wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2017 – 01:21 AM EDT

PDB ID	:	3LIB
Title	:	Crystal Structure of the extracellular domain of the putative histidine kinase mmHK1S-Z3
Authors	:	Zhang, Z.; Hendrickson, W.A.
Deposited on	:	unknown
Resolution	:	2.99 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:

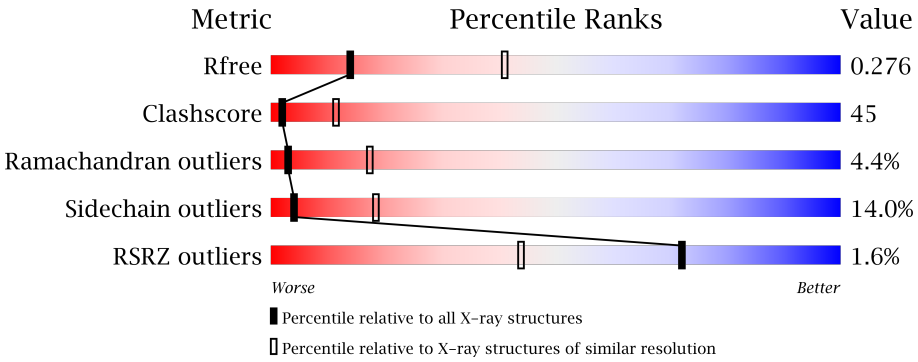
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.99 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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	290	.% 41% 42% 10% 7%
1	B	290	2% 37% 45% 11% • 7%
1	C	290	.% 34% 44% 12% • 8%
1	D	290	.% 39% 44% 10% 7%
1	E	290	.% 46% 37% 9% • 8%

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Mol	Chain	Length	Quality of chain
1	F	290	.% 51% 34% 9% 7%
1	G	290	.% 47% 33% 12% 7%
1	H	290	2% 39% 41% 11% 8%
1	I	290	2% 45% 38% 10% 7%
1	J	290	.% 43% 40% 8% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21176 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 Hypothetical sensory transduction histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	B	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	C	268	Total	C	N	O	S	0	0	0
			2092	1333	329	422	8			
1	D	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	E	268	Total	C	N	O	S	0	0	0
			2094	1335	329	422	8			
1	F	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	G	270	Total	C	N	O	S	0	0	0
			2113	1347	334	424	8			
1	H	267	Total	C	N	O	S	0	0	0
			2086	1331	328	419	8			
1	I	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	J	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
A	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
A	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
A	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
B	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
B	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
B	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
C	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
C	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
C	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
D	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
D	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
D	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
E	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
E	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
E	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
F	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
F	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
F	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
G	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
G	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
G	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
H	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
H	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
H	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
I	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
I	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
I	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
J	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
J	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
J	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total K 1 1	0	0
2	J	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	I	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0

- Molecule 3 is water.

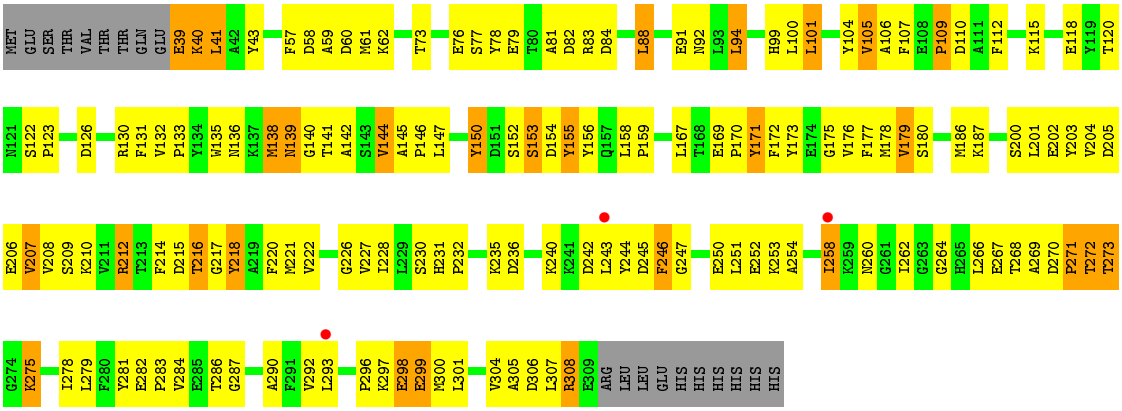
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	C	7	Total O 7 7	0	0
3	D	7	Total O 7 7	0	0
3	E	6	Total O 6 6	0	0
3	F	8	Total O 8 8	0	0
3	G	3	Total O 3 3	0	0
3	H	3	Total O 3 3	0	0
3	I	2	Total O 2 2	0	0
3	J	8	Total O 8 8	0	0

