



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2018 – 09:38 PM EDT

PDB ID : 1FC7
Title : PHOTOSYSTEM II D1 C-TERMINAL PROCESSING PROTEASE
Authors : Liao, D.I.; Qian, J.; Chisholm, D.A.; Jordan, D.B.; Diner, B.A.
Deposited on : 2000-07-18
Resolution : 2.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

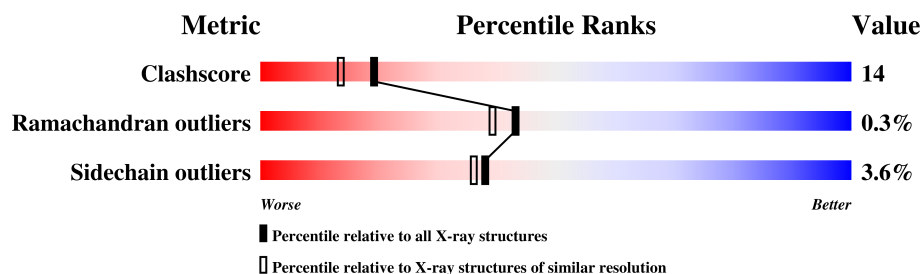
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)

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 $\leq 5\%$.

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 3178 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
1	A	386	Total	C	N	O	S	0	0	0
			2853	1786	505	558	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	initiating methionine	UNP O04073

- Molecule 2 is water.

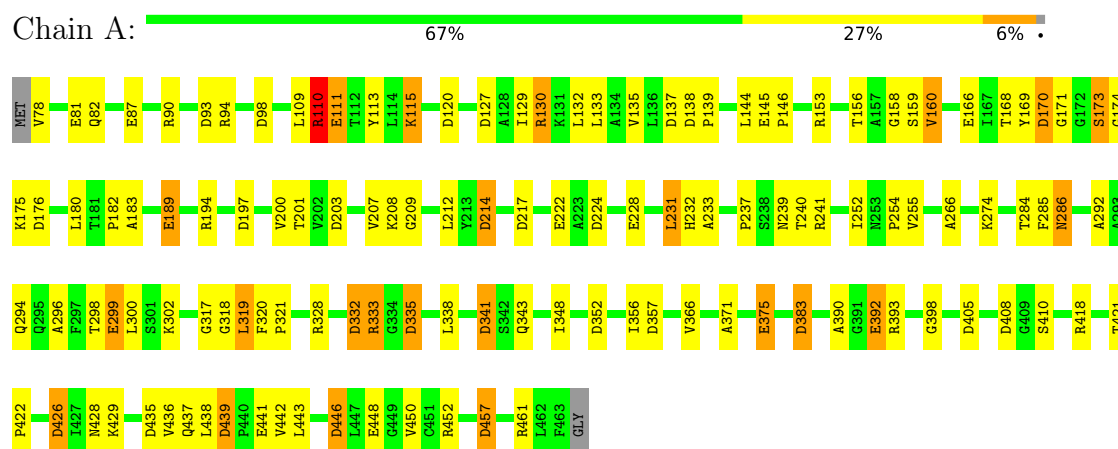
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	325	Total	O	0	0
			325	325		

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 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: PHOTOSYSTEM II D1 PROTEASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.80Å 64.10Å 63.40Å 90.00° 122.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.187 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3178	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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	0.97	12/2894 (0.4%)	1.40	56/3938 (1.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLU	CD-OE2	7.18	1.33	1.25
1	A	111	GLU	CD-OE2	6.88	1.33	1.25
1	A	166	GLU	CD-OE2	6.63	1.32	1.25
1	A	441	GLU	CD-OE2	6.61	1.32	1.25
1	A	299	GLU	CD-OE2	6.30	1.32	1.25
1	A	222	GLU	CD-OE2	6.23	1.32	1.25
1	A	87	GLU	CD-OE2	6.04	1.32	1.25
1	A	145	GLU	CD-OE2	5.69	1.31	1.25
1	A	228	GLU	CD-OE2	5.69	1.31	1.25
1	A	392	GLU	CD-OE2	5.22	1.31	1.25
1	A	448	GLU	CD-OE2	5.21	1.31	1.25
1	A	375	GLU	CD-OE2	5.18	1.31	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	A	341	ASP	CB-CG-OD1	9.38	126.75	118.30
1	A	130	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	138	ASP	CB-CG-OD2	-8.74	110.43	118.30
1	A	435	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	A	197	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	A	446	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	A	170	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	A	217	ASP	CB-CG-OD1	7.94	125.45	118.30
1	A	137	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	408	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	217	ASP	CB-CG-OD2	-7.79	111.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	A	439	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	241	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	A	241	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	224	ASP	CB-CG-OD1	7.23	124.80	118.30
1	A	176	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	461	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	439	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	332	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	197	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	446	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	137	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	452	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	408	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	335	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	A	138	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	176	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	457	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	352	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	332	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	127	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	383	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	120	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	93	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	214	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	94	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	405	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	435	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	224	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	98	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	90	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	93	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	130	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	335	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	426	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	328	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	127	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	457	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	333	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	203	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	418	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	110	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	214	ASP	CB-CG-OD2	-5.05	113.75	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	2893	80	1
2	A	325	0	0	20	1
All	All	3178	0	2893	80	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 14.

