wwPDB X-ray Structure Validation Summary Report (i)

Oct 7, 2023 – 10:20 PM EDT

PDB ID	:	6DV5
Title	:	Oligomeric complex of a Hsp27 24-mer at 3.6 A resolution
Authors	:	Aguda, A.H.; Brayer, G.D.
Deposited on	:	2018-06-22
Resolution	:	3.58 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:

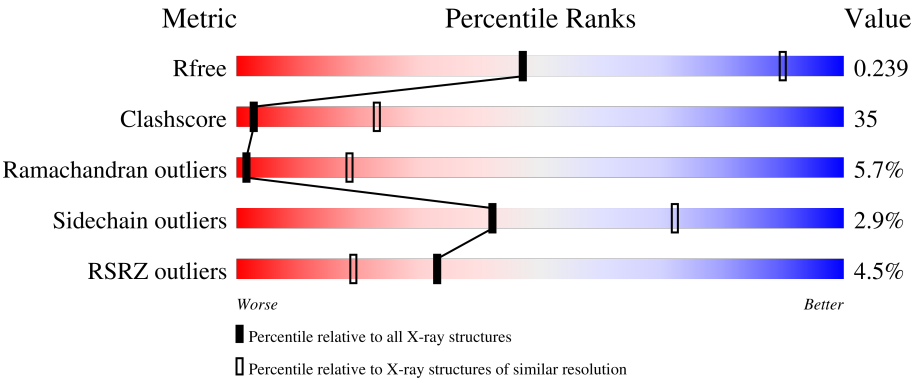
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.58 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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 <=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	205	7% 47% 34% 7% 12%
1	B	205	7% 41% 32% • 24%
1	C	205	% 44% 30% 6% • 19%
1	D	205	% 41% 35% • 20%
1	E	205	5% 46% 32% 6% 16%

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Mol	Chain	Length	Quality of chain
1	F	205	3% 55% 24% 20%
1	G	205	4% 55% 25% 7% 13%
1	H	205	7% 52% 21% 5% 22%
1	I	205	2% 47% 32% 18%
1	J	205	4% 51% 26% 21%
1	K	205	5% 60% 22% 15%
1	L	205	% 57% 22% 20%
1	M	205	6% 45% 33% 8% 14%
1	N	205	4% 53% 24% 21%
1	O	205	4% 46% 33% 6% 15%
1	P	205	% 52% 26% 20%
1	Q	205	2% 49% 22% 6% 21%
1	R	205	3% 60% 20% 19%
1	S	205	5% 50% 33% 5% 12%
1	T	205	2% 54% 25% 19%
1	U	205	2% 41% 37% 7% 15%
1	V	205	% 51% 25% 21%
1	W	205	5% 52% 27% 18%
1	X	205	2% 52% 26% 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 32356 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 Heat shock protein beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	156	Total	C	N	O	S	0	0	0
			1256	799	219	236	2			
1	A	181	Total	C	N	O	S	0	0	0
			1442	909	256	274	3			
1	D	165	Total	C	N	O	S	0	0	0
			1335	844	240	249	2			
1	F	163	Total	C	N	O	S	0	0	0
			1307	826	233	246	2			
1	H	160	Total	C	N	O	S	0	0	0
			1292	815	232	242	3			
1	J	162	Total	C	N	O	S	0	0	0
			1307	827	232	246	2			
1	L	165	Total	C	N	O	S	0	0	0
			1321	835	232	251	3			
1	N	162	Total	C	N	O	S	0	0	0
			1302	822	232	245	3			
1	P	164	Total	C	N	O	S	0	0	0
			1316	832	233	248	3			
1	R	167	Total	C	N	O	S	0	0	0
			1339	846	237	253	3			
1	T	166	Total	C	N	O	S	0	0	0
			1331	841	236	252	2			
1	V	161	Total	C	N	O	S	0	0	0
			1295	820	229	243	3			
1	X	166	Total	C	N	O	S	0	0	0
			1334	843	236	252	3			
1	C	166	Total	C	N	O	S	0	0	0
			1335	845	236	251	3			
1	E	173	Total	C	N	O	S	0	0	0
			1378	873	241	262	2			
1	G	179	Total	C	N	O	S	0	0	0
			1427	900	254	271	2			

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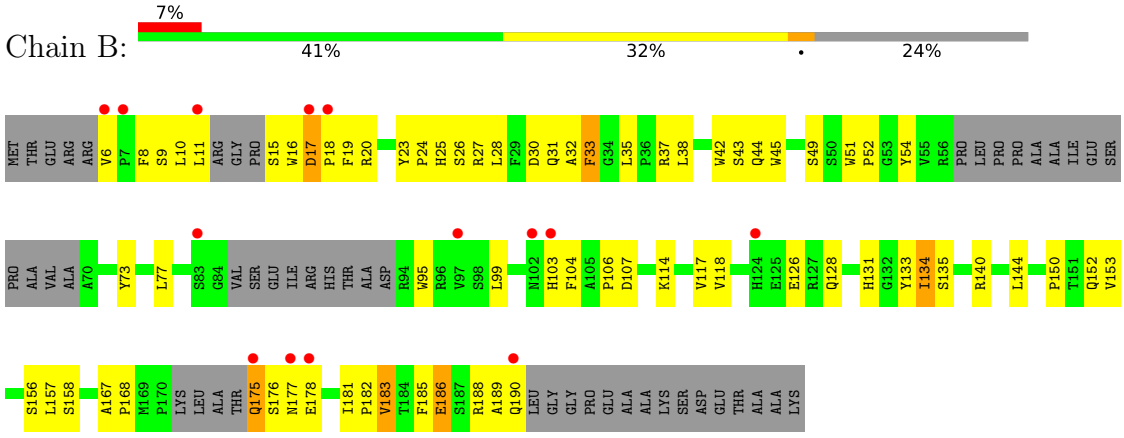
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	169	Total	C	N	O	S	0	0	0
			1347	855	237	253	2			
1	K	175	Total	C	N	O	S	0	0	0
			1403	884	249	267	3			
1	M	177	Total	C	N	O	S	0	0	0
			1411	891	252	266	2			
1	O	174	Total	C	N	O	S	0	0	0
			1388	878	247	260	3			
1	Q	161	Total	C	N	O	S	0	0	0
			1301	823	232	243	3			
1	S	180	Total	C	N	O	S	0	0	0
			1435	905	255	272	3			
1	U	175	Total	C	N	O	S	0	0	0
			1395	881	249	262	3			
1	W	169	Total	C	N	O	S	0	0	0
			1359	861	242	253	3			

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.

