wwPDB X-ray Structure Validation Summary Report (i)

May 2, 2024 – 04:22 PM JST

PDB ID	:	5YB0
Title	:	Crystal Structure of Wild Type Phosphoserine aminotransferase (PSAT) from E. histolytica
Authors	:	Singh, R.K.; Gourinath, S.
Deposited on	:	2017-09-02
Resolution	:	2.94 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:

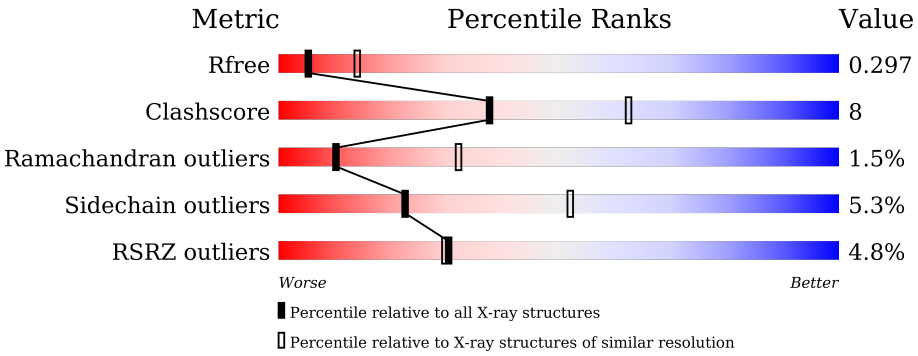
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	358	78% 15%
1	B	358	3% 75% 18%
1	C	358	75% 20%
1	D	358	5% 79% 16%
1	E	358	3% 81% 13%
1	F	358	78% 10% 10%

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Mol	Chain	Length	Quality of chain
1	G	358	2% 84% 10% 5%
1	H	358	8% 87% 9%
1	I	358	9% 84% 8% 6%
1	J	358	9% 66% 29%
1	K	358	8% 82% 5% 12%
1	L	358	3% 56% 40%

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	PLP	A	401	-	-	X	-
2	PLP	F	401	-	-	X	-

2 Entry composition (i)

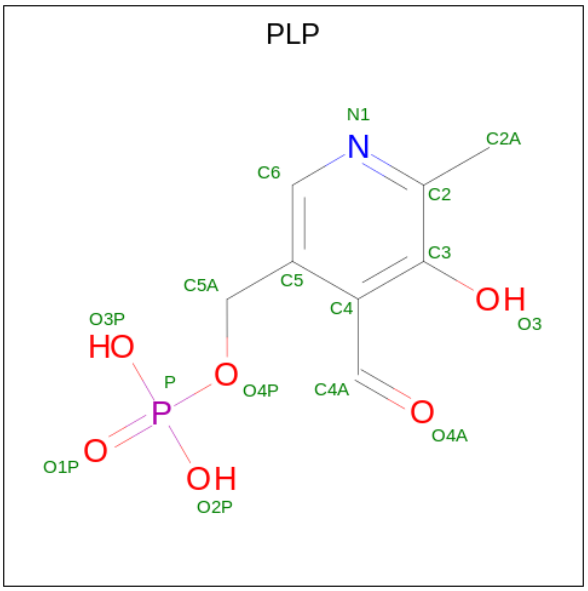
There are 4 unique types of molecules in this entry. The entry contains 27402 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoserine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2751	1765	458	513	15			
1	B	349	Total	C	N	O	S	0	0	0
			2759	1771	459	514	15			
1	C	349	Total	C	N	O	S	0	0	0
			2703	1734	450	504	15			
1	D	345	Total	C	N	O	S	0	0	0
			2603	1666	438	485	14			
1	E	342	Total	C	N	O	S	0	0	0
			2477	1579	419	464	15			
1	F	322	Total	C	N	O	S	0	0	0
			2300	1466	380	442	12			
1	G	341	Total	C	N	O	S	0	0	0
			2506	1600	425	466	15			
1	H	349	Total	C	N	O	S	0	0	0
			2225	1401	394	419	11			
1	I	336	Total	C	N	O	S	0	0	0
			2246	1407	395	431	13			
1	J	253	Total	C	N	O	S	0	0	0
			1491	926	265	291	9			
1	K	316	Total	C	N	O	S	0	0	0
			1752	1075	326	347	4			
1	L	216	Total	C	N	O	S	0	0	0
			1269	790	230	245	4			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 16 8 1 6 1	0	0
2	B	1	Total C N O P 16 8 1 6 1	0	0
2	C	1	Total C N O P 16 8 1 6 1	0	0
2	D	1	Total C N O P 16 8 1 6 1	0	0
2	E	1	Total C N O P 16 8 1 6 1	0	0
2	F	1	Total C N O P 16 8 1 6 1	0	0
2	G	1	Total C N O P 16 8 1 6 1	0	0
2	H	1	Total C N O P 16 8 1 6 1	0	0
2	I	1	Total C N O P 16 8 1 6 1	0	0
2	K	1	Total C N O P 16 8 1 6 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

- Molecule 4 is water.

