



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:22 PM GMT

PDB ID : 1FC6  
Title : PHOTOSYSTEM II D1 C-TERMINAL PROCESSING PROTEASE  
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Deposited on : 2000-07-18  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

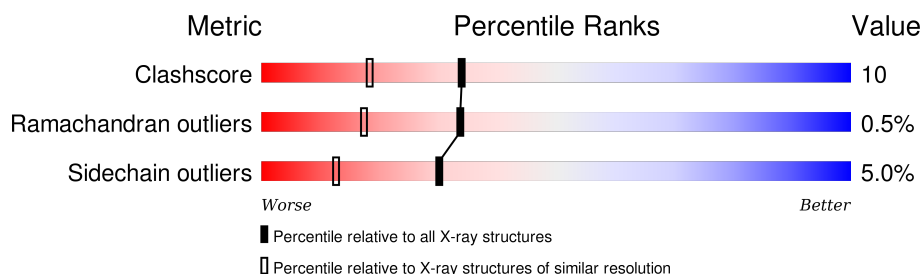
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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  $\geq 3$ , 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	388	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3205 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 PHOTOSYSTEM II D1 PROTEASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	386	2853	1784	505	558	2	4	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MSE	-	initiating MSE	UNP O04073
A	132	MSE	LEU	ENGINEERED	UNP O04073
A	210	MSE	LEU	ENGINEERED	UNP O04073
A	119	MSE	MET	MODIFIED RESIDUE	UNP O04073
A	329	MSE	MET	MODIFIED RESIDUE	UNP O04073

- Molecule 2 is water.

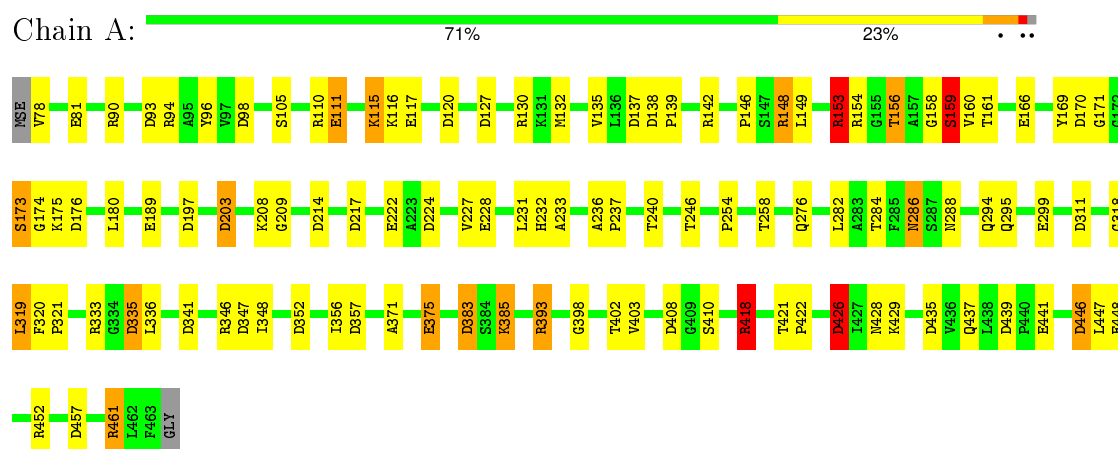
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	352	Total	O	0	0
			352	352		

### 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.

Note EDS was not executed.

#### • Molecule 1: PHOTOSYSTEM II D1 PROTEASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.30Å 64.45Å 63.73Å 90.00° 122.11° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	99.1 (30.00-1.80)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.168 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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	1.10	10/2890 (0.3%)	1.50	66/3924 (1.7%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	GLU	CD-OE2	7.31	1.33	1.25
1	A	375	GLU	CD-OE2	7.11	1.33	1.25
1	A	117	GLU	CD-OE2	7.04	1.33	1.25
1	A	228	GLU	CD-OE2	6.63	1.32	1.25
1	A	189	GLU	CD-OE2	6.54	1.32	1.25
1	A	166	GLU	CD-OE2	6.46	1.32	1.25
1	A	299	GLU	CD-OE2	6.43	1.32	1.25
1	A	222	GLU	CD-OE2	5.76	1.31	1.25
1	A	448	GLU	CD-OE2	5.60	1.31	1.25
1	A	111	GLU	CD-OE2	5.01	1.31	1.25

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	ASP	CB-CG-OD2	-11.10	108.31	118.30
1	A	90	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	A	93	ASP	CB-CG-OD2	-9.77	109.50	118.30
1	A	341	ASP	CB-CG-OD1	9.34	126.70	118.30
1	A	341	ASP	CB-CG-OD2	-9.17	110.05	118.30
1	A	94	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	A	130	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	138	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	A	93	ASP	CB-CG-OD1	8.52	125.97	118.30
1	A	197	ASP	CB-CG-OD1	8.26	125.74	118.30
1	A	352	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	A	214	ASP	CB-CG-OD1	7.89	125.40	118.30
1	A	127	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	A	217	ASP	CB-CG-OD1	7.69	125.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	138	ASP	CB-CG-OD1	7.43	124.98	118.30
1	A	333	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	A	94	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	457	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	142	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	A	224	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	418	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	148	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	439	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	A	203	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	98	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	A	98	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	130	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	176	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	105	SER	N-CA-CB	6.30	119.95	110.50
1	A	137	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	457	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	127	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	154	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	426	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	408	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	357	ASP	CB-CG-OD1	5.97	123.68	118.30
1	A	383	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	418	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	346	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	A	148	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	217	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	335	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	439	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	96	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	224	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	393	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	408	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	446	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	153	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	426	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	393	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	357	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	120	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	110	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	335	ASP	CB-CG-OD1	5.32	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	452	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	347	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	311	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	461	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	346	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	203	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	435	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	197	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	214	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2853	0	2891	58	0
2	A	352	0	0	17	0
All	All	3205	0	2891	58	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 10.

