



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3JQZ  
Title : Crystal Structure of Human serum albumin complexed with Lidocaine  
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Deposited on : 2009-09-08  
Resolution : 3.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

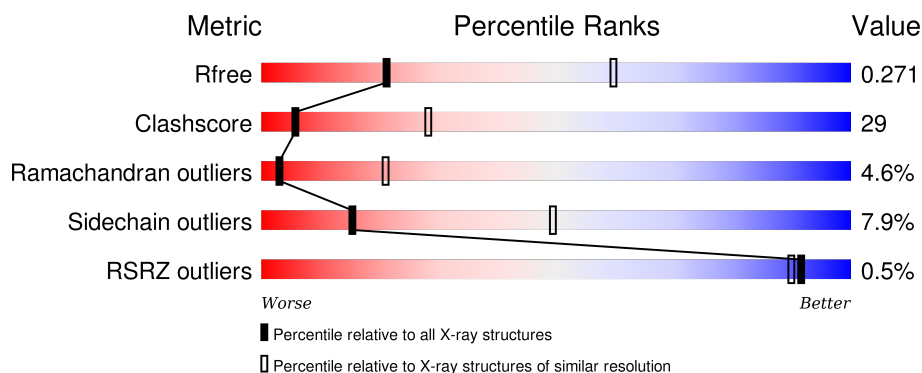
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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  $\geq 3$ , 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	585	 45% 46% 7% ..
1	B	585	 48% 43% 7% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LQZ	A	586	-	-	X	-

## 2 Entry composition [i](#)

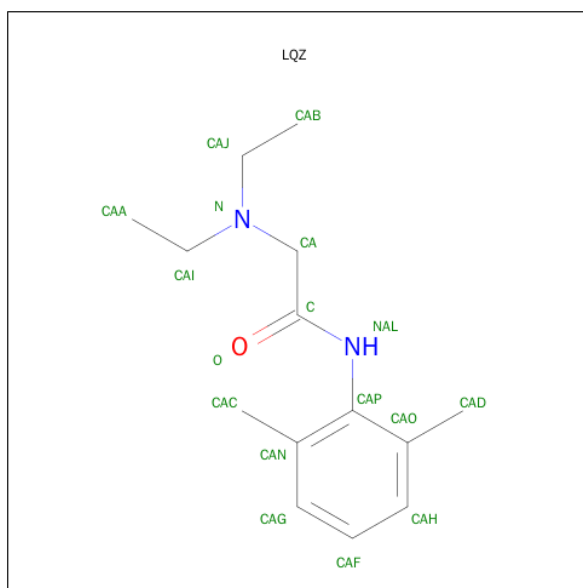
There are 2 unique types of molecules in this entry. The entry contains 9279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4631	2922	783	885	41			
1	B	582	Total	C	N	O	S	0	0	0
			4631	2922	783	885	41			

- Molecule 2 is 2-(DIETHYLAMINO)-N-(2,6-DIMETHYLPHENYL)ETHANAMIDE (three-letter code: LQZ) (formula: C<sub>14</sub>H<sub>22</sub>N<sub>2</sub>O).