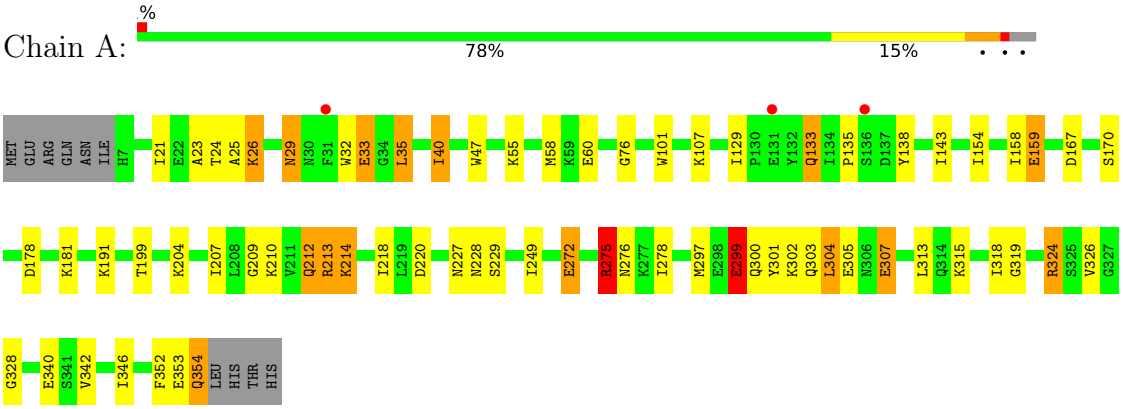
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	12	Total O 12 12	0	0
4	C	16	Total O 16 16	0	0
4	D	11	Total O 11 11	0	0
4	E	18	Total O 18 18	0	0
4	F	9	Total O 9 9	0	0
4	G	13	Total O 13 13	0	0
4	H	19	Total O 19 19	0	0
4	I	23	Total O 23 23	0	0
4	J	10	Total O 10 10	0	0
4	K	8	Total O 8 8	0	0
4	L	2	Total O 2 2	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.

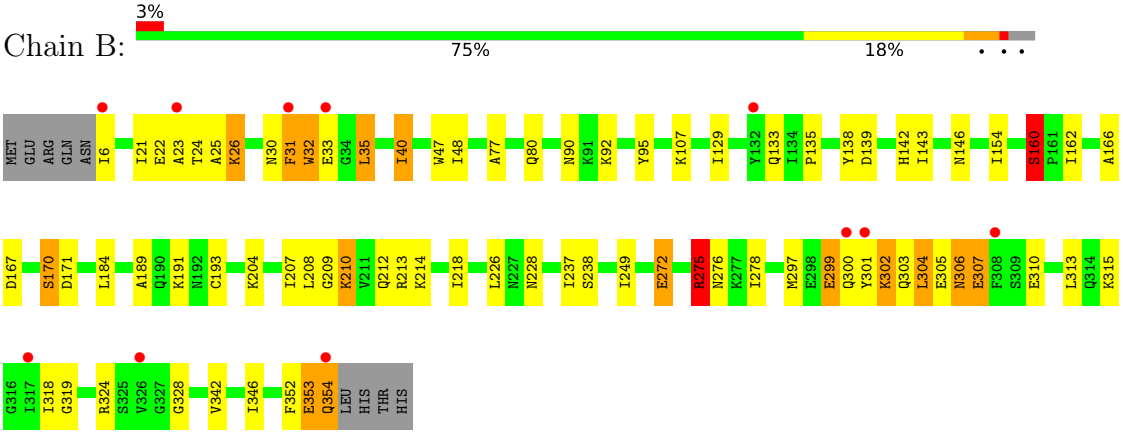
• Molecule 1: Phosphoserine aminotransferase

Chain A:



