



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 02:07 am BST

PDB ID : 3JQZ
Title : Crystal Structure of Human serum albumin complexed with Lidocaine
Authors : Hein, K.L.; Kragh-Hansen, U.; Morth, J.P.; Nissen, P.
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

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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

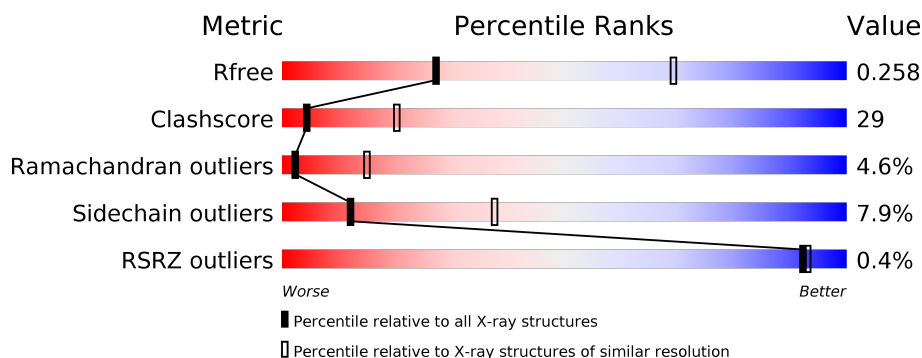
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 $\leq 5\%$. 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	<div> <div>45%</div> <div>46%</div> <div>7% ..</div> </div>
1	B	585	<div> <div>%</div> <div>48%</div> <div>43%</div> <div>7% .</div> </div>

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](#)

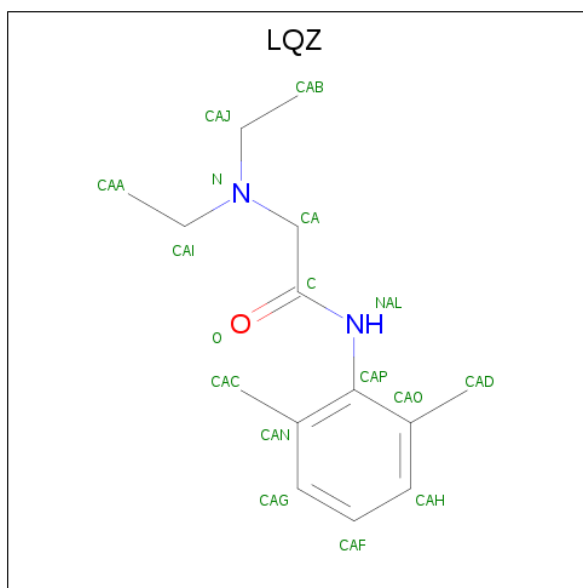
There are 2 unique types of molecules in this entry. The entry contains 9279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₁₄H₂₂N₂O).