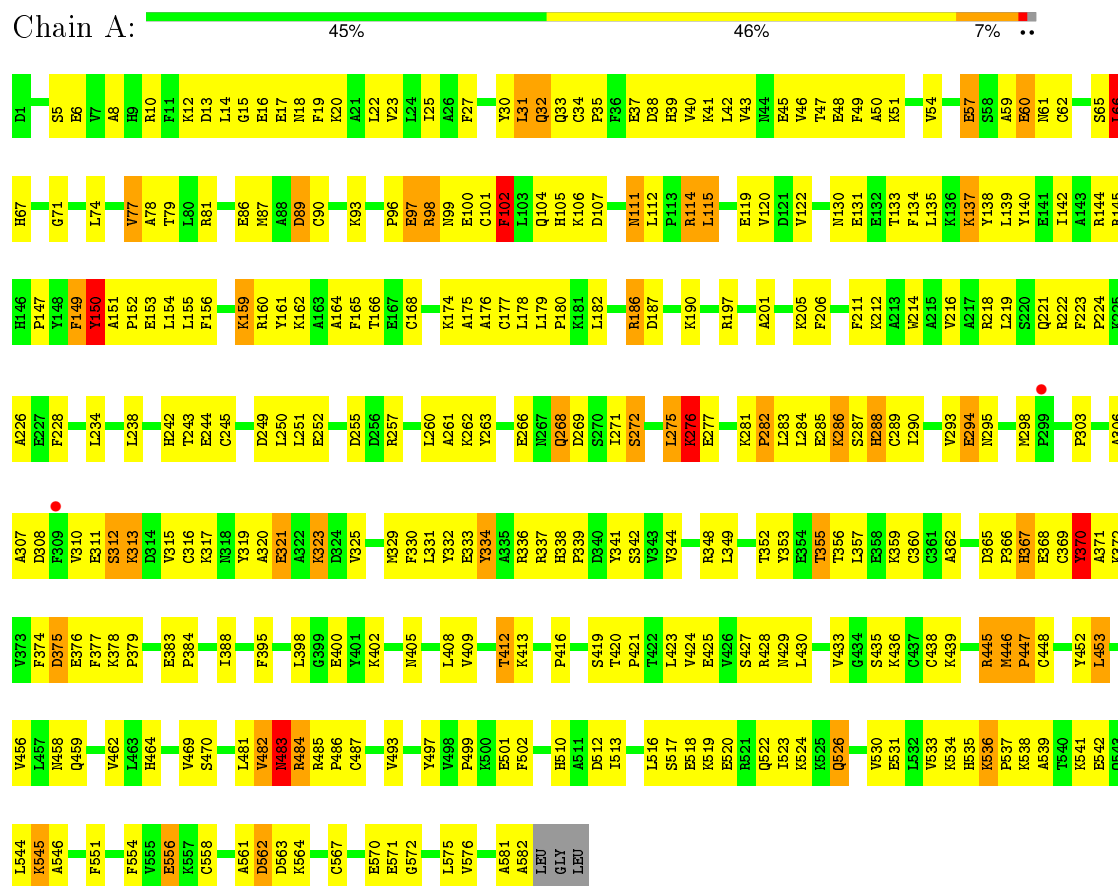


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	14	2	1		

### 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 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.

#### • Molecule 1: Serum albumin



E571	Y497	V415	K329	L250	H145
K574	V498	P416	F330	L251	H146
L575	K500	Q417	E333	E252	F149
A581	F501	V418	Y334	R257	Y150
A582	N503	T420	A335	A258	A151
LEU	A504	P421	R336	E152	E153
GLY	L423	T422	R337	K262	L154
LEU	F509	G431	H338	E266	L155
	H510	K432	D340	N267	F156
	A511	V433	Y341	F157	F157
	D512	V433	S342	I271	A158
	I513	G434	V343	S272	K159
	T515	S435	V344	S273	R160
	L516	K436		K274	Y161
	S517	C437	R348	L275	K162
	F518	C438	Y353	K276	
	K519	K439		E277	A175
	E520	K444	T356	P282	A176
	R521	R445	L357	L283	C177
	Q522	N446	E358	L178	L178
	I523	P447	K359	L179	L179
	K524	C448		K286	P180
	K525	A449	A364	S287	
	Q526	E450	D365	R288	K190
		D451	P366	C289	
	V530	Y452	B367	I290	K195
		L453		V293	K199
	H535	V456	X370	E294	C200
	K536	L457	A371	N295	A201
	P537	N458	K372	D296	S202
	K538	Q459	V373	E297	L203
	A539	L460	F374	N298	Q204
	T540	C461	D375	P299	K205
	Q543	V462	E376	L302	
		L463	F377		F211
	V547	H464	K378		W214
	N548	E465	P379	L305	A215
				A306	V216
	F551	V469	E383	F309	A217
	F554	S470	P384	V310	R218
	V555	D471	G385	E311	
	E556	R472	N386	S312	R222
	K557	K475	L387	K313	F223
	C558		I388	D314	K225
		S480	L398	V315	A226
	A561	L481	G399	C316	E227
	D562	V482	E400	K317	F228
	D563	N483	Y401	N318	
	K564	R484	K402	Y319	
	E565	R485	F403	K233	K233
	T566	P486	Q404	D324	L234
	C567		L408	V325	V235
	F568	E492	T412	F326	
	A569	V493		L327	T243
	E570			G328	D249

