wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1XDH / pdb_00001xdh
Title	:	Structure of plasmepsin II in complex with pepstatin A
Authors	:	Prade, L.
Deposited on	:	2004-09-06
Resolution	:	1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

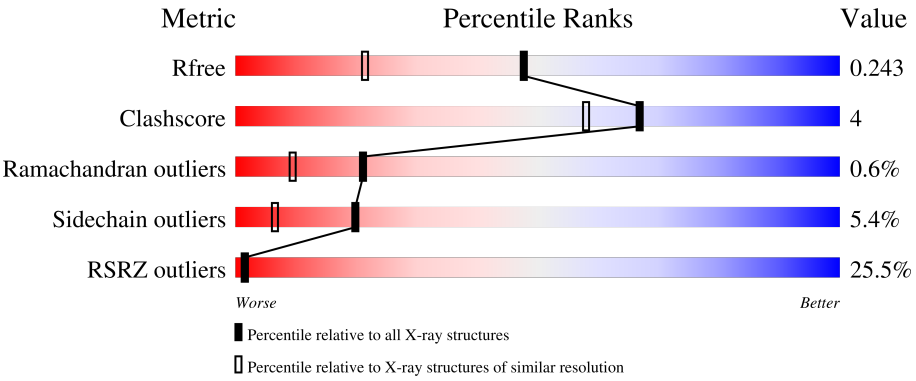
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	331	16% 92% 6% ··
1	B	331	35% 86% 11% ··
2	C	6	67% 17% 17%
2	D	6	33% 50% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6046 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 Plasmepsin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2607	1689	404	503	11			
1	B	329	Total	C	N	O	S	0	0	0
			2607	1689	404	503	11			

- Molecule 2 is a protein called Pepstatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			48	34	5	9			
2	D	6	Total	C	N	O	0	0	0
			48	34	5	9			

- Molecule 3 is water.

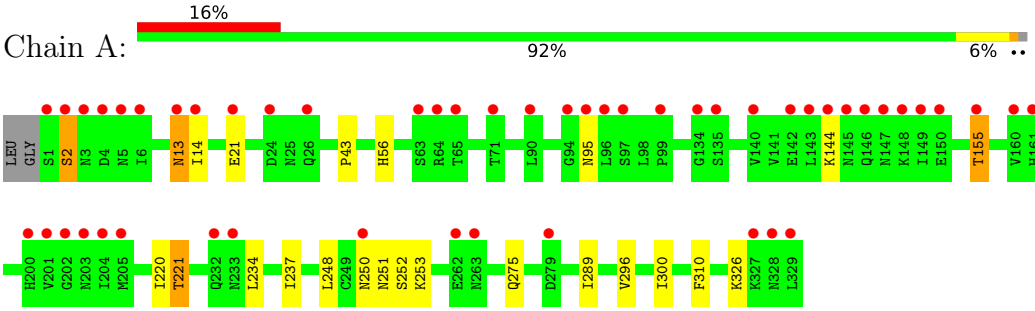
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	413	Total	O	0	0
			413	413		
3	B	317	Total	O	0	0
			317	317		
3	C	1	Total	O	0	0
			1	1		
3	D	5	Total	O	0	0
			5	5		

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.

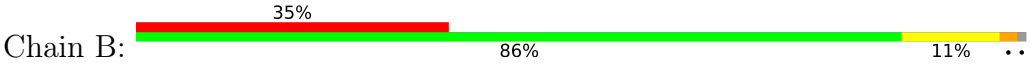
• Molecule 1: Plasmepsin 2

Chain A:



• Molecule 1: Plasmepsin 2

Chain B:



• Molecule 2: Pepstatin

Chain C:

• Molecule 2: Pepstatin

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.11Å 141.11Å 97.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 1.70 119.52 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (119.52-1.70) 98.8 (119.52-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.214 , 0.237 0.221 , 0.243	Depositor DCC
R_{free} test set	6068 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6046	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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

Bond lengths and bond angles in the following residue types are not validated in this section: STA, IVA

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	0.51	0/2674	0.78	0/3638
1	B	0.47	0/2674	0.79	5/3638 (0.1%)
2	C	0.60	0/17	1.03	0/21
2	D	0.84	0/17	1.01	0/21
All	All	0.49	0/5382	0.79	5/7318 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	2	0
2	C	0	2
2	D	0	2
All	All	2	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	221	THR	CA-CB-CG2	6.42	121.41	110.50
1	B	247	THR	CA-CB-OG1	6.22	118.94	109.60
1	B	247	THR	CA-CB-CG2	5.99	120.68	110.50
1	B	221	THR	CA-CB-OG1	5.64	118.06	109.60
1	B	247	THR	OG1-CB-CG2	5.32	119.95	109.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	221	THR	CB
1	B	247	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1350	STA	Mainchain,Peptide
2	D	1350	STA	Mainchain,Peptide

