W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:35 PM GMT

PDB ID	:	1UD0
Title	:	CRYSTAL STRUCTURE OF THE C-TERMINAL 10-kDA SUBDOMAIN OF HSC70
Authors	:	Chou, C.C.; Forouhar, F.; Yeh, Y.H.; Wang, C.; Hsiao, C.D.
Deposited on	:	2003-04-24
Resolution	:	3.45 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.

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 3.45 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.
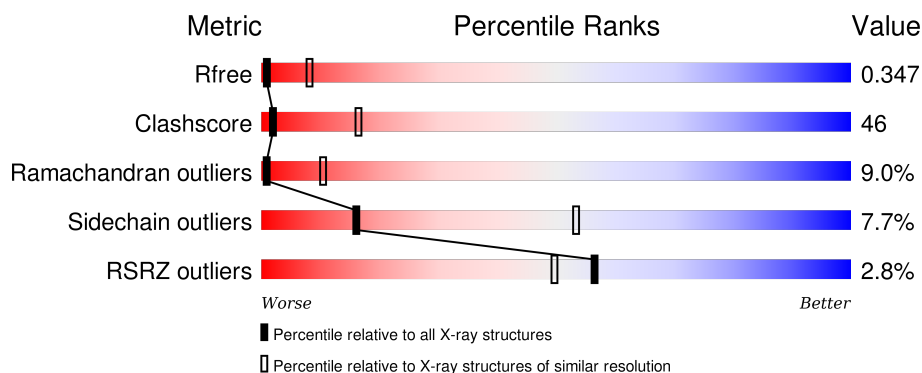
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	113	
1	B	113	
1	C	113	
1	D	113	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2705 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 70 kDa heat-shock-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	84	Total	C	N	O	S	Se	0	0	0
			672	417	114	136	2	3			
1	B	82	Total	C	N	O	S	Se	0	0	0
			664	413	112	134	2	3			
1	C	88	Total	C	N	O	S	Se	0	0	0
			702	438	118	140	2	4			
1	D	78	Total	C	N	O	S	Se	0	0	0
			641	399	108	130	2	2			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	LEU	-	CLONING ARTIFACT	UNP P63018
A	535	VAL	-	CLONING ARTIFACT	UNP P63018
A	536	PRO	-	CLONING ARTIFACT	UNP P63018
A	537	ARG	-	CLONING ARTIFACT	UNP P63018
A	538	GLY	-	CLONING ARTIFACT	UNP P63018
A	539	SER	-	CLONING ARTIFACT	UNP P63018
A	540	HIS	-	CLONING ARTIFACT	UNP P63018
A	541	MSE	-	CLONING ARTIFACT	UNP P63018
A	549	MSE	MET	MODIFIED RESIDUE	UNP P63018
A	617	MSE	MET	MODIFIED RESIDUE	UNP P63018
A	621	MSE	MET	MODIFIED RESIDUE	UNP P63018
B	534	LEU	-	CLONING ARTIFACT	UNP P63018
B	535	VAL	-	CLONING ARTIFACT	UNP P63018
B	536	PRO	-	CLONING ARTIFACT	UNP P63018
B	537	ARG	-	CLONING ARTIFACT	UNP P63018
B	538	GLY	-	CLONING ARTIFACT	UNP P63018
B	539	SER	-	CLONING ARTIFACT	UNP P63018
B	540	HIS	-	CLONING ARTIFACT	UNP P63018
B	541	MSE	-	CLONING ARTIFACT	UNP P63018
B	549	MSE	MET	MODIFIED RESIDUE	UNP P63018
B	617	MSE	MET	MODIFIED RESIDUE	UNP P63018

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Chain	Residue	Modelled	Actual	Comment	Reference
B	621	MSE	MET	MODIFIED RESIDUE	UNP P63018
C	534	LEU	-	CLONING ARTIFACT	UNP P63018
C	535	VAL	-	CLONING ARTIFACT	UNP P63018
C	536	PRO	-	CLONING ARTIFACT	UNP P63018
C	537	ARG	-	CLONING ARTIFACT	UNP P63018
C	538	GLY	-	CLONING ARTIFACT	UNP P63018
C	539	SER	-	CLONING ARTIFACT	UNP P63018
C	540	HIS	-	CLONING ARTIFACT	UNP P63018
C	541	MSE	-	CLONING ARTIFACT	UNP P63018
C	549	MSE	MET	MODIFIED RESIDUE	UNP P63018
C	617	MSE	MET	MODIFIED RESIDUE	UNP P63018
C	621	MSE	MET	MODIFIED RESIDUE	UNP P63018
D	534	LEU	-	CLONING ARTIFACT	UNP P63018
D	535	VAL	-	CLONING ARTIFACT	UNP P63018
D	536	PRO	-	CLONING ARTIFACT	UNP P63018
D	537	ARG	-	CLONING ARTIFACT	UNP P63018
D	538	GLY	-	CLONING ARTIFACT	UNP P63018
D	539	SER	-	CLONING ARTIFACT	UNP P63018
D	540	HIS	-	CLONING ARTIFACT	UNP P63018
D	541	MSE	-	CLONING ARTIFACT	UNP P63018
D	549	MSE	MET	MODIFIED RESIDUE	UNP P63018
D	617	MSE	MET	MODIFIED RESIDUE	UNP P63018
D	621	MSE	MET	MODIFIED RESIDUE	UNP P63018

