



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:14 PM UTC

PDB ID : 3JQZ / pdb_00003jqz
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

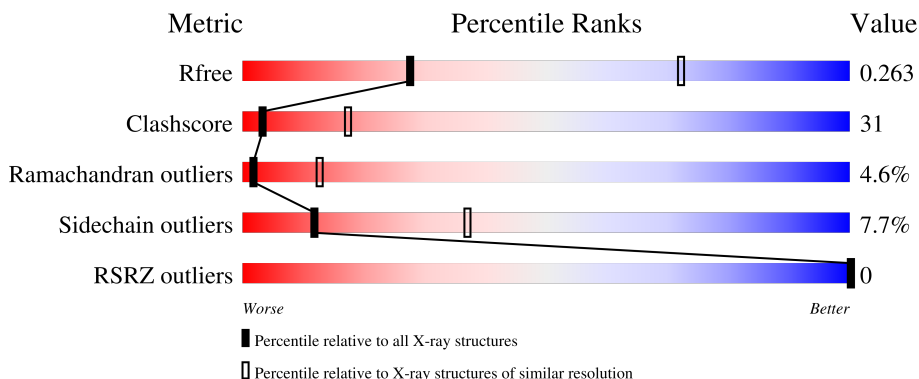
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

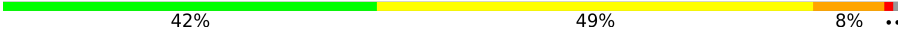
The reported resolution of this entry is 3.30 Å.

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 of 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	
1	B	585	

2 Entry composition [i](#)

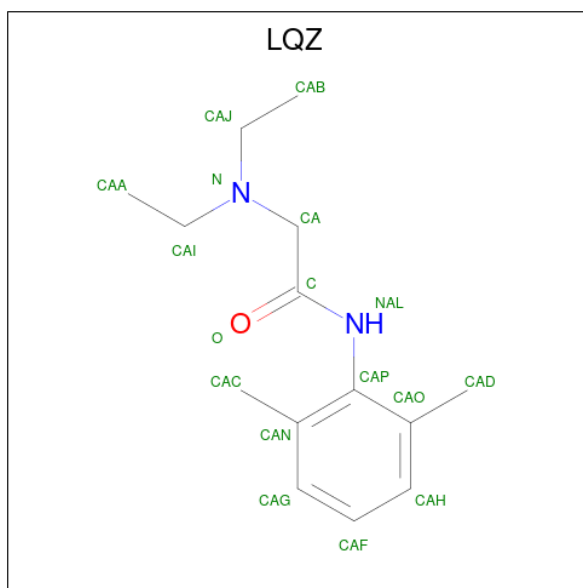
There are 2 unique types of molecules in this entry. The entry contains 9279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: LQZ) (formula: C₁₄H₂₂N₂O).