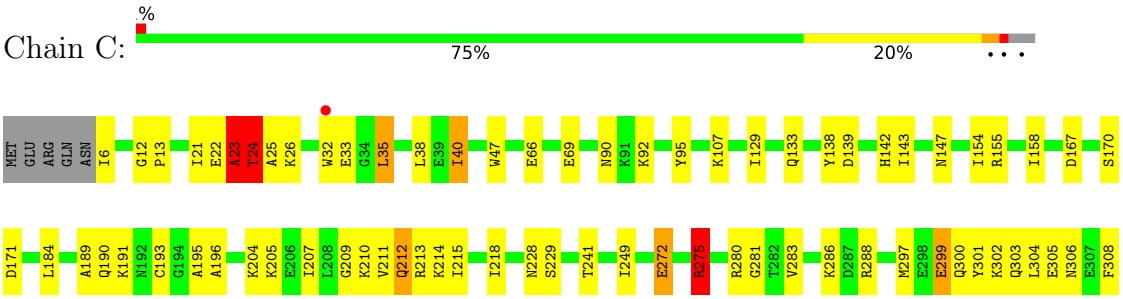
• Molecule 1: Phosphoserine aminotransferase

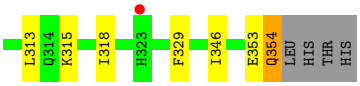
Chain B:



• Molecule 1: Phosphoserine aminotransferase

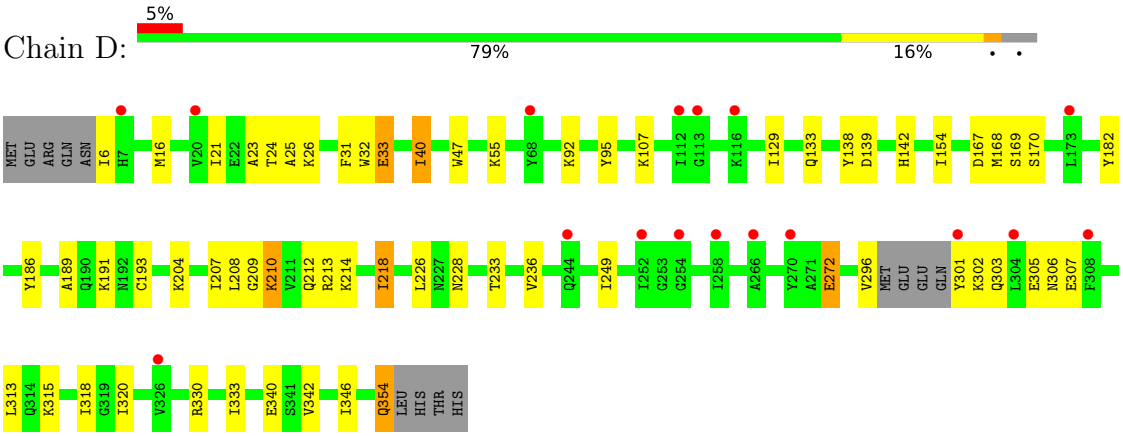
Chain C:





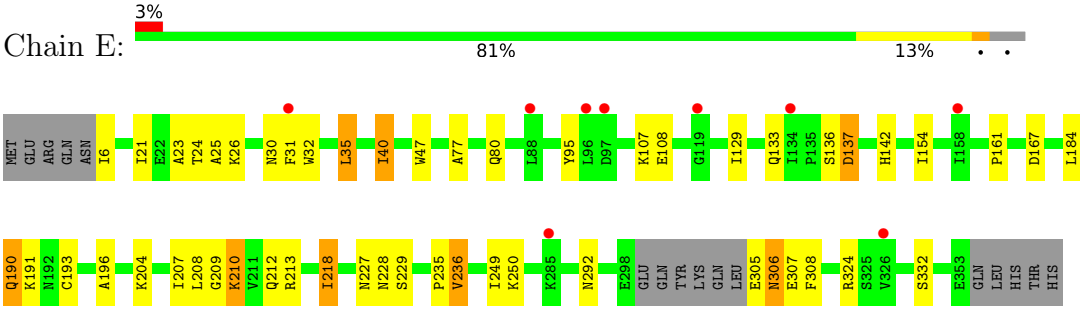
• Molecule 1: Phosphoserine aminotransferase

Chain D:



