

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2020 – 04:11 PM BST

PDB ID 5R36

> Title PanDDA analysis group deposition – Auto-refined data of Endothiapepsin for

> > ground state model 30, DMSO-Free

Wollenhaupt, J.; Metz, A.; Barthel, T.; Lima, G.M.A.; Heine, A.; Mueller, U.; Authors

Klebe, G.; Weiss, M.S.

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Resolution 1.01 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

4.02b-467MolProbity Xtriage (Phenix) 1.13

EDS 2.13.1

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

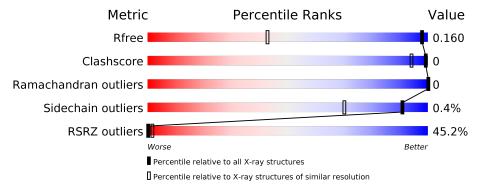
Validation Pipeline (wwPDB-VP) 2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.01 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1050 (1.06-0.94)
Clashscore	141614	1117 (1.06-0.94)
Ramachandran outliers	138981	1043 (1.06-0.94)
Sidechain outliers	138945	1045 (1.06-0.94)
RSRZ outliers	127900	1023 (1.06-0.94)

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 <=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			
			36%			
1	A	419	78%	•	21%	



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5130 atoms, of which 2341 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 Endothiapepsin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	A	330	Total 4803	C 1566	H 2341	N 367	O 527	S 2	0	25	0

• Molecule 2 is water.

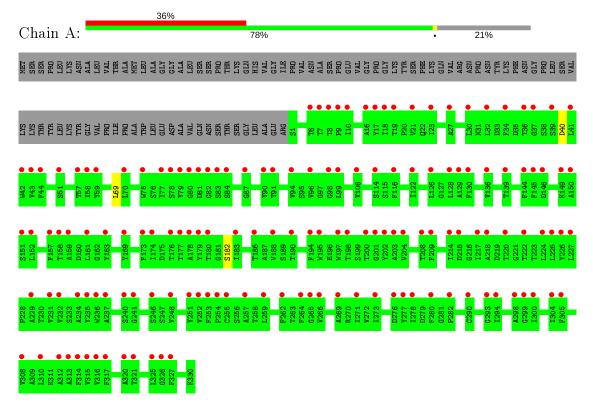
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	327	Total O 327 327	0	0



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 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: Endothiapepsin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	45.20Å 73.41Å 52.48Å	Depositor
a, b, c, α , β , γ	90.00° 109.33° 90.00°	Depositor
Resolution (Å)	42.66 - 1.01	Depositor
Resolution (A)	42.66 - 1.01	EDS
% Data completeness	95.2 (42.66-1.01)	Depositor
(in resolution range)	95.3 (42.66-1.01)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.97 (at 1.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
D D.	0.132 , 0.141	Depositor
R, R_{free}	0.148 , 0.160	DCC
R_{free} test set	2101 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.44, 56.7	EDS
L-test for twinning ²	$ < L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5130	wwPDB-VP
Average B, all atoms $(Å^2)$	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.30% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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	Mol Chain		lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.33	0/2594	0.62	0/3553	

There are no bond length outliers.

There are no bond angle outliers.

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	Α	2462	2341	2300	1	1
2	A	327	0	0	1	4
All	All	2789	2341	2300	1	4

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 0.

All (1) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:69:LEU:HD21	2:A:611:HOH:O	2.18	0.43

All (4) 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	$egin{array}{l} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	Clash overlap (Å)
2:A:687:HOH:O	2:A:693:HOH:O[1_554]	1.94	0.26
2:A:677:HOH:O	2:A:682:HOH:O[2_757]	2.06	0.14
2:A:611:HOH:O	2:A:687:HOH:O[1_556]	2.11	0.09
1:A:182[B]:SER:OG	2:A:611:HOH:O[1_554]	2.15	0.05

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	Perce	$_{ m ntiles}$
1	A	353/419 (84%)	349 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	273/336 (81%)	272 (100%)	1 (0%)	91 70

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP

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



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 (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, 95^{th} 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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	330/419 (78%)	1.97	149 (45%) 0 2	10, 14, 21, 32	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	GLY	5.6
1	A	300[A]	ILE	5.0
1	A	77	ILE	4.9
1	A	259	LEU	4.2
1	A	79	TYR	4.2
1	A	150[A]	ALA	4.0
1	A	82	GLY	3.9
1	A	83	SER	3.9
1	A	321	THR	3.6
1	A	246[A]	SER	3.5
1	A	236	TRP	3.5
1	A	78	SER	3.4
1	A	81	ASP	3.4
1	A	241	GLY	3.3
1	A	188	VAL	3.3
1	A	290	CYS	3.2
1	A	231	VAL	3.2
1	A	276[A]	ASP	3.1
1	A	269	ALA	3.1
1	A	314	PHE	3.1
1	A	149[A]	LYS	3.0
1	A	84	SER	3.0
1	A	114	SER	3.0
1	A	37	GLY	2.9
1	A	169	TYR	2.9
1	A	161	LEU	2.9
1	A	174[A]	ILE	2.9