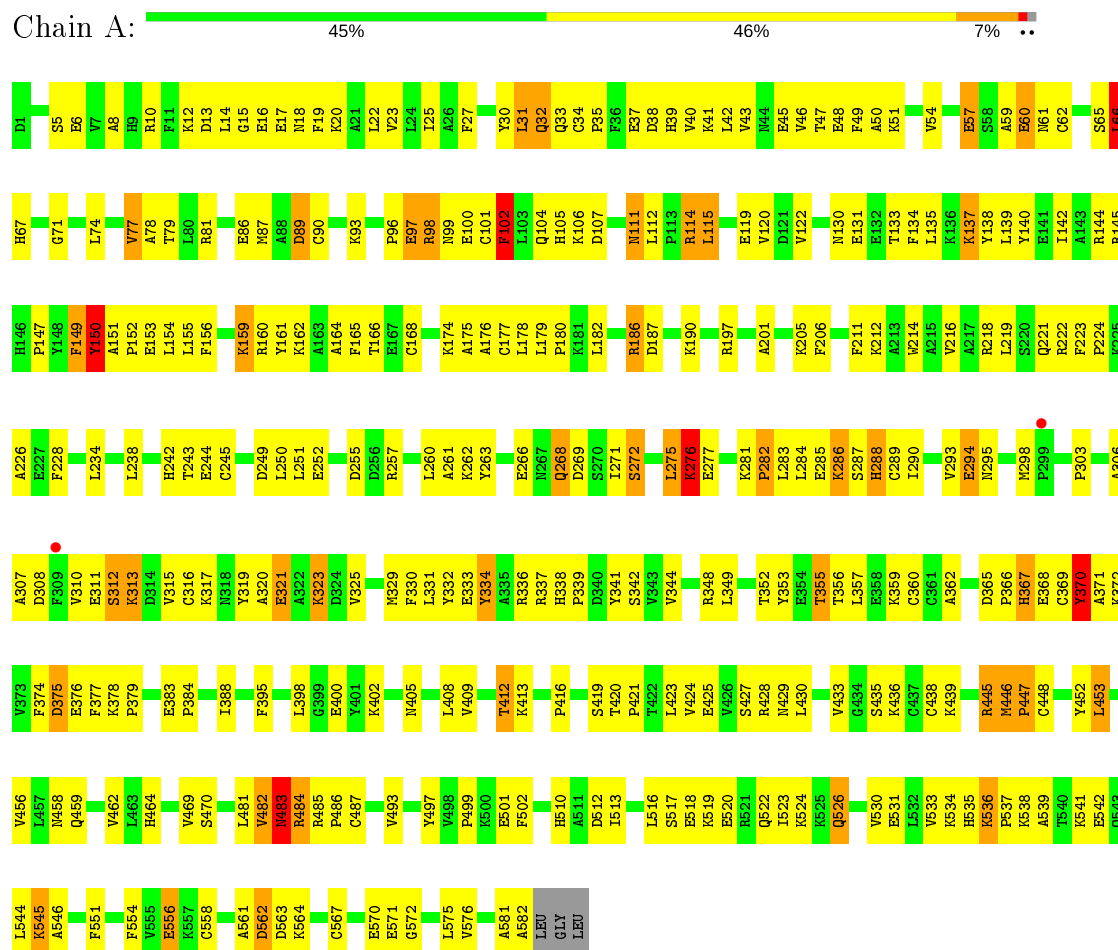


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	14	2	1		

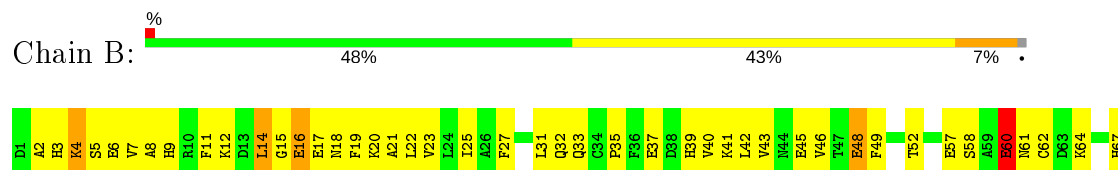
3 Residue-property plots

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



• Molecule 1: Serum albumin



E571	Y497	V415	K329	L250	R145	T68
K574	V498	P416	F330	L251	H146	L69
L575	P499	Q417	E333	E252	F149	F70
A581	E501	V418	E334	R257	Y150	G71
A582	F502	S419	A335	A258	A151	D72
LEU	U503	T420	R336	K262	P152	K73
GLY	A504	P421	R337	K266	E153	L74
LEU	F509	T422	R338	E267	L154	T75
	H510	L423	P339	N267	F155	V76
	H511	Q431	D340	E266	F156	V77
	D512	K432	Y341	N267	F157	A78
	I513	V433	S342	I271	A158	T79
	C514	G434	V345	S272	K159	L80
	T515	S435	V344	S273	R160	R81
	L516	K436	V348	K274	Y161	Y84
	S517	C437	R348	L275	K162	G85
	E518	K439	Y353	E277	A175	E86
	H519	K444	T356	P282	A176	M87
	H520	R445	L357	L283	C177	A88
	H521	N446	E358	K286	L178	K93
	Q522	P447	K359	S287	L179	Q94
	I523	A449	A364	H288	P180	E95
	K524	E450	D365	C289	K190	R98
	K525	D451	P366	I290	K195	M99
	Q526	Y452	R367	V293	E100	C101
	V530	L453	Y370	E294	F102	F102
	H535	V456	A371	I295	I103	L103
	K536	L457	K372	D296	Q104	Q104
	K537	N458	V373	E297	H105	H105
	K538	Q459	F374	M298	K106	K106
	A539	L460	D375	P299	D107	D107
	T540	C461	E376	L302	D108	D108
	Q543	V462	F377	L305	N111	N111
	V547	L463	K378	A306	R114	R114
	H548	H464	P379	E383	L115	L115
	F551	V469	E384	F309	V116	V116
	F554	S470	R385	V310	E119	E119
	V555	D471	R386	E311	V120	V120
	E556	R472	L387	S312	D121	D121
	K557	K475	I388	D314	V122	V122
	C558	S480	L398	V315	E131	E131
	A561	L481	G399	C316	L135	L135
	D562	V482	E400	K317	K136	K136
	D563	N483	Y401	R318	K137	K137
	K564	R484	R402	Y319	Y138	Y138
	E565	F403	Q404	K323	L139	L139
	T566	R485	Q404	D324	Y140	Y140
	C567	P486	L408	V325	E141	E141
	F568	E492	T412	F326	I142	I142
	A569	V493	L327	L327	A143	A143
	E570		G328	G328	R144	R144

4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	168.48 Å 168.48 Å 97.02 Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.32 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.268 0.213 , 0.258	Depositor DCC