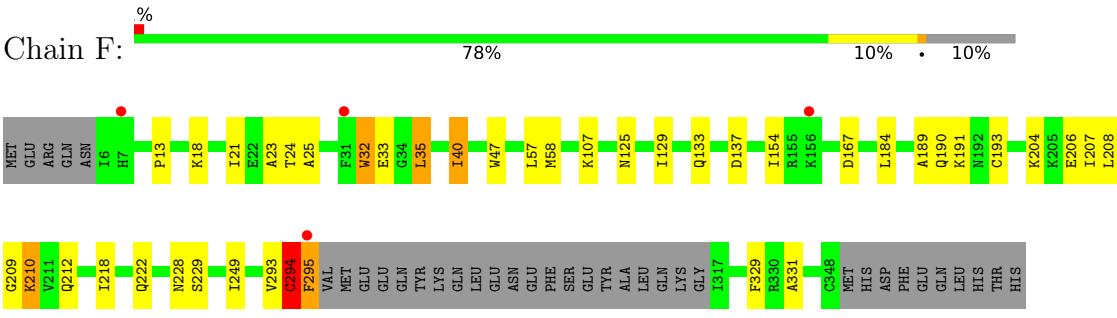
• Molecule 1: Phosphoserine aminotransferase

Chain E:



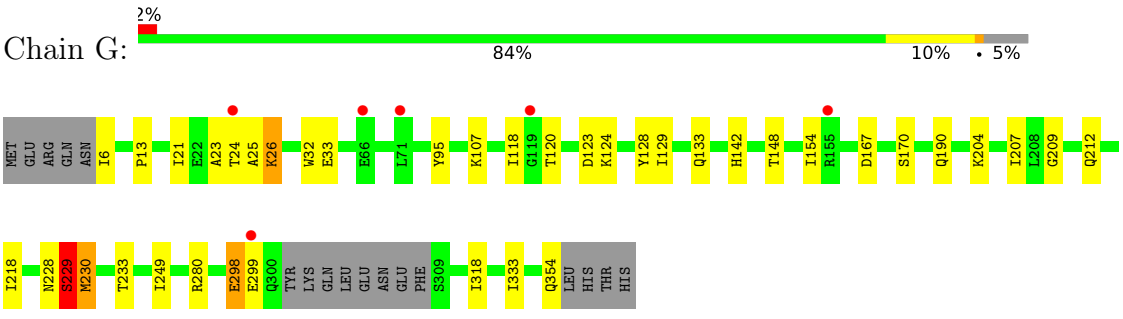
• Molecule 1: Phosphoserine aminotransferase

Chain F:



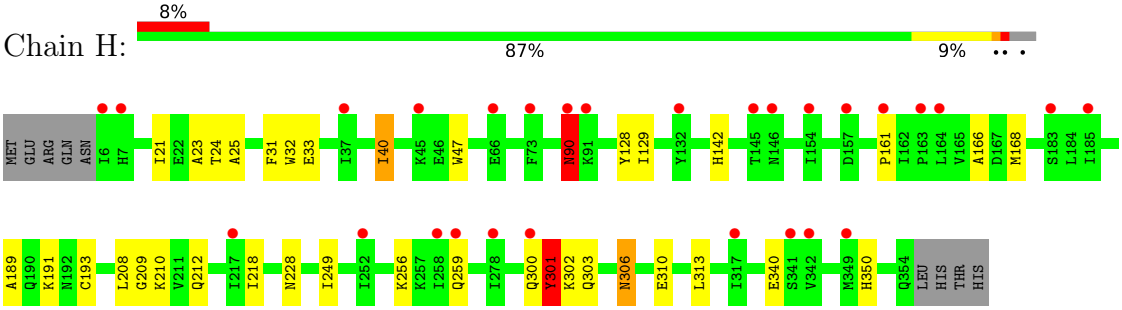
• Molecule 1: Phosphoserine aminotransferase

Chain G:



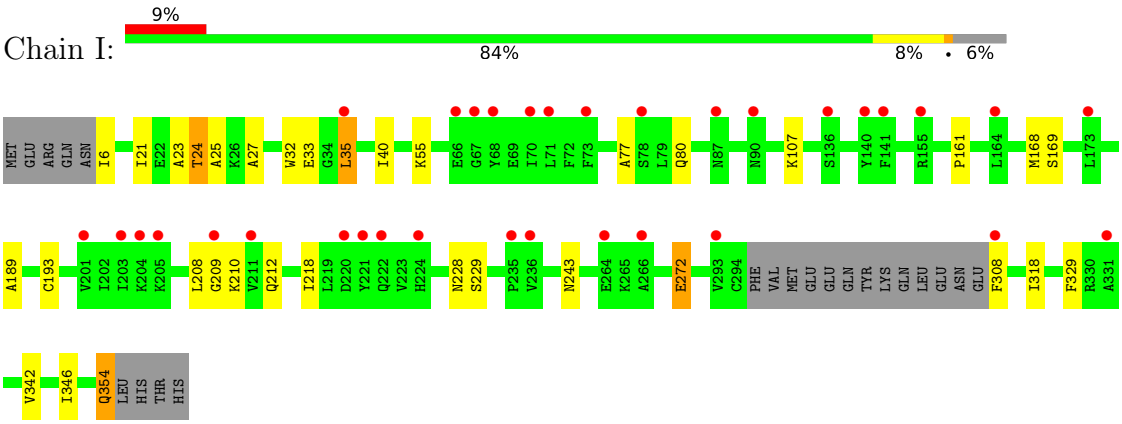
• Molecule 1: Phosphoserine aminotransferase