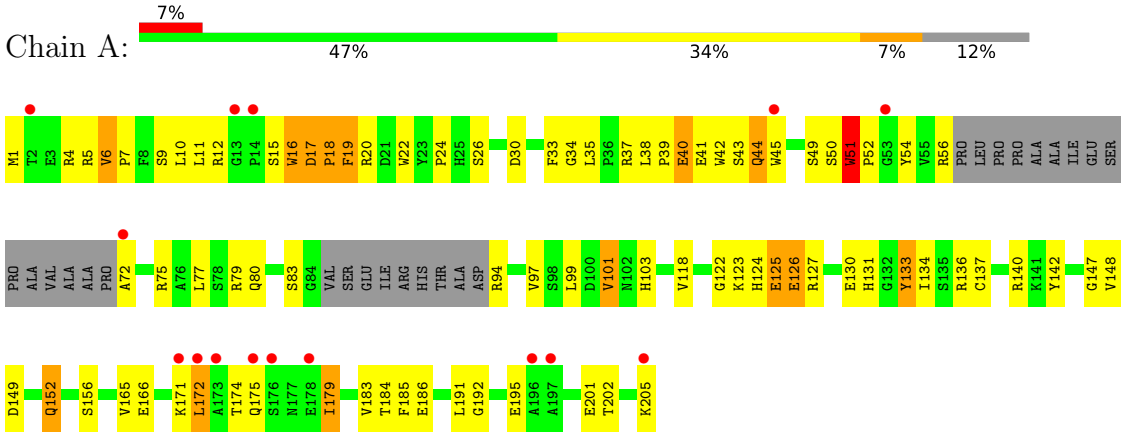
• Molecule 1: Heat shock protein beta-1

Chain B:



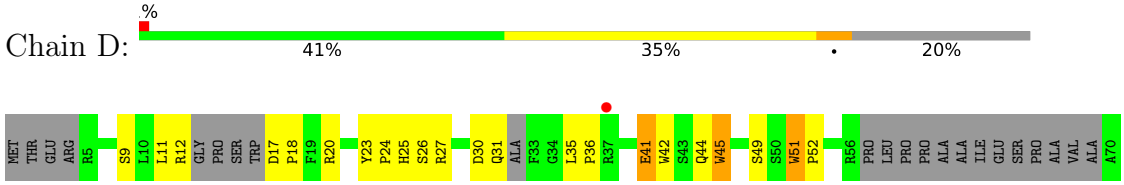
• Molecule 1: Heat shock protein beta-1

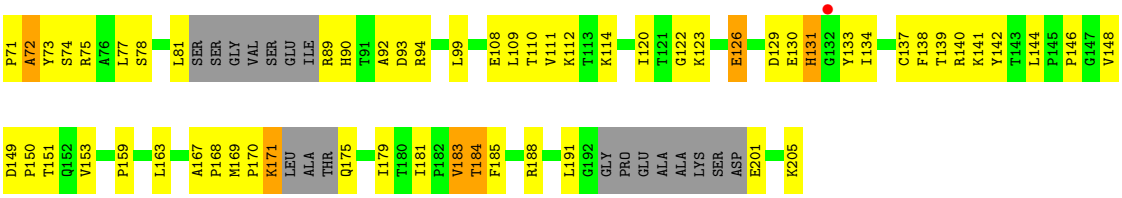
Chain A:



• Molecule 1: Heat shock protein beta-1

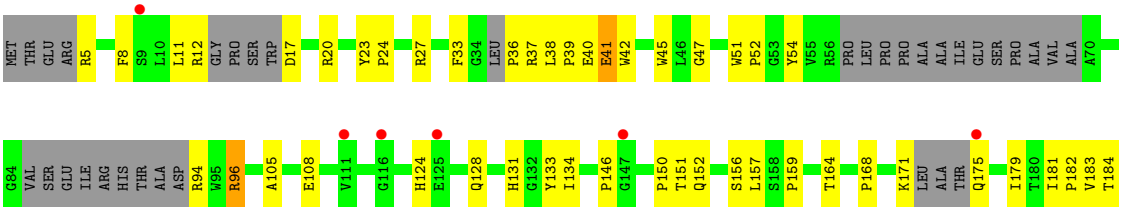
Chain D:

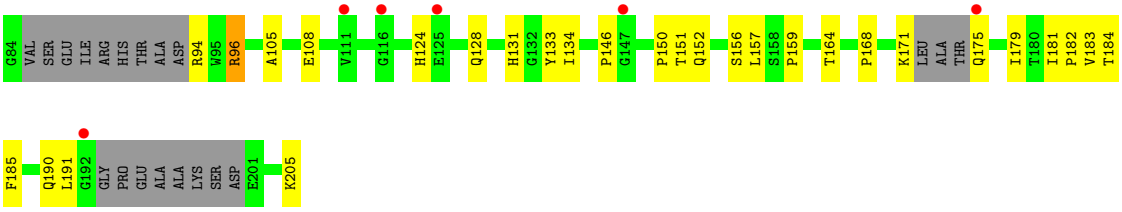




• Molecule 1: Heat shock protein beta-1

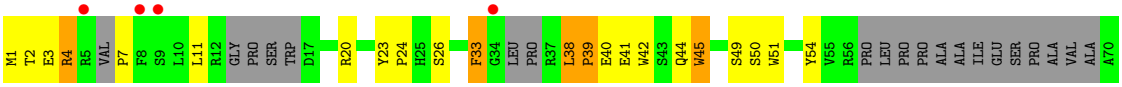
Chain F:

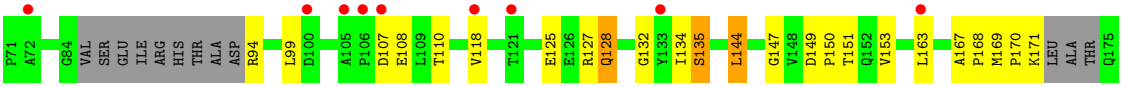


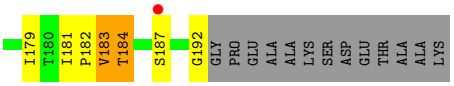


• Molecule 1: Heat shock protein beta-1

Chain H:

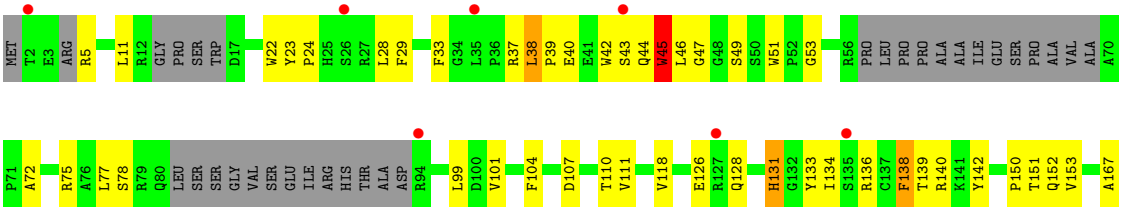


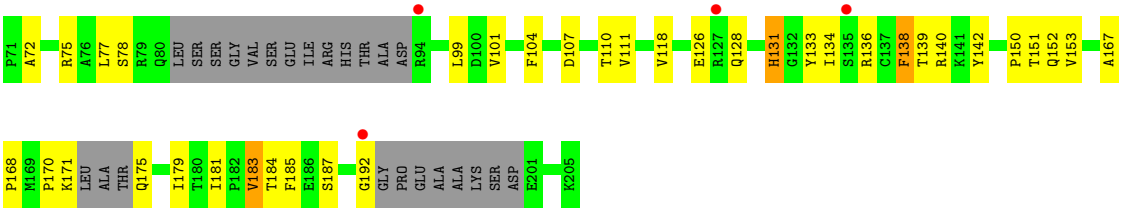




• Molecule 1: Heat shock protein beta-1

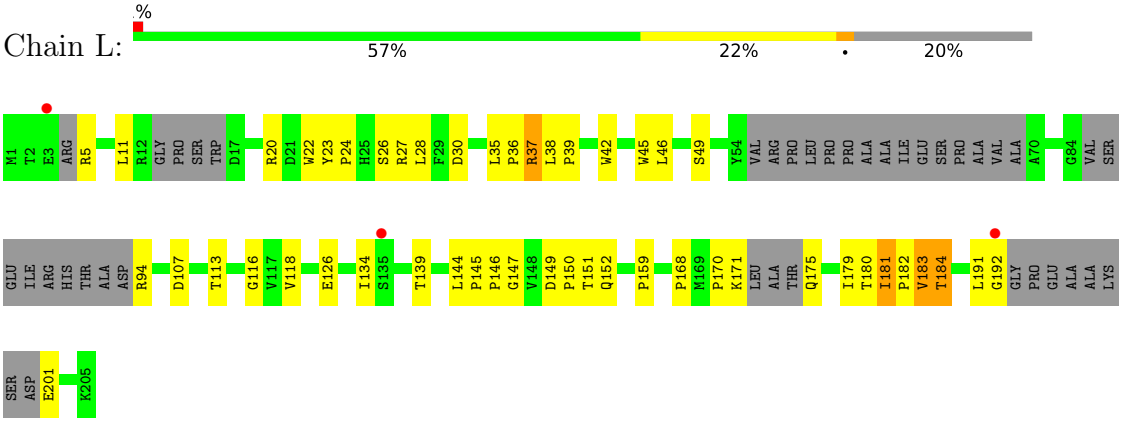
Chain J:





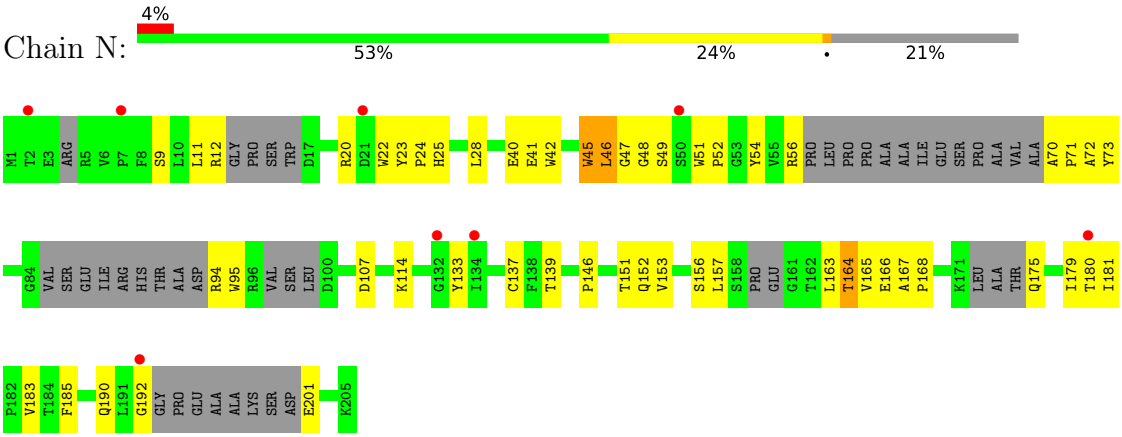
• Molecule 1: Heat shock protein beta-1

Chain L:



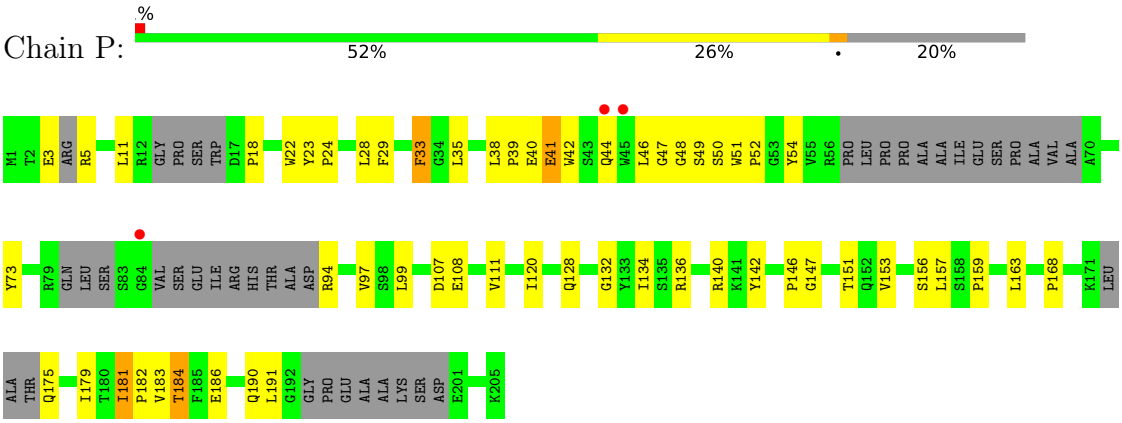
• Molecule 1: Heat shock protein beta-1

Chain N:



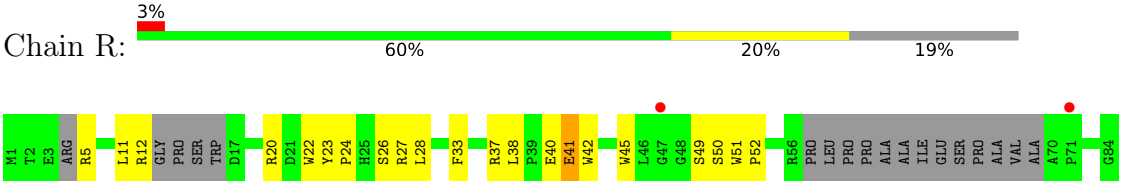
• Molecule 1: Heat shock protein beta-1

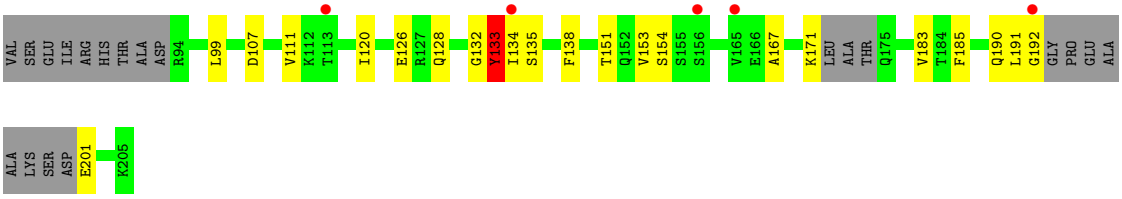
Chain P:



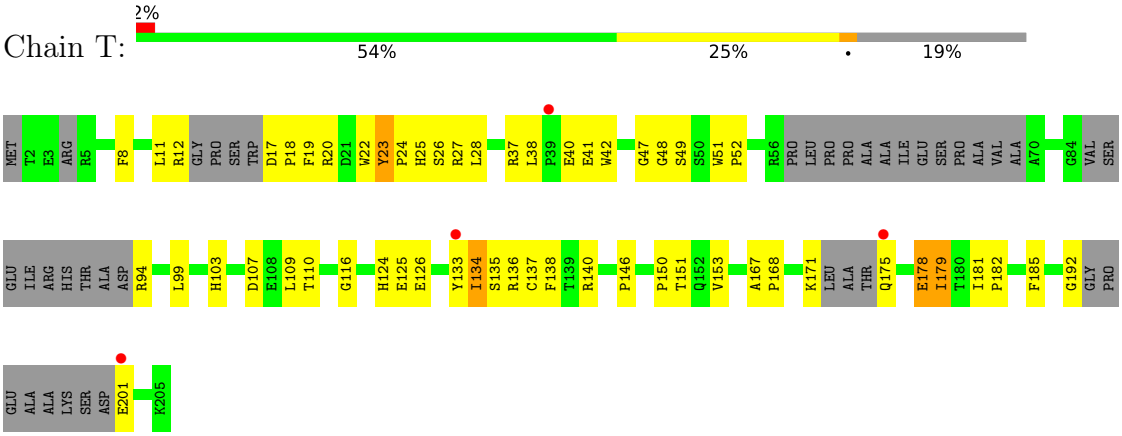
• Molecule 1: Heat shock protein beta-1

Chain R:

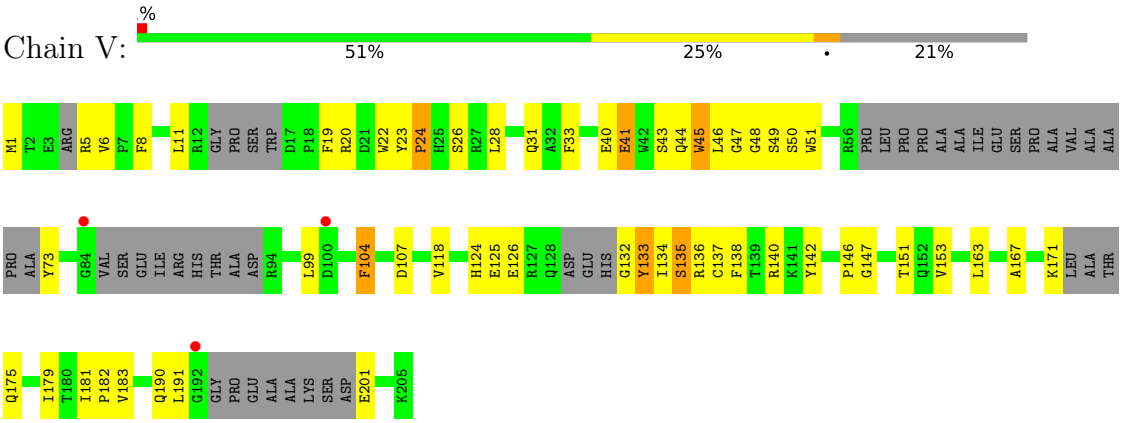




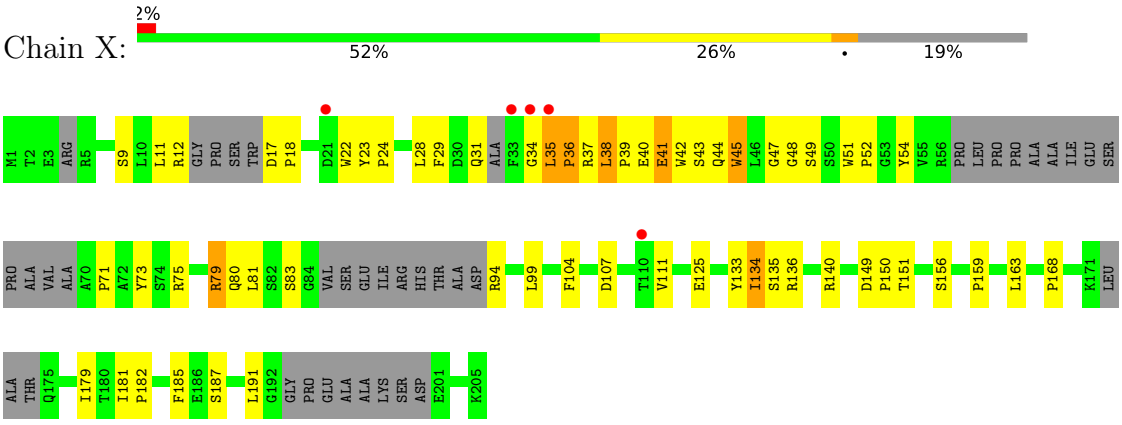
• Molecule 1: Heat shock protein beta-1



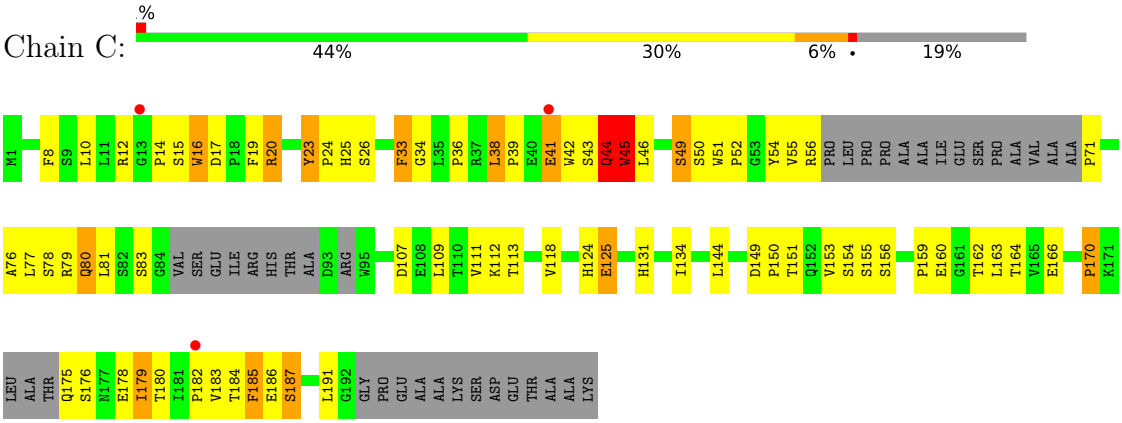
• Molecule 1: Heat shock protein beta-1



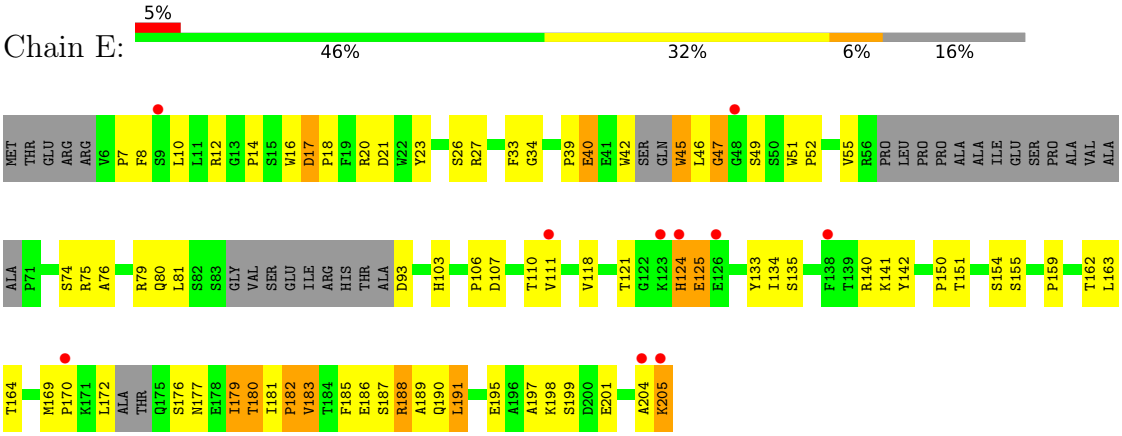
• Molecule 1: Heat shock protein beta-1



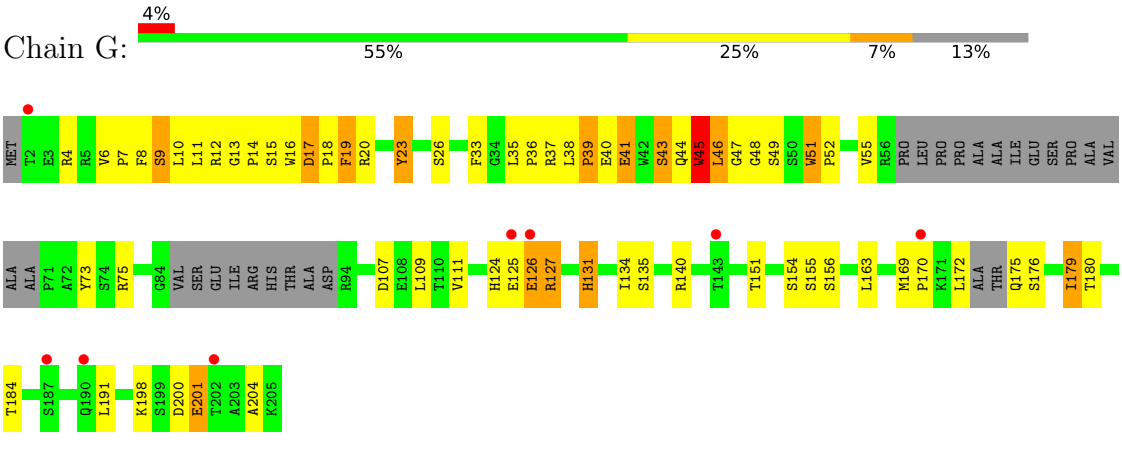
• Molecule 1: Heat shock protein beta-1



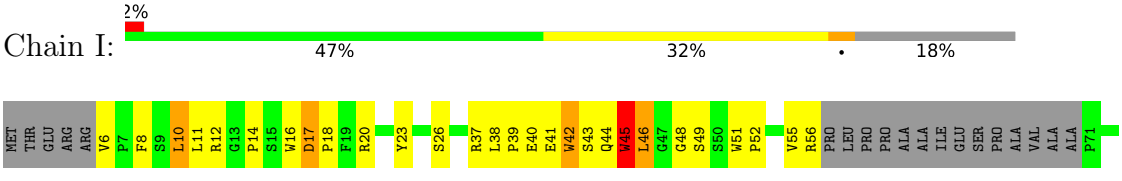
• Molecule 1: Heat shock protein beta-1

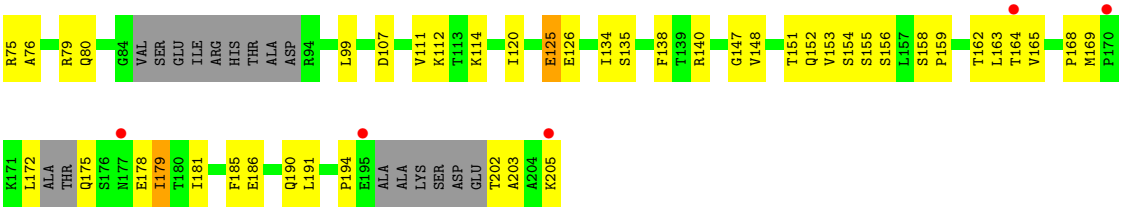


• Molecule 1: Heat shock protein beta-1



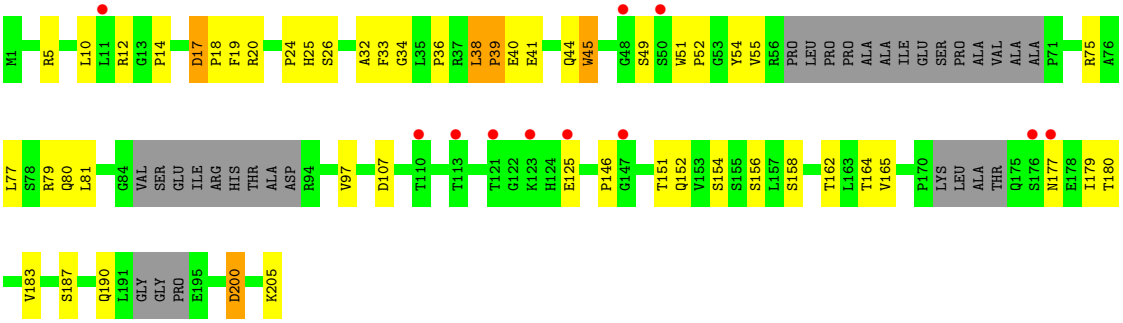
• Molecule 1: Heat shock protein beta-1





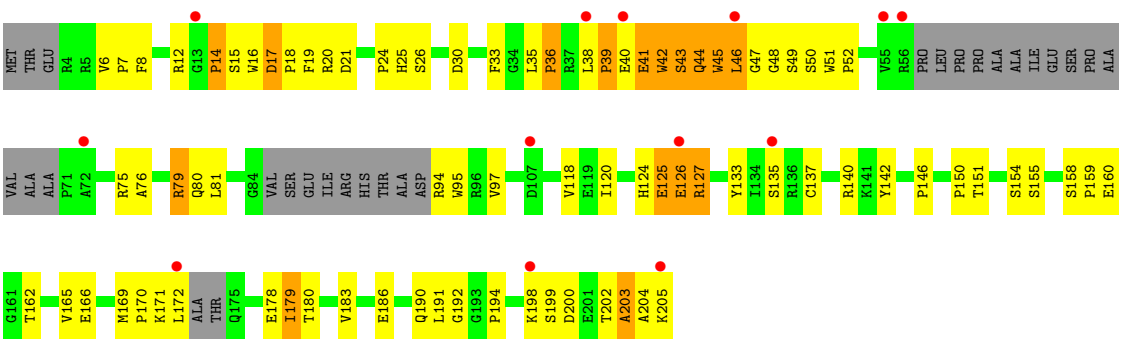
• Molecule 1: Heat shock protein beta-1

Chain K:



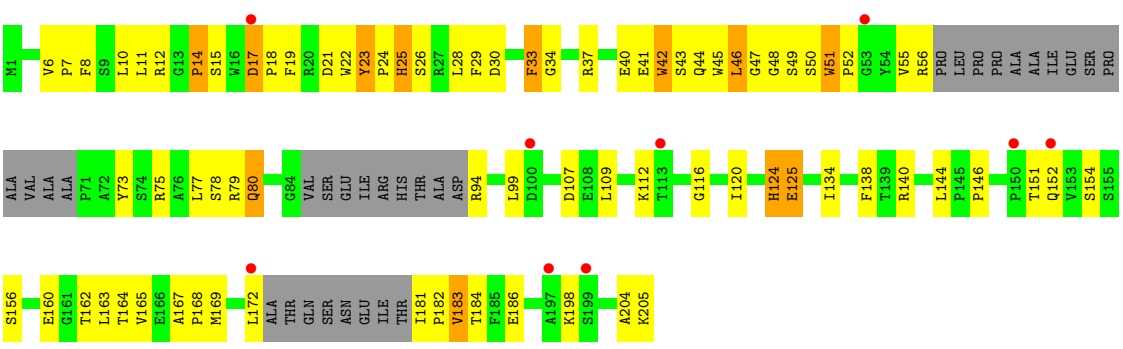
• Molecule 1: Heat shock protein beta-1

Chain M:



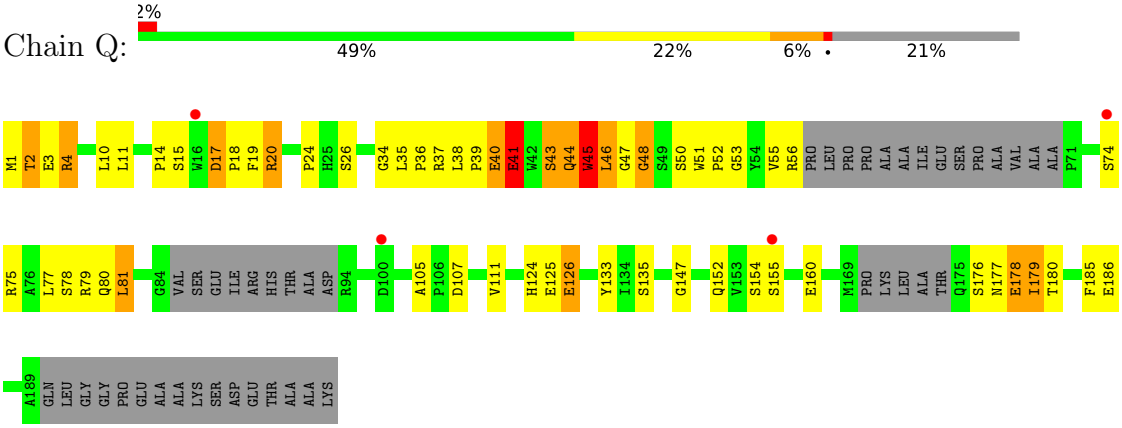
• Molecule 1: Heat shock protein beta-1

Chain O:



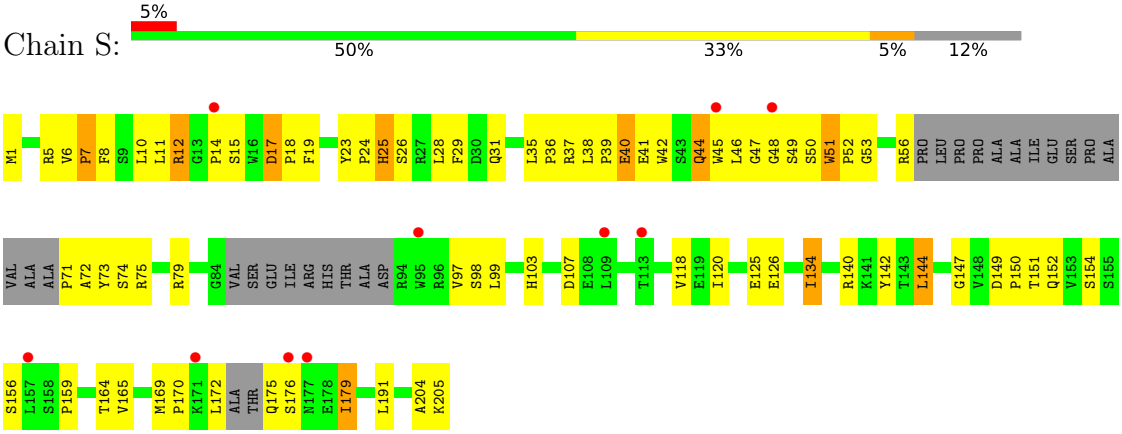
• Molecule 1: Heat shock protein beta-1

Chain Q:



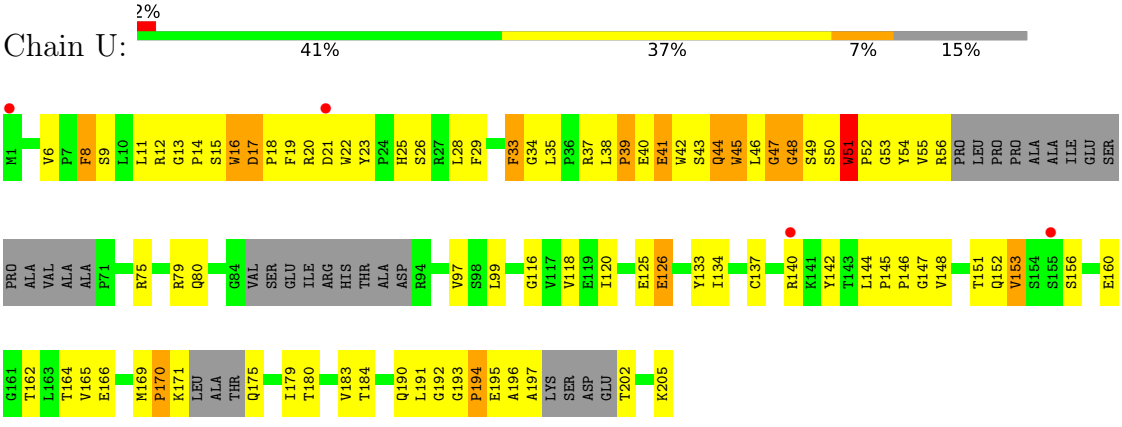
• Molecule 1: Heat shock protein beta-1

Chain S:



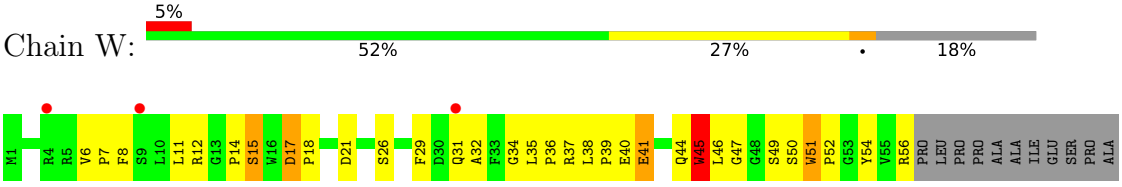
• Molecule 1: Heat shock protein beta-1

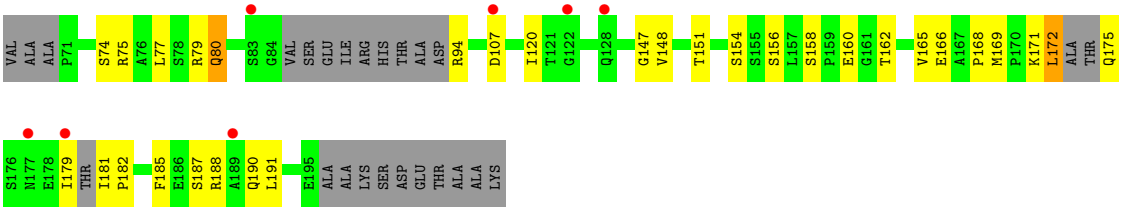
Chain U:



• Molecule 1: Heat shock protein beta-1

Chain W:




VAL ALA ALA P71 S74 R75 A76 L77 S78 R79 Q80 S83 G84 VAL SER GLU ILE ARG HIS THR ALA ASP R94 D107 I120 T121 G122 Q128 G147 V148 T151 S154 S155 S156 L157 S158 P159 E160 G161 T162 V165 E166 A167 P168 M169 P170 K171 L172 ALA THR Q175
S176 N177 E178 I179 THR I181 P182 F185 E186 S187 R188 A189 Q190 L191 E195 ALA ALA LYS SER ASP GLU THR ALA ALA LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	324.70Å 324.70Å 198.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.73 – 3.58 93.73 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.8 (93.73-3.58) 99.8 (93.73-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	18.26 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.238 , 0.242 0.235 , 0.239	Depositor DCC
R_{free} test set	4645 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 26.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.000 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.000 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.000 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.002 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.000 for h,-h-k,-l	Xtriage

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[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.

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Property	Value	Source
Reported twinning fraction	0.580 for H, K, L 0.057 for K, H, -L 0.062 for -K, -1/3H+1/3K+4/3L, -2/3H-1/3K-1/3L 0.061 for -1/3H+1/3K+4/3L, -K, 2/3H+1/3K+1/3L 0.062 for 1/3H-1/3K-4/3L, -H, 1/3H+2/3K-1/3L 0.061 for -H, 1/3H-1/3K-4/3L, -1/3H-2/3K+1/3L 0.059 for -1/3H-2/3K+4/3L, H+K, -1/3H+1/3K+1/3L 0.059 for -2/3H-1/3K-4/3L, H+K, 1/3H-1/3K-1/3L	Depositor
Outliers	0 of 91924 reflections	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	32356	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality (i)

5.1 Standard geometry (i)

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	0/1483	0.84	0/2014
1	B	0.69	0/1294	0.80	0/1761
1	C	0.71	0/1373	0.81	1/1863 (0.1%)
1	D	0.68	0/1370	0.79	0/1855
1	E	0.71	0/1417	0.84	1/1923 (0.1%)
1	F	0.67	0/1341	0.79	0/1814
1	G	0.70	0/1467	0.83	0/1990
1	H	0.68	0/1325	0.77	0/1791
1	I	0.68	0/1386	0.84	1/1881 (0.1%)
1	J	0.67	0/1341	0.79	0/1816
1	K	0.69	0/1441	0.83	1/1953 (0.1%)
1	L	0.66	0/1355	0.74	0/1834
1	M	0.69	0/1451	0.78	1/1968 (0.1%)
1	N	0.69	0/1333	0.81	0/1799
1	O	0.64	0/1428	0.81	1/1936 (0.1%)
1	P	0.67	0/1349	0.78	0/1824
1	Q	0.71	0/1339	0.84	1/1818 (0.1%)
1	R	0.65	0/1373	0.80	0/1858
1	S	0.68	0/1475	0.84	1/2000 (0.1%)
1	T	0.70	0/1365	0.78	0/1848
1	U	0.73	0/1434	0.87	1/1944 (0.1%)
1	V	0.70	0/1326	0.80	0/1791
1	W	0.71	0/1398	0.83	1/1896 (0.1%)
1	X	0.68	0/1367	0.80	0/1848
All	All	0.69	0/33231	0.81	10/45025 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	14	PRO	N-CA-CB	7.01	111.71	103.30
1	W	14	PRO	N-CA-CB	6.96	111.65	103.30
1	E	14	PRO	N-CA-CB	6.79	111.45	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	14	PRO	N-CA-CB	6.67	111.31	103.30
1	O	14	PRO	N-CA-CB	6.66	111.29	103.30

There are no chirality outliers.

There are no planarity outliers.

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	1442	0	1393	195	0
1	B	1256	0	1195	132	0
1	C	1335	0	1277	146	0
1	D	1335	0	1285	194	0
1	E	1378	0	1318	158	0
1	F	1307	0	1257	113	0
1	G	1427	0	1370	102	0
1	H	1292	0	1243	88	0
1	I	1347	0	1292	119	0
1	J	1307	0	1256	77	0
1	K	1403	0	1344	86	0
1	L	1321	0	1270	73	0
1	M	1411	0	1357	149	0
1	N	1302	0	1252	117	0
1	O	1388	0	1339	174	0
1	P	1316	0	1267	73	0
1	Q	1301	0	1245	113	0
1	R	1339	0	1292	86	0
1	S	1435	0	1382	163	0
1	T	1331	0	1280	95	0
1	U	1395	0	1342	144	0
1	V	1295	0	1257	113	0
1	W	1359	0	1306	127	0
1	X	1334	0	1286	84	0
All	All	32356	0	31105	2239	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 35.

