
3	I	45	0	0	7	0
3	J	78	0	0	17	0
3	K	71	0	0	6	0
3	L	28	0	0	2	0
3	M	81	0	0	9	0
3	N	53	0	0	5	0
3	O	37	0	0	8	0
3	P	78	0	0	11	0
3	Q	80	0	0	10	0
3	R	72	0	0	10	0
All	All	49278	0	48270	3485	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 36.

The worst 5 of 3485 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:CA	1:D:70:ASN:CB	1.74	1.64
1:D:70:ASN:CA	1:D:70:ASN:HD22	1.30	1.41
1:E:89:GLN:OE1	1:E:89:GLN:CB	1.72	1.36
1:D:70:ASN:CA	1:D:70:ASN:ND2	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%)	6	10
1	B	346/363 (95%)	300 (87%)	35 (10%)	11 (3%)	3	4
1	C	343/363 (94%)	317 (92%)	22 (6%)	4 (1%)	10	20
1	D	354/363 (98%)	319 (90%)	24 (7%)	11 (3%)	3	5
1	E	344/363 (95%)	308 (90%)	25 (7%)	11 (3%)	3	4
1	F	351/363 (97%)	315 (90%)	25 (7%)	11 (3%)	3	5
1	G	342/363 (94%)	311 (91%)	25 (7%)	6 (2%)	6	12
1	H	355/363 (98%)	319 (90%)	22 (6%)	14 (4%)	2	3
1	I	342/363 (94%)	300 (88%)	34 (10%)	8 (2%)	5	8
1	J	354/363 (98%)	320 (90%)	24 (7%)	10 (3%)	4	6
1	K	352/363 (97%)	325 (92%)	22 (6%)	5 (1%)	9	17
1	L	342/363 (94%)	307 (90%)	30 (9%)	5 (2%)	8	16
1	M	358/363 (99%)	318 (89%)	29 (8%)	11 (3%)	3	5
1	N	342/363 (94%)	307 (90%)	29 (8%)	6 (2%)	6	12
1	O	342/363 (94%)	305 (89%)	33 (10%)	4 (1%)	10	20
1	P	358/363 (99%)	328 (92%)	23 (6%)	7 (2%)	6	10
1	Q	342/363 (94%)	319 (93%)	18 (5%)	5 (2%)	8	16
1	R	342/363 (94%)	316 (92%)	23 (7%)	3 (1%)	14	27
All	All	6267/6534 (96%)	5658 (90%)	470 (8%)	139 (2%)	5	9

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 ⓘ

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%)	245 (85%)	42 (15%)	3	6
1	B	279/290 (96%)	237 (85%)	42 (15%)	3	5
1	C	277/290 (96%)	231 (83%)	46 (17%)	2	4
1	D	284/290 (98%)	248 (87%)	36 (13%)	4	9
1	E	282/290 (97%)	244 (86%)	38 (14%)	4	8
1	F	282/290 (97%)	236 (84%)	46 (16%)	2	4
1	G	276/290 (95%)	234 (85%)	42 (15%)	3	5
1	H	285/290 (98%)	241 (85%)	44 (15%)	2	5
1	I	276/290 (95%)	231 (84%)	45 (16%)	2	4
1	J	284/290 (98%)	247 (87%)	37 (13%)	4	8
1	K	283/290 (98%)	246 (87%)	37 (13%)	4	8
1	L	276/290 (95%)	234 (85%)	42 (15%)	3	5
1	M	287/290 (99%)	249 (87%)	38 (13%)	4	8
1	N	276/290 (95%)	240 (87%)	36 (13%)	4	8
1	O	276/290 (95%)	234 (85%)	42 (15%)	3	5
1	P	287/290 (99%)	250 (87%)	37 (13%)	4	9
1	Q	276/290 (95%)	241 (87%)	35 (13%)	4	9
1	R	276/290 (95%)	241 (87%)	35 (13%)	4	9
All	All	5049/5220 (97%)	4329 (86%)	720 (14%)	3	6

5 of 720 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	69	ILE
1	O	9	GLN
1	L	176	ILE
1	L	51	THR
1	M	245	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	166	ASN
1	L	217	ASN
1	R	231	ASN
1	Q	125	GLN

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Mol	Chain	Res	Type
1	J	217	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	401	-	4,4,4	0.77	0	6,6,6	1.06	0
2	SO4	G	401	-	4,4,4	1.25	1 (25%)	6,6,6	0.42	0
2	SO4	G	403	-	4,4,4	0.63	0	6,6,6	0.73	0
2	SO4	K	400	-	4,4,4	1.18	1 (25%)	6,6,6	1.27	0
2	SO4	O	401	-	4,4,4	0.73	0	6,6,6	0.72	0
2	SO4	D	400	-	4,4,4	1.50	1 (25%)	6,6,6	3.07	3 (50%)
2	SO4	E	400	-	4,4,4	0.97	0	6,6,6	0.40	0
2	SO4	J	400	-	4,4,4	0.88	0	6,6,6	0.64	0
2	SO4	P	402	-	4,4,4	0.54	0	6,6,6	0.54	0
2	SO4	R	402	-	4,4,4	0.66	0	6,6,6	1.04	0
2	SO4	G	402	-	4,4,4	0.81	0	6,6,6	0.93	0
2	SO4	M	401	-	4,4,4	0.72	0	6,6,6	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	R	401	-	4,4,4	1.05	0	6,6,6	1.50	1 (16%)
2	SO4	A	402	-	4,4,4	0.95	0	6,6,6	1.18	1 (16%)
2	SO4	P	401	-	4,4,4	1.03	0	6,6,6	1.21	1 (16%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	SO4	O2-S	2.26	1.58	1.44
2	D	400	SO4	O1-S	2.23	1.58	1.44
2	K	400	SO4	O2-S	2.18	1.57	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	SO4	O4-S-O1	6.32	142.60	109.56
2	D	400	SO4	O4-S-O2	-2.95	94.16	109.56
2	D	400	SO4	O4-S-O3	-2.55	94.46	108.54
2	R	401	SO4	O4-S-O3	2.54	122.56	108.54
2	A	402	SO4	O4-S-O1	-2.47	96.66	109.56

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	401	SO4	2	0
2	R	402	SO4	1	0
2	A	402	SO4	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.