Chain H:



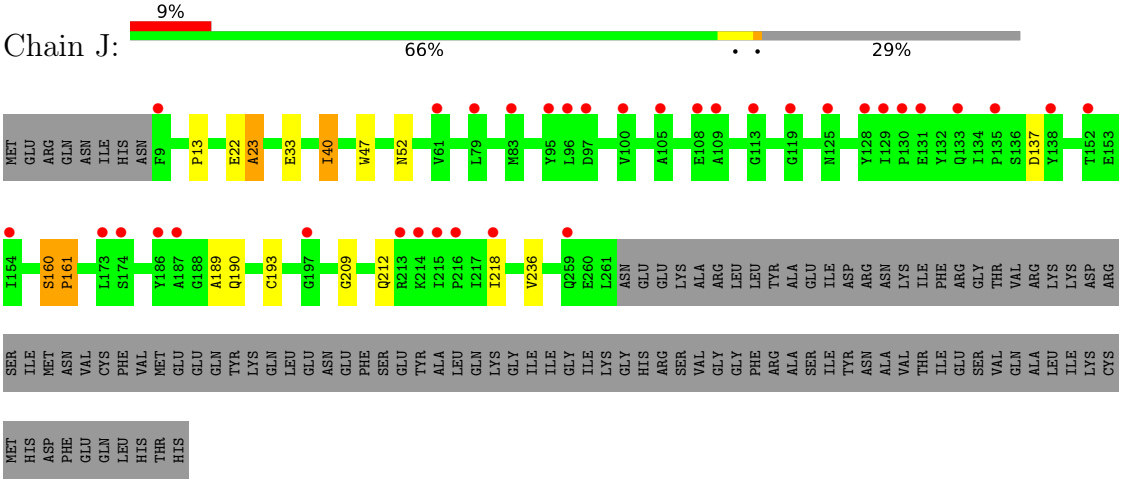
• Molecule 1: Phosphoserine aminotransferase

Chain I:



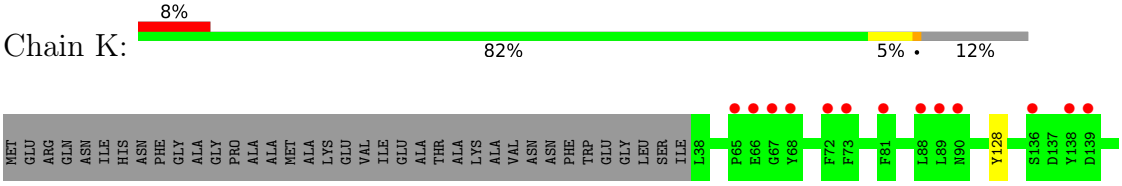
• Molecule 1: Phosphoserine aminotransferase

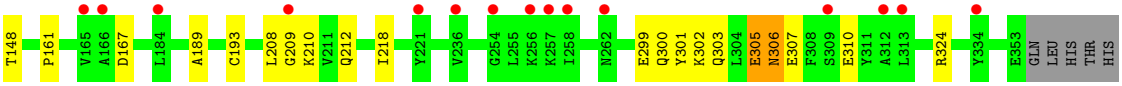
Chain J:



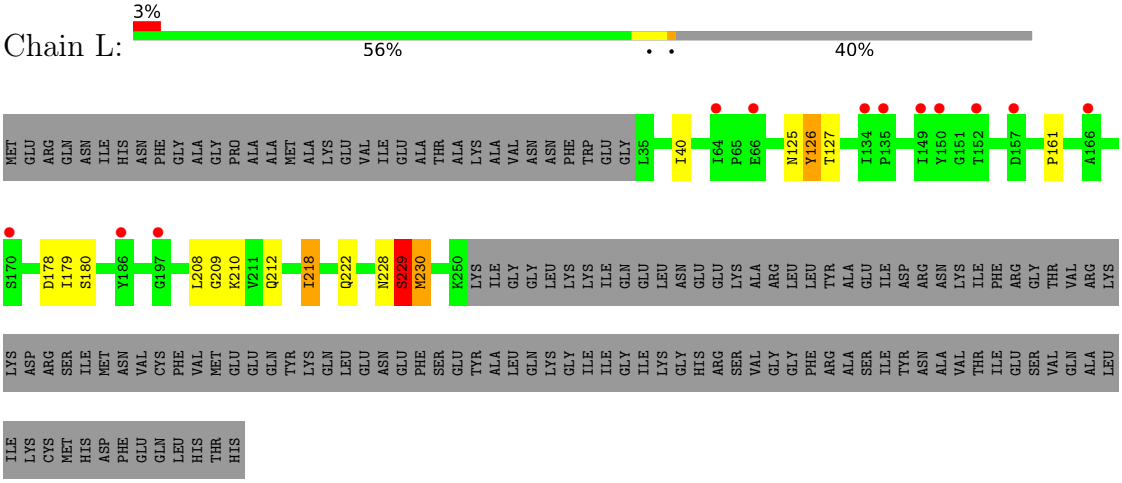
• Molecule 1: Phosphoserine aminotransferase

