



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:07 AM GMT

PDB ID : 2JXR
Title : STRUCTURE OF YEAST PROTEINASE A
Authors : Aguilar, C.F.; Badasso, M.; Dreyer, T.; Cronin, N.B.; Newman, M.P.; Cooper, J.B.; Hoover, D.J.; Wood, S.P.; Johnson, M.S.; Blundell, T.L.
Deposited on : 1997-04-24
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

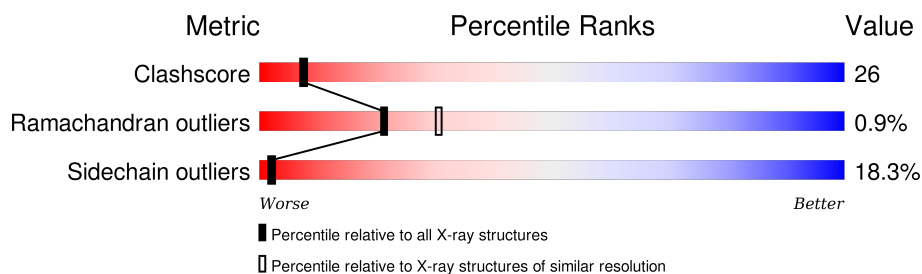
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	329	 45% 40% 11% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	A	336	X	-	-	-
4	NDG	A	337	X	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2768 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.

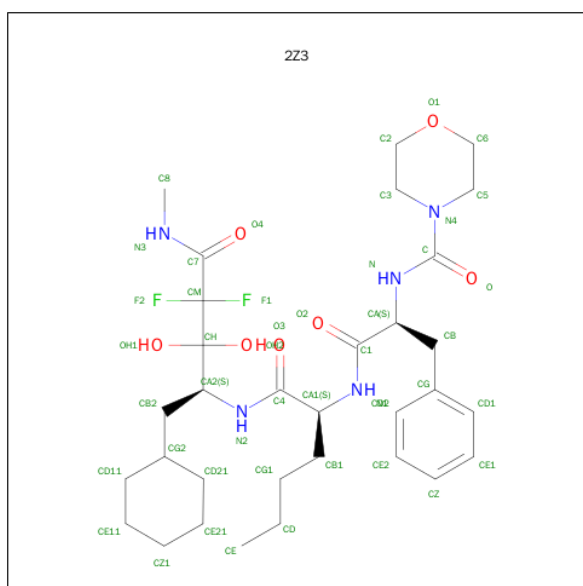
- Molecule 1 is a protein called PROTEINASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2528	1618	396	508	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ILE	LEU	ENGINEERED	UNP P07267

- Molecule 2 is N-(MORPHOLIN-4-YLCARBONYL)-L-PHENYLALANYL-N-[(1R)-1-(CYCLOHEXYLMETHYL)-3,3-DIFLUORO-2,2-DIHYDROXY-4-(METHYLAMINO)-4-OXOBUTYL]-L-NORLEUCINAMIDE (three-letter code: 2Z3) (formula: $C_{32}H_{49}F_2N_5O_7$).

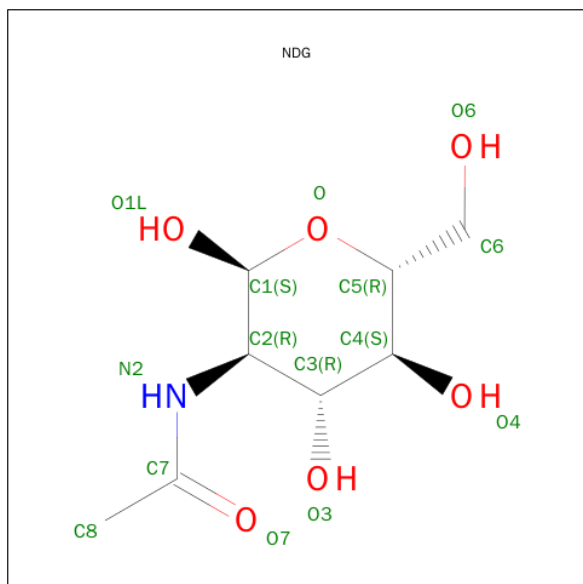


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			46	32	2	5	7		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

