



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:25 am GMT

PDB ID : 1PV2
Title : Native Form 2 E.coli Chaperone Hsp31
Authors : Quigley, P.M.; Korotkov, K.; Baneyx, F.; Hol, W.G.J.
Deposited on : 2003-06-26
Resolution : 2.71 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

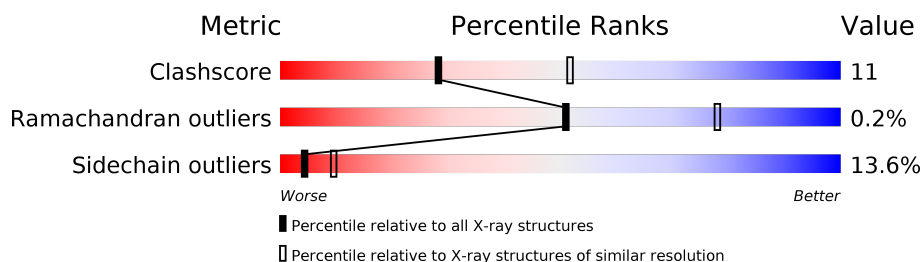
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	112137	2993 (2.74-2.70)
Ramachandran outliers	110173	2946 (2.74-2.70)
Sidechain outliers	110143	2947 (2.74-2.70)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	283	
1	B	283	
1	C	283	
1	D	283	
1	E	283	
1	F	283	
1	G	283	

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Mol	Chain	Length	Quality of chain
1	H	283	<div><div></div><div>65%</div><div>26%</div><div>6%</div><div>••</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16233 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 Chaperone protein hchA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1864	1203	309	344	8			
1	B	257	Total	C	N	O	S	0	0	0
			2008	1297	337	365	9			
1	C	249	Total	C	N	O	S	0	0	0
			1940	1252	323	356	9			
1	D	264	Total	C	N	O	S	0	0	0
			2048	1319	342	378	9			
1	E	270	Total	C	N	O	S	0	0	0
			2091	1341	352	389	9			
1	F	261	Total	C	N	O	S	0	0	0
			2031	1310	339	373	9			
1	G	260	Total	C	N	O	S	0	0	0
			2023	1305	338	371	9			
1	H	277	Total	C	N	O	S	0	0	0
			2156	1386	359	402	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING MET	UNP P31658
B	1	MET	-	INITIATING MET	UNP P31658
C	1	MET	-	INITIATING MET	UNP P31658
D	1	MET	-	INITIATING MET	UNP P31658
E	1	MET	-	INITIATING MET	UNP P31658
F	1	MET	-	INITIATING MET	UNP P31658
G	1	MET	-	INITIATING MET	UNP P31658
H	1	MET	-	INITIATING MET	UNP P31658

- Molecule 2 is water.

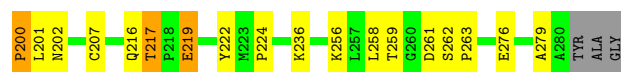
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	O 7	0	0
2	B	7	Total 7	O 7	0	0
2	C	13	Total 13	O 13	0	0
2	D	7	Total 7	O 7	0	0
2	E	6	Total 6	O 6	0	0
2	F	8	Total 8	O 8	0	0
2	G	11	Total 11	O 11	0	0
2	H	13	Total 13	O 13	0	0

Note EDS was not executed.

- [illegible]

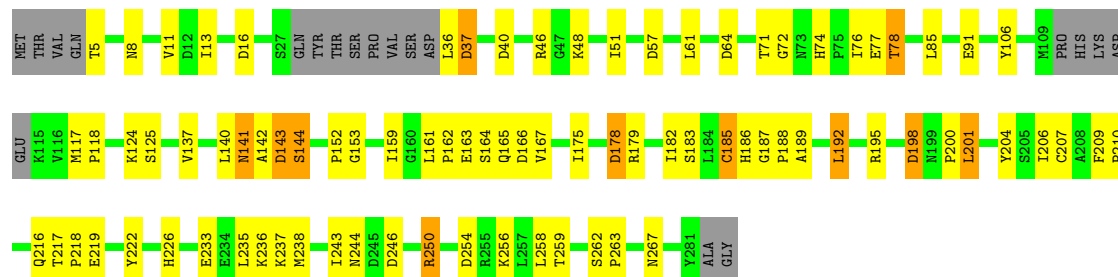
- Chain B:
-
- 65% 20% 5% 9%
- MET THR VAL GLN THR S6 K7 T113 D16 S25 L26 S27 Q28 Y29 THR SER PRO VAL SER ASP LEU ASP GLY VAL ASP TYR PRO K43 P44 Y45 R46 G47 K48 H49 R50 I51 L52 D57 L61 P62 M65 T71 G72 N73 H74 P75 I76 E77 T78 F90 L100 M101 T102 K103 F104 E105 M109 PRO HIS LYS ASP GLI K115 R128 V137 M141 ALA ASP S144 A147 A148 I149 G153 L161 P162 E163 S164 Q165 D166 V167 A168 A169 Q172 K176 M177 D178 R179 S183 L184 C185 H186 G187 P188 A189 L192 R195 D198

