wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:05 PM GMT

PDB ID	:	4UQV
Title	:	methanococcus jannaschii serine hydroxymethyl-transferase in complex with PLP
Authors	:	Saccoccia, F.; Angelucci, F.; Ilari, A.
Deposited on	:	2014-06-25
Resolution	:	3.00 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 (1)) were used in the production of this report:

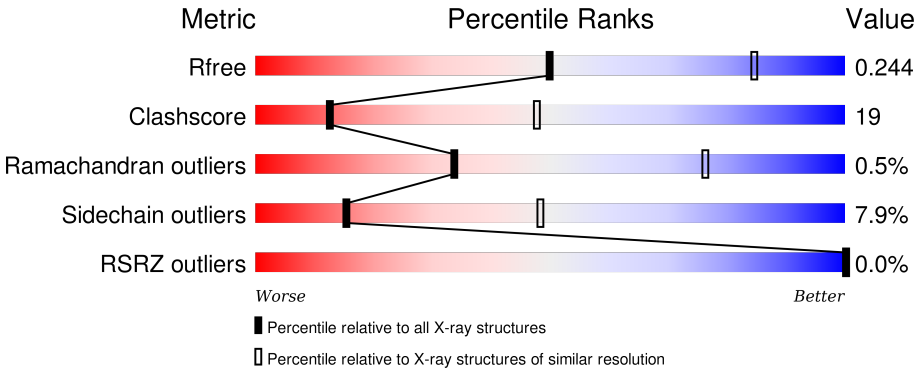
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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.

Mol	Chain	Length	Quality of chain
1	A	429	61% 34%
1	B	429	60% 36%
1	C	429	59% 36%
1	D	429	57% 36% 6%
1	E	429	52% 43%

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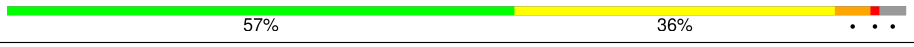
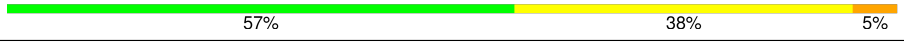
Mol	Chain	Length	Quality of chain
1	F	429	
1	G	429	
1	H	429	
1	I	429	
1	J	429	
1	K	429	
1	L	429	

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	C	1430	-	-	-	X
2	PLP	I	1430	-	-	-	X

2 Entry composition (i)

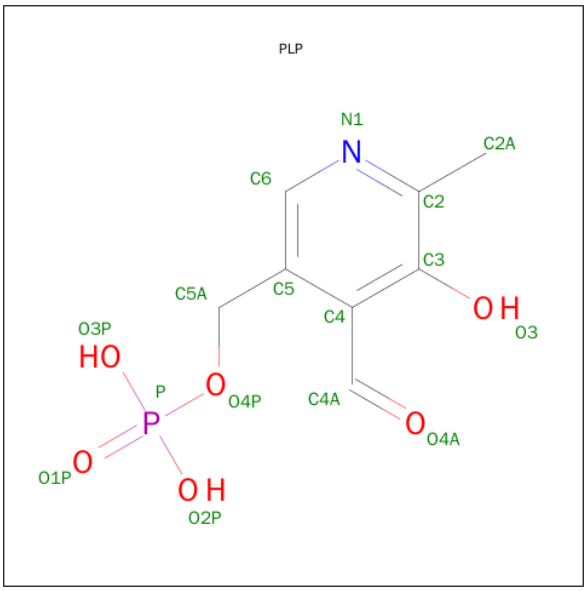
There are 2 unique types of molecules in this entry. The entry contains 40370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERINE HYDROXYMETHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3362	2146	560	639	17			
1	B	424	Total	C	N	O	S	0	0	0
			3344	2133	558	636	17			
1	C	420	Total	C	N	O	S	0	0	0
			3308	2112	552	628	16			
1	D	425	Total	C	N	O	S	0	0	0
			3354	2141	559	638	16			
1	E	427	Total	C	N	O	S	0	0	0
			3369	2150	565	638	16			
1	F	418	Total	C	N	O	S	0	0	0
			3300	2107	554	623	16			
1	G	429	Total	C	N	O	S	0	0	0
			3386	2160	567	642	17			
1	H	427	Total	C	N	O	S	0	0	0
			3366	2146	564	639	17			
1	I	427	Total	C	N	O	S	0	0	0
			3369	2150	565	638	16			
1	J	429	Total	C	N	O	S	0	0	0
			3386	2160	567	642	17			
1	K	422	Total	C	N	O	S	0	0	0
			3329	2125	559	629	16			
1	L	420	Total	C	N	O	S	0	0	0
			3317	2122	555	624	16			

