



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 07:48 pm BST

PDB ID : 1JYI
Title : CONCAVALIN A/12-MER PEPTIDE COMPLEX
Authors : Jain, D.; Kaur, K.J.; Sundaravadivel, B.; Salunke, D.M.
Deposited on : 2001-09-12
Resolution : 2.75 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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

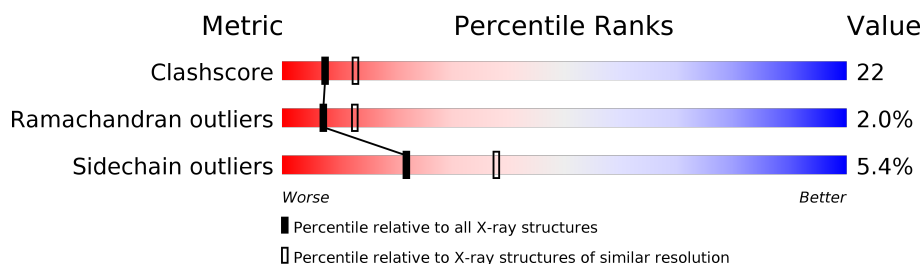
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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	64% 32% .
1	B	237	70% 29% .
1	C	237	71% 27% .
1	D	237	67% 30% .
2	P	12	17% 50% 17% 17%
2	Q	12	25% 25% 42% 8%
2	R	12	25% 42% 25% 8%
2	S	12	33% 25% 33% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7925 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 Concanavalin-Br.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	B	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	C	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	D	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ASP	GLY	conflict	UNP P55915
A	70	ALA	GLY	conflict	UNP P55915
A	151	ASP	GLU	conflict	UNP P55915
A	155	GLU	ARG	conflict	UNP P55915
B	58	ASP	GLY	conflict	UNP P55915
B	70	ALA	GLY	conflict	UNP P55915
B	151	ASP	GLU	conflict	UNP P55915
B	155	GLU	ARG	conflict	UNP P55915
C	58	ASP	GLY	conflict	UNP P55915
C	70	ALA	GLY	conflict	UNP P55915
C	151	ASP	GLU	conflict	UNP P55915
C	155	GLU	ARG	conflict	UNP P55915
D	58	ASP	GLY	conflict	UNP P55915
D	70	ALA	GLY	conflict	UNP P55915
D	151	ASP	GLU	conflict	UNP P55915
D	155	GLU	ARG	conflict	UNP P55915

- Molecule 2 is a protein called 12-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	12	Total	C	N	O	0	0	0
			98	66	12	20			
2	Q	12	Total	C	N	O	0	0	0
			98	66	12	20			
2	R	12	Total	C	N	O	0	0	0
			98	66	12	20			
2	S	12	Total	C	N	O	0	0	0
			98	66	12	20			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	66	Total	O	0	0
			66	66		
5	C	84	Total	O	0	0
			84	84		

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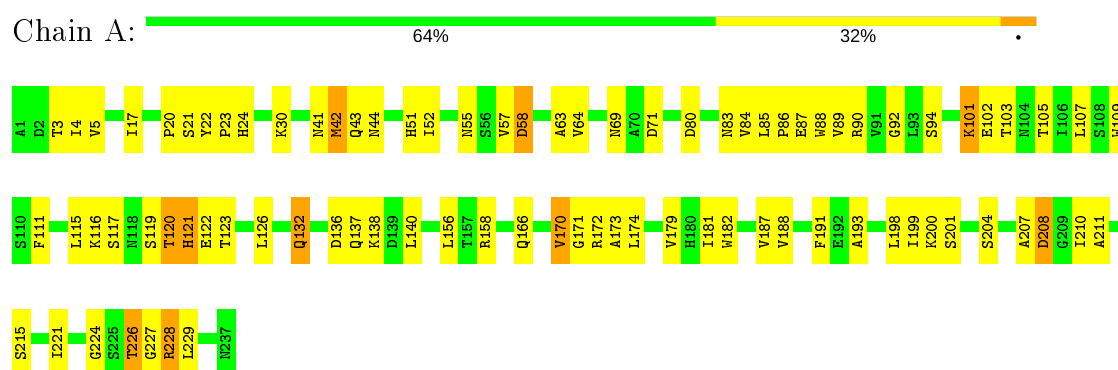
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	60	Total 60	O 60	0	0
5	P	1	Total 1	O 1	0	0
5	Q	1	Total 1	O 1	0	0
5	R	3	Total 3	O 3	0	0
5	S	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