R_{free} test set	1054 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	115.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9279	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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%)	2	15
1	B	580/585 (99%)	459 (79%)	94 (16%)	27 (5%)	2	14
All	All	1160/1170 (99%)	927 (80%)	180 (16%)	53 (5%)	2	15

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%)	11	36
1	B	509/511 (100%)	471 (92%)	38 (8%)	13	39
All	All	1018/1022 (100%)	938 (92%)	80 (8%)	12	37

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	5.98	9 (52%)	22,22,22	1.52	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	-	-	6/12/12/12	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	CAP-CAO	13.53	1.60	1.40
2	A	586	LQZ	CAP-CAN	10.56	1.56	1.40
2	A	586	LQZ	CAF-CAG	8.78	1.57	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	586	LQZ	CAF-CAH	8.71	1.57	1.38
2	A	586	LQZ	CAG-CAN	7.77	1.56	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	586	LQZ	CA-C-NAL	4.36	122.32	114.12
2	A	586	LQZ	O-C-NAL	-2.29	119.45	123.63
2	A	586	LQZ	CAH-CAO-CAP	2.11	120.90	117.77
2	A	586	LQZ	CAN-CAP-NAL	2.07	122.21	119.00

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	586	LQZ	CAN-CAP-NAL-C
2	A	586	LQZ	CAA-CAI-N-CAJ
2	A	586	LQZ	CAA-CAI-N-CA
2	A	586	LQZ	CAB-CAJ-N-CA
2	A	586	LQZ	CAB-CAJ-N-CAI

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, 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	582/585 (99%)	-0.29	2 (0%) 94 94	75, 135, 213, 291	0
1	B	582/585 (99%)	-0.31	3 (0%) 91 91	78, 140, 213, 306	0
All	All	1164/1170 (99%)	-0.30	5 (0%) 92 93	75, 137, 213, 306	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	GLY	3.7
1	B	150	TYR	3.4
1	B	86	GLU	3.1
1	A	299	PRO	2.4
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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
2	LQZ	A	586	17/17	0.87	0.31	113,113,113,113	0

6.5 Other polymers ⓘ

There are no such residues in this entry.