Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	5RCM
Title	:	PanDDA analysis group deposition – Endothiapepsin ground state model 07
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Deposited on	:	2020-03-24
Resolution	:	1.03 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:

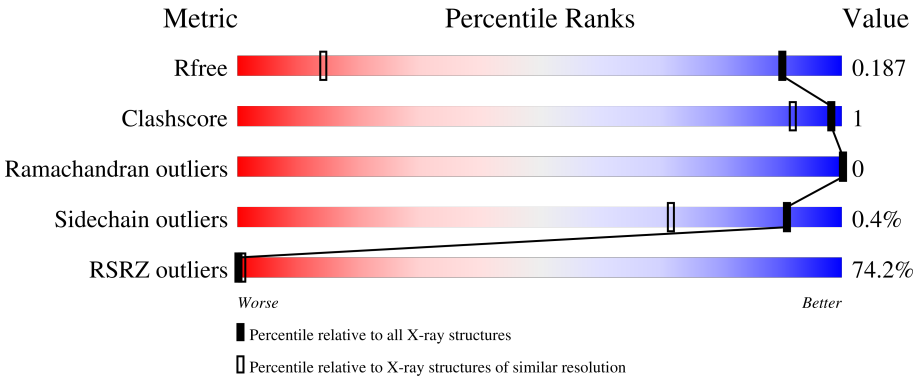
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.03 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	1596 (1.10-0.98)
Clashscore	141614	1677 (1.10-0.98)
Ramachandran outliers	138981	1591 (1.10-0.98)
Sidechain outliers	138945	1589 (1.10-0.98)
RSRZ outliers	127900	1557 (1.10-0.98)

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 <=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	58%, 78%, ·, 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2736 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
			Total	C	N	O	S			
1	A	330	2462	1566	367	527	2	0	19	0

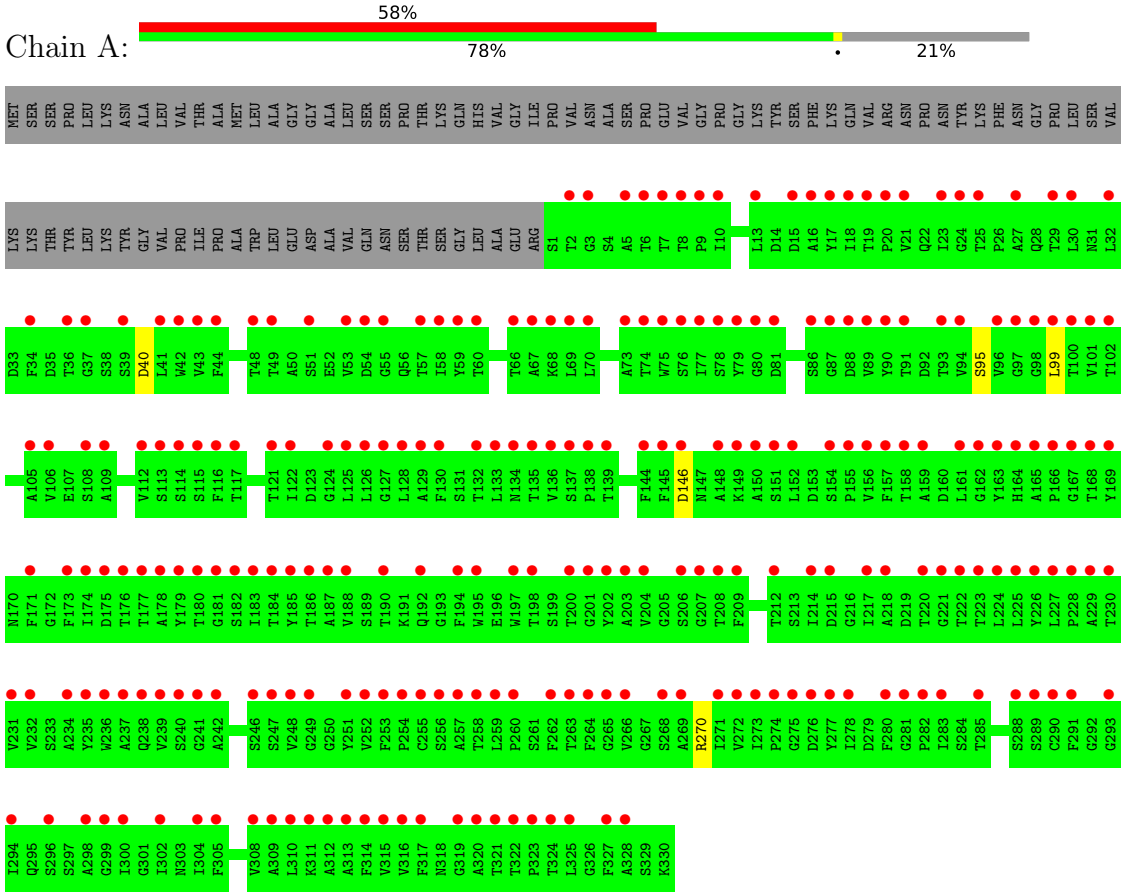
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	274	274	274	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 a, b, c, α, β, γ	45.26Å 72.90Å 52.46Å 90.00° 109.26° 90.00°	Depositor
Resolution (Å)	49.57 – 1.03 49.52 – 1.03	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.57-1.03) 99.3 (49.52-1.03)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 1.03Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.16.3549	Depositor
R, R_{free}	0.188 , 0.189 0.190 , 0.187	Depositor DCC
R_{free} test set	7854 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.6	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	0.97	EDS
Total number of atoms	2736	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