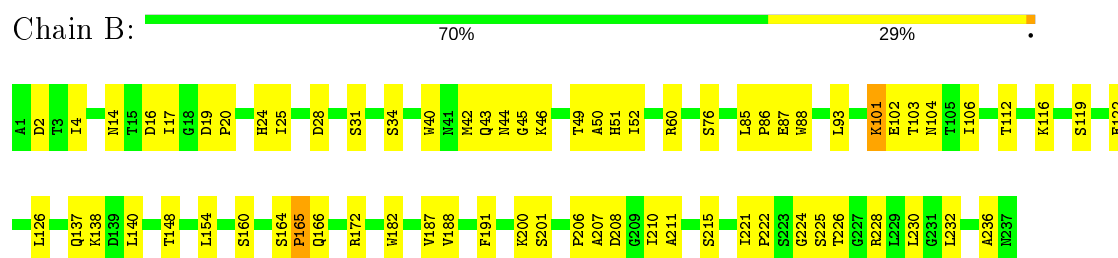
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

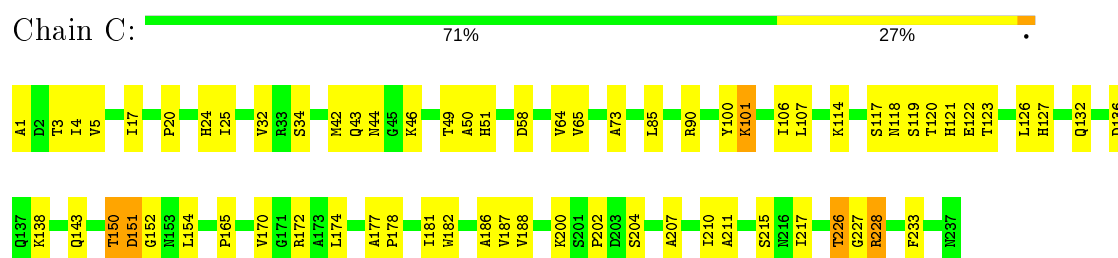
- Molecule 1: Concanavalin-Br



- Molecule 1: Concanavalin-Br

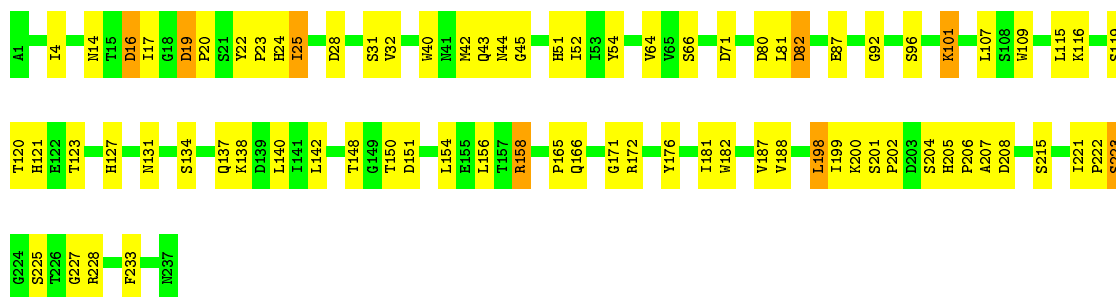


- Molecule 1: Concanavalin-Br

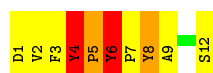
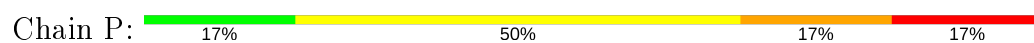


- Molecule 1: Concanavalin-Br

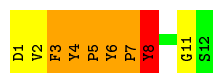
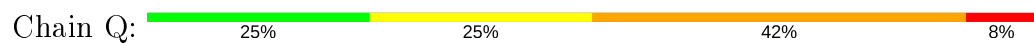




