



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5RE2 / pdb_00005re2
Title : PanDDA analysis group deposition – Endothiapepsin ground state model 59
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Deposited on : 2020-03-24
Resolution : 1.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

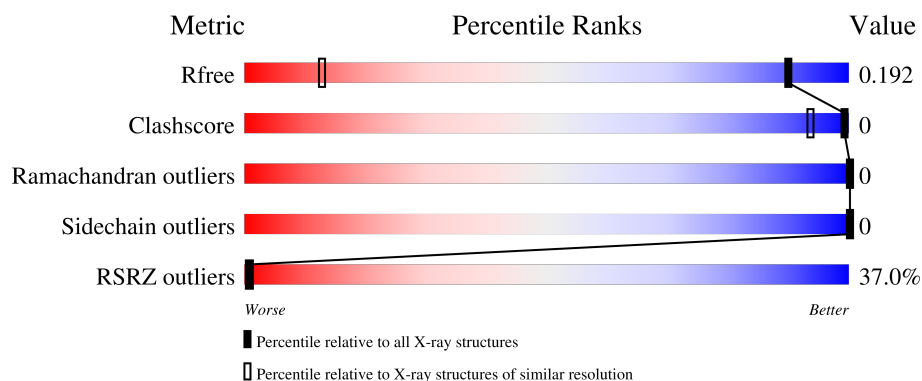
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.00 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))
R_{free}	180053	1358 (1.04-0.96)
Clashscore	190562	1411 (1.04-0.96)
Ramachandran outliers	187476	1347 (1.04-0.96)
Sidechain outliers	187428	1348 (1.04-0.96)
RSRZ outliers	180081	1355 (1.04-0.96)

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 of 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	419	29% 77% . 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2717 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 Endothiapepsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	19	0
			2462	1566	367	527	2			

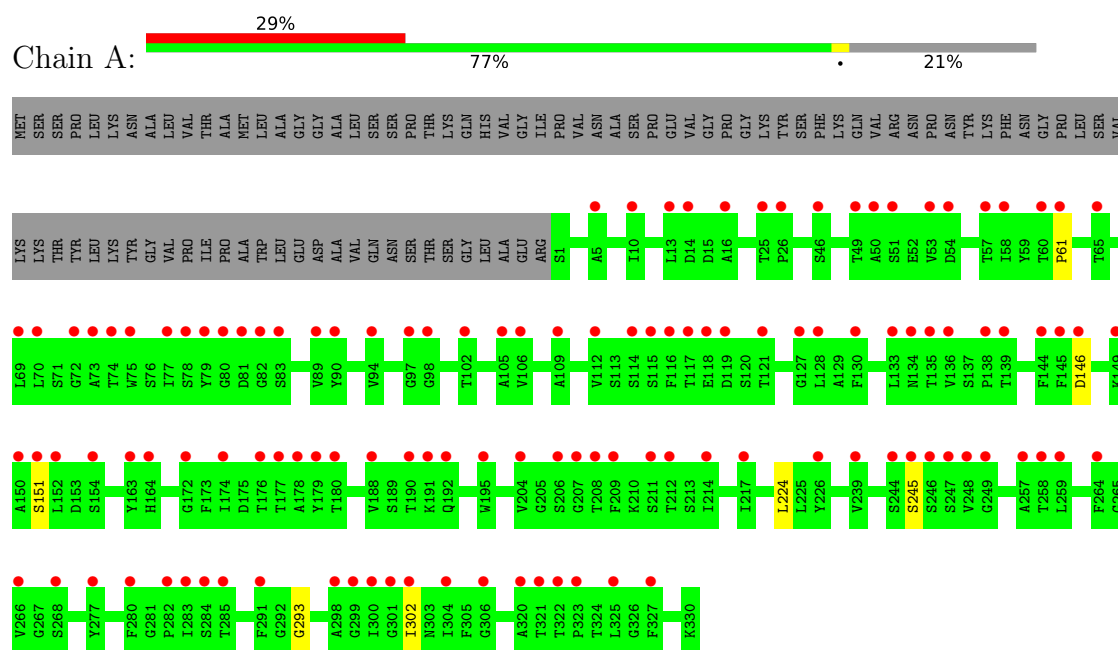
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	255	Total	O	0	0
			255	255		

3 Residue-property plots

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.29Å 72.85Å 52.46Å 90.00° 109.22° 90.00°	Depositor
Resolution (Å)	42.80 – 1.00 42.80 – 1.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.80-1.00) 98.5 (42.80-1.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.16.3549	Depositor
R, R_{free}	0.184 , 0.184 0.189 , 0.192	Depositor DCC
R_{free} test set	8532 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2717	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% 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	1.14	4/2552 (0.2%)	0.97	1/3496 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	PRO	C-O	-5.79	1.17	1.24
1	A	302	ILE	C-O	-5.76	1.17	1.23
1	A	245	SER	CA-CB	-5.62	1.45	1.53
1	A	151	SER	CA-CB	-5.13	1.44	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ASP	CA-CB-CG	7.43	120.03	112.60