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Mol	Chain	Res	Type	RSRZ			
1	A	197	TRP	2.9			
1	A	75	TRP	2.9			
1	A	34	PHE	2.9			
1	A	255	CYS	2.8			
1	A	299[A]	GLY	2.8			
1	A	315	VAL	2.8			
1	A	98	GLY	2.8			
1	A	32	LEU	2.8			
1	A	51	SER	2.8			
1	A	240[A]	SER	2.8			
1	A	194	PHE	2.8			
1	A	313	ALA	2.8			
1	A	271	ILE	2.7			
1	A	44	PHE	2.7			
1	A	145	PHE	2.7			
1	A	253	PHE	2.7			
1	A	294	ILE	2.7			
1	A	126	LEU	2.7			
1	A	59	TYR	2.7			
1	A	18	ILE	2.7			
1	A	310	LEU	2.6			
1	A	208	THR	2.6			
1	A	277[A]	TYR	2.6			
1	A	312	ALA	2.6			
1	A	8	THR	2.6			
1	A	10	ILE	2.6			
1	A	21	VAL	2.6			
1	A	139	THR	2.6			
1	A	225	LEU	2.6			
1	A	325[A]	LEU	2.6			
1	A	173	PHE	2.6			
1	A	305	PHE	2.6			
1	A	190	THR	2.5			
1	A	23	ILE	2.5			
1	A	58	ILE	2.5			
1	A	304	ILE	2.5			
1	A	195	TRP	2.5			
1	A	178	ALA	2.5			
1	A	163	TYR	2.5			
1	A	130	PHE	2.5			
1	A	264	PHE	2.5			
1	A	234	ALA	2.5			

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Mol	Chain	Res	Type	RSRZ
1	A	237	ALA	2.5
1	A	96	VAL	2.5
1	A	146	ASP	2.5
1	A	128	LEU	2.5
1	A	7	THR	2.5
1	A	136	VAL	2.4
1	A	266	VAL	2.4
1	A	122	ILE	2.4
1	A	183[A]	ILE	2.4
1	A	201	GLY	2.4
1	A	27	ALA	2.4
1	A	252	VAL	2.4
1	A	177	THR	2.4
1	A	217	ILE	2.4
1	A	257	ALA	2.4
1	A	144	PHE	2.4
1	A	157	PHE	2.4
1	A	316	VAL	2.4
1	A	273	ILE	2.4
1	A	152	LEU	2.4
1	A	17	TYR	2.4
1	A	179	TYR	2.4
1	A	235	TYR	2.4
1	A	280	PHE	2.4
1	A	220	THR	2.3
1	A	232	VAL	2.3
1	A	308	VAL	2.3
1	A	320	ALA	2.3
1	A	202	TYR	2.3
1	A	226	TYR	2.3
1	A	6	THR	2.3
1	A	222	THR	2.3
1	A	326[A]	GLY	2.3
1	A	224	LEU	2.3
1	A	251	TYR	2.3
1	A	57	THR	2.3
1	A	91	THR	2.3
1	A	176	THR	2.3
1	A	90	TYR	2.3
1	A	227	LEU	2.3
1	A	282	PRO	2.3
1	A	262	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	317	PHE	2.3
1	A	327	PHE	2.3
1	A	42	TRP	2.2
1	A	198	THR	2.2
1	A	36	THR	2.2
1	A	200	THR	2.2
1	A	87	GLY	2.2
1	A	293	GLY	2.2
1	A	16	ALA	2.2
1	A	214	ILE	2.2
1	A	209	PHE	2.2
1	A	254	PRO	2.2
1	A	94	VAL	2.2
1	A	151	SER	2.2
1	A	41	LEU	2.2
1	A	278	ILE	2.2
1	A	158	THR	2.1
1	A	70	LEU	2.1
1	A	116	PHE	2.1
1	A	265	GLY	2.1
1	A	43	VAL	2.1
1	A	106	VAL	2.1
1	A	248	VAL	2.1
1	A	203	ALA	2.1
1	A	229	ALA	2.1
1	A	30	LEU	2.1
1	A	99	LEU	2.1
1	A	129	ALA	2.1
1	A	159	ALA	2.1
1	A	215[A]	ASP	2.1
1	A	19	THR	2.1
1	A	204	VAL	2.1
1	A	218	ALA	2.0
1	A	298[A]	ALA	2.0
1	A	180	THR	2.0
1	A	39	SER	2.0
1	A	186	THR	2.0
1	A	9[A]	PRO	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 monosaccharides 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.