All (58) 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:175:LYS:HB3	1:A:209:GLY:HA2	1.58	0.84
1:A:319:LEU:HD22	1:A:321:PRO:HD2	1.61	0.83
1:A:232:HIS:HB3	1:A:240:THR:HG22	1.63	0.78
1:A:175:LYS:HG2	2:A:768:HOH:O	1.89	0.73
1:A:319:LEU:CD2	1:A:321:PRO:HD2	2.20	0.72
1:A:398:GLY:H	1:A:428:ASN:HD22	1.43	0.67
1:A:153:ARG:HD2	2:A:653:HOH:O	1.94	0.66
1:A:111:GLU:O	1:A:115:LYS:HE2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:HB2	2:A:764:HOH:O	1.94	0.66
1:A:231:LEU:HD12	1:A:231:LEU:N	2.12	0.65
1:A:418:ARG:HD2	1:A:426:ASP:OD1	1.96	0.64
1:A:446:ASP:HB2	2:A:623:HOH:O	1.98	0.63
1:A:156:THR:HG22	1:A:160:VAL:O	2.00	0.62
1:A:232:HIS:HD2	1:A:233:ALA:O	1.82	0.62
1:A:175:LYS:HA	2:A:768:HOH:O	2.00	0.61
1:A:258:THR:HB	1:A:447:LEU:HD13	1.80	0.61
1:A:294:GLN:NE2	2:A:761:HOH:O	2.33	0.61
1:A:175:LYS:HB3	1:A:209:GLY:CA	2.30	0.61
1:A:149:LEU:O	1:A:153:ARG:HG3	2.02	0.60
1:A:161:THR:HG22	2:A:684:HOH:O	2.01	0.59
1:A:254:PRO:HA	1:A:284:THR:HG22	1.85	0.58
1:A:319:LEU:HD22	1:A:321:PRO:CD	2.34	0.56
1:A:146:PRO:HD3	1:A:410:SER:HB3	1.88	0.55
1:A:174:GLY:O	1:A:208:LYS:HE3	2.08	0.54
1:A:286:ASN:HD22	1:A:286:ASN:C	2.10	0.54
1:A:174:GLY:O	1:A:175:LYS:HB2	2.09	0.52
1:A:385:LYS:HE3	2:A:536:HOH:O	2.08	0.51
1:A:318:GLY:N	2:A:782:HOH:O	2.21	0.51
1:A:203:ASP:OD2	1:A:227:VAL:HG23	2.12	0.50
1:A:446:ASP:OD2	2:A:623:HOH:O	2.20	0.48
1:A:383:ASP:OD2	1:A:421:THR:HB	2.14	0.48
1:A:159:SER:HA	2:A:773:HOH:O	2.14	0.48
1:A:159:SER:OG	1:A:159:SER:O	2.30	0.48
1:A:385:LYS:HA	1:A:385:LYS:HE2	1.96	0.47
1:A:246:THR:HB	2:A:685:HOH:O	2.14	0.47
1:A:158:GLY:C	1:A:160:VAL:H	2.19	0.46
1:A:232:HIS:CG	1:A:237:PRO:HA	2.50	0.46
1:A:115:LYS:O	1:A:116:LYS:HE2	2.16	0.46
1:A:171:GLY:HA3	2:A:781:HOH:O	2.16	0.46
1:A:78:VAL:O	1:A:78:VAL:HG13	2.16	0.46
1:A:402:THR:HG22	1:A:403:VAL:N	2.31	0.46
1:A:139:PRO:HB2	1:A:169:TYR:CE1	2.51	0.45
1:A:336:LEU:O	1:A:422:PRO:HD3	2.15	0.45
1:A:335:ASP:CG	1:A:348:ILE:HD11	2.37	0.45
1:A:371:ALA:HA	1:A:375:GLU:HG3	1.99	0.45
1:A:170:ASP:HB3	1:A:173:SER:HA	1.98	0.44
1:A:171:GLY:N	2:A:781:HOH:O	2.48	0.44
1:A:428:ASN:O	1:A:429:LYS:HB2	2.17	0.44
1:A:393:ARG:NE	2:A:668:HOH:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:HH11	1:A:153:ARG:HD2	1.63	0.43
1:A:286:ASN:ND2	1:A:288:ASN:H	2.17	0.43
1:A:294:GLN:HG3	1:A:356:ILE:HD11	2.02	0.42
1:A:429:LYS:HE2	2:A:767:HOH:O	2.20	0.41
1:A:148:ARG:HA	1:A:148:ARG:NE	2.36	0.41
1:A:132:MSE:O	1:A:135:VAL:HG22	2.21	0.41
1:A:320:PHE:HB3	1:A:321:PRO:HD3	2.03	0.41
1:A:81:GLU:HG2	2:A:705:HOH:O	2.21	0.40
1:A:233:ALA:HB3	1:A:236:ALA:HB3	2.04	0.40

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	384/388 (99%)	374 (97%)	8 (2%)	2 (0%)	34 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	SER
1	A	159	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	302/298 (101%)	287 (95%)	15 (5%)	30 13

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LYS
1	A	153	ARG
1	A	156	THR
1	A	159	SER
1	A	180	LEU
1	A	276	GLN
1	A	282	LEU
1	A	286	ASN
1	A	295	GLN
1	A	319	LEU
1	A	385	LYS
1	A	418	ARG
1	A	426	ASP
1	A	437	GLN
1	A	461	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	226	GLN
1	A	232	HIS
1	A	286	ASN
1	A	294	GLN
1	A	428	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 [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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.