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	2462	0	2329	1	0
2	A	255	0	0	0	2
All	All	2717	0	2329	1	2

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD22	1:A:293:GLY:HA2	2.02	0.41

All (2) 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)
2:A:641:HOH:O	2:A:645:HOH:O[2_747]	1.96	0.24
2:A:422:HOH:O	2:A:622:HOH:O[1_556]	2.12	0.08

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	347/419 (83%)	344 (99%)	3 (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	270/336 (80%)	270 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	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 oligosaccharides 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 ⓘ

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	330/419 (78%)	1.90	122 (36%) 1 1	5, 11, 18, 24	19 (5%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300[A]	ILE	8.2
1	A	82	GLY	6.8
1	A	246[A]	SER	6.6
1	A	150	ALA	6.1
1	A	321	THR	6.1
1	A	10	ILE	5.9
1	A	178	ALA	5.9
1	A	322	THR	5.6
1	A	121	THR	5.4
1	A	80	GLY	5.4
1	A	208	THR	5.3
1	A	145	PHE	5.1
1	A	74	THR	5.0
1	A	72	GLY	4.9
1	A	211	SER	4.7
1	A	135	THR	4.6
1	A	149[A]	LYS	4.5
1	A	302	ILE	4.4
1	A	13	LEU	4.4
1	A	53	VAL	4.4
1	A	248	VAL	4.3
1	A	46	SER	4.3
1	A	247	SER	4.3
1	A	152	LEU	4.2
1	A	116	PHE	4.0
1	A	50	ALA	3.9
1	A	258	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	285	THR	3.9
1	A	51	SER	3.7
1	A	320	ALA	3.7
1	A	112	VAL	3.7
1	A	163	TYR	3.6
1	A	139	THR	3.6
1	A	90	TYR	3.6
1	A	115	SER	3.6
1	A	65	THR	3.6
1	A	130	PHE	3.6
1	A	299[A]	GLY	3.5
1	A	244	SER	3.5
1	A	304	ILE	3.4
1	A	284	SER	3.4
1	A	98	GLY	3.4
1	A	75	TRP	3.3
1	A	70	LEU	3.3
1	A	306	GLY	3.2
1	A	79	TYR	3.1
1	A	177	THR	3.1
1	A	138	PRO	3.1
1	A	176	THR	3.1
1	A	291	PHE	3.0
1	A	268[A]	SER	3.0
1	A	164	HIS	2.9
1	A	323	PRO	2.9
1	A	174[A]	ILE	2.9
1	A	128	LEU	2.9
1	A	117	THR	2.9
1	A	109	ALA	2.9
1	A	257	ALA	2.9
1	A	191	LYS	2.8
1	A	217	ILE	2.8
1	A	207	GLY	2.8
1	A	119	ASP	2.8
1	A	209	PHE	2.8
1	A	188	VAL	2.8
1	A	133	LEU	2.8
1	A	102	THR	2.8
1	A	190	THR	2.8
1	A	206[A]	SER	2.8
1	A	69	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	89	VAL	2.8
1	A	25	THR	2.7
1	A	298[A]	ALA	2.7
1	A	212	THR	2.7
1	A	118	GLU	2.7
1	A	81	ASP	2.6
1	A	136	VAL	2.6
1	A	54	ASP	2.6
1	A	78	SER	2.6
1	A	60	THR	2.5
1	A	114	SER	2.5
1	A	73	ALA	2.5
1	A	94	VAL	2.5
1	A	61	PRO	2.4
1	A	58	ILE	2.4
1	A	249	GLY	2.4
1	A	325[A]	LEU	2.4
1	A	151	SER	2.4
1	A	179	TYR	2.4
1	A	264	PHE	2.4
1	A	26	PRO	2.3
1	A	127	GLY	2.3
1	A	154[A]	SER	2.3
1	A	192	GLN	2.3
1	A	283	ILE	2.3
1	A	106	VAL	2.3
1	A	266	VAL	2.3
1	A	49	THR	2.3
1	A	77	ILE	2.3
1	A	214	ILE	2.3
1	A	239	VAL	2.3
1	A	134	ASN	2.2
1	A	172	GLY	2.2
1	A	280	PHE	2.2
1	A	105	ALA	2.2
1	A	226	TYR	2.2
1	A	277	TYR	2.2
1	A	245	SER	2.2
1	A	97	GLY	2.2
1	A	204	VAL	2.2
1	A	16	ALA	2.1
1	A	146	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	259	LEU	2.1
1	A	57	THR	2.1
1	A	180	THR	2.1
1	A	5	ALA	2.1
1	A	327	PHE	2.1
1	A	14	ASP	2.0
1	A	301	GLY	2.0
1	A	282	PRO	2.0
1	A	83	SER	2.0
1	A	195	TRP	2.0
1	A	144	PHE	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 oligosaccharides 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.