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



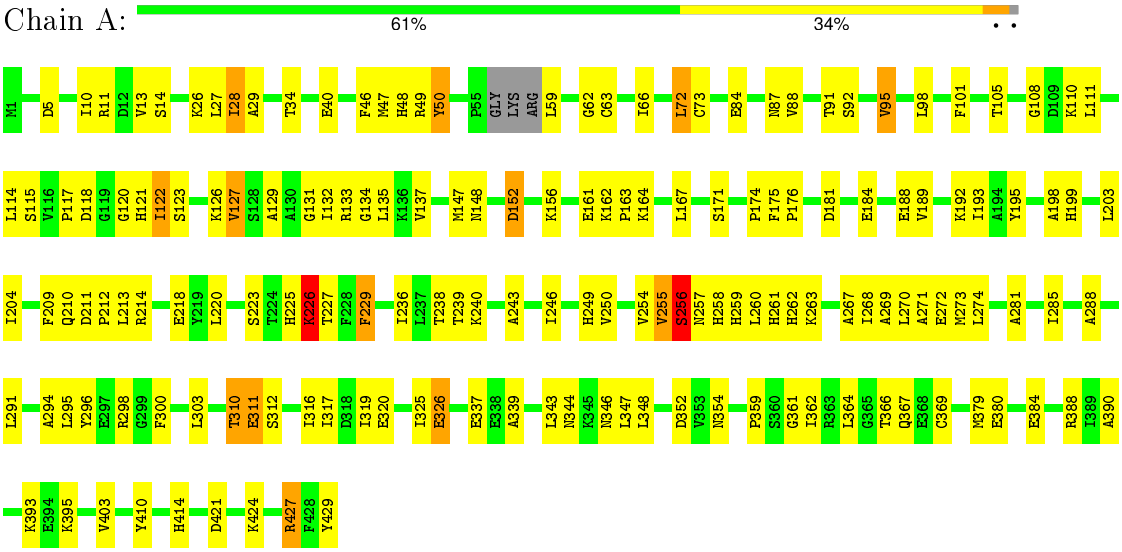
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	L	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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.

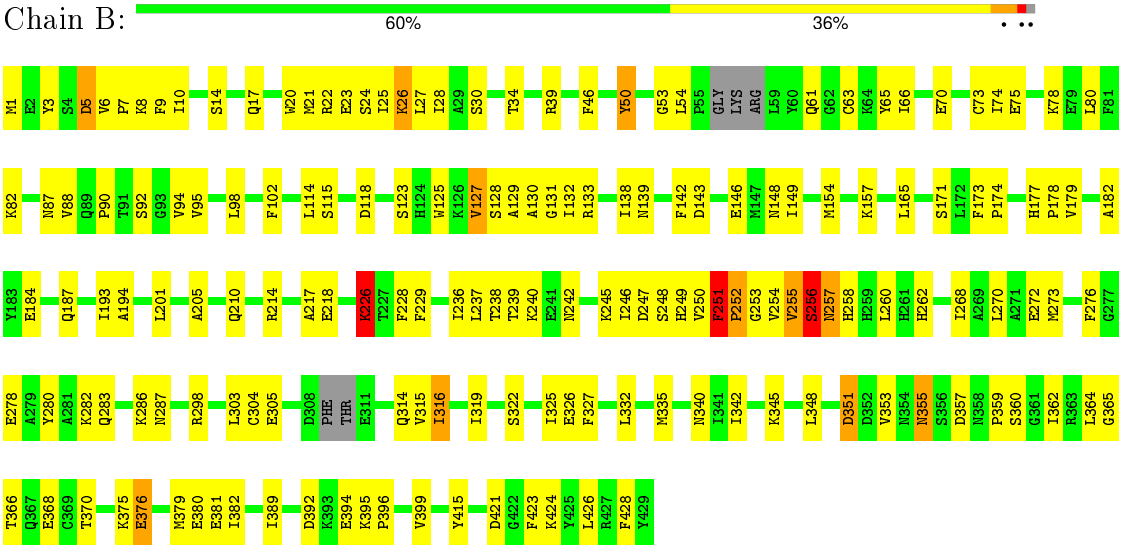
- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain A:



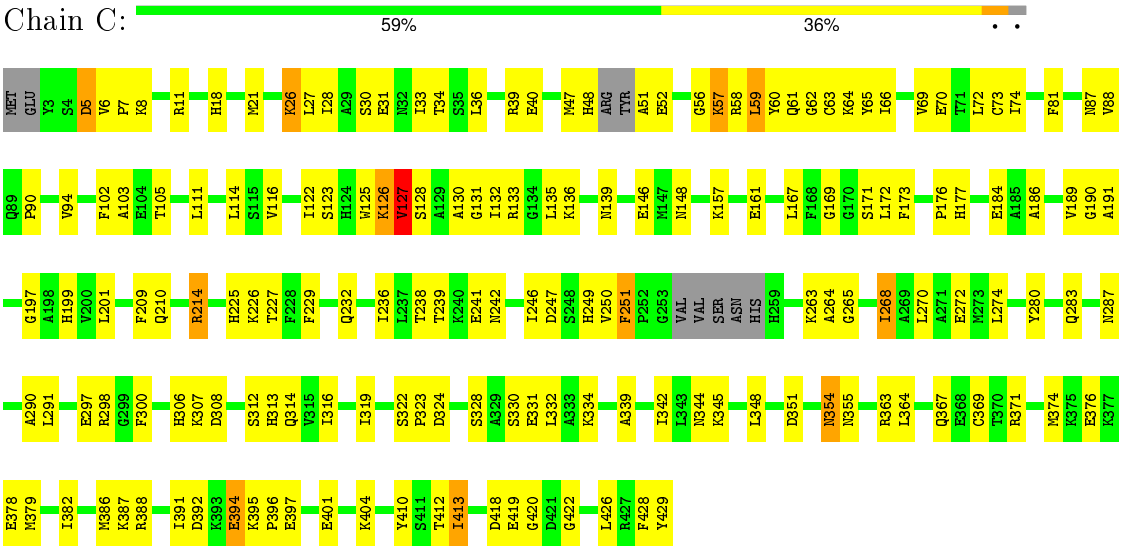
- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain B:



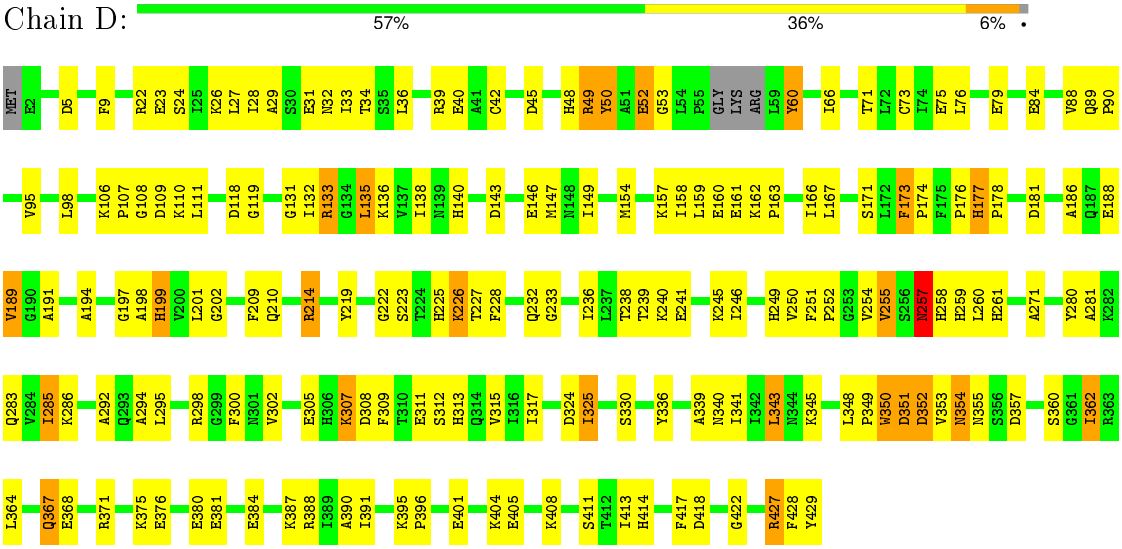
- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain C:



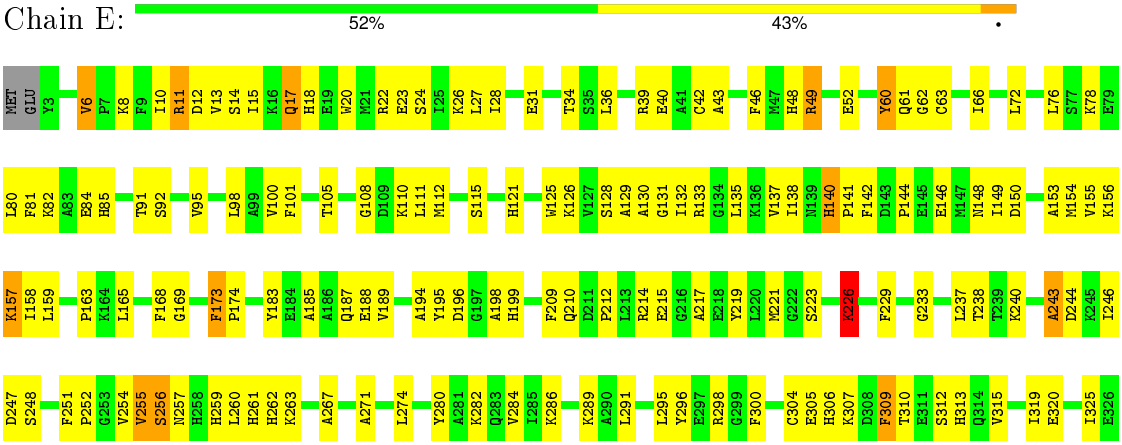
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

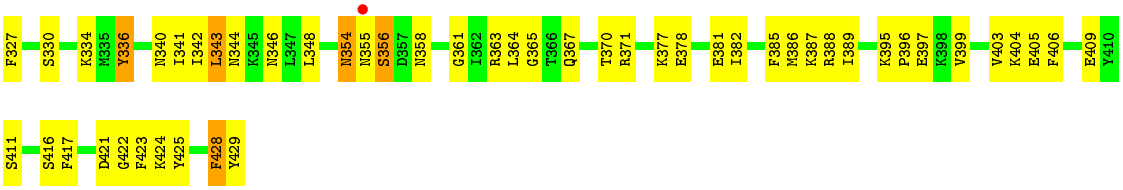
Chain D:



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

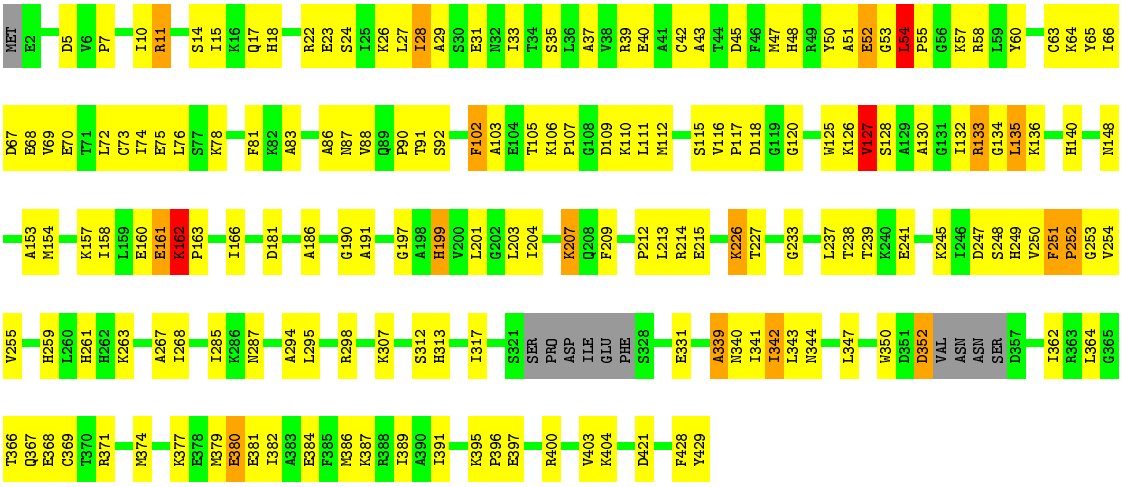
Chain E:





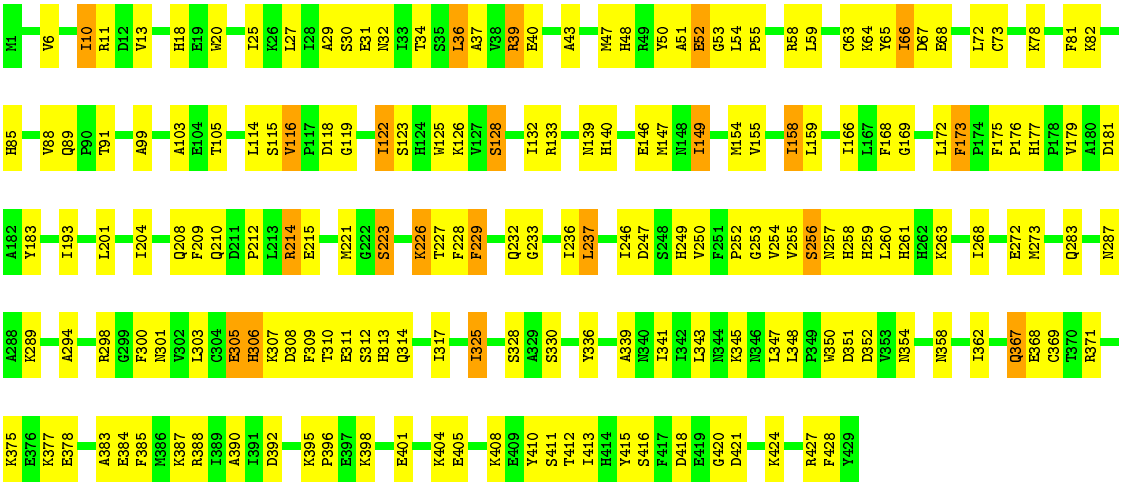
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain F:



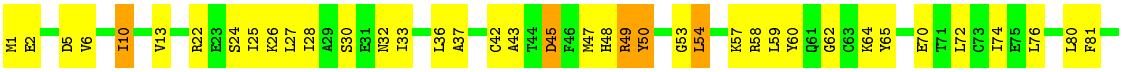
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

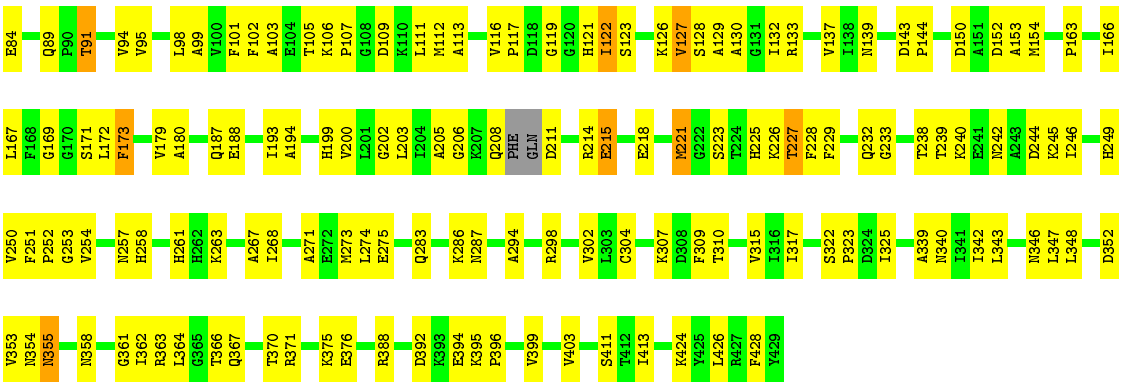
Chain G:



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

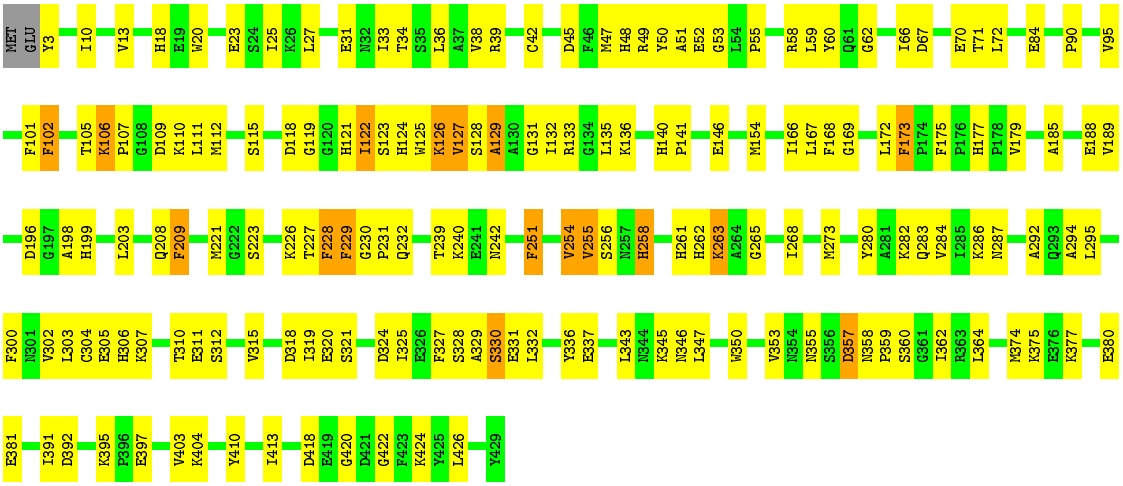
Chain H:





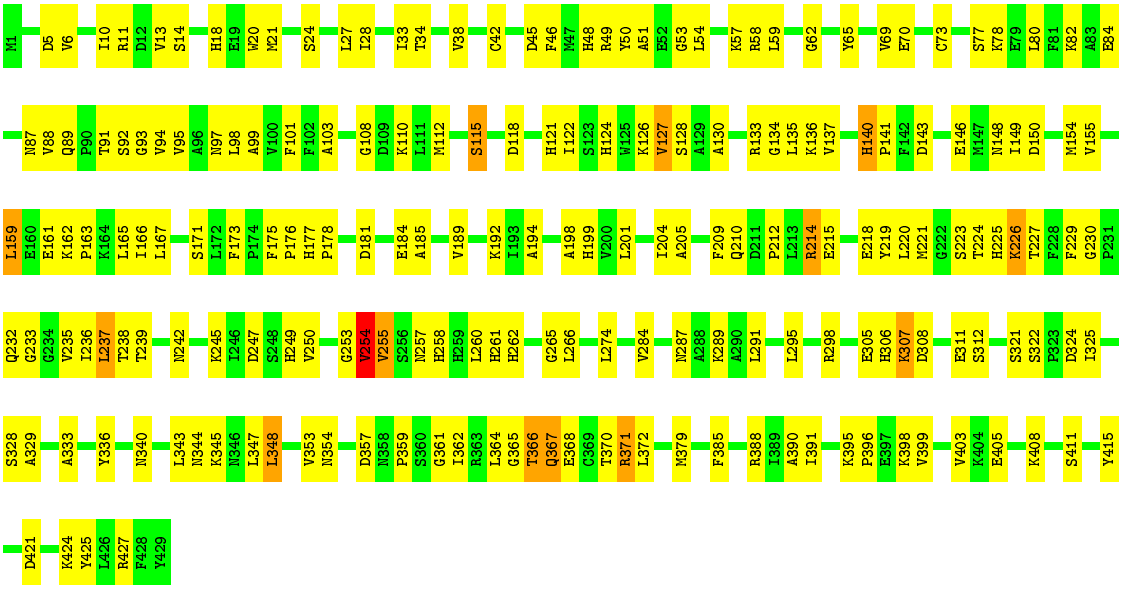
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain I:



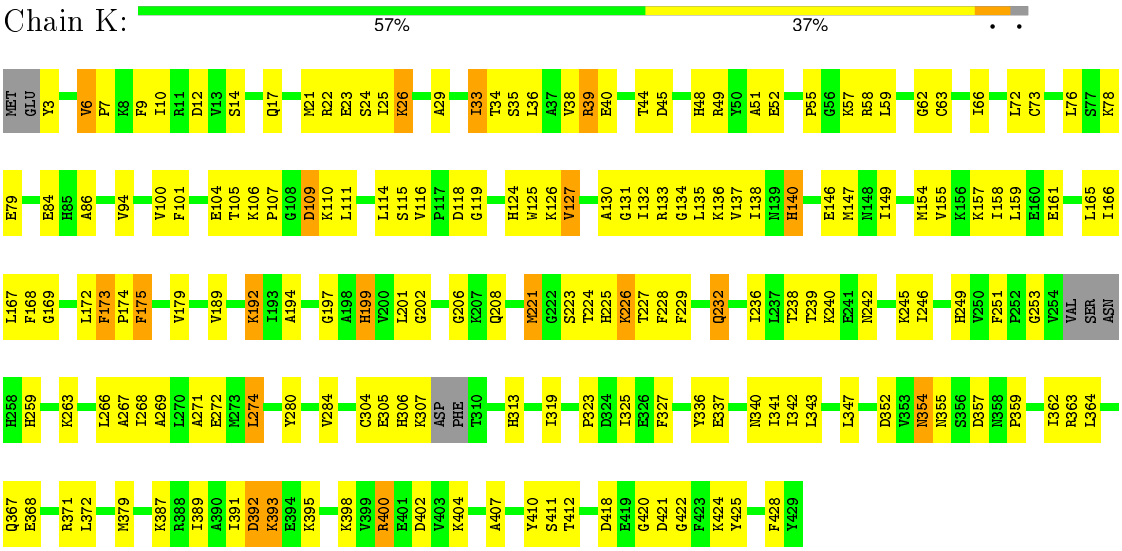
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain J:



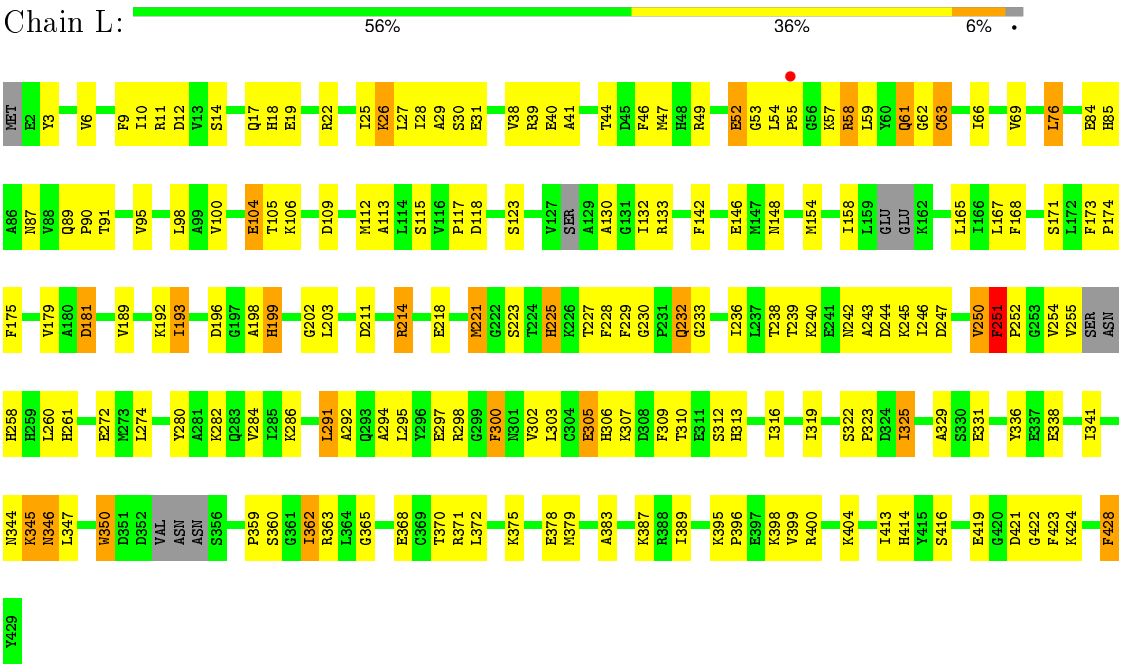
- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain K:



- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

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	123.13Å 47.16Å 344.08Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	49.15 – 3.00 49.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-3.00) 90.7 (49.15-3.00)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1702)	Depositor
R, R_{free}	0.198 , 0.243 0.204 , 0.244	Depositor DCC
R_{free} test set	3660 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 29.6	EDS
Estimated twinning fraction	0.500 for -H,-K,L 0.438 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for -H,-K,L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 80986 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	40370	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.25	0/3437	0.48	0/4635
1	B	0.28	1/3417 (0.0%)	0.54	6/4606 (0.1%)
1	C	0.26	0/3380	0.49	1/4554 (0.0%)
1	D	0.26	0/3429	0.52	0/4625
1	E	0.25	0/3445	0.55	3/4646 (0.1%)
1	F	0.26	0/3372	0.53	2/4542 (0.0%)
1	G	0.26	0/3462	0.47	0/4668
1	H	0.25	0/3440	0.50	1/4637 (0.0%)
1	I	0.25	0/3445	0.52	3/4646 (0.1%)
1	J	0.27	0/3462	0.55	3/4668 (0.1%)
1	K	0.25	0/3402	0.50	1/4584 (0.0%)
1	L	0.24	0/3389	0.47	0/4563
All	All	0.26	1/41080 (0.0%)	0.51	20/55374 (0.0%)