Chain K:





• Molecule 1: Phosphoserine aminotransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.45Å 134.07Å 139.06Å 62.85° 88.58° 74.92°	Depositor
Resolution (Å)	50.15 – 2.94 50.08 – 3.01	Depositor EDS
% Data completeness (in resolution range)	87.9 (50.15-2.94) 87.9 (50.08-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.265 , 0.301 0.259 , 0.297	Depositor DCC
R_{free} test set	3837 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	76.4	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,h-k,-l	Xtriage
Reported twinning fraction	0.888 for H, K, L 0.112 for H, H-K, -L	Depositor
Outliers	0 of 76766 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	27402	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CL, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.67	0/2799	0.85	4/3771 (0.1%)
1	B	0.60	0/2807	0.86	4/3782 (0.1%)
1	C	0.57	0/2749	0.76	2/3710 (0.1%)
1	D	0.51	0/2644	0.70	1/3571 (0.0%)
1	E	0.54	0/2515	0.67	0/3410
1	F	1.04	8/2336 (0.3%)	0.82	9/3178 (0.3%)
1	G	0.48	0/2547	0.66	0/3448
1	H	0.47	1/2255 (0.0%)	0.72	5/3096 (0.2%)
1	I	0.43	0/2275	0.59	0/3100
1	J	0.50	0/1508	0.68	3/2082 (0.1%)
1	K	0.42	0/1769	0.63	0/2455
1	L	0.43	0/1285	0.63	1/1778 (0.1%)
All	All	0.59	9/27489 (0.0%)	0.73	29/37381 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	1
1	H	0	5
1	I	0	1
1	J	0	2
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	27

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	295	PHE	CA-C	23.87	2.15	1.52
1	F	295	PHE	C-O	22.02	1.65	1.23
1	F	295	PHE	N-CA	17.75	1.81	1.46
1	F	294	CYS	CA-C	16.00	1.94	1.52
1	F	294	CYS	C-N	10.57	1.58	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	160	SER	C-N-CD	-17.05	83.08	120.60
1	F	294	CYS	N-CA-CB	-10.71	91.33	110.60
1	B	160	SER	C-N-CA	10.64	166.68	122.00
1	H	32	TRP	N-CA-C	-10.57	82.47	111.00
1	F	295	PHE	CA-C-O	-10.31	98.44	120.10

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	GLN	Peptide
1	A	299	GLU	Peptide
1	B	160	SER	Peptide
1	B	212	GLN	Peptide
1	B	299	GLU	Peptide

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	2751	0	2813	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2759	0	2823	82	1
1	C	2703	0	2726	64	0
1	D	2603	0	2592	33	0
1	E	2477	0	2358	40	0
1	F	2300	0	2138	35	0
1	G	2506	0	2407	25	1
1	H	2225	0	1837	21	0
1	I	2246	0	1931	24	0
1	J	1491	0	1103	10	0
1	K	1752	0	1108	11	0
1	L	1269	0	893	8	0
2	A	16	0	7	9	0
2	B	16	0	8	4	0
2	C	16	0	7	3	0
2	D	16	0	8	3	0
2	E	16	0	8	3	0
2	F	16	0	8	6	0
2	G	16	0	7	1	0
2	H	16	0	7	4	0
2	I	16	0	8	0	0
2	K	16	0	7	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	14	0	0	1	0
4	B	12	0	0	0	0
4	C	16	0	0	2	0
4	D	11	0	0	0	0
4	E	18	0	0	1	0
4	F	9	0	0	2	0
4	G	13	0	0	2	0
4	H	19	0	0	6	0
4	I	23	0	0	3	0
4	J	10	0	0	3	0
4	K	8	0	0	2	0
4	L	2	0	0	0	0
All	All	27402	0	24804	400	1

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 8.