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.48Å 168.48Å 97.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.93 – 3.30 44.93 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.93-3.30) 99.9 (44.93-3.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.220 , 0.268 0.219 , 0.271	Depositor DCC
$R_{free}$ test set	1054 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	115.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 91.3	EDS
Estimated twinning fraction	0.044 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 20505 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: LQZ

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	0.27	2/4721 (0.0%)	0.43	1/6368 (0.0%)
1	B	0.22	0/4721	0.40	0/6368
All	All	0.25	2/9442 (0.0%)	0.41	1/12736 (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	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ASN	C-N	6.13	1.48	1.34
1	A	182	LEU	C-N	-5.64	1.21	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ASN	O-C-N	-6.61	112.12	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASN	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	4631	0	4552	287	0
1	B	4631	0	4552	255	0
2	A	17	0	22	8	0
All	All	9279	0	9126	534	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 29.

The worst 5 of 534 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:B:179:LEU:HD22	1:B:180:PRO:HD3	1.37	1.03
1:A:77:VAL:HG23	1:A:78:ALA:H	1.34	0.91
1:B:348:ARG:HG3	1:B:482:VAL:HG12	1.54	0.90
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.54	0.88
1:A:276:LYS:HD2	1:A:277:GLU:H	1.37	0.88

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	580/585 (99%)	468 (81%)	86 (15%)	26 (4%)	3	21
1	B	580/585 (99%)	459 (79%)	94 (16%)	27 (5%)	3	20
All	All	1160/1170 (99%)	927 (80%)	180 (16%)	53 (5%)	3	21

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	60	GLU
1	A	66	LEU
1	A	89	ASP
1	A	97	GLU

### 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	509/511 (100%)	467 (92%)	42 (8%)	14	47
1	B	509/511 (100%)	471 (92%)	38 (8%)	17	52
All	All	1018/1022 (100%)	938 (92%)	80 (8%)	15	49

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	ARG
1	B	57	GLU
1	B	446	MET
1	A	512	ASP
1	A	536	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	522	GLN
1	B	61	ASN
1	B	464	HIS
1	A	535	HIS
1	B	18	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	LQZ	A	586	-	17,17,17	5.72	9 (52%)	22,22,22	1.46	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LQZ	A	586	-	-	0/12/12/12	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	586	LQZ	O-C	-2.27	1.18	1.23
2	A	586	LQZ	CAP-NAL	2.65	1.48	1.43
2	A	586	LQZ	C-NAL	4.77	1.47	1.35
2	A	586	LQZ	CAH-CAO	6.63	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	586	LQZ	CAG-CAN	7.26	1.56	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	586	LQZ	O-C-NAL	-2.39	119.45	123.72
2	A	586	LQZ	CAH-CAO-CAP	2.00	120.90	117.78
2	A	586	LQZ	CAN-CAP-NAL	2.16	122.21	118.99
2	A	586	LQZ	CA-C-NAL	3.86	122.32	114.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	586	LQZ	8	0

## 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	582/585 (99%)	-0.27	2 (0%)	94 94	75, 135, 213, 291	0
1	B	582/585 (99%)	-0.30	4 (0%)	89 86	78, 140, 213, 306	0
All	All	1164/1170 (99%)	-0.28	6 (0%)	91 90	75, 137, 213, 306	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	GLY	3.8
1	B	150	TYR	3.6
1	B	86	GLU	3.1
1	A	299	PRO	2.5
1	A	309	PHE	2.1

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LQZ	A	586	17/17	0.87	0.31	1.10	113,113,113,113	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.