The worst 5 of 2239 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:A:33:PHE:CE1	1:A:35:LEU:HG	1.31	1.62
1:O:94:ARG:HB2	1:O:169:MET:CG	1.39	1.52
1:O:45:TRP:HB2	1:O:50:SER:CB	1.37	1.50
1:A:35:LEU:HB3	1:Q:46:LEU:CD2	1.42	1.45
1:A:15:SER:HB2	1:A:16:TRP:CE3	1.52	1.40

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	175/205 (85%)	124 (71%)	37 (21%)	14 (8%)	1 11
1	B	146/205 (71%)	112 (77%)	28 (19%)	6 (4%)	3 26
1	C	157/205 (77%)	107 (68%)	36 (23%)	14 (9%)	1 9
1	D	151/205 (74%)	129 (85%)	15 (10%)	7 (5%)	2 23
1	E	163/205 (80%)	120 (74%)	29 (18%)	14 (9%)	1 10
1	F	149/205 (73%)	125 (84%)	22 (15%)	2 (1%)	12 49
1	G	171/205 (83%)	125 (73%)	31 (18%)	15 (9%)	1 9
1	H	146/205 (71%)	122 (84%)	14 (10%)	10 (7%)	1 15
1	I	159/205 (78%)	119 (75%)	30 (19%)	10 (6%)	1 17
1	J	148/205 (72%)	126 (85%)	17 (12%)	5 (3%)	3 31
1	K	165/205 (80%)	124 (75%)	35 (21%)	6 (4%)	3 29
1	L	151/205 (74%)	129 (85%)	15 (10%)	7 (5%)	2 23
1	M	169/205 (82%)	123 (73%)	29 (17%)	17 (10%)	0 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	144/205 (70%)	117 (81%)	22 (15%)	5 (4%)	3 30
1	O	166/205 (81%)	119 (72%)	36 (22%)	11 (7%)	1 16
1	P	148/205 (72%)	125 (84%)	18 (12%)	5 (3%)	3 31
1	Q	153/205 (75%)	113 (74%)	26 (17%)	14 (9%)	1 9
1	R	153/205 (75%)	131 (86%)	19 (12%)	3 (2%)	7 41
1	S	172/205 (84%)	129 (75%)	34 (20%)	9 (5%)	2 20
1	T	152/205 (74%)	125 (82%)	22 (14%)	5 (3%)	4 31
1	U	165/205 (80%)	111 (67%)	39 (24%)	15 (9%)	1 9
1	V	145/205 (71%)	124 (86%)	15 (10%)	6 (4%)	3 26
1	W	159/205 (78%)	120 (76%)	33 (21%)	6 (4%)	3 27
1	X	150/205 (73%)	127 (85%)	14 (9%)	9 (6%)	1 17
All	All	3757/4920 (76%)	2926 (78%)	616 (16%)	215 (6%)	1 18

5 of 215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	ASP
1	B	134	ILE
1	B	177	ASN
1	B	189	ALA
1	A	44	GLN

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	157/175 (90%)	151 (96%)	6 (4%)	33 66
1	B	139/175 (79%)	134 (96%)	5 (4%)	35 67
1	C	147/175 (84%)	138 (94%)	9 (6%)	18 53
1	D	146/175 (83%)	141 (97%)	5 (3%)	37 69
1	E	150/175 (86%)	145 (97%)	5 (3%)	38 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	143/175 (82%)	143 (100%)	0	100	100
1	G	155/175 (89%)	149 (96%)	6 (4%)	32	65
1	H	142/175 (81%)	138 (97%)	4 (3%)	43	73
1	I	147/175 (84%)	144 (98%)	3 (2%)	55	79
1	J	143/175 (82%)	138 (96%)	5 (4%)	36	68
1	K	153/175 (87%)	149 (97%)	4 (3%)	46	74
1	L	145/175 (83%)	143 (99%)	2 (1%)	67	85
1	M	153/175 (87%)	148 (97%)	5 (3%)	38	69
1	N	142/175 (81%)	142 (100%)	0	100	100
1	O	150/175 (86%)	144 (96%)	6 (4%)	31	65
1	P	144/175 (82%)	141 (98%)	3 (2%)	53	79
1	Q	143/175 (82%)	136 (95%)	7 (5%)	25	59
1	R	147/175 (84%)	145 (99%)	2 (1%)	67	85
1	S	156/175 (89%)	150 (96%)	6 (4%)	33	66
1	T	146/175 (83%)	144 (99%)	2 (1%)	67	85
1	U	151/175 (86%)	145 (96%)	6 (4%)	31	65
1	V	143/175 (82%)	139 (97%)	4 (3%)	43	73
1	W	149/175 (85%)	144 (97%)	5 (3%)	37	69
1	X	147/175 (84%)	145 (99%)	2 (1%)	67	85
All	All	3538/4200 (84%)	3436 (97%)	102 (3%)	42	72

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	107	ASP
1	M	133	TYR
1	W	107	ASP
1	G	198	LYS
1	K	107	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	25	HIS

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Mol	Chain	Res	Type
1	S	31	GLN
1	U	190	GLN
1	R	175	GLN
1	P	177	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	181/205 (88%)	0.82	15 (8%) 11 6	27, 61, 113, 195	0
1	B	156/205 (76%)	0.86	14 (8%) 9 5	47, 60, 112, 161	0
1	C	166/205 (80%)	0.50	3 (1%) 68 51	28, 60, 95, 158	0
1	D	165/205 (80%)	0.57	2 (1%) 79 64	13, 65, 104, 165	0
1	E	173/205 (84%)	0.79	10 (5%) 23 12	24, 65, 99, 131	0
1	F	163/205 (79%)	0.74	7 (4%) 35 21	27, 65, 112, 138	0
1	G	179/205 (87%)	0.69	8 (4%) 33 19	16, 64, 105, 133	0
1	H	160/205 (78%)	0.89	14 (8%) 10 5	24, 66, 100, 166	0
1	I	169/205 (82%)	0.59	5 (2%) 50 32	18, 61, 99, 152	0
1	J	162/205 (79%)	0.73	8 (4%) 29 17	26, 65, 101, 136	0
1	K	175/205 (85%)	0.75	11 (6%) 20 10	19, 68, 100, 135	0
1	L	165/205 (80%)	0.64	3 (1%) 68 51	16, 61, 95, 177	0
1	M	177/205 (86%)	0.68	13 (7%) 15 8	29, 65, 123, 159	0
1	N	162/205 (79%)	0.71	8 (4%) 29 17	31, 67, 112, 156	0
1	O	174/205 (84%)	0.68	9 (5%) 27 16	27, 66, 107, 146	0
1	P	164/205 (80%)	0.53	3 (1%) 68 51	25, 65, 108, 137	0
1	Q	161/205 (78%)	0.51	4 (2%) 57 39	27, 63, 102, 175	0
1	R	167/205 (81%)	0.77	7 (4%) 36 22	20, 64, 97, 138	0
1	S	180/205 (87%)	0.71	10 (5%) 24 13	28, 67, 106, 141	0
1	T	166/205 (80%)	0.55	4 (2%) 59 41	23, 67, 97, 151	0
1	U	175/205 (85%)	0.57	4 (2%) 60 42	26, 64, 108, 246	0
1	V	161/205 (78%)	0.57	3 (1%) 66 49	29, 63, 106, 156	0
1	W	169/205 (82%)	0.69	10 (5%) 22 11	24, 65, 114, 159	0
1	X	166/205 (80%)	0.61	5 (3%) 50 32	32, 63, 98, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	4036/4920 (82%)	0.67	180 (4%)	33	19	13, 64, 107, 246	0

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	192	GLY	6.9
1	L	192	GLY	4.7
1	I	195	GLU	4.4
1	A	172	LEU	4.1
1	A	14	PRO	4.0

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

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.