wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 07:49 PM EDT

PDB ID	:	2F1Z
Title	:	Crystal structure of HAUSP
Authors	:	Hu, M.; Gu, L.; Jeffrey, P.D.; Shi, Y.
Deposited on	:	2005-11-15
Resolution	:	3.20 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:

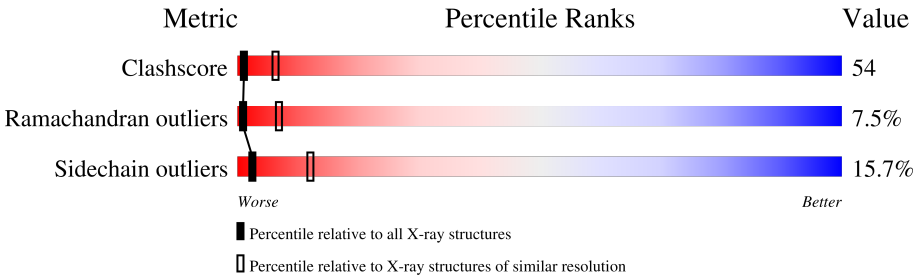
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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	522	22% 52% 15% • 10%
1	B	522	29% 48% 14% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8015 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3842	2442	652	726	22			
1	B	481	Total	C	N	O	S	0	0	0
			3933	2500	668	743	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	cloning artifact	UNP Q93009
A	40	SER	-	cloning artifact	UNP Q93009
A	41	HIS	-	cloning artifact	UNP Q93009
A	42	MET	-	cloning artifact	UNP Q93009
B	39	GLY	-	cloning artifact	UNP Q93009
B	40	SER	-	cloning artifact	UNP Q93009
B	41	HIS	-	cloning artifact	UNP Q93009
B	42	MET	-	cloning artifact	UNP Q93009

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	118	Total	O	0	0
			118	118		
2	B	122	Total	O	0	0
			122	122		

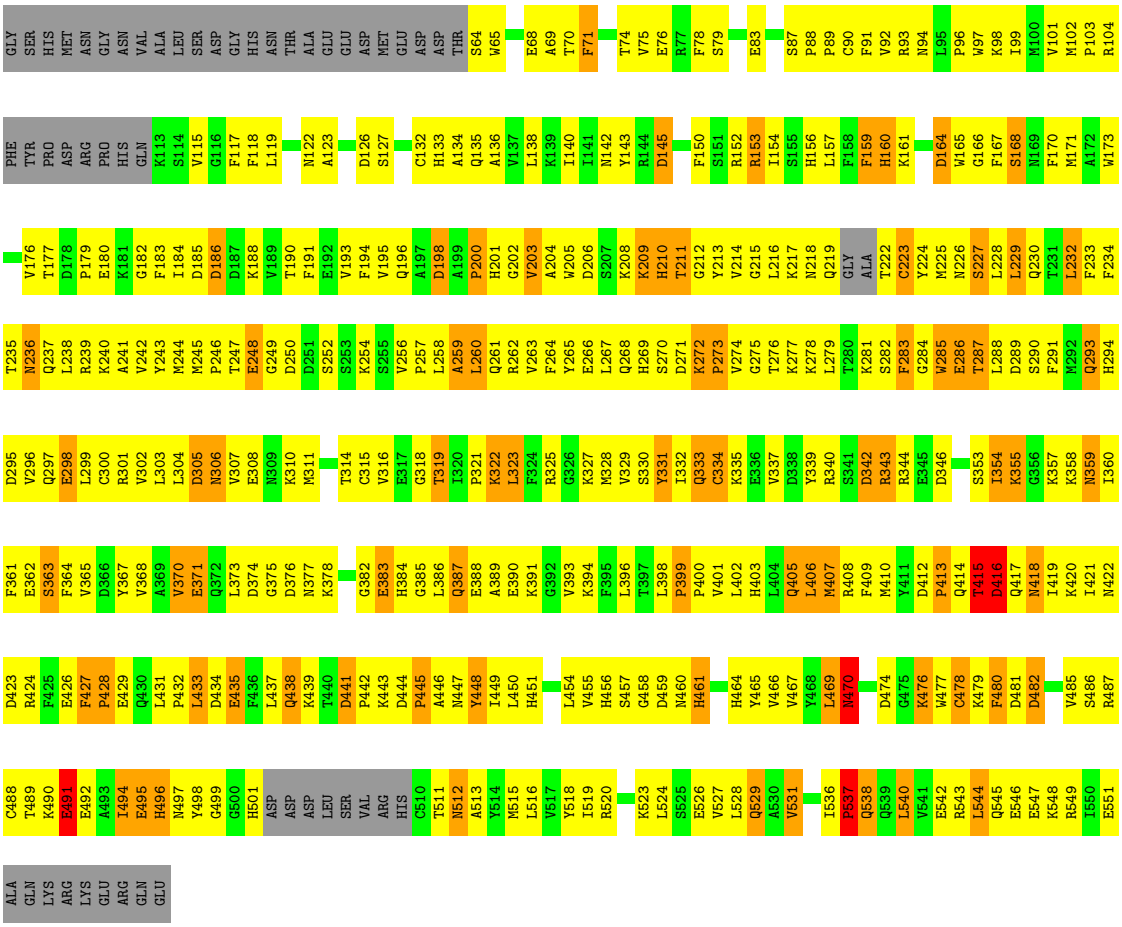
3 Residue-property plots (i)

