



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2017 – 09:44 PM EDT

PDB ID : 1JQU
Title : Are Carboxy Terminii of Helices Coded by the Local Sequence or by Tertiary Structure Contacts
Authors : Sagermann, M.; Martensson, L.-G.; Baase, W.A.; Matthews, B.W.
Deposited on : unknown
Resolution : 2.60 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

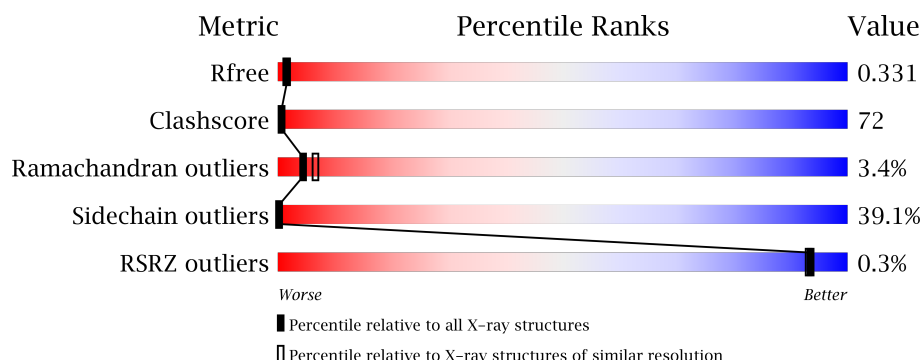
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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.

Mol	Chain	Length	Quality of chain
1	A	164	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 31% 52% 16% </div> </div>
1	B	164	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 25% 44% 29% </div> </div>
1	C	164	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 21% 48% 28% </div> </div>
1	D	164	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 16% 49% 30% 5% </div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5241 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 Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1303	819	237	242	5			
1	B	164	Total	C	N	O	S	0	0	0
			1303	819	237	242	5			
1	C	164	Total	C	N	O	S	0	0	0
			1303	819	237	242	5			
1	D	164	Total	C	N	O	S	0	0	0
			1303	819	237	242	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	THR	CIS	ENGINEERED	UNP P00720
A	97	ALA	CIS	ENGINEERED	UNP P00720
A	158	LEU	TRP	ENGINEERED	UNP P00720
B	54	THR	CIS	ENGINEERED	UNP P00720
B	97	ALA	CIS	ENGINEERED	UNP P00720
B	158	LEU	TRP	ENGINEERED	UNP P00720
C	54	THR	CIS	ENGINEERED	UNP P00720
C	97	ALA	CIS	ENGINEERED	UNP P00720
C	158	LEU	TRP	ENGINEERED	UNP P00720
D	54	THR	CIS	ENGINEERED	UNP P00720
D	97	ALA	CIS	ENGINEERED	UNP P00720
D	158	LEU	TRP	ENGINEERED	UNP P00720

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		
2	B	9	Total	O	0	0
			9	9		

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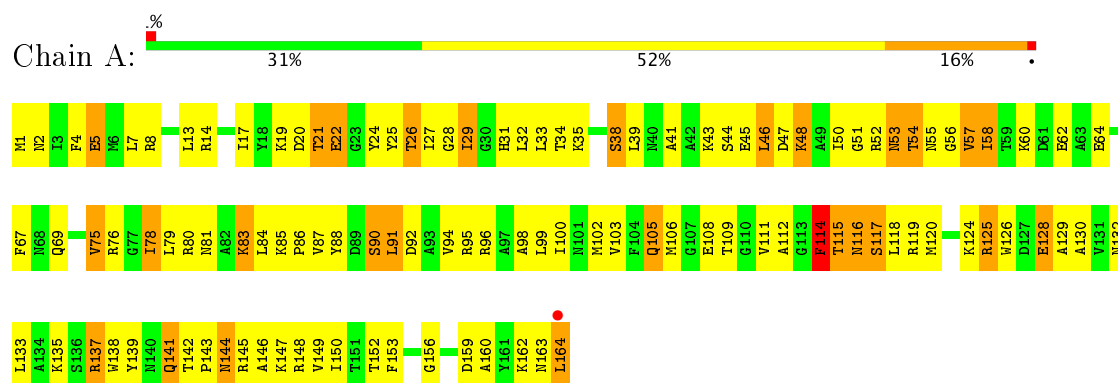
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	13	Total	O	0	0
			13	13		
2	D	2	Total	O	0	0
			2	2		

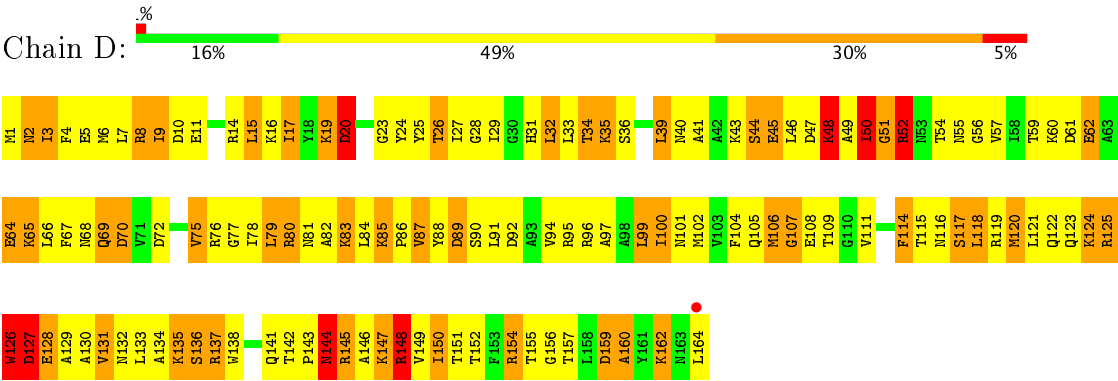
3 Residue-property plots

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 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.