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	2607	0	2536	16	0
1	B	2607	0	2536	23	0
2	C	48	0	60	0	0
2	D	48	0	60	3	0
3	A	413	0	0	6	0
3	B	317	0	0	5	0
3	C	1	0	0	0	0
3	D	5	0	0	0	0
All	All	6046	0	5192	39	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 4.

The worst 5 of 39 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:221:THR:HB	1:A:300:ILE:HB	1.72	0.71
1:A:155:THR:HG22	3:A:1348:HOH:O	1.92	0.69
1:A:155:THR:HG21	3:A:1354:HOH:O	1.93	0.69
1:B:155:THR:HG21	3:B:1352:HOH:O	1.92	0.68
1:B:221:THR:HG23	3:B:1364:HOH:O	1.92	0.68

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	A	327/331 (99%)	311 (95%)	15 (5%)	1 (0%)	36 22
1	B	327/331 (99%)	315 (96%)	9 (3%)	3 (1%)	14 4
2	C	3/6 (50%)	3 (100%)	0	0	100 100
2	D	3/6 (50%)	3 (100%)	0	0	100 100
All	All	660/674 (98%)	632 (96%)	24 (4%)	4 (1%)	21 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	B	2	SER
1	B	26	GLN
1	B	135	SER

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	294/295 (100%)	282 (96%)	12 (4%)	27 11
1	B	294/295 (100%)	274 (93%)	20 (7%)	14 4
2	C	2/2 (100%)	2 (100%)	0	100 100
2	D	2/2 (100%)	2 (100%)	0	100 100
All	All	592/594 (100%)	560 (95%)	32 (5%)	20 6

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	248	LEU
1	B	284	LEU
1	B	21	GLU
1	A	326	LYS
1	B	327	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	161	HIS
1	B	232	GLN
1	B	251	ASN
1	A	250	ASN
1	A	251	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	STA	C	1350	2	10,10,11	0.47	0	9,12,14	0.92	1 (11%)
2	STA	C	1352	2	11,11,11	1.27	2 (18%)	11,14,14	1.10	1 (9%)
2	STA	D	1350	2	10,10,11	0.35	0	9,12,14	0.70	0
2	STA	D	1352	2	11,11,11	1.33	2 (18%)	11,14,14	1.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STA	C	1350	2	-	2/11/11/12	-
2	STA	C	1352	2	-	0/12/12/12	-
2	STA	D	1350	2	-	1/11/11/12	-
2	STA	D	1352	2	-	1/12/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1352	STA	O-C	3.51	1.33	1.22
2	C	1352	STA	O-C	3.39	1.33	1.22
2	D	1352	STA	OXT-C	-2.54	1.22	1.30
2	C	1352	STA	OXT-C	-2.42	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1352	STA	OXT-C-CM	2.24	120.97	114.00
2	C	1350	STA	CH-CM-C	-2.06	109.51	113.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1350	STA	O-C-CM-CH
2	D	1350	STA	O-C-CM-CH
2	D	1352	STA	OXT-C-CM-CH
2	C	1350	STA	OH-CH-CM-C

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1350	STA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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	329/331 (99%)	0.84	54 (16%) 4 4	12, 21, 35, 58	0
1	B	329/331 (99%)	1.54	115 (34%) 1 1	14, 28, 49, 62	0
2	C	3/6 (50%)	-0.34	0 100 100	13, 13, 15, 20	0
2	D	3/6 (50%)	0.52	0 100 100	20, 20, 23, 28	0
All	All	664/674 (98%)	1.18	169 (25%) 1 1	12, 24, 45, 62	0

The worst 5 of 169 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	7.4
1	B	26	GLN	6.2
1	B	1	SER	6.1
1	A	162	ASP	5.8
1	A	202	GLY	5.7

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	STA	D	1352	12/12	0.84	0.17	32,37,40,41	0
2	STA	C	1352	12/12	0.85	0.17	25,33,39,39	0
2	STA	D	1350	11/12	0.95	0.07	19,20,21,23	0
2	STA	C	1350	11/12	0.97	0.06	12,13,15,15	0

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.