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.

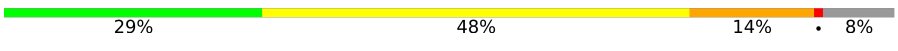
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

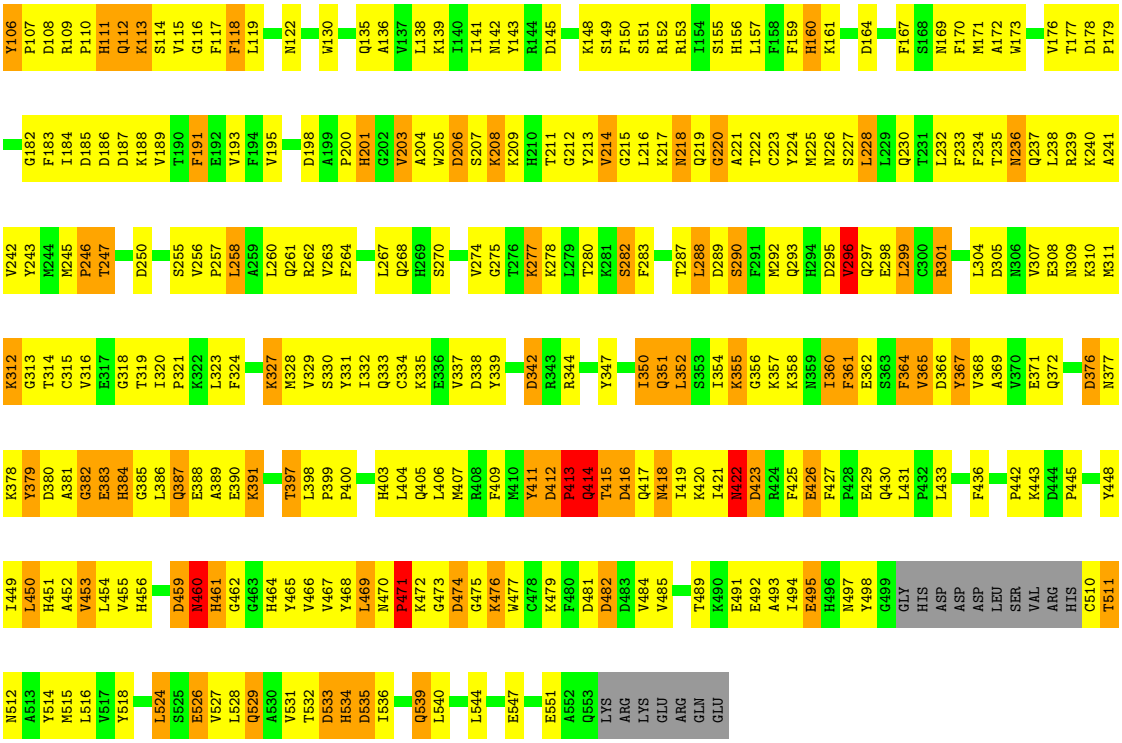
Chain A:



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain B:




Y106 P107 D108 R109 P110 H111 Q112 K113 S114 V115 G116 F117 F118 L119 N122 W130 Q135 A136 V137 L138 K139 I140 I141 N142 Y143 R144 D145 K148 S149 F150 S151 R152 R153 I154 S155 H156 L157 F158 F159 H160 K161 D164 F167 S168 N169 F170 M171 A172 W173 V176 T177 D178 P179
G182 F183 I184 D185 D186 D187 K188 V189 T190 F191 E192 V193 F194 V195 D198 A199 P200 H201 G202 V203 A204 W205 D206 S207 K208 K209 H210 T211 G212 Y213 V214 G215 L216 K217 N218 Q219 G220 A221 T222 C223 Y224 M225 N226 S227 L228 L229 Q230 T231 L232 F233 F234 T235 N236 Q237 L238 R239 K240 A241
V242 Y243 M244 M245 P246 T247 D250 S255 V256 P257 L258 A259 L260 Q261 R262 V263 F264 L267 Q268 H269 S270 V274 G275 T276 K277 K278 L279 T280 K281 S282 F283 T287 L288 D289 S290 F291 M292 Q293 H294 D295 V296 Q297 E298 L299 C300 R301 L304 D305 N306 V307 E308 N309 K310 M311
K312 G313 T314 C315 V316 E317 G318 T319 I320 P321 K322 L323 F324 K327 M328 V329 S330 Y331 I332 Q333 C334 K335 E336 V337 D338 Y339 D342 R343 R344 Y347 I350 Q351 L352 S353 I354 K355 G356 K357 K358 N359 I360 F361 E362 S363 F364 V365 D366 Y367 V368 A369 V370 E371 Q372 D376 N377
K378 Y379 D380 A381 G382 E383 H384 G385 L386 Q387 E388 A389 E390 K391 T397 L398 P399 P400 H403 L404 Q405 L406 M407 R408 F409 M410 Y411 D412 P413 Q414 T415 D416 Q417 M418 I419 K420 I421 N422 D423 R424 F425 E426 F427 P428 E429 Q430 L431 P432 L433 F436 P442 K443 D444 P445 Y448
I449 L450 H451 A452 V453 L454 V455 H456 D459 N460 H461 G462 G463 H464 Y465 V466 V467 Y468 L469 N470 P471 K472 G473 D474 G475 K476 W477 C478 K479 F480 D481 D482 D483 V484 V485 T489 K490 E491 E492 A493 I494 E495 H496 N497 Y498 G499 GLY HIS ASP ASP ASP LEU SER VAL ARG HIS C510 T511
N512 A513 Y514 M515 L516 V517 Y518 L524 S525 E526 V527 L528 Q529 A530 V531 T532 D533 H534 D535 I536 Q539 L540 L544 E547 E551 A552 Q553 LYS ARG LYS GLU ARG GLN GLU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.62Å 219.86Å 130.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8015	wwPDB-VP
Average B, all atoms (Å^2)	56.0	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	0.46	0/3935	0.74	1/5312 (0.0%)
1	B	0.50	2/4032 (0.0%)	0.81	9/5449 (0.2%)
All	All	0.48	2/7967 (0.0%)	0.78	10/10761 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	ARG	CZ-NH1	5.37	1.40	1.33
1	B	104	ARG	CB-CG	5.26	1.66	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	104	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	B	414	GLN	N-CA-C	-9.00	86.71	111.00
1	B	104	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	105	PHE	N-CA-C	7.61	131.54	111.00
1	B	387	GLN	CB-CA-C	-6.44	97.52	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	TYR	Sidechain

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	3842	0	3710	428	1
1	B	3933	0	3794	406	0
2	A	118	0	0	44	0
2	B	122	0	0	41	0
All	All	8015	0	7504	821	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 54.

The worst 5 of 821 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:109:ARG:HE	1:B:110:PRO:HD2	1.21	1.04
1:B:491:GLU:HA	1:B:495:GLU:HG3	1.39	1.03
1:A:501:HIS:HB3	1:B:413:PRO:HG3	1.38	1.01
1:B:214:VAL:HG22	1:B:215:GLY:H	1.27	1.00
1:A:294:HIS:HB3	1:A:298:GLU:HG3	1.47	0.97

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:A:287:THR:O	1:A:287:THR:O[4_555]	1.83	0.37

5.3 Torsion angles

5.3.1 Protein backbone

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	462/522 (88%)	356 (77%)	71 (15%)	35 (8%)	1 7
1	B	477/522 (91%)	364 (76%)	78 (16%)	35 (7%)	1 7
All	All	939/1044 (90%)	720 (77%)	149 (16%)	70 (8%)	1 7

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	183	PHE
1	A	203	VAL
1	A	277	LYS
1	A	334	CYS

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	428/472 (91%)	355 (83%)	73 (17%)	2 10
1	B	437/472 (93%)	374 (86%)	63 (14%)	3 15
All	All	865/944 (92%)	729 (84%)	136 (16%)	2 12

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	418	ASN
1	B	450	LEU
1	B	533	ASP
1	A	415	THR
1	A	407	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	372	GLN

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Mol	Chain	Res	Type
1	B	464	HIS
1	B	387	GLN
1	B	417	GLN
1	B	539	GLN

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.