The worst 5 of 400 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:F:295:PHE:N	1:F:295:PHE:CA	1.81	1.42
1:F:295:PHE:O	1:F:295:PHE:C	1.65	1.35
1:F:294:CYS:C	1:F:294:CYS:CA	1.94	1.35
1:B:354:GLN:O	1:B:354:GLN:NE2	1.62	1.33
1:F:295:PHE:CA	1:F:295:PHE:C	2.15	1.15

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLU:OE1	1:G:128:TYR:OH[1_455]	2.17	0.03

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	346/358 (97%)	321 (93%)	21 (6%)	4 (1%)	13 38
1	B	347/358 (97%)	319 (92%)	22 (6%)	6 (2%)	9 29
1	C	347/358 (97%)	327 (94%)	15 (4%)	5 (1%)	11 34
1	D	341/358 (95%)	318 (93%)	17 (5%)	6 (2%)	8 27
1	E	338/358 (94%)	314 (93%)	17 (5%)	7 (2%)	7 24
1	F	318/358 (89%)	301 (95%)	15 (5%)	2 (1%)	25 56
1	G	337/358 (94%)	321 (95%)	11 (3%)	5 (2%)	10 32
1	H	347/358 (97%)	322 (93%)	18 (5%)	7 (2%)	7 25
1	I	332/358 (93%)	314 (95%)	15 (4%)	3 (1%)	17 46
1	J	251/358 (70%)	237 (94%)	12 (5%)	2 (1%)	19 49
1	K	314/358 (88%)	294 (94%)	14 (4%)	6 (2%)	8 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	214/358 (60%)	201 (94%)	8 (4%)	5 (2%)	6 22
All	All	3832/4296 (89%)	3589 (94%)	185 (5%)	58 (2%)	10 32

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLU
1	B	31	PHE
1	B	32	TRP
1	B	160	SER
1	B	306	ASN

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	299/310 (96%)	273 (91%)	26 (9%)	10 29
1	B	300/310 (97%)	280 (93%)	20 (7%)	16 41
1	C	286/310 (92%)	268 (94%)	18 (6%)	18 44
1	D	267/310 (86%)	250 (94%)	17 (6%)	17 43
1	E	235/310 (76%)	225 (96%)	10 (4%)	29 60
1	F	214/310 (69%)	206 (96%)	8 (4%)	34 65
1	G	242/310 (78%)	233 (96%)	9 (4%)	34 65
1	H	159/310 (51%)	153 (96%)	6 (4%)	33 64
1	I	179/310 (58%)	171 (96%)	8 (4%)	27 58
1	J	86/310 (28%)	84 (98%)	2 (2%)	50 78
1	K	67/310 (22%)	66 (98%)	1 (2%)	65 85
1	L	66/310 (21%)	63 (96%)	3 (4%)	27 58
All	All	2400/3720 (64%)	2272 (95%)	128 (5%)	22 52

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	35	LEU
1	I	229	SER
1	C	26	LYS
1	C	24	THR
1	I	354	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	292	ASN
1	G	350	HIS
1	K	350	HIS
1	I	354	GLN
1	J	52	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)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PLP	D	401	1	16,16,16	2.58	3 (18%)	20,23,23	1.91	4 (20%)
2	PLP	I	401	1	16,16,16	2.96	3 (18%)	20,23,23	1.97	5 (25%)
2	PLP	B	401	1	16,16,16	2.77	3 (18%)	20,23,23	2.13	5 (25%)
2	PLP	H	401	-	16,16,16	2.66	4 (25%)	20,23,23	2.37	6 (30%)
2	PLP	A	401	-	16,16,16	2.47	3 (18%)	20,23,23	1.75	7 (35%)
2	PLP	E	401	1	16,16,16	2.79	3 (18%)	20,23,23	2.28	8 (40%)
2	PLP	C	401	1	16,16,16	2.75	3 (18%)	20,23,23	1.58	5 (25%)
2	PLP	G	401	1	16,16,16	2.49	3 (18%)	20,23,23	1.87	5 (25%)
2	PLP	F	401	1	16,16,16	2.69	3 (18%)	20,23,23	2.02	6 (30%)
2	PLP	K	401	-	16,16,16	2.72	3 (18%)	20,23,23	1.83	6 (30%)