- Molecule 2: 12-mer peptide



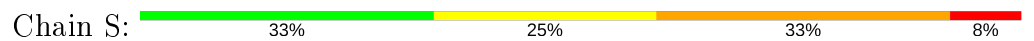
- Molecule 2: 12-mer peptide



- Molecule 2: 12-mer peptide



- Molecule 2: 12-mer peptide



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.55Å 118.32Å 252.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.75	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.75)	Depositor
R_{merge}	0.67	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.192 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7925	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: CA, MN

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	0.39	0/1851	0.70	1/2522 (0.0%)
1	B	0.36	0/1851	0.67	0/2522
1	C	0.38	0/1851	0.69	1/2522 (0.0%)
1	D	0.37	0/1851	0.66	0/2522
2	P	0.47	0/103	0.61	0/140
2	Q	0.50	0/103	0.72	0/140
2	R	0.54	0/103	0.73	0/140
2	S	0.46	0/103	0.56	0/140
All	All	0.38	0/7816	0.68	2/10648 (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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ASP	CB-CA-C	-5.54	99.32	110.40
1	C	58	ASP	CA-CB-CG	5.35	125.16	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	207	ALA	Peptide

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	1809	0	1755	99	0
1	B	1809	0	1755	64	0
1	C	1809	0	1755	53	0
1	D	1809	0	1755	75	0
2	P	98	0	83	34	0
2	Q	98	0	83	25	0
2	R	98	0	83	21	0
2	S	98	0	83	24	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	72	0	0	6	0
5	B	66	0	0	7	0
5	C	84	0	0	7	0
5	D	60	0	0	7	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
5	R	3	0	0	0	0
5	S	2	0	0	1	0
All	All	7925	0	7352	329	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 22.

The worst 5 of 329 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:204:SER:HA	2:P:5:PRO:HB3	1.11	1.10
2:R:6:TYR:CG	2:R:7:PRO:HD2	1.98	0.98
1:A:172:ARG:HD2	1:A:221:ILE:HG12	1.47	0.95
1:D:204:SER:HA	2:S:5:PRO:HB3	1.46	0.95
1:A:43:GLN:HG2	2:P:9:ALA:HA	1.50	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	210 (89%)	22 (9%)	3 (1%)	12	21
1	B	235/237 (99%)	210 (89%)	23 (10%)	2 (1%)	17	31
1	C	235/237 (99%)	215 (92%)	16 (7%)	4 (2%)	9	16
1	D	235/237 (99%)	201 (86%)	33 (14%)	1 (0%)	34	53
2	P	10/12 (83%)	4 (40%)	4 (40%)	2 (20%)	0	0
2	Q	10/12 (83%)	3 (30%)	3 (30%)	4 (40%)	0	0
2	R	10/12 (83%)	4 (40%)	3 (30%)	3 (30%)	0	0
2	S	10/12 (83%)	8 (80%)	1 (10%)	1 (10%)	0	0
All	All	980/996 (98%)	855 (87%)	105 (11%)	20 (2%)	7	13

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	A	121	HIS
1	C	118	ASN
1	D	120	THR
2	Q	8	TYR

5.3.2 Protein sidechains ⓘ

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%)	194 (96%)	9 (4%)	28	47
1	B	203/203 (100%)	199 (98%)	4 (2%)	55	72
1	C	203/203 (100%)	196 (97%)	7 (3%)	37	58
1	D	203/203 (100%)	192 (95%)	11 (5%)	22	38
2	P	10/10 (100%)	6 (60%)	4 (40%)	0	0
2	Q	10/10 (100%)	6 (60%)	4 (40%)	0	0
2	R	10/10 (100%)	8 (80%)	2 (20%)	1	1
2	S	10/10 (100%)	5 (50%)	5 (50%)	0	0
All	All	852/852 (100%)	806 (95%)	46 (5%)	22	38

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	16	ASP
1	D	101	LYS
2	S	3	PHE
1	D	19	ASP
1	D	66	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	ASN
1	C	43	GLN
1	D	205	HIS
1	B	166	GLN
1	B	237	ASN

5.3.3 RNA ⓘ

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](#)

Of 8 ligands modelled in this entry, 8 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.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.