- [illegible]



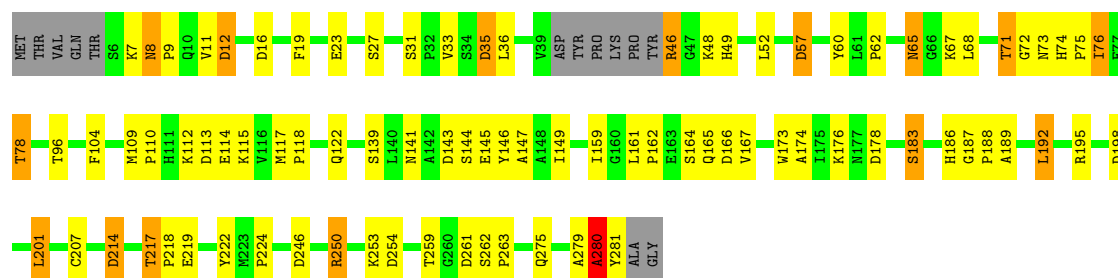
• Molecule 1: Chaperone protein hchA

Chain D: 63% 26% 7%



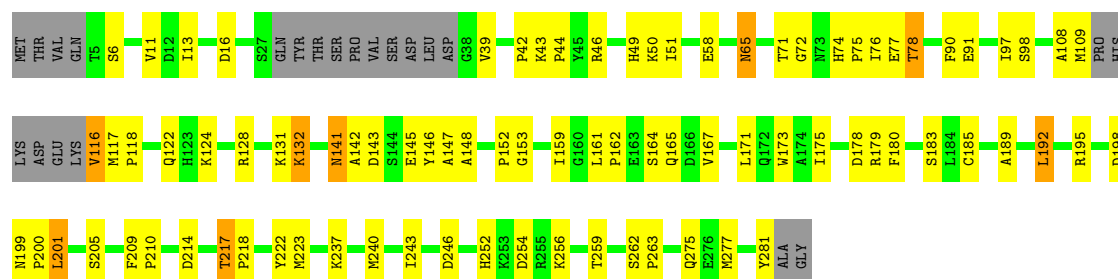
• Molecule 1: Chaperone protein hchA

Chain E: 64% 25% 5% 5%



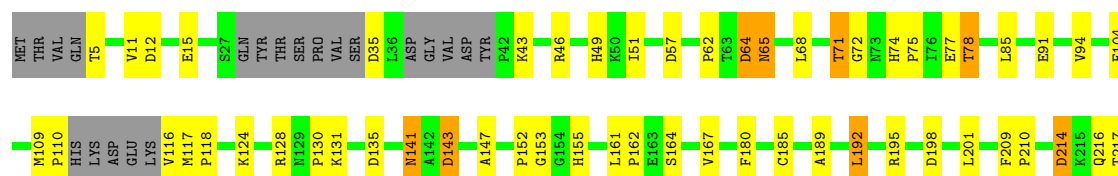
• Molecule 1: Chaperone protein hchA

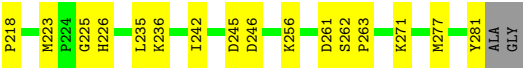
Chain F: 62% 28% 8%



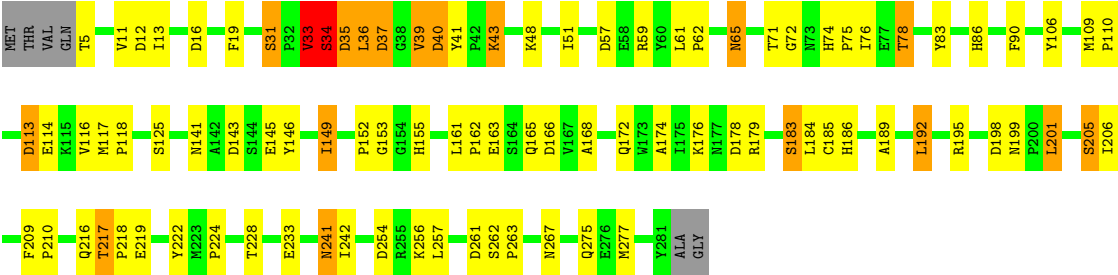
• Molecule 1: Chaperone protein hchA

Chain G: 66% 23% 8%





● Molecule 1: Chaperone protein hchA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.49Å 99.02Å 116.80Å 102.95° 101.52° 94.19°	Depositor
Resolution (Å)	48.80 – 2.71	Depositor
% Data completeness (in resolution range)	94.0 (48.80-2.71)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.221 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16233	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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	0.42	0/1912	0.98	24/2591 (0.9%)
1	B	0.26	0/2062	0.60	8/2792 (0.3%)
1	C	0.39	2/1991 (0.1%)	0.61	6/2698 (0.2%)
1	D	0.26	0/2104	0.62	10/2853 (0.4%)
1	E	0.32	0/2147	0.68	16/2912 (0.5%)
1	F	0.26	0/2087	0.61	6/2831 (0.2%)
1	G	0.26	0/2078	0.61	11/2817 (0.4%)
1	H	0.30	1/2218 (0.0%)	0.65	12/3014 (0.4%)
All	All	0.31	3/16599 (0.0%)	0.68	93/22508 (0.4%)

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	4
1	C	0	1
1	E	0	2
1	H	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	7	LYS	C-N	-10.12	1.10	1.34
1	C	200	PRO	C-N	8.60	1.53	1.34
1	H	34	SER	C-N	-6.46	1.19	1.34

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	TYR	CB-CG-CD2	18.61	132.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ALA	C-N-CA	12.80	153.70	121.70
1	A	146	TYR	CB-CG-CD1	-12.66	113.40	121.00
1	A	87	ALA	N-CA-CB	8.19	121.56	110.10
1	A	146	TYR	CZ-CE2-CD2	-7.67	112.89	119.80

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	TYR	Sidechain
1	A	148	ALA	Mainchain,Peptide
1	A	85	LEU	Peptide
1	C	7	LYS	Mainchain
1	E	280	ALA	Mainchain

5.2 Too-close contacts

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	1864	0	1818	76	0
1	B	2008	0	1965	45	0