All (80) 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:232:HIS:HB3	1:A:240:THR:HG22	1.51	0.91
1:A:319:LEU:HD22	1:A:321:PRO:HD2	1.58	0.83
1:A:443:LEU:HD21	1:A:450:VAL:HG13	1.59	0.83
1:A:170:ASP:HB3	1:A:173:SER:HA	1.62	0.80
1:A:254:PRO:HA	1:A:284:THR:HG22	1.66	0.78
1:A:111:GLU:O	1:A:115:LYS:HE2	1.87	0.74
1:A:274:LYS:HD2	2:A:524:HOH:O	1.89	0.72
1:A:175:LYS:HG2	2:A:748:HOH:O	1.90	0.70
1:A:319:LEU:CD2	1:A:321:PRO:HD2	2.21	0.69
1:A:285:PHE:HB2	1:A:317:GLY:O	1.92	0.69
1:A:231:LEU:N	1:A:231:LEU:HD12	2.10	0.67
1:A:175:LYS:HA	2:A:748:HOH:O	1.94	0.67
1:A:146:PRO:HD3	1:A:410:SER:HB3	1.77	0.67
1:A:109:LEU:O	1:A:109:LEU:HD23	1.97	0.65
1:A:212:LEU:HD12	2:A:750:HOH:O	1.96	0.64
1:A:318:GLY:N	2:A:760:HOH:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASP:HB2	2:A:622:HOH:O	1.99	0.62
1:A:109:LEU:C	1:A:109:LEU:HD23	2.20	0.62
1:A:298:THR:O	1:A:302:LYS:HG3	1.99	0.62
1:A:254:PRO:HG3	1:A:286:ASN:HD21	1.65	0.61
1:A:132:LEU:O	1:A:135:VAL:HG22	2.02	0.59
1:A:175:LYS:HB3	1:A:209:GLY:HA2	1.85	0.58
1:A:437:GLN:O	1:A:438:LEU:HD23	2.03	0.58
1:A:194:ARG:HG2	2:A:591:HOH:O	2.02	0.58
1:A:109:LEU:HD22	1:A:132:LEU:CD1	2.35	0.57
1:A:232:HIS:HB3	1:A:240:THR:CG2	2.31	0.56
1:A:109:LEU:HD21	1:A:113:TYR:CE1	2.41	0.56
1:A:286:ASN:HD22	1:A:286:ASN:C	2.08	0.55
1:A:183:ALA:HB1	1:A:252:ILE:HD11	1.88	0.55
1:A:109:LEU:HD22	1:A:132:LEU:HD13	1.88	0.54
1:A:446:ASP:O	1:A:450:VAL:HG23	2.08	0.53
1:A:174:GLY:O	1:A:208:LYS:HE3	2.08	0.53
1:A:207:VAL:N	2:A:598:HOH:O	2.39	0.53
1:A:383:ASP:OD2	1:A:421:THR:HB	2.09	0.52
1:A:398:GLY:H	1:A:428:ASN:HD22	1.58	0.52
1:A:139:PRO:HB2	1:A:169:TYR:CE1	2.44	0.52
1:A:232:HIS:CD2	1:A:237:PRO:HA	2.45	0.52
1:A:174:GLY:O	1:A:175:LYS:HB2	2.11	0.51
1:A:296:ALA:O	1:A:300:LEU:HG	2.11	0.51
1:A:129:ILE:O	1:A:133:LEU:HG	2.11	0.50
1:A:317:GLY:HA3	2:A:760:HOH:O	2.10	0.50
1:A:393:ARG:NE	2:A:662:HOH:O	2.32	0.50
1:A:320:PHE:HB3	1:A:321:PRO:HD3	1.94	0.49
1:A:294:GLN:HG3	1:A:356:ILE:HD11	1.95	0.49
1:A:371:ALA:HA	1:A:375:GLU:HG3	1.95	0.49
1:A:109:LEU:HG	2:A:766:HOH:O	2.12	0.49
1:A:144:LEU:O	1:A:410:SER:HB2	2.13	0.49
1:A:428:ASN:O	1:A:429:LYS:HB2	2.12	0.49
1:A:169:TYR:CE1	1:A:212:LEU:HG	2.49	0.48
1:A:81:GLU:HG2	2:A:690:HOH:O	2.13	0.48
1:A:194:ARG:NH2	2:A:606:HOH:O	2.37	0.47
1:A:110:ARG:HG2	1:A:111:GLU:N	2.29	0.47
1:A:171:GLY:N	2:A:759:HOH:O	2.36	0.47
1:A:319:LEU:HD22	1:A:321:PRO:CD	2.38	0.47
1:A:341:ASP:OD1	1:A:343:GLN:HB3	2.14	0.47
1:A:338:LEU:HD23	1:A:338:LEU:N	2.30	0.46
1:A:158:GLY:C	1:A:160:VAL:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD23	1:A:113:TYR:CD1	2.51	0.45
1:A:78:VAL:HA	1:A:82:GLN:OE1	2.16	0.45
1:A:232:HIS:HD2	1:A:233:ALA:O	1.99	0.45
1:A:266:ALA:HB2	2:A:529:HOH:O	2.16	0.45
1:A:335:ASP:CG	1:A:348:ILE:HD11	2.37	0.44
1:A:153:ARG:HB2	2:A:744:HOH:O	2.17	0.44
1:A:171:GLY:HA3	2:A:759:HOH:O	2.18	0.44
1:A:439:ASP:HB3	1:A:442:VAL:HG23	1.99	0.44
1:A:232:HIS:HB2	1:A:239:ASN:O	2.19	0.43
1:A:390:ALA:HA	1:A:436:VAL:O	2.18	0.43
1:A:366:VAL:HG23	1:A:392:GLU:O	2.18	0.43
1:A:130:ARG:HG2	2:A:481:HOH:O	2.18	0.42
1:A:182:PRO:HB2	1:A:189:GLU:HB2	2.01	0.42
1:A:168:THR:HA	1:A:212:LEU:HD11	2.01	0.42
1:A:158:GLY:O	1:A:160:VAL:N	2.48	0.41
1:A:255:VAL:HB	1:A:292:ALA:HB1	2.02	0.41
1:A:437:GLN:NE2	2:A:687:HOH:O	2.50	0.41
1:A:200:VAL:HG12	1:A:201:THR:HG23	2.02	0.41
1:A:214:ASP:OD1	2:A:715:HOH:O	2.21	0.41
1:A:232:HIS:CG	1:A:237:PRO:HA	2.56	0.41
1:A:109:LEU:CD2	1:A:113:TYR:CD1	3.04	0.40
1:A:421:THR:HB	1:A:422:PRO:HD2	2.04	0.40
1:A:332:ASP:HB3	1:A:333:ARG:NH1	2.36	0.40

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:457:ASP:O	2:A:666:HOH:O[2_655]	2.03	0.17

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	384/388 (99%)	370 (96%)	13 (3%)	1 (0%)	43	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	SER

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	302/303 (100%)	291 (96%)	11 (4%)	38	36

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	115	LYS
1	A	156	THR
1	A	159	SER
1	A	160	VAL
1	A	180	LEU
1	A	231	LEU
1	A	286	ASN
1	A	299	GLU
1	A	319	LEU
1	A	426	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	232	HIS
1	A	286	ASN
1	A	294	GLN

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Mol	Chain	Res	Type
1	A	428	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

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.