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	0.82	0/2552	0.91	2/3496 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	270	ARG	NE-CZ-NH2	-5.93	117.33	120.30

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	2462	0	2329	3	0
2	A	274	0	0	2	1
All	All	2736	0	2329	3	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 1.

All (3) 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:146:ASP:CG	2:A:402:HOH:O	2.20	0.80
1:A:146:ASP:CB	2:A:402:HOH:O	2.49	0.60
1:A:95:SER:HA	1:A:99:LEU:O	2.21	0.41

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)
2:A:401:HOH:O	2:A:502:HOH:O[1_655]	2.13	0.07

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%)	343 (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	270/336 (80%)	269 (100%)	1 (0%)	91 72

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

Mol	Chain	Res	Type
1	A	40	ASP

Sometimes 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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	330/419 (78%)	2.64	245 (74%)	0	1	8, 11, 19, 25	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300[A]	ILE	7.5
1	A	299[A]	GLY	6.8
1	A	150	ALA	6.1
1	A	321	THR	5.6
1	A	246[A]	SER	4.7
1	A	312	ALA	4.5
1	A	80	GLY	4.4
1	A	322	THR	4.4
1	A	43	VAL	4.4
1	A	105	ALA	4.3
1	A	320	ALA	4.3
1	A	10	ILE	4.3
1	A	58	ILE	4.2
1	A	241	GLY	4.1
1	A	248	VAL	4.1
1	A	259	LEU	4.1
1	A	316	VAL	4.1
1	A	190	THR	4.1
1	A	188	VAL	4.0
1	A	236	TRP	4.0
1	A	122	ILE	4.0
1	A	273	ILE	4.0
1	A	174[A]	ILE	3.9
1	A	145	PHE	3.9
1	A	231	VAL	3.9
1	A	290	CYS	3.9
1	A	77	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	128	LEU	3.9
1	A	313	ALA	3.8
1	A	41	LEU	3.8
1	A	294	ILE	3.8
1	A	204	VAL	3.8
1	A	252	VAL	3.7
1	A	278	ILE	3.7
1	A	283	ILE	3.7
1	A	197	TRP	3.7
1	A	285	THR	3.7
1	A	161	LEU	3.7
1	A	183	ILE	3.7
1	A	139	THR	3.7
1	A	225	LEU	3.7
1	A	23	ILE	3.7
1	A	271	ILE	3.7
1	A	239	VAL	3.6
1	A	276[A]	ASP	3.6
1	A	255	CYS	3.6
1	A	266	VAL	3.6
1	A	208	THR	3.6
1	A	126	LEU	3.6
1	A	152	LEU	3.5
1	A	325[A]	LEU	3.5
1	A	315	VAL	3.5
1	A	227	LEU	3.5
1	A	44	PHE	3.5
1	A	264	PHE	3.5
1	A	186	THR	3.4
1	A	214	ILE	3.4
1	A	209	PHE	3.4
1	A	178	ALA	3.4
1	A	169	TYR	3.4
1	A	304	ILE	3.4
1	A	177	THR	3.4
1	A	30	LEU	3.4
1	A	224	LEU	3.4
1	A	89	VAL	3.3
1	A	298[A]	ALA	3.3
1	A	144	PHE	3.3
1	A	79	TYR	3.3
1	A	277	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	96	VAL	3.3
1	A	253	PHE	3.3
1	A	57	THR	3.3
1	A	258	THR	3.3
1	A	49	THR	3.2
1	A	327	PHE	3.2
1	A	7	THR	3.2
1	A	121	THR	3.2
1	A	302	ILE	3.2
1	A	112	VAL	3.2
1	A	310	LEU	3.2
1	A	42	TRP	3.2
1	A	151	SER	3.2
1	A	222	THR	3.2
1	A	156	VAL	3.2
1	A	232	VAL	3.2
1	A	305	PHE	3.1
1	A	73	ALA	3.1
1	A	229	ALA	3.1
1	A	234	ALA	3.1
1	A	230	THR	3.1
1	A	195	TRP	3.1
1	A	269	ALA	3.1
