

Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 02:00 PM BST

PDB ID	:	5R3X
Title	:	PanDDA analysis group deposition – Auto-refined data of Endothiapepsin for
		ground state model 57, DMSO-Free
Authors	:	Wollenhaupt, J.; Metz, A.; Barthel, T.; Lima, G.M.A.; Heine, A.; Mueller, U.;
		Klebe, G.; Weiss, M.S.
Deposited on		
$\operatorname{Resolution}$:	1.17 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:

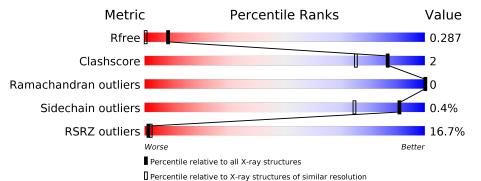
MolProbity Xtriage (Phenix) EDS		
Percentile statistics	-	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac		5.8.0158
CCP4	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.17 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	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f Similar\ resolution}\ (\#{ m Entries}, { m resolution\ range}({ m \AA}))$
R_{free}	130704	1758 (1.20-1.12)
Clashscore	141614	1832 (1.20-1.12)
Ramachandran outliers	138981	1768 (1.20-1.12)
Sidechain outliers	138945	1768 (1.20-1.12)
RSRZ outliers	127900	1724 (1.20-1.12)

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					
1	А	419	13%	·	21%			



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4937 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	А	330	Total 4803	m C 1566	Н 2341	N 367	О 527	${ m S} 2$	0	25	0

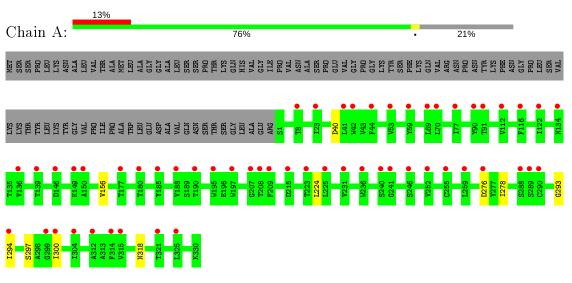
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	134	Total O 134 134	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	45.18Å 7 3.14 Å 5 2.57 Å	Depositor
a, b, c, α , β , γ	90.00° 109.14° 90.00°	Depositor
Resolution (Å)	42.68 - 1.17	Depositor
Resolution (A)	49.67 - 1.16	EDS
% Data completeness	98.7 (42.68-1.17)	Depositor
(in resolution range)	98.7(49.67-1.16)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.94 (at 1.16 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
D D.	0.245 , 0.288	Depositor
R, R_{free}	0.260 , 0.287	DCC
R_{free} test set	2088 reflections (1.92%)	wwPDB-VP
Wilson B-factor $(Å^2)$	18.9	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	$0.45 \;, 50.5$	EDS
L-test for twinning ²	$ \langle L \rangle = 0.54, \langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4937	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.94% of the height of the origin peak. No significant pseudotranslation is detected.

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.



 $^{^1 {\}rm Intensities}$ 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	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.43	0/2594	0.68	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	А	2462	2341	2300	10	0
2	А	134	0	0	0	0
All	All	2596	2341	2300	10	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 2.

All (10) 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:278:ILE:HG23	1:A:294:ILE:HD13	1.76	0.67
1:A:278:ILE:CG2	1:A:294:ILE:HD13	2.34	0.57
1:A:276[B]:ASP:N	1:A:276[B]:ASP:OD1	2.38	0.57
1:A:293:GLY:C	1:A:294:ILE:HD12	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD22	1:A:293:GLY:HA2	1.99	0.44
1:A:278:ILE:HG12	1:A:294:ILE:HD11	1.99	0.44
1:A:278:ILE:HG12	1:A:294:ILE:CD1	2.46	0.44
1:A:294:ILE:HD12	1:A:294:ILE:N	2.34	0.43
1:A:156:VAL:HG12	1:A:318:ASN:HA	2.00	0.43
1:A:297:SER:HA	1:A:300[A]:ILE:HD12	2.02	0.42

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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	А	353/419~(84%)	349~(99%)	4 (1%)	0	100 10	0

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	А	273/336~(81%)	272~(100%)	1 (0%)	91 75

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



Mol	Chain	Res	Type
1	А	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, 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 $>$	# RSR	Z>	2	$OWAB(Å^2)$	Q<0.9
1	А	330/419~(78%)	1.46	55~(16%)	1	2	15, 19, 27, 36	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	150[A]	ALA	6.3
1	А	300[A]	ILE	5.2
1	А	321	THR	4.6
1	А	246[A]	SER	3.3
1	А	299[A]	GLY	3.2
1	А	208	THR	3.1
1	А	136	VAL	3.0
1	А	289[A]	SER	2.9
1	А	294	ILE	2.9
1	А	188	VAL	2.8
1	А	209	PHE	2.8
1	А	231	VAL	2.8
1	А	276[A]	ASP	2.7
1	А	240[A]	SER	2.6
1	А	42	TRP	2.6
1	А	149[A]	LYS	2.5
1	А	325[A]	LEU	2.5
1	А	197	TRP	2.5
1	А	177	THR	2.5
1	А	215[A]	ASP	2.5
1	А	53	VAL	2.4
1	А	69	LEU	2.4
1	А	70	LEU	2.4
1	А	134	ASN	2.4
1	А	77	ILE	2.4
1	А	304	ILE	2.4
1	А	315	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	А	290	CYS	2.3
1	А	288	SER	2.3
1	А	223	THR	2.3
1	А	312	ALA	2.2
1	А	241	GLY	2.2
1	А	8	THR	2.2
1	А	112	VAL	2.2
1	А	190	THR	2.2
1	А	116	PHE	2.2
1	А	314	PHE	2.2
1	А	59	TYR	2.2
1	А	180	THR	2.2
1	А	41	LEU	2.2
1	А	259	LEU	2.2
1	А	139	THR	2.2
1	А	44	PHE	2.2
1	А	255	CYS	2.1
1	А	23	ILE	2.1
1	А	185	TYR	2.1
1	А	236	TRP	2.1
1	А	122	ILE	2.1
1	А	91	THR	2.1
1	А	207	GLY	2.1
1	А	90	TYR	2.1
1	А	252	VAL	2.0
1	А	225	LEU	2.0
1	А	146	ASP	2.0
1	А	195	TRP	2.0

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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.

