



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:33 pm BST

PDB ID : 3NUM
Title : Substrate induced remodeling of the active site regulates HtrA1 activity
Authors : Truebestein, L.; Tennstaedt, A.; Hauske, P.; Krojer, T.; Kaiser, M.; Clausen, T.; Ehrmann, M.
Deposited on : 2010-07-07
Resolution : 2.75 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) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

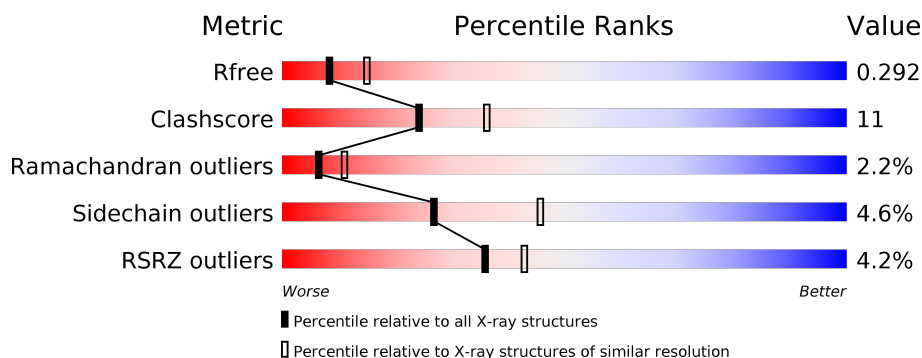
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	332	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>15%</div> <div>43%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1407 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 Serine protease HTRA1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	0	0	0
			1407	900	236	271			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	MET	-	INITIATING METHIONINE	UNP Q92743
A	328	ALA	SER	ENGINEERED MUTATION	UNP Q92743
A	481	LEU	-	EXPRESSION TAG	UNP Q92743
A	482	GLU	-	EXPRESSION TAG	UNP Q92743
A	483	HIS	-	EXPRESSION TAG	UNP Q92743
A	484	HIS	-	EXPRESSION TAG	UNP Q92743
A	485	HIS	-	EXPRESSION TAG	UNP Q92743
A	486	HIS	-	EXPRESSION TAG	UNP Q92743
A	487	HIS	-	EXPRESSION TAG	UNP Q92743
A	488	HIS	-	EXPRESSION TAG	UNP Q92743

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	109.48Å 109.48Å 113.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.32 – 2.75 34.18 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.7 (19.32-2.75) 95.7 (34.18-2.75)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.6.0066	Depositor
R, R_{free}	0.242 , 0.287 0.241 , 0.292	Depositor DCC
R_{free} test set	630 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	84.3	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1407	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.66	0/1428	0.77	1/1942 (0.1%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	320	ASP	CB-CA-C	-5.83	98.74	110.40

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	1407	0	1410	31	0
All	All	1407	0	1410	31	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.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:A:344:THR:HG22	1:A:346:LYS:H	1.52	0.73
1:A:323:ILE:HD13	1:A:343:ASN:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:THR:HB	1:A:353:PHE:O	1.98	0.64
1:A:340:ILE:HD12	1:A:340:ILE:C	2.20	0.61
1:A:283:GLY:HA3	1:A:327:ASN:HA	1.84	0.59
1:A:259:GLN:OE1	1:A:259:GLN:N	2.34	0.58
1:A:172:ILE:O	1:A:176:VAL:HG12	2.04	0.58
1:A:207:PHE:HE1	1:A:342:ILE:CD1	2.17	0.58
1:A:207:PHE:CE1	1:A:342:ILE:CD1	2.92	0.53
1:A:258:HIS:CG	1:A:262:LEU:HD21	2.44	0.53
1:A:272:GLU:HA	1:A:272:GLU:OE1	2.09	0.52
1:A:232:LEU:O	1:A:235:GLY:N	2.42	0.51
1:A:272:GLU:CA	1:A:272:GLU:OE1	2.60	0.50
1:A:232:LEU:HD12	1:A:232:LEU:N	2.26	0.49
1:A:340:ILE:C	1:A:340:ILE:CD1	2.82	0.49
1:A:357:SER:HA	1:A:360:ILE:HD12	1.95	0.48
1:A:180:ALA:HB3	1:A:181:PRO:HD3	1.95	0.48
1:A:219:ALA:HB3	1:A:250:ASP:OD1	2.14	0.47
1:A:279:VAL:CG2	1:A:332:LEU:HD11	2.44	0.47
1:A:173:ALA:HA	1:A:176:VAL:CG1	2.45	0.47
1:A:340:ILE:HD12	1:A:341:GLY:N	2.30	0.47
1:A:188:LEU:HB3	1:A:202:ALA:HB3	1.97	0.46
1:A:230:VAL:HG23	1:A:240:ALA:HB2	1.98	0.45
1:A:323:ILE:HD13	1:A:343:ASN:CB	2.43	0.44
1:A:317:ILE:HD12	1:A:356:PRO:HG3	2.02	0.42
1:A:179:ILE:HD13	1:A:333:VAL:HG21	2.01	0.42
1:A:232:LEU:N	1:A:232:LEU:CD1	2.84	0.41
1:A:334:ASN:HD21	1:A:338:GLU:HB2	1.86	0.41
1:A:182:ALA:HA	1:A:208:ILE:HD12	2.03	0.41
1:A:360:ILE:HG22	1:A:364:LEU:CD1	2.51	0.41
1:A:207:PHE:CE1	1:A:342:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

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	184/332 (55%)	172 (94%)	8 (4%)	4 (2%)	6	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	ASP
1	A	233	LYS
1	A	225	LYS
1	A	193	PRO

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	151/285 (53%)	144 (95%)	7 (5%)	27	46

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	GLU
1	A	201	VAL
1	A	271	SER
1	A	274	ARG
1	A	291	THR
1	A	320	ASP
1	A	369	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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](#)

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	190/332 (57%)	0.18	8 (4%) 36 43	52, 91, 123, 159	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	PRO	3.4
1	A	294	THR	2.4
1	A	325	TYR	2.4
1	A	200	PRO	2.3
1	A	161	ASP	2.1
1	A	224	ASN	2.1
1	A	283	GLY	2.0
1	A	300	THR	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.