1	A	106	VAL	3.1
1	A	91	THR	3.1
1	A	93	THR	3.1
1	A	163	TYR	3.1
1	A	180	THR	3.1
1	A	226	TYR	3.1
1	A	125	LEU	3.1
1	A	37	GLY	3.1
1	A	176	THR	3.1
1	A	18	ILE	3.0
1	A	29	THR	3.0
1	A	75	TRP	3.0
1	A	21	VAL	3.0
1	A	136	VAL	3.0
1	A	155	PRO	3.0
1	A	70	LEU	3.0
1	A	217	ILE	3.0
1	A	78	SER	3.0
1	A	34	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	94	VAL	3.0
1	A	27	ALA	3.0
1	A	129	ALA	3.0
1	A	220	THR	3.0
1	A	280	PHE	3.0
1	A	69	LEU	2.9
1	A	173	PHE	2.9
1	A	257	ALA	2.9
1	A	114	SER	2.9
1	A	256	SER	2.9
1	A	157	PHE	2.9
1	A	215[A]	ASP	2.9
1	A	20	PRO	2.9
1	A	19	THR	2.9
1	A	36	THR	2.9
1	A	165	ALA	2.9
1	A	218	ALA	2.9
1	A	13	LEU	2.8
1	A	32	LEU	2.8
1	A	99	LEU	2.8
1	A	314	PHE	2.8
1	A	289[A]	SER	2.8
1	A	74	THR	2.8
1	A	117	THR	2.8
1	A	198	THR	2.8
1	A	228	PRO	2.8
1	A	235	TYR	2.8
1	A	149[A]	LYS	2.8
1	A	184	THR	2.8
1	A	200	THR	2.8
1	A	51	SER	2.8
1	A	59	TYR	2.8
1	A	185	TYR	2.8
1	A	194	PHE	2.8
1	A	251	TYR	2.8
1	A	272	VAL	2.7
1	A	60	THR	2.7
1	A	138	PRO	2.7
1	A	323	PRO	2.7
1	A	130	PHE	2.7
1	A	317	PHE	2.7
1	A	9[A]	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	282	PRO	2.7
1	A	5	ALA	2.7
1	A	67	ALA	2.7
1	A	6	THR	2.7
1	A	202	TYR	2.7
1	A	167	GLY	2.7
1	A	159	ALA	2.7
1	A	133	LEU	2.7
1	A	146	ASP	2.7
1	A	166	PRO	2.7
1	A	249	GLY	2.7
1	A	247	SER	2.7
1	A	192	GLN	2.6
1	A	158	THR	2.6
1	A	324	THR	2.6
1	A	90	TYR	2.6
1	A	76	SER	2.5
1	A	308	VAL	2.5
1	A	293	GLY	2.5
1	A	16	ALA	2.5
1	A	66	THR	2.5
1	A	281	GLY	2.5
1	A	134	ASN	2.5
1	A	237	ALA	2.5
1	A	135	THR	2.5
1	A	127	GLY	2.5
1	A	116	PHE	2.5
1	A	171	PHE	2.5
1	A	97	GLY	2.5
1	A	179	TYR	2.5
1	A	154[A]	SER	2.5
1	A	262	PHE	2.5
1	A	162	GLY	2.4
1	A	212	THR	2.4
1	A	109	ALA	2.4
1	A	187	ALA	2.4
1	A	328	ALA	2.4
1	A	137	SER	2.4
1	A	254	PRO	2.4
1	A	203	ALA	2.4
1	A	48	THR	2.3
1	A	100	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	88	ASP	2.3
1	A	182[A]	SER	2.3
1	A	15	ASP	2.3
1	A	291	PHE	2.3
1	A	55	GLY	2.3
1	A	164	HIS	2.3
1	A	8	THR	2.3
1	A	102	THR	2.3
1	A	288	SER	2.3
1	A	24	GLY	2.3
1	A	175	ASP	2.3
1	A	17	TYR	2.3
1	A	108	SER	2.2
1	A	148	ALA	2.2
1	A	309	ALA	2.2
1	A	68[A]	LYS	2.2
1	A	132	THR	2.2
1	A	39	SER	2.2
1	A	206[A]	SER	2.2
1	A	223	THR	2.2
1	A	274	PRO	2.2
1	A	296	SER	2.2
1	A	260	PRO	2.2
1	A	2	THR	2.2
1	A	86	SER	2.2
1	A	81	ASP	2.2
1	A	221	GLY	2.2
1	A	319	GLY	2.2
1	A	240[A]	SER	2.2
1	A	168	THR	2.2
1	A	263	THR	2.2
1	A	98	GLY	2.1
1	A	207	GLY	2.1
1	A	53	VAL	2.1
1	A	101	VAL	2.1
1	A	265	GLY	2.1
1	A	115	SER	2.1
1	A	268[A]	SER	2.1
1	A	311[A]	LYS	2.1
1	A	242	ALA	2.1
1	A	275	GLY	2.1
1	A	113	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLY	2.1
1	A	124	GLY	2.1
1	A	201	GLY	2.1
1	A	25	THR	2.0
1	A	87	GLY	2.0
1	A	181	GLY	2.0
1	A	238	GLN	2.0
1	A	54	ASP	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.