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Na 1	0	0
2	D	2	Total 2	Na 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	7	Total 7	O 7	0	0
3	C	5	Total 5	O 5	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

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.
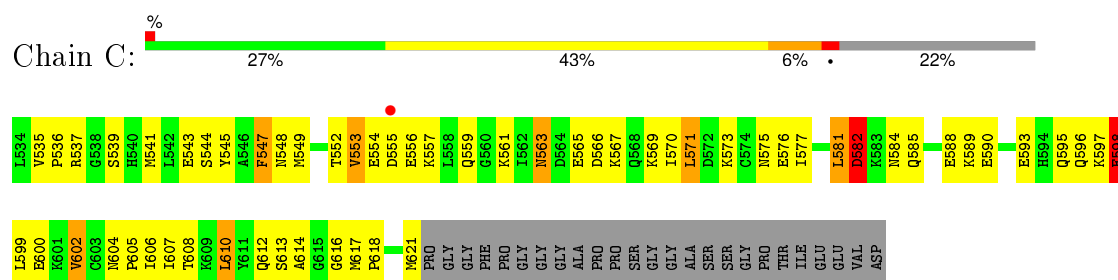
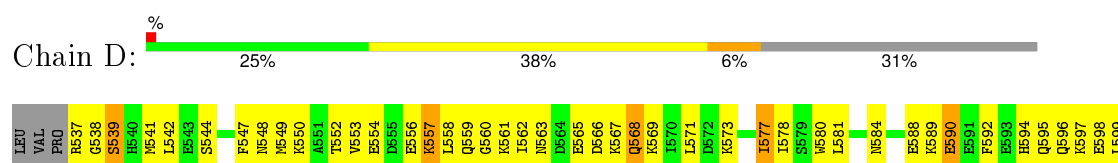- Molecule 1: 70 kDa heat-shock-like protein
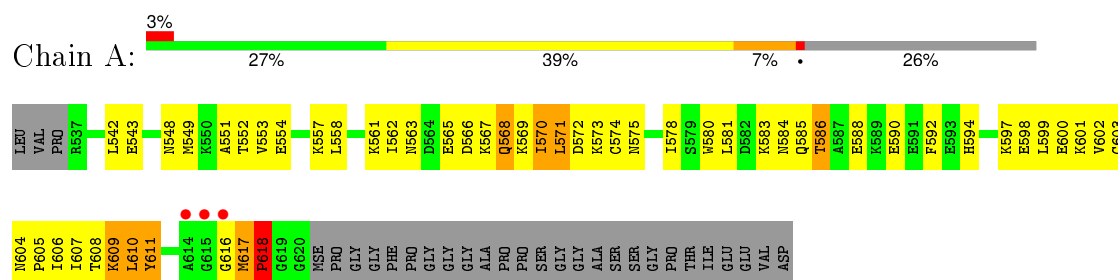
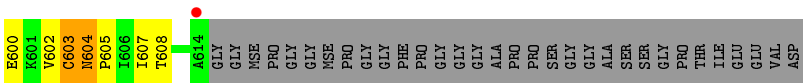- Molecule 1: 70 kDa heat-shock-like protein
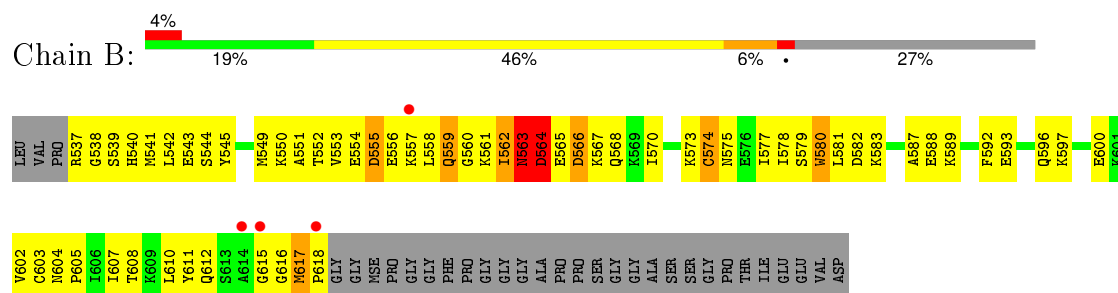
- Molecule 1: 70 kDa heat-shock-like protein

