wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1FWL
Title	:	CRYSTAL STRUCTURE OF HOMOSERINE KINASE
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Deposited on	:	2000-09-22
Resolution	:	2.25 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:

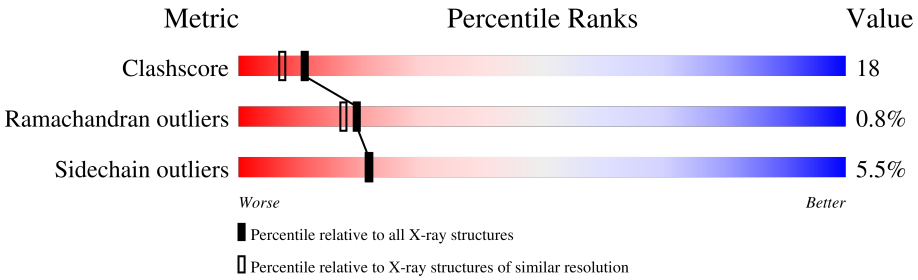
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.25 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	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	296	79% 18% .
1	B	296	61% 33% 5%
1	C	296	75% 22% .
1	D	296	71% 26% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9582 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 HOMOSERINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2269	1460	366	434	9			
1	B	296	Total	C	N	O	S	0	0	0
			2269	1460	366	434	9			
1	C	296	Total	C	N	O	S	0	0	0
			2269	1460	366	434	9			
1	D	296	Total	C	N	O	S	0	0	0
			2269	1460	366	434	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	164	Total	O	0	0
			164	164		
2	B	77	Total	O	0	0
			77	77		
2	C	142	Total	O	0	0
			142	142		
2	D	123	Total	O	0	0
			123	123		

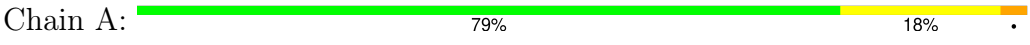
3 Residue-property plots (i)

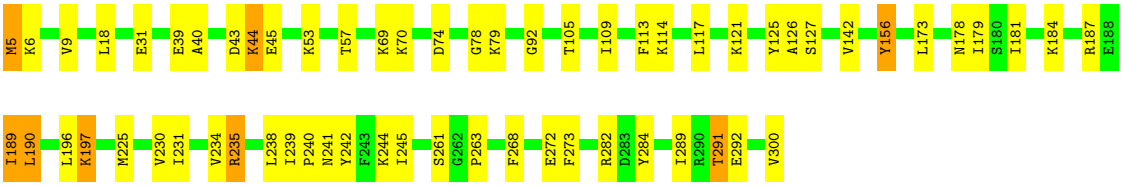
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: HOMOSERINE KINASE

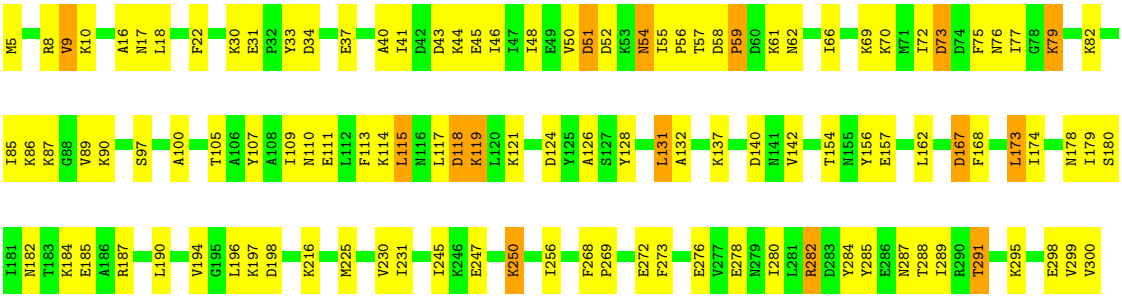
Chain A:





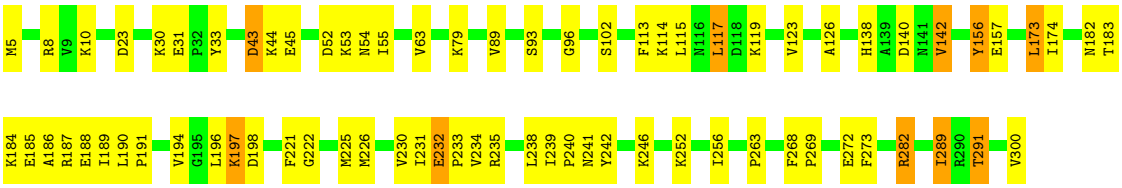
• Molecule 1: HOMOSERINE KINASE

Chain B:



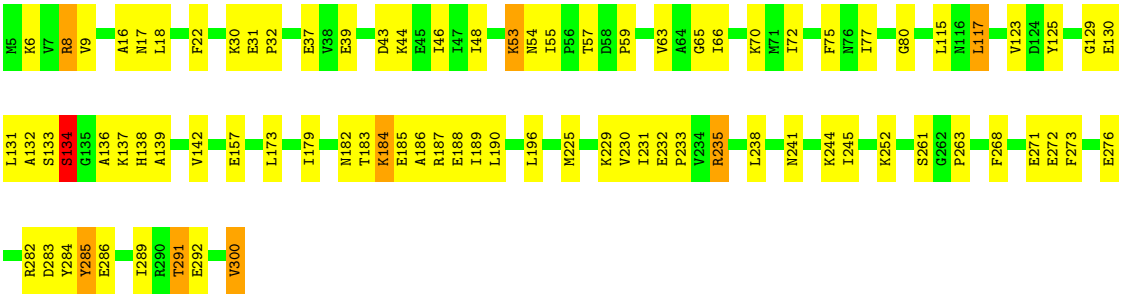
• Molecule 1: HOMOSERINE KINASE

Chain C:



• Molecule 1: HOMOSERINE KINASE

Chain D:


M5
K6
V7
R8
V9
A16
N17
L18
F22
K30
E31
P32
E37
V38
E39
D43
K44
E45
I46
I47
I48
K53
N54
I55
P56
T57
D58
P59
V63
A64
G65
I66
K70
M71
I72
F75
N76
I77
G80
L115
N116
L117
V123
D124
Y125
G129
E130
L131
A132
S133
S134
G135
A136
K137
H138
A139
V142
E157
L173
I179
N182
T183
K184
E185
A186
R187
E188
I189
L190
L196
M225
K229
V230
I231
E232
P233
V234
R235
L238
N241
K244
I245
K252
S261
G262
P263
F268
E271
E272
F273
E276
R282
D283
Y284
Y285
E286
I289
R290
T291
E292
V300

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.99Å 128.72Å 109.42Å 90.00° 105.57° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25	Depositor
% Data completeness (in resolution range)	97.9 (20.00-2.25)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9582	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.65	0/2306	0.78	0/3112
1	B	0.55	0/2306	0.73	1/3112 (0.0%)
1	C	0.68	0/2306	0.80	1/3112 (0.0%)
1	D	0.64	0/2306	0.79	2/3112 (0.1%)
All	All	0.63	0/9224	0.78	4/12448 (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	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	156	TYR	N-CA-C	-5.77	95.43	111.00
1	D	80	GLY	N-CA-C	-5.55	99.21	113.10
1	D	285	TYR	N-CA-C	-5.44	96.32	111.00
1	B	54	ASN	N-CA-C	-5.43	96.34	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	TYR	Sidechain

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	2269	0	2339	49	0
1	B	2269	0	2339	130	0
1	C	2269	0	2339	69	0
1	D	2269	0	2339	89	0
2	A	164	0	0	6	0
2	B	77	0	0	3	0
2	C	142	0	0	5	0
2	D	123	0	0	7	0
All	All	9582	0	9356	336	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 18.

The worst 5 of 336 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ASP:HB3	1:B:61:LYS:HE2	1.26	1.09
1:D:130:GLU:HB3	1:D:138:HIS:HB2	1.35	1.03
1:B:119:LYS:H	1:B:119:LYS:HD2	1.22	1.00
1:D:31:GLU:H	1:D:291:THR:HG21	1.26	0.99
1:B:167:ASP:HB3	2:B:329:HOH:O	1.67	0.94

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/296 (99%)	286 (97%)	7 (2%)	1 (0%)	41 46
1	B	294/296 (99%)	272 (92%)	18 (6%)	4 (1%)	11 7
1	C	294/296 (99%)	274 (93%)	18 (6%)	2 (1%)	22 21
1	D	294/296 (99%)	277 (94%)	15 (5%)	2 (1%)	22 21
All	All	1176/1184 (99%)	1109 (94%)	58 (5%)	9 (1%)	19 17

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	134	SER
1	A	44	LYS
1	B	51	ASP
1	C	44	LYS
1	B	44	LYS

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	248/248 (100%)	234 (94%)	14 (6%)	21 21
1	B	248/248 (100%)	233 (94%)	15 (6%)	19 18
1	C	248/248 (100%)	235 (95%)	13 (5%)	23 24
1	D	248/248 (100%)	235 (95%)	13 (5%)	23 24
All	All	992/992 (100%)	937 (94%)	55 (6%)	21 21

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	291	THR
1	C	196	LEU
1	D	300	VAL
1	D	190	LEU
1	C	23	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	141	ASN
1	A	178	ASN
1	A	215	ASN
1	C	138	HIS

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)

There are no ligands in this entry.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.