• Molecule 1: Lysozyme



● Molecule 1: Lysozyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.30 Å 77.20 Å 138.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.60 34.92 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.60) 78.8 (34.92-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 2.48 Å)	Xtriage
Refinement program	CNS, TNT	Depositor
R, R_{free}	0.229 , 0.316 0.213 , 0.331	Depositor DCC
R_{free} test set	2090 reflections (9.96%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 127.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5241	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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

5.1 Standard geometry

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	0.59	0/1321	0.61	1/1777 (0.1%)
1	B	0.54	0/1321	0.85	1/1777 (0.1%)
1	C	1.22	14/1321 (1.1%)	1.25	18/1777 (1.0%)
1	D	1.28	10/1321 (0.8%)	1.57	19/1777 (1.1%)
All	All	0.97	24/5284 (0.5%)	1.13	39/7108 (0.5%)

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	C	0	7
1	D	0	5
All	All	0	12

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	PHE	CB-CG	-23.47	1.11	1.51
1	D	127	ASP	CB-CG	21.39	1.96	1.51
1	D	50	ILE	CB-CG1	17.73	2.03	1.54
1	D	50	ILE	C-N	-16.20	1.03	1.33
1	D	124	LYS	CB-CG	14.27	1.91	1.52

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	TRP	O-C-N	-26.84	79.76	122.70
1	B	36	SER	C-N-CD	-24.21	67.34	120.60
1	D	50	ILE	O-C-N	-24.16	82.12	123.20
1	C	114	PHE	CB-CG-CD2	-20.01	106.79	120.80
1	D	50	ILE	C-N-CA	19.23	162.69	122.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	MET	Mainchain,Peptide
1	C	2	ASN	Mainchain
1	C	30	GLY	Mainchain
1	C	33	LEU	Mainchain
1	C	34	THR	Mainchain

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	1303	0	1337	139	0
1	B	1303	0	1337	205	0
1	C	1303	0	1333	200	0
1	D	1303	0	1335	240	0
2	A	5	0	0	4	0
2	B	9	0	0	6	0
2	C	13	0	0	12	0
2	D	2	0	0	2	0
All	All	5241	0	5342	762	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 72.

The worst 5 of 762 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:C:32:LEU:CB	1:C:32:LEU:CG	1.75	1.57
1:D:125:ARG:CB	1:D:125:ARG:CG	1.85	1.52
1:C:34:THR:CG2	1:C:34:THR:CB	1.88	1.50
1:D:124:LYS:CB	1:D:124:LYS:CG	1.91	1.48
1:D:50:ILE:CG1	1:D:50:ILE:CB	2.03	1.34

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	162/164 (99%)	143 (88%)	16 (10%)	3 (2%)	9	18
1	B	162/164 (99%)	132 (82%)	23 (14%)	7 (4%)	3	4
1	C	162/164 (99%)	136 (84%)	21 (13%)	5 (3%)	5	8
1	D	162/164 (99%)	127 (78%)	28 (17%)	7 (4%)	3	4
All	All	648/656 (99%)	538 (83%)	88 (14%)	22 (3%)	4	6

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	B	37	PRO
1	B	136	SER
1	C	21	THR
1	C	163	ASN

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	137/137 (100%)	93 (68%)	44 (32%)	0	0
1	B	137/137 (100%)	79 (58%)	58 (42%)	0	0
1	C	137/137 (100%)	87 (64%)	50 (36%)	0	0
1	D	137/137 (100%)	75 (55%)	62 (45%)	0	0
All	All	548/548 (100%)	334 (61%)	214 (39%)	0	0

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	157	THR
1	C	61	ASP
1	D	126	TRP
1	B	162	LYS
1	C	14	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	ASN
1	C	2	ASN
1	D	140	ASN
1	B	163	ASN
1	C	69	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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	126:TRP	C	127:ASP	N	1.18
1	D	50:ILE	C	51:GLY	N	1.03

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	164/164 (100%)	-0.73	1 (0%) 89 88	8, 28, 57, 98	0
1	B	164/164 (100%)	-0.55	0 100 100	13, 37, 66, 102	0
1	C	164/164 (100%)	-0.60	0 100 100	13, 31, 62, 109	0
1	D	164/164 (100%)	-0.28	1 (0%) 89 88	19, 49, 79, 94	0
All	All	656/656 (100%)	-0.54	2 (0%) 93 93	8, 36, 71, 109	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	LEU	5.5
1	D	164	LEU	2.4

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 [i](#)

There are no such residues in this entry.