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	PLP	D	401	1	-	0/8/8/8	0/1/1/1
2	PLP	I	401	1	-	0/8/8/8	0/1/1/1
2	PLP	B	401	1	-	0/8/8/8	0/1/1/1
2	PLP	H	401	-	-	1/8/8/8	0/1/1/1
2	PLP	A	401	-	-	3/8/8/8	0/1/1/1
2	PLP	E	401	1	-	0/8/8/8	0/1/1/1
2	PLP	C	401	1	-	0/8/8/8	0/1/1/1
2	PLP	G	401	1	-	0/8/8/8	0/1/1/1
2	PLP	F	401	1	-	3/8/8/8	0/1/1/1
2	PLP	K	401	-	-	0/8/8/8	0/1/1/1

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	PLP	C3-C2	9.14	1.50	1.40
2	B	401	PLP	C3-C2	8.22	1.49	1.40
2	K	401	PLP	C3-C2	7.89	1.48	1.40
2	C	401	PLP	C3-C2	7.88	1.48	1.40
2	D	401	PLP	C3-C2	7.40	1.48	1.40

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	401	PLP	C3-C4-C4A	6.43	129.01	119.90
2	E	401	PLP	C4-C3-C2	-5.99	116.48	120.19
2	B	401	PLP	C4-C3-C2	-5.96	116.50	120.19
2	D	401	PLP	C4-C3-C2	-5.76	116.62	120.19
2	I	401	PLP	C4-C3-C2	-4.97	117.11	120.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PLP	C5A-O4P-P-O2P
2	A	401	PLP	C5A-O4P-P-O3P
2	F	401	PLP	C4-C5-C5A-O4P
2	F	401	PLP	C6-C5-C5A-O4P
2	A	401	PLP	C5A-O4P-P-O1P

There are no ring outliers.

9 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	PLP	3	0
2	B	401	PLP	4	0
2	H	401	PLP	4	0
2	A	401	PLP	9	0
2	E	401	PLP	3	0
2	C	401	PLP	3	0
2	G	401	PLP	1	0
2	F	401	PLP	6	0
2	K	401	PLP	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

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	348/358 (97%)	-0.19	3 (0%) 84 85	36, 60, 97, 137	0
1	B	349/358 (97%)	-0.08	11 (3%) 47 46	37, 66, 111, 163	0
1	C	349/358 (97%)	-0.10	2 (0%) 89 90	35, 68, 102, 127	0
1	D	345/358 (96%)	0.14	17 (4%) 29 29	42, 86, 125, 153	0
1	E	342/358 (95%)	-0.09	9 (2%) 56 56	45, 75, 115, 131	0
1	F	322/358 (89%)	-0.11	4 (1%) 79 80	43, 78, 121, 146	0
1	G	341/358 (95%)	0.06	6 (1%) 68 69	48, 90, 125, 155	0
1	H	349/358 (97%)	0.20	28 (8%) 12 10	62, 100, 136, 160	0
1	I	336/358 (93%)	0.36	33 (9%) 7 6	55, 94, 137, 156	0
1	J	253/358 (70%)	0.50	34 (13%) 3 2	61, 100, 158, 199	0
1	K	316/358 (88%)	0.29	28 (8%) 9 8	68, 104, 143, 163	0
1	L	216/358 (60%)	0.16	12 (5%) 24 23	58, 107, 146, 165	0
All	All	3866/4296 (89%)	0.08	187 (4%) 30 30	35, 85, 133, 199	0

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	187	ALA	11.1
1	F	295	PHE	8.2
1	A	31	PHE	8.0
1	I	35	LEU	7.0
1	I	224	HIS	6.4

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 (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	PLP	I	401	16/16	0.89	0.16	75,89,94,97	0
2	PLP	H	401	16/16	0.91	0.26	75,85,94,97	0
2	PLP	A	401	16/16	0.91	0.24	56,75,92,101	0
3	CL	A	402	1/1	0.92	0.09	74,74,74,74	0
2	PLP	G	401	16/16	0.93	0.24	69,86,89,91	0
2	PLP	C	401	16/16	0.93	0.15	61,69,76,79	0
3	CL	E	402	1/1	0.93	0.12	92,92,92,92	0
3	CL	C	402	1/1	0.94	0.28	81,81,81,81	0
2	PLP	K	401	16/16	0.95	0.12	62,70,73,74	0
2	PLP	E	401	16/16	0.95	0.20	64,71,78,79	0
2	PLP	B	401	16/16	0.96	0.15	49,64,70,75	0
2	PLP	F	401	16/16	0.96	0.17	64,71,74,75	0
2	PLP	D	401	16/16	0.96	0.21	57,86,93,95	0
3	CL	D	402	1/1	0.97	0.14	78,78,78,78	0
3	CL	B	402	1/1	0.98	0.16	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.