wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:20 PM GMT

PDB ID	:	1JUI
Title	:	CONCANAVALIN A-CARBOHYDRATE MIMICKING 10-MER PEPTIDE COMPLEX
Authors	:	Jain, D.; Kaur, K.J.; Salunke, D.M.
Deposited on	:	2001-08-24
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

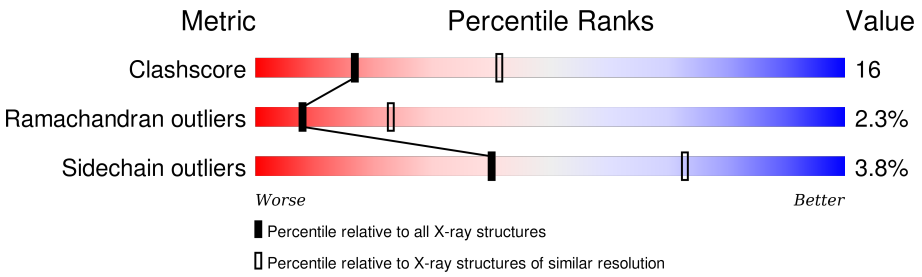
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)

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 <=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	237	81% 17% •
1	B	237	74% 24% •
1	C	237	80% 17% •
1	D	237	74% 24% •
2	P	10	30% 30% 20% 20%
2	Q	10	40% 40% 10% 10%
2	R	10	30% 50% 10% 10%

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Mol	Chain	Length	Quality of chain
2	S	10	10% 30% 50% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7899 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 A.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ASP	GLU	SEE REMARK 999	UNP P02866
A	155	GLU	ARG	SEE REMARK 999	UNP P02866
B	151	ASP	GLU	SEE REMARK 999	UNP P02866
B	155	GLU	ARG	SEE REMARK 999	UNP P02866
C	151	ASP	GLU	SEE REMARK 999	UNP P02866
C	155	GLU	ARG	SEE REMARK 999	UNP P02866
D	151	ASP	GLU	SEE REMARK 999	UNP P02866
D	155	GLU	ARG	SEE REMARK 999	UNP P02866

- Molecule 2 is a protein called 10-mer Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	P	10	87	59	11	16	1	0	0	0
2	Q	10	87	59	11	16	1	0	0	0
2	R	10	87	59	11	16	1	0	0	0
2	S	10	87	59	11	16	1	0	0	0

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

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

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	66	Total O 66 66	0	0
5	B	70	Total O 70 70	0	0
5	C	77	Total O 77 77	0	0
5	D	86	Total O 86 86	0	0
5	P	1	Total O 1 1	0	0
5	Q	2	Total O 2 2	0	0
5	R	3	Total O 3 3	0	0
5	S	2	Total O 2 2	0	0

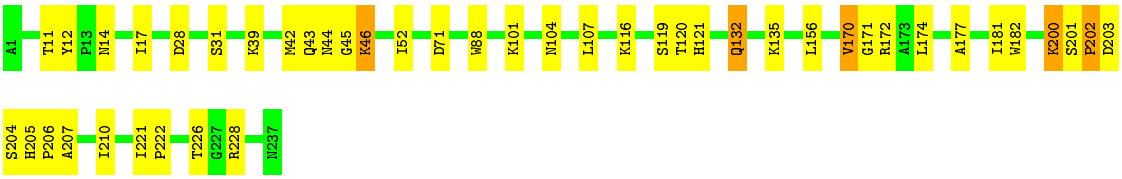
3 Residue-property plots (i)

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

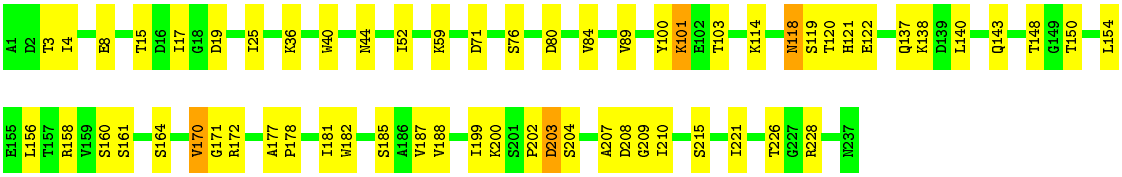
- Molecule 1: Concanavalin A

Chain A:



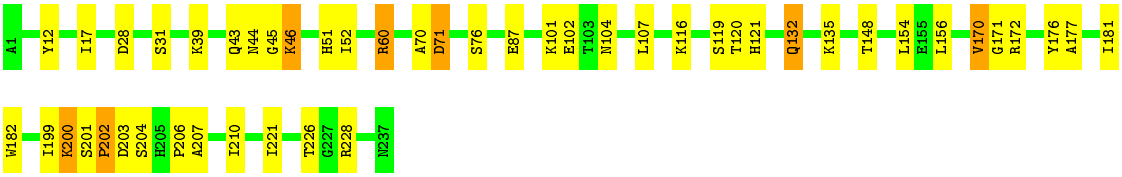
- Molecule 1: Concanavalin A

Chain B:



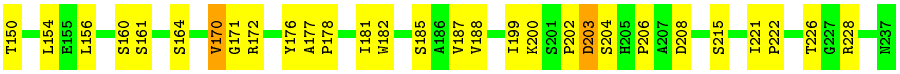
- Molecule 1: Concanavalin A

Chain C:



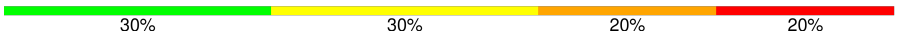
- Molecule 1: Concanavalin A

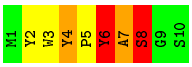
Chain D:



- Molecule 2: 10-mer Peptide

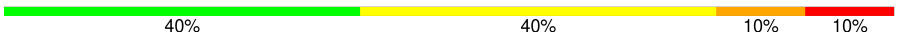
Chain P:

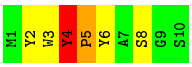




- Molecule 2: 10-mer Peptide

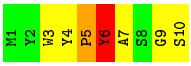
Chain Q:





- Molecule 2: 10-mer Peptide

Chain R:



- Molecule 2: 10-mer Peptide

Chain S:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	102.97Å 118.33Å 253.60Å 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}	0.60	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.188 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7899	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.67	0/2522
1	B	0.37	0/1851	0.68	0/2522
1	C	0.39	0/1851	0.68	0/2522
1	D	0.41	0/1851	0.69	0/2522
2	P	1.03	0/92	1.49	3/124 (2.4%)
2	Q	0.90	0/92	1.68	4/124 (3.2%)
2	R	0.85	0/92	1.20	2/124 (1.6%)
2	S	0.61	0/92	1.17	1/124 (0.8%)
All	All	0.42	0/7772	0.73	10/10584 (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
2	R	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	2	TYR	N-CA-C	-8.13	89.05	111.00
2	Q	3	TRP	CA-CB-CG	6.52	126.09	113.70
2	R	6	TYR	N-CA-C	6.15	127.62	111.00
2	P	8	SER	N-CA-C	5.66	126.29	111.00
2	Q	3	TRP	CB-CA-C	-5.62	99.16	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	R	6	TYR	Sidechain

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	1809	0	1755	42	0
1	B	1809	0	1755	52	0
1	C	1809	0	1755	56	0
1	D	1809	0	1755	73	0
2	P	87	0	73	14	0
2	Q	87	0	73	14	0
2	R	87	0	73	17	0
2	S	87	0	73	36	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	66	0	0	2	0
5	B	70	0	0	6	0
5	C	77	0	0	9	0
5	D	86	0	0	6	0
5	P	1	0	0	0	0
5	Q	2	0	0	0	0
5	R	3	0	0	0	0
5	S	2	0	0	0	0
All	All	7899	0	7312	245	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 16.

The worst 5 of 245 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:44:ASN:HB3	2:P:4:TYR:HB3	1.23	1.09
1:C:60:ARG:HD2	1:C:76:SER:HB3	1.39	1.05
1:D:44:ASN:HB3	2:S:4:TYR:CA	1.90	1.01
1:D:118:ASN:HD22	1:D:185:SER:HB2	1.34	0.91
1:D:172:ARG:HD2	1:D:221:ILE:HG12	1.51	0.90

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	235/237 (99%)	215 (92%)	17 (7%)	3 (1%)	15 40
1	B	235/237 (99%)	213 (91%)	20 (8%)	2 (1%)	21 52
1	C	235/237 (99%)	214 (91%)	18 (8%)	3 (1%)	15 40
1	D	235/237 (99%)	213 (91%)	20 (8%)	2 (1%)	21 52
2	P	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0 0
2	Q	8/10 (80%)	3 (38%)	2 (25%)	3 (38%)	0 0
2	R	8/10 (80%)	3 (38%)	2 (25%)	3 (38%)	0 0
2	S	8/10 (80%)	1 (12%)	3 (38%)	4 (50%)	0 0
All	All	972/988 (98%)	866 (89%)	84 (9%)	22 (2%)	8 23

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	A	204	SER
1	C	120	THR
1	C	204	SER
2	P	6	TYR

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	203/203 (100%)	196 (97%)	7 (3%)	44	76
1	B	203/203 (100%)	197 (97%)	6 (3%)	48	80
1	C	203/203 (100%)	196 (97%)	7 (3%)	44	76
1	D	203/203 (100%)	197 (97%)	6 (3%)	48	80
2	P	8/8 (100%)	5 (62%)	3 (38%)	0	0
2	Q	8/8 (100%)	7 (88%)	1 (12%)	6	15
2	R	8/8 (100%)	8 (100%)	0	100	100
2	S	8/8 (100%)	6 (75%)	2 (25%)	1	2
All	All	844/844 (100%)	812 (96%)	32 (4%)	40	73

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

Mol	Chain	Res	Type
1	C	60	ARG
1	C	132	GLN
2	Q	4	TYR
1	C	101	LYS
1	C	170	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	237	ASN
1	C	43	GLN
1	D	69	ASN
1	B	118	ASN
1	D	104	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)

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 (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.