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	3
1	B	0	2
1	C	0	5
1	D	0	3
1	E	0	2
1	F	0	2
1	G	0	1
1	I	0	3
1	J	0	1
1	K	0	3
1	L	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	27

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	PRO	N-CD	5.21	1.55	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	226	LYS	N-CA-C	9.70	137.19	111.00
1	E	226	LYS	N-CA-C	9.53	136.72	111.00
1	B	226	LYS	N-CA-C	9.24	135.94	111.00
1	I	226	LYS	N-CA-C	8.29	133.38	111.00
1	J	254	VAL	CB-CA-C	-7.69	96.79	111.40

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	VAL	Peptide
1	A	255	VAL	Peptide
1	A	256	SER	Peptide
1	B	226	LYS	Peptide
1	B	256	SER	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	3362	0	3304	132	0
1	B	3344	0	3288	149	0
1	C	3308	0	3257	134	0
1	D	3354	0	3292	177	0
1	E	3369	0	3316	157	0
1	F	3300	0	3252	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3386	0	3334	152	0
1	H	3366	0	3316	132	0
1	I	3369	0	3316	147	0
1	J	3386	0	3335	137	0
1	K	3329	0	3281	134	0
1	L	3317	0	3269	135	0
2	A	15	0	7	2	0
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	0	0
2	E	15	0	7	2	0
2	F	15	0	7	2	0
2	G	15	0	7	1	0
2	H	15	0	7	0	0
2	I	15	0	7	0	0
2	J	15	0	7	1	0
2	K	15	0	7	0	0
2	L	15	0	7	0	0
All	All	40370	0	39644	1550	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 19.

The worst 5 of 1550 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:I:52:GLU:HG2	1:I:60:TYR:CD1	1.70	1.24
1:D:351:ASP:HB2	1:D:352:ASP:OD1	1.44	1.16
1:A:310:THR:HG23	1:A:311:GLU:N	1.55	1.12
1:C:47:MET:HE1	1:D:34:THR:HG21	1.25	1.11
1:A:147:MET:HB2	1:A:175:PHE:HE2	1.08	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	422/429 (98%)	391 (93%)	28 (7%)	3 (1%)	26	70
1	B	418/429 (97%)	382 (91%)	32 (8%)	4 (1%)	19	61
1	C	414/429 (96%)	375 (91%)	38 (9%)	1 (0%)	52	88
1	D	421/429 (98%)	375 (89%)	44 (10%)	2 (0%)	34	76
1	E	425/429 (99%)	380 (89%)	43 (10%)	2 (0%)	34	76
1	F	412/429 (96%)	368 (89%)	38 (9%)	6 (2%)	13	50
1	G	427/429 (100%)	394 (92%)	33 (8%)	0	100	100
1	H	423/429 (99%)	378 (89%)	44 (10%)	1 (0%)	52	88
1	I	425/429 (99%)	398 (94%)	26 (6%)	1 (0%)	52	88
1	J	427/429 (100%)	383 (90%)	41 (10%)	3 (1%)	26	70
1	K	416/429 (97%)	377 (91%)	38 (9%)	1 (0%)	52	88
1	L	410/429 (96%)	368 (90%)	40 (10%)	2 (0%)	34	76
All	All	5040/5148 (98%)	4569 (91%)	445 (9%)	26 (0%)	34	76

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	B	127	VAL
1	C	127	VAL
1	F	54	LEU
1	F	127	VAL

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	357/359 (99%)	332 (93%)	25 (7%)	19	55
1	B	355/359 (99%)	334 (94%)	21 (6%)	24	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	350/359 (98%)	327 (93%)	23 (7%)	21 57
1	D	356/359 (99%)	325 (91%)	31 (9%)	13 43
1	E	357/359 (99%)	327 (92%)	30 (8%)	14 45
1	F	348/359 (97%)	320 (92%)	28 (8%)	15 47
1	G	359/359 (100%)	327 (91%)	32 (9%)	12 42
1	H	357/359 (99%)	328 (92%)	29 (8%)	15 47
1	I	357/359 (99%)	334 (94%)	23 (6%)	22 59
1	J	359/359 (100%)	334 (93%)	25 (7%)	19 55
1	K	352/359 (98%)	323 (92%)	29 (8%)	14 46
1	L	350/359 (98%)	309 (88%)	41 (12%)	7 27
All	All	4257/4308 (99%)	3920 (92%)	337 (8%)	15 48

5 of 337 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	331	GLU
1	G	398	LYS
1	L	181	ASP
1	F	352	ASP
1	G	181	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	32	ASN
1	G	225	HIS
1	K	262	HIS
1	G	210	GLN
1	G	258	HIS