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 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.

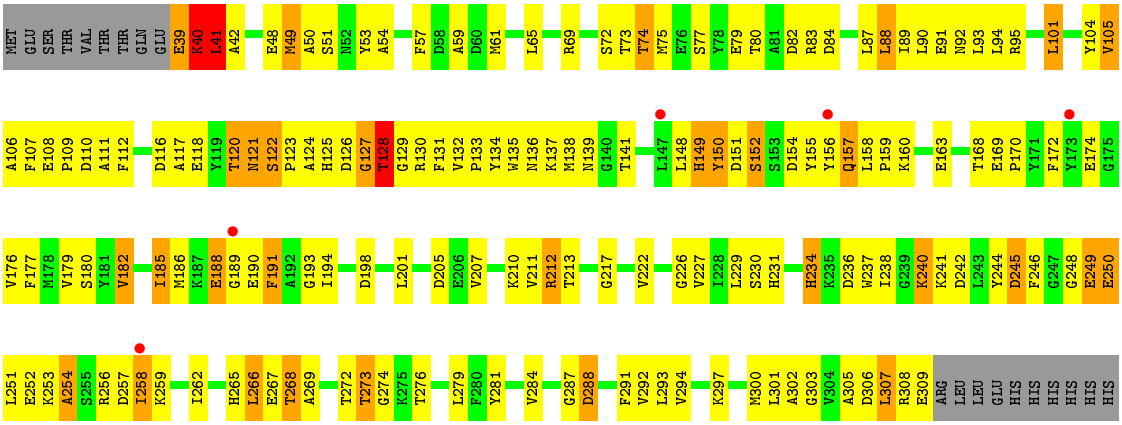
- Molecule 1: Hypothetical sensory transduction histidine kinase

Chain A:



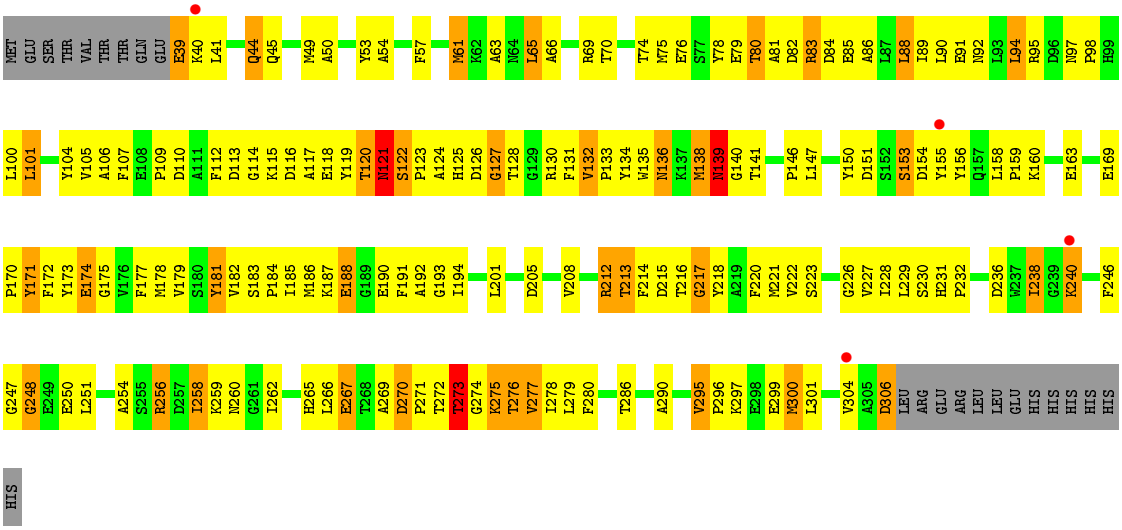
- Molecule 1: Hypothetical sensory transduction histidine kinase