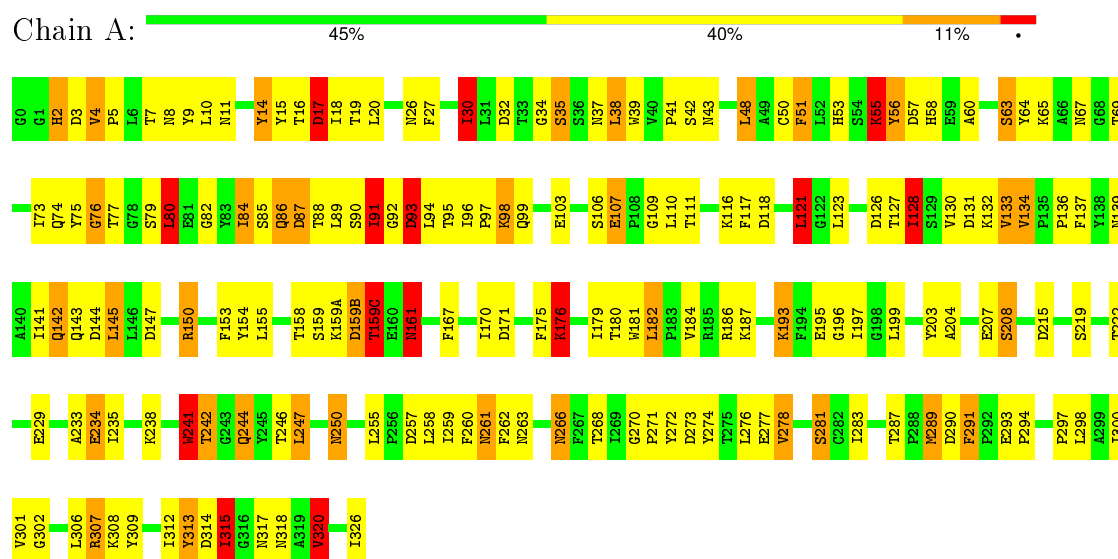
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: PROTEINASE A



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.70Å 86.70Å 110.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.193 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2768	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 2Z3, NAG, NDG, MAN

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	1.23	7/2592 (0.3%)	2.28	105/3526 (3.0%)

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	A	5	0
3	A	3	0
All	All	8	0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	PHE	CE2-CZ	6.31	1.49	1.37
1	A	301	VAL	CB-CG1	-6.11	1.40	1.52
1	A	63	SER	CA-CB	-5.82	1.44	1.52
1	A	175	PHE	CE1-CZ	5.78	1.48	1.37
1	A	229	GLU	CB-CG	5.72	1.63	1.52

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH1	-21.91	109.34	120.30
1	A	244	GLN	CA-CB-CG	17.52	151.94	113.40
1	A	4	VAL	CA-CB-CG2	15.27	133.81	110.90
1	A	320	VAL	CG1-CB-CG2	14.34	133.84	110.90
1	A	241	TRP	C-N-CA	13.45	155.32	121.70

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	16	THR	CB
1	A	43	ASN	CA
1	A	63	SER	CA
1	A	161	ASN	CA
1	A	241	TRP	CA

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	2528	0	2398	129	0
2	A	46	0	49	4	0
3	A	61	0	52	3	0
4	A	14	0	12	10	0
5	A	119	0	0	7	0
All	All	2768	0	2511	132	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 26.

