



Full wwPDB Geometry-Only Validation Report ⓘ

May 29, 2020 – 01:53 am BST

PDB ID : 2YZ4
Title : The neutron structure of concanavalin A at 2.2 Angstroms
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Deposited on : 2007-05-02
Resolution : 2.20 Å(reported)

This is a Full wwPDB Geometry-Only 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

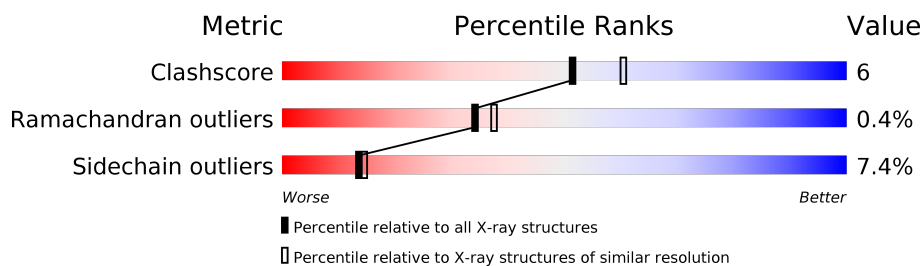
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

NEUTRON DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	237	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3810 atoms, of which 1356 are hydrogens and 559 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 Concanavalin A.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	237	Total	C	D	H	N	O	S	0	0	0
			3564	1141	399	1356	302	364	2			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

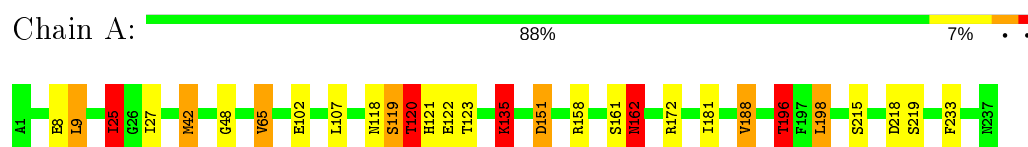
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	84	Total	D	O	0	0
			244	160	84		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Concanavalin A



4 Model quality ⓘ

4.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MN, DOD

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	0.95	2/1851 (0.1%)	1.44	23/2522 (0.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	VAL	CB-CG1	15.25	1.84	1.52
1	A	102	GLU	CD-OE2	8.42	1.34	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	THR	C-N-CA	13.82	156.24	121.70
1	A	65	VAL	CG1-CB-CG2	-12.25	91.30	110.90
1	A	172	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	A	135	LYS	CB-CG-CD	10.32	138.43	111.60
1	A	158	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	A	196	THR	N-CA-CB	9.14	127.66	110.30
1	A	218	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	A	65	VAL	CA-CB-CG1	-8.79	97.71	110.90
1	A	25	ILE	N-CA-CB	8.25	129.78	110.80
1	A	25	ILE	CA-CB-CG1	7.87	125.95	111.00
1	A	158	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	42	MET	CG-SD-CE	-7.40	88.36	100.20
1	A	27	ILE	CA-CB-CG1	6.73	123.78	111.00
1	A	151	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	188	VAL	CB-CA-C	6.17	123.11	111.40
1	A	172	ARG	NH1-CZ-NH2	6.07	126.07	119.40
1	A	188	VAL	CA-CB-CG1	5.93	119.80	110.90
1	A	162	ASN	OD1-CG-ND2	5.72	135.05	121.90
1	A	198	LEU	CB-CG-CD2	5.60	120.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ILE	CB-CG1-CD1	5.50	129.31	113.90
1	A	196	THR	CA-CB-OG1	5.49	120.53	109.00
1	A	233	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	A	119	SER	N-CA-CB	-5.08	102.89	110.50

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2208	1356	1754	20	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	244	0	0	1	0
All	All	2454	1356	1754	20	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 6.

All (20) 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:65:VAL:CG1	1:A:65:VAL:CB	1.84	1.50
1:A:162:ASN:O	1:A:162:ASN:ND2	1.81	1.13
1:A:65:VAL:CG1	1:A:65:VAL:CG2	2.43	0.95
1:A:162:ASN:C	1:A:162:ASN:ND2	2.20	0.93
1:A:65:VAL:CG1	1:A:65:VAL:CA	2.53	0.86
1:A:9:LEU:HD11	1:A:65:VAL:HG11	1.42	0.86
1:A:48:GLY:O	1:A:196:THR:HB	1.92	0.64
1:A:215:SER:OG	1:A:219:SER:CB	2.46	0.64
1:A:215:SER:OG	1:A:219:SER:HB2	1.96	0.60
1:A:65:VAL:CG1	1:A:65:VAL:HG22	2.30	0.56
1:A:9:LEU:CD1	1:A:65:VAL:HG11	2.25	0.55
1:A:25:ILE:HD12	1:A:65:VAL:CG1	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HD12	1:A:65:VAL:HG13	1.80	0.54
1:A:8:GLU:O	1:A:25:ILE:HB	2.03	0.53
1:A:119:SER:O	1:A:122:GLU:HB2	2.06	0.51
1:A:25:ILE:CD1	1:A:65:VAL:HG13	2.35	0.50
1:A:120:THR:O	1:A:122:GLU:OE1	2.29	0.50
1:A:135:LYS:H	1:A:135:LYS:CD	2.18	0.49
1:A:9:LEU:HD12	1:A:25:ILE:CG2	2.38	0.48
1:A:181:ILE:HD12	4:A:580:DOD:O	2.09	0.46

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	235/237 (99%)	229 (97%)	5 (2%)	1 (0%)	34	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	THR

4.3.2 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	203/203 (100%)	188 (93%)	15 (7%)	13 14

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	25	ILE
1	A	42	MET
1	A	107	LEU
1	A	118	ASN
1	A	120	THR
1	A	121	HIS
1	A	123	THR
1	A	135	LYS
1	A	151	ASP
1	A	161	SER
1	A	162	ASN
1	A	188	VAL
1	A	196	THR
1	A	198	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	118	ASN
1	A	237	ASN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

4.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.