Chain B:



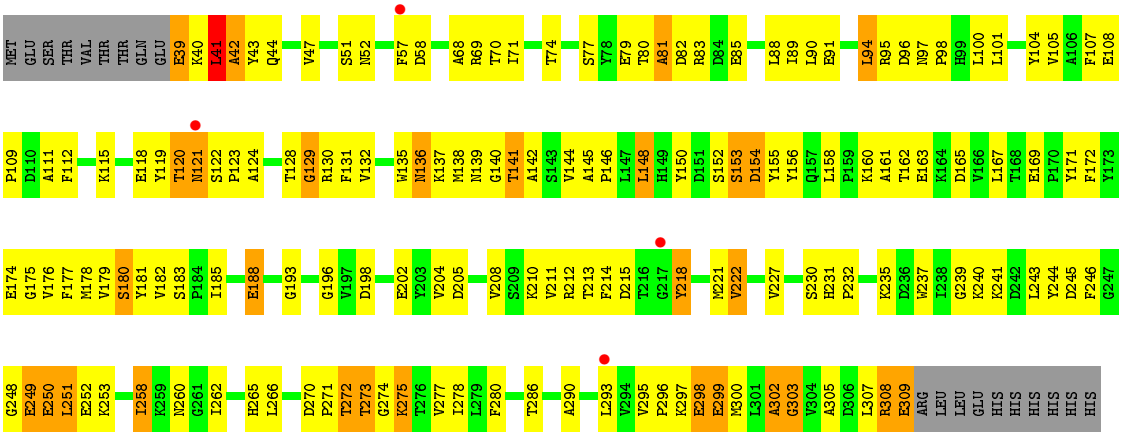
- Molecule 1: Hypothetical sensory transduction histidine kinase

Chain C:



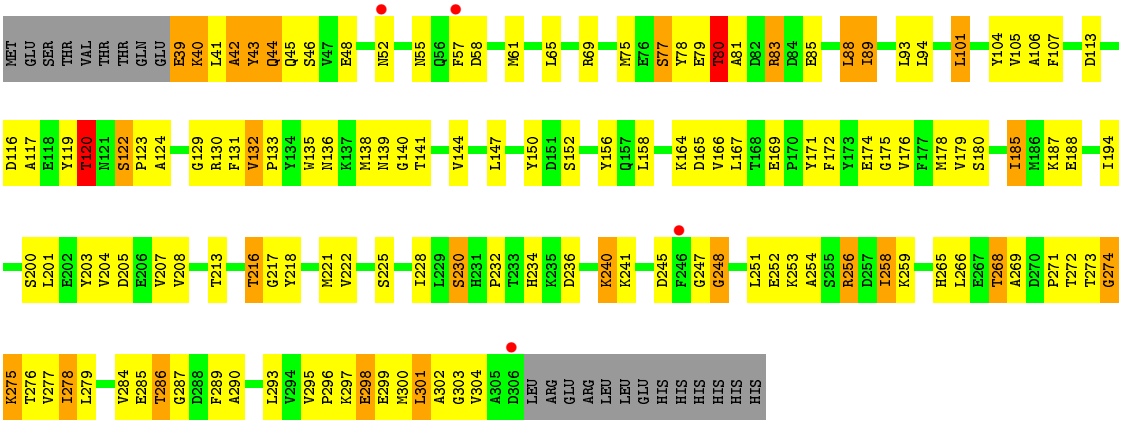
• Molecule 1: Hypothetical sensory transduction histidine kinase

Chain D:



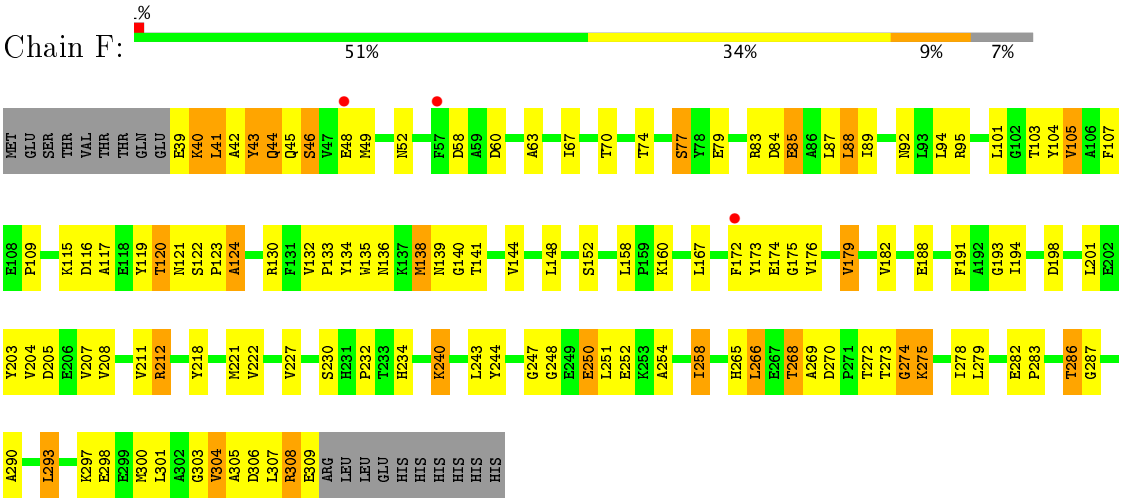
• Molecule 1: Hypothetical sensory transduction histidine kinase

Chain E:



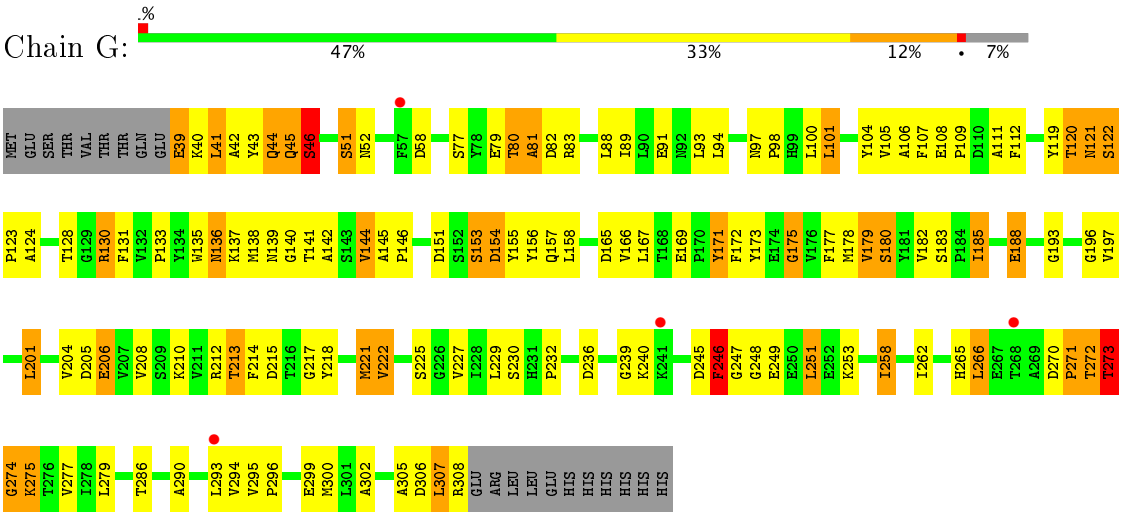
• Molecule 1: Hypothetical sensory transduction histidine kinase

Chain F:



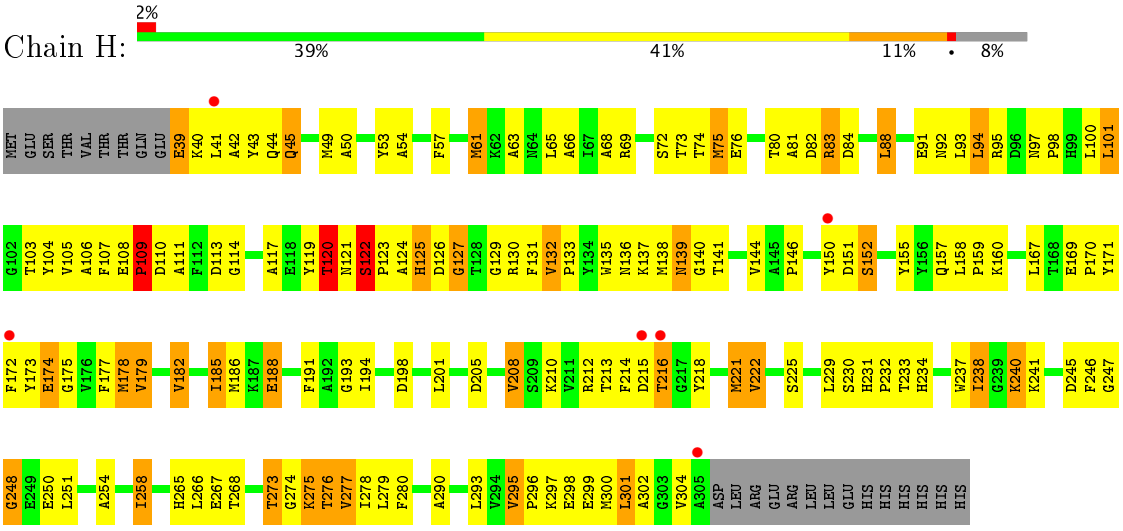
- Molecule 1: Hypothetical sensory transduction histidine kinase

Chain G:



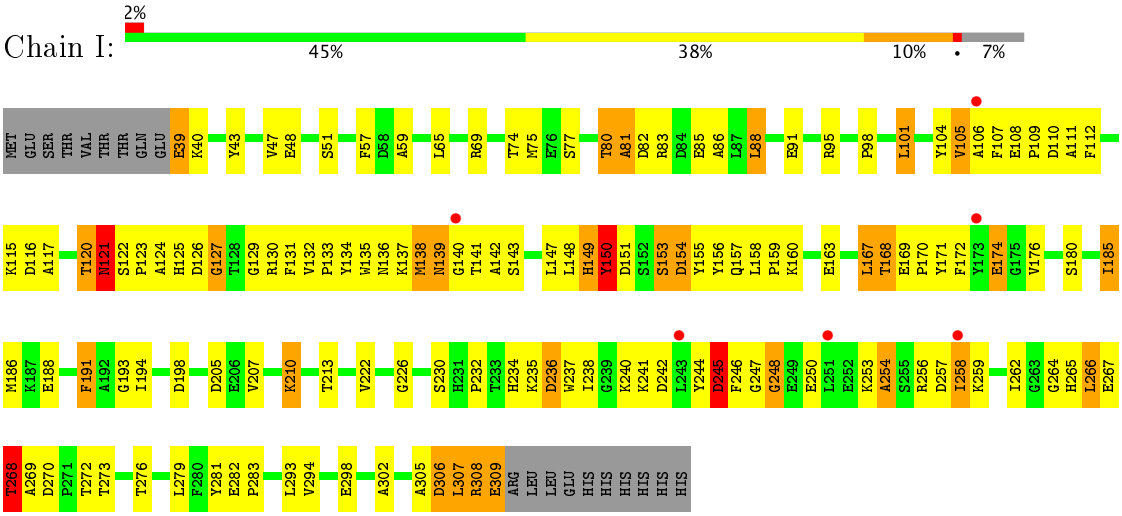
- Molecule 1: Hypothetical sensory transduction histidine kinase

Chain H:



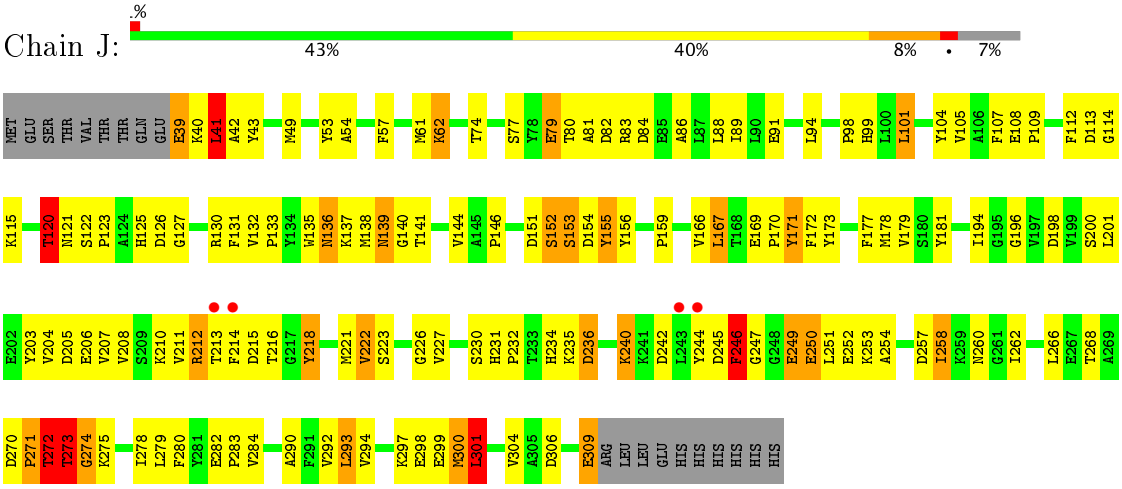
- Molecule 1: Hypothetical sensory transduction histidine kinase

Chain I:



• Molecule 1: Hypothetical sensory transduction histidine kinase

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	129.52Å 129.52Å 404.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.72 – 2.99 46.12 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.72-2.99) 99.3 (46.12-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.197 , 0.272 0.202 , 0.276	Depositor DCC
R_{free} test set	3839 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	76.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21176	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: K

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	0.75	0/2172	0.83	0/2950
1	B	0.70	0/2172	0.77	0/2950
1	C	0.83	1/2142 (0.0%)	0.86	1/2910 (0.0%)
1	D	0.75	0/2172	0.84	1/2950 (0.0%)
1	E	0.77	1/2144 (0.0%)	0.85	0/2913
1	F	0.74	0/2172	0.83	1/2950 (0.0%)
1	G	0.73	0/2163	0.84	1/2938 (0.0%)
1	H	0.80	0/2136	0.84	2/2902 (0.1%)
1	I	0.68	0/2172	0.74	0/2950
1	J	0.77	0/2172	0.84	0/2950
All	All	0.75	2/21617 (0.0%)	0.83	6/29363 (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	D	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	52	ASN	CG-OD1	5.32	1.35	1.24
1	C	139	ASN	CG-OD1	5.01	1.34	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	45	GLN	N-CA-C	6.15	127.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	83	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	H	178	MET	CB-CG-SD	-5.24	96.67	112.40
1	F	274	GLY	N-CA-C	-5.24	100.00	113.10
1	H	75	MET	CG-SD-CE	-5.12	92.00	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	297	LYS	Peptide
1	D	298	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	2122	0	2022	192	0
1	B	2122	0	2022	200	0
1	C	2092	0	1985	235	0
1	D	2122	0	2022	197	0
1	E	2094	0	1991	158	0
1	F	2122	0	2022	142	0
1	G	2113	0	2016	193	0
1	H	2086	0	1988	215	0
1	I	2122	0	2022	172	0
1	J	2122	0	2022	222	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	7	0	0	4	0
3	D	7	0	0	0	0
3	E	6	0	0	0	0
3	F	8	0	0	1	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	2	0	0	0	0
3	J	8	0	0	0	0
All	All	21176	0	20112	1852	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 45.

The worst 5 of 1852 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:41:LEU:CD2	1:D:42:ALA:H	1.17	1.56
1:D:39:GLU:N	1:D:40:LYS:CG	1.71	1.50
1:C:270:ASP:CB	1:C:271:PRO:HA	1.32	1.44
1:E:39:GLU:N	1:E:40:LYS:HB3	1.31	1.42
1:D:41:LEU:CD2	1:D:42:ALA:N	1.77	1.41

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	269/290 (93%)	230 (86%)	29 (11%)	10 (4%)	4 22
1	B	269/290 (93%)	209 (78%)	46 (17%)	14 (5%)	2 14
1	C	266/290 (92%)	221 (83%)	33 (12%)	12 (4%)	3 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	269/290 (93%)	224 (83%)	34 (13%)	11 (4%)	3 19
1	E	266/290 (92%)	221 (83%)	34 (13%)	11 (4%)	3 19
1	F	269/290 (93%)	231 (86%)	30 (11%)	8 (3%)	5 27
1	G	268/290 (92%)	225 (84%)	28 (10%)	15 (6%)	2 12
1	H	265/290 (91%)	219 (83%)	37 (14%)	9 (3%)	4 24
1	I	269/290 (93%)	217 (81%)	38 (14%)	14 (5%)	2 14
1	J	269/290 (93%)	222 (82%)	32 (12%)	15 (6%)	2 12
All	All	2679/2900 (92%)	2219 (83%)	341 (13%)	119 (4%)	3 17

5 of 119 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
1	A	299	GLU
1	B	120	THR
1	B	149	HIS
1	B	188	GLU

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	227/246 (92%)	197 (87%)	30 (13%)	5 20
1	B	227/246 (92%)	194 (86%)	33 (14%)	4 17
1	C	223/246 (91%)	187 (84%)	36 (16%)	3 14
1	D	227/246 (92%)	194 (86%)	33 (14%)	4 17
1	E	224/246 (91%)	193 (86%)	31 (14%)	4 19
1	F	227/246 (92%)	202 (89%)	25 (11%)	7 28
1	G	226/246 (92%)	192 (85%)	34 (15%)	3 16
1	H	223/246 (91%)	189 (85%)	34 (15%)	3 16
1	I	227/246 (92%)	198 (87%)	29 (13%)	5 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	227/246 (92%)	195 (86%)	32 (14%)	4 18
All	All	2258/2460 (92%)	1941 (86%)	317 (14%)	4 18

5 of 317 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	152	SER
1	F	221	MET
1	J	136	ASN
1	E	185	ILE
1	E	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	271/290 (93%)	0.31	3 (1%)	80	55	57, 74, 97, 127	0
1	B	271/290 (93%)	0.31	5 (1%)	69	40	62, 80, 102, 115	0
1	C	268/290 (92%)	0.29	4 (1%)	74	47	50, 70, 100, 113	0
1	D	271/290 (93%)	0.29	4 (1%)	74	47	20, 71, 97, 113	0
1	E	268/290 (92%)	0.29	4 (1%)	74	47	43, 66, 98, 119	0
1	F	271/290 (93%)	0.27	3 (1%)	80	55	42, 67, 96, 130	0
1	G	270/290 (93%)	0.31	4 (1%)	74	47	48, 71, 94, 107	0
1	H	267/290 (92%)	0.28	6 (2%)	62	33	51, 70, 97, 108	0
1	I	271/290 (93%)	0.31	6 (2%)	62	33	62, 80, 103, 113	0
1	J	271/290 (93%)	0.33	4 (1%)	74	47	58, 74, 97, 123	0
All	All	2699/2900 (93%)	0.30	43 (1%)	72	44	20, 73, 99, 130	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	305	ALA	4.5
1	I	251	LEU	3.6
1	A	293	LEU	3.2
1	I	140	GLY	3.1
1	B	147	LEU	2.8

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	K	B	10	1/1	0.89	0.38	-	130,130,130,130	0
2	K	A	1	1/1	0.94	0.37	-	91,91,91,91	0
2	K	D	5	1/1	0.92	0.34	-	131,131,131,131	0
2	K	G	4	1/1	0.94	0.42	-	122,122,122,122	0
2	K	I	9	1/1	0.90	0.35	-	113,113,113,113	0
2	K	C	3	1/1	0.77	0.41	-	112,112,112,112	0
2	K	F	8	1/1	0.90	0.40	-	107,107,107,107	0
2	K	J	2	1/1	0.91	0.40	-	85,85,85,85	0
2	K	H	7	1/1	0.66	0.42	-	119,119,119,119	0
2	K	E	6	1/1	0.74	0.27	-	104,104,104,104	0

6.5 Other polymers (i)

There are no such residues in this entry.