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

12 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	PLP	A	1430	1	15,15,16	1.20	1 (6%)	21,22,23	1.55	3 (14%)
2	PLP	B	1430	1	15,15,16	1.19	1 (6%)	21,22,23	1.73	2 (9%)
2	PLP	C	1430	1	15,15,16	1.12	1 (6%)	21,22,23	2.03	3 (14%)
2	PLP	D	1430	1	15,15,16	1.35	1 (6%)	21,22,23	1.85	3 (14%)
2	PLP	E	1430	1	15,15,16	1.37	1 (6%)	21,22,23	2.48	4 (19%)
2	PLP	F	1430	1	15,15,16	1.12	1 (6%)	21,22,23	1.83	2 (9%)
2	PLP	G	1430	1	15,15,16	1.18	1 (6%)	21,22,23	1.68	2 (9%)
2	PLP	H	1430	1	15,15,16	1.10	1 (6%)	21,22,23	1.57	2 (9%)
2	PLP	I	1430	1	15,15,16	1.18	1 (6%)	21,22,23	1.77	2 (9%)
2	PLP	J	1430	1	15,15,16	1.17	1 (6%)	21,22,23	1.71	1 (4%)
2	PLP	K	1430	1	15,15,16	1.19	1 (6%)	21,22,23	1.61	2 (9%)
2	PLP	L	1430	1	15,15,16	1.12	1 (6%)	21,22,23	1.74	2 (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
2	PLP	A	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	C	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	E	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	F	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	G	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	H	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	I	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	J	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	K	1430	1	-	0/6/6/8	0/1/1/1
2	PLP	L	1430	1	-	0/6/6/8	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1430	PLP	C3-C2	-4.45	1.37	1.40
2	E	1430	PLP	C3-C2	-4.32	1.37	1.40
2	K	1430	PLP	C3-C2	-3.69	1.38	1.40
2	B	1430	PLP	C3-C2	-3.61	1.38	1.40
2	G	1430	PLP	C3-C2	-3.60	1.38	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1430	PLP	C4A-C4-C3	-2.65	115.56	120.36
2	D	1430	PLP	C2A-C2-C3	-2.20	118.39	121.04
2	A	1430	PLP	C5-C6-N1	-2.11	120.19	123.86
2	A	1430	PLP	C6-C5-C4	2.01	119.85	118.15
2	H	1430	PLP	C4A-C4-C5	2.46	123.44	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1430	PLP	2	0
2	B	1430	PLP	1	0
2	C	1430	PLP	1	0
2	E	1430	PLP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1430	PLP	2	0
2	G	1430	PLP	1	0
2	J	1430	PLP	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	426/429 (99%)	-0.79	0 100 100	30, 45, 66, 73	0
1	B	424/429 (98%)	-0.78	0 100 100	31, 47, 68, 80	0
1	C	420/429 (97%)	-0.77	0 100 100	34, 52, 67, 79	0
1	D	425/429 (99%)	-0.64	0 100 100	33, 61, 78, 85	0
1	E	427/429 (99%)	-0.62	1 (0%) 95 87	40, 62, 80, 95	0
1	F	418/429 (97%)	-0.63	0 100 100	43, 62, 76, 93	0
1	G	429/429 (100%)	-0.83	0 100 100	30, 45, 61, 71	0
1	H	427/429 (99%)	-0.77	0 100 100	29, 47, 71, 79	0
1	I	427/429 (99%)	-0.82	0 100 100	33, 48, 64, 71	0
1	J	429/429 (100%)	-0.71	0 100 100	37, 53, 72, 78	0
1	K	422/429 (98%)	-0.61	0 100 100	45, 62, 76, 91	0
1	L	420/429 (97%)	-0.52	1 (0%) 95 87	51, 66, 79, 93	0
All	All	5094/5148 (98%)	-0.71	2 (0%) 100 100	29, 55, 74, 95	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	355	ASN	3.1
1	L	55	PRO	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
2	PLP	I	1430	15/16	0.93	0.22	2.04	41,42,42,43	0
2	PLP	C	1430	15/16	0.94	0.20	2.02	45,46,46,47	0
2	PLP	D	1430	15/16	0.94	0.19	0.77	53,56,59,60	0
2	PLP	G	1430	15/16	0.97	0.18	0.67	37,37,39,39	0
2	PLP	B	1430	15/16	0.97	0.14	0.49	41,43,44,44	0
2	PLP	L	1430	15/16	0.92	0.21	0.47	65,66,66,66	0
2	PLP	F	1430	15/16	0.97	0.20	0.43	51,54,56,57	0
2	PLP	E	1430	15/16	0.97	0.17	0.01	43,44,46,47	0
2	PLP	H	1430	15/16	0.98	0.14	-0.04	42,44,45,46	0
2	PLP	K	1430	15/16	0.94	0.18	-0.06	58,59,59,60	0
2	PLP	A	1430	15/16	0.96	0.15	-0.13	36,37,39,39	0
2	PLP	J	1430	15/16	0.95	0.13	-0.47	47,47,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.