1	C	1940	0	1898	37	0
1	D	2048	0	1987	41	0
1	E	2091	0	2034	37	0
1	F	2031	0	1979	44	0
1	G	2023	0	1976	32	0
1	H	2156	0	2087	48	0
2	A	7	0	0	1	0
2	B	7	0	0	0	0
2	C	13	0	0	1	0
2	D	7	0	0	0	0
2	E	6	0	0	0	0
2	F	8	0	0	0	0
2	G	11	0	0	0	0
2	H	13	0	0	0	0
All	All	16233	0	15744	354	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 11.

The worst 5 of 354 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:74:HIS:O	1:A:78:THR:HG22	1.59	1.00
1:A:50:LYS:N	1:A:51:ILE:HA	1.72	0.99
1:A:85:LEU:O	1:A:90:PHE:HB2	1.74	0.86
1:B:49:HIS:HB3	1:B:147:ALA:HB2	1.59	0.85
1:A:75:PRO:HG2	1:A:109:MET:HB3	1.59	0.85

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	233/283 (82%)	204 (88%)	27 (12%)	2 (1%)	20	45
1	B	249/283 (88%)	232 (93%)	17 (7%)	0	100	100
1	C	241/283 (85%)	226 (94%)	14 (6%)	1 (0%)	38	65
1	D	258/283 (91%)	248 (96%)	10 (4%)	0	100	100
1	E	266/283 (94%)	251 (94%)	14 (5%)	1 (0%)	38	65
1	F	255/283 (90%)	242 (95%)	13 (5%)	0	100	100
1	G	252/283 (89%)	242 (96%)	10 (4%)	0	100	100
1	H	275/283 (97%)	256 (93%)	18 (6%)	1 (0%)	38	65
All	All	2029/2264 (90%)	1901 (94%)	123 (6%)	5 (0%)	51	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	36	LEU

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Mol	Chain	Res	Type
1	A	86	HIS
1	A	87	ALA
1	E	280	ALA
1	C	279	ALA

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	192/230 (84%)	166 (86%)	26 (14%)	4	10
1	B	207/230 (90%)	178 (86%)	29 (14%)	4	9
1	C	202/230 (88%)	177 (88%)	25 (12%)	5	12
1	D	211/230 (92%)	185 (88%)	26 (12%)	5	12
1	E	218/230 (95%)	182 (84%)	36 (16%)	2	6
1	F	210/230 (91%)	179 (85%)	31 (15%)	3	8
1	G	210/230 (91%)	191 (91%)	19 (9%)	11	25
1	H	225/230 (98%)	190 (84%)	35 (16%)	3	7
All	All	1675/1840 (91%)	1448 (86%)	227 (14%)	4	9

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	236	LYS
1	E	141	ASN
1	H	145	GLU
1	D	250	ARG
1	E	46	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	267	ASN

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Mol	Chain	Res	Type
1	E	196	HIS
1	H	196	HIS
1	E	65	ASN
1	E	141	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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.