



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:01 pm BST

PDB ID : 2WXX
Title : Crystal structure of mouse angiotensinogen in the oxidised form
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Deposited on : 2009-11-11
Resolution : 2.95 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 ⓘ symbol.

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 : 2.11
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) : 2.11

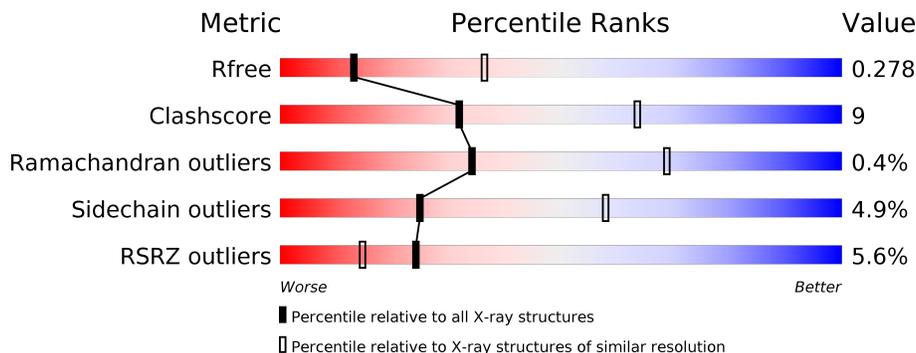
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 $\leq 5\%$. 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	453	 2% 71% 18% • 9%
1	B	453	 4% 75% 18% • 6%
1	C	453	 3% 71% 20% • 7%
1	D	453	 11% 73% 17% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12945 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 ANGIOTENSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	412	3181	2036	535	600	10	0	1	0
1	B	428	3314	2117	558	629	10	0	2	0
1	C	422	3274	2095	550	619	10	0	3	0
1	D	411	3176	2036	533	597	10	0	2	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	THR	ALA	conflict	UNP P11859
A	174	VAL	MET	conflict	UNP P11859
A	317	ILE	THR	conflict	UNP P11859
A	329	GLN	ARG	conflict	UNP P11859
A	379	ASN	SER	conflict	UNP P11859
B	77	THR	ALA	conflict	UNP P11859
B	174	VAL	MET	conflict	UNP P11859
B	317	ILE	THR	conflict	UNP P11859
B	329	GLN	ARG	conflict	UNP P11859
B	379	ASN	SER	conflict	UNP P11859
C	77	THR	ALA	conflict	UNP P11859
C	174	VAL	MET	conflict	UNP P11859
C	317	ILE	THR	conflict	UNP P11859
C	329	GLN	ARG	conflict	UNP P11859
C	379	ASN	SER	conflict	UNP P11859
D	77	THR	ALA	conflict	UNP P11859
D	174	VAL	MET	conflict	UNP P11859
D	317	ILE	THR	conflict	UNP P11859
D	329	GLN	ARG	conflict	UNP P11859
D	379	ASN	SER	conflict	UNP P11859

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	95.37Å 99.42Å 425.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	213.20 – 2.95 68.82 – 2.95	Depositor EDS
% Data completeness (in resolution range)	84.5 (213.20-2.95) 84.5 (68.82-2.95)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.96Å)	Xtrriage
Refinement program	REFMAC 5.5.0099	Depositor
R, R_{free}	0.223 , 0.271 0.230 , 0.278	Depositor DCC
R_{free} test set	1850 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtrriage
Anisotropy	0.474	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.055 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12945	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.40	1/3251 (0.0%)	0.54	1/4427 (0.0%)
1	B	0.38	0/3392	0.56	0/4621
1	C	0.34	0/3353	0.50	0/4567
1	D	0.31	0/3250	0.47	0/4424
All	All	0.36	1/13246 (0.0%)	0.52	1/18039 (0.0%)

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	2	0
1	B	1	0
1	C	1	0
1	D	1	0
All	All	5	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	THR	CB-OG1	5.40	1.54	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	LEU	CA-CB-CG	-5.03	103.73	115.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	167	THR	CB

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Mol	Chain	Res	Type	Atom
1	A	327	ILE	CB
1	B	327	ILE	CB
1	C	327	ILE	CB
1	D	327	ILE	CB

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	3181	0	3179	66	0
1	B	3314	0	3308	56	0
1	C	3274	0	3261	67	0
1	D	3176	0	3173	46	0
All	All	12945	0	12921	230	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 9.

The worst 5 of 230 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:367:LYS:C	1:A:368:LEU:HD23	1.50	1.29
1:A:371:LEU:O	1:A:371:LEU:HD23	1.48	1.12
1:A:367:LYS:O	1:A:368:LEU:HD23	1.62	1.00
1:C:448:ASN:C	1:C:448:ASN:HD22	1.66	0.97
1:C:193:LEU:HD23	1:C:200:LEU:HD11	1.47	0.94

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	403/453 (89%)	383 (95%)	17 (4%)	3 (1%)	22	56
1	B	422/453 (93%)	402 (95%)	17 (4%)	3 (1%)	22	56
1	C	415/453 (92%)	393 (95%)	22 (5%)	0	100	100
1	D	403/453 (89%)	385 (96%)	18 (4%)	0	100	100
All	All	1643/1812 (91%)	1563 (95%)	74 (4%)	6 (0%)	34	69

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ALA
1	B	449	PRO
1	B	199	ALA
1	B	336	ILE
1	A	449	PRO

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	354/394 (90%)	334 (94%)	20 (6%)	21	53
1	B	371/394 (94%)	356 (96%)	15 (4%)	31	64
1	C	364/394 (92%)	342 (94%)	22 (6%)	19	50
1	D	352/394 (89%)	339 (96%)	13 (4%)	34	66
All	All	1441/1576 (91%)	1371 (95%)	70 (5%)	25	58

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	293	GLN
1	C	105	LEU
1	D	315	HIS
1	B	316	CYS
1	C	1	ASP

Some 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	447	ASN
1	C	9	HIS
1	C	448	ASN
1	B	393	ASN
1	C	350	GLN

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 carbohydrates 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

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>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	412/453 (90%)	0.28	11 (2%) 54 38	50, 76, 114, 130	9 (2%)
1	B	428/453 (94%)	0.33	20 (4%) 31 20	46, 77, 113, 142	9 (2%)
1	C	422/453 (93%)	0.29	13 (3%) 49 32	26, 89, 118, 138	9 (2%)
1	D	411/453 (90%)	0.65	49 (11%) 4 2	52, 118, 182, 230	9 (2%)
All	All	1673/1812 (92%)	0.38	93 (5%) 24 15	26, 87, 148, 230	36 (2%)

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	GLY	6.5
1	D	335	TRP	6.3
1	D	440	LEU	5.1
1	D	336	ILE	4.4
1	D	337	GLU	4.4

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.