The worst 5 of 132 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:242:THR:CG2	1:A:242:THR:O	1.97	1.13
1:A:242:THR:HG22	1:A:242:THR:O	1.50	1.10
1:A:4:VAL:HG23	1:A:16:THR:HG21	1.30	1.09
1:A:84:ILE:HD12	1:A:84:ILE:N	1.75	1.00
1:A:128:ILE:O	1:A:128:ILE:HG12	1.64	0.96

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	327/329 (99%)	305 (93%)	19 (6%)	3 (1%)	21	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	TRP
1	A	159(C)	THR
1	A	161	ASN

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	268/268 (100%)	219 (82%)	49 (18%)	2	2

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ASP
1	A	161	ASN
1	A	300	ILE
1	A	158	THR
1	A	170	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	317	ASN
1	A	244	GLN
1	A	139	ASN
1	A	232	ASN

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 ⓘ

5 carbohydrates 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	$\# Z > 2$
3	NAG	A	332	1,3	14,14,15	1.38	2 (14%)	15,19,21	2.83	5 (33%)
3	NAG	A	333	3	14,14,15	1.31	2 (14%)	15,19,21	3.00	9 (60%)
3	BMA	A	334	3	11,11,12	1.69	3 (27%)	14,15,17	3.33	6 (42%)
3	BMA	A	335	3	11,11,12	1.83	5 (45%)	14,15,17	2.71	6 (42%)
3	MAN	A	336	3	11,11,12	1.51	1 (9%)	14,15,17	2.51	6 (42%)

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
3	NAG	A	332	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	333	3	-	0/6/23/26	0/1/1/1
3	BMA	A	334	3	-	0/2/19/22	0/1/1/1
3	BMA	A	335	3	-	0/2/19/22	0/1/1/1
3	MAN	A	336	3	3/3/4/5	0/2/19/22	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	333	NAG	C2-N2	2.17	1.50	1.46
3	A	334	BMA	O4-C4	2.21	1.48	1.43
3	A	335	BMA	O2-C2	2.22	1.48	1.43
3	A	335	BMA	O3-C3	2.36	1.48	1.43
3	A	335	BMA	O5-C5	2.55	1.49	1.43

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	332	NAG	C2-N2-C7	-7.49	113.42	123.04
3	A	335	BMA	C1-O5-C5	-6.50	104.00	112.25
3	A	332	NAG	O7-C7-C8	-4.78	113.28	122.06
3	A	333	NAG	C2-N2-C7	-4.74	116.95	123.04
3	A	335	BMA	O5-C1-C2	-4.65	103.31	110.86

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	336	MAN	C2
3	A	336	MAN	C5
3	A	336	MAN	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	334	BMA	1	0
3	A	335	BMA	3	0

5.6 Ligand geometry

2 ligands 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	2Z3	A	327	-	43,48,48	1.36	4 (9%)	51,66,66	2.33	18 (35%)
4	NDG	A	337	1	14,14,15	1.39	1 (7%)	15,19,21	3.93	9 (60%)

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	2Z3	A	327	-	-	0/44/75/75	0/3/3/3
4	NDG	A	337	1	1/1/5/7	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	327	2Z3	CB2-CA2	-5.70	1.48	1.53
4	A	337	NDG	C3-C2	-3.00	1.45	1.52
2	A	327	2Z3	CD11-CG2	-2.37	1.46	1.52
2	A	327	2Z3	CE2-CD2	2.31	1.43	1.38
2	A	327	2Z3	O4-C7	2.85	1.28	1.22

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	337	NDG	C2-N2-C7	-9.45	110.89	123.04
2	A	327	2Z3	CZ-CE2-CD2	-4.30	113.89	120.19
4	A	337	NDG	O-C5-C6	-3.66	99.42	107.35
2	A	327	2Z3	F2-CM-C7	-3.26	105.77	109.88
2	A	327	2Z3	F2-CM-F1	-3.24	98.94	106.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	337	NDG	C2

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	327	2Z3	4	0
4	A	337	NDG	10	0

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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.