- Molecule 1: 70 kDa heat-shock-like protein

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	117.48Å 117.48Å 163.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.93 – 3.45 14.92 – 3.45	Depositor EDS
% Data completeness (in resolution range)	90.3 (14.93-3.45) 99.0 (14.92-3.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.30 (at 3.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.249 , 0.309 0.305 , 0.347	Depositor DCC
R_{free} test set	450 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	63.0	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 22.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	1 of 16440 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	2705	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.51	0/678	0.69	0/900
1	B	0.49	0/670	0.69	0/890
1	C	0.51	0/708	0.65	0/940
1	D	0.62	1/647 (0.2%)	0.71	1/861 (0.1%)
All	All	0.53	1/2703 (0.0%)	0.68	1/3591 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	544	SER	C-N	7.58	1.51	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	544	SER	O-C-N	-5.38	114.08	122.70

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	672	0	659	65	0
1	B	664	0	653	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	702	0	695	62	0
1	D	641	0	631	66	1
2	B	1	0	0	0	0
2	D	2	0	0	0	0
3	A	8	0	0	0	0
3	B	7	0	0	0	0
3	C	5	0	0	0	0
3	D	3	0	0	0	0
All	All	2705	0	2638	247	1

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 46.

The worst 5 of 247 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:537:ARG:HG2	1:D:538:GLY:H	1.15	1.08
1:B:617:MSE:H	1:B:618:PRO:HD2	1.18	1.05
1:B:562:ILE:HB	1:B:566:ASP:HB3	1.48	0.93
1:A:558:LEU:HD23	1:A:562:ILE:HB	1.53	0.91
1:A:549:MSE:HE3	1:A:549:MSE:HA	1.54	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:GLU:OE2	1:D:554:GLU:OE2[7_556]	1.50	0.70

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	82/113 (73%)	54 (66%)	17 (21%)	11 (13%)	0	4
1	B	80/113 (71%)	49 (61%)	23 (29%)	8 (10%)	1	9
1	C	86/113 (76%)	61 (71%)	20 (23%)	5 (6%)	2	21
1	D	76/113 (67%)	51 (67%)	20 (26%)	5 (7%)	1	18
All	All	324/452 (72%)	215 (66%)	80 (25%)	29 (9%)	1	10

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	618	PRO
1	B	559	GLN
1	B	563	ASN
1	B	617	MSE
1	D	539	SER

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	74/89 (83%)	68 (92%)	6 (8%)	15	51
1	B	74/89 (83%)	71 (96%)	3 (4%)	37	74
1	C	78/89 (88%)	68 (87%)	10 (13%)	5	27
1	D	72/89 (81%)	68 (94%)	4 (6%)	26	66
All	All	298/356 (84%)	275 (92%)	23 (8%)	16	53

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	555	ASP
1	C	581	LEU
1	D	603	CYS
1	C	563	ASN
1	C	582	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	612	GLN
1	C	604	ASN
1	D	584	ASN
1	B	604	ASN
1	D	563	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)

Of 3 ligands modelled in this entry, 3 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 (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)

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, 95th 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	81/113 (71%)	0.01	3 (3%)	45	39	44, 44, 44, 44	0
1	B	79/113 (69%)	0.20	4 (5%)	32	27	44, 44, 44, 44	0
1	C	84/113 (74%)	-0.01	1 (1%)	81	74	44, 44, 44, 44	0
1	D	76/113 (67%)	-0.12	1 (1%)	79	72	44, 44, 44, 44	0
All	All	320/452 (70%)	0.02	9 (2%)	56	50	44, 44, 44, 44	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	615	GLY	4.1
1	B	618	PRO	4.0
1	B	615	GLY	3.5
1	C	555	ASP	3.4
1	A	614	ALA	3.2

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 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, 95th 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	NA	B	701	1/1	0.54	0.29	-	34,34,34,34	1
2	NA	D	702	1/1	0.88	0.19	-	25,25,25,25	0
2	NA	D	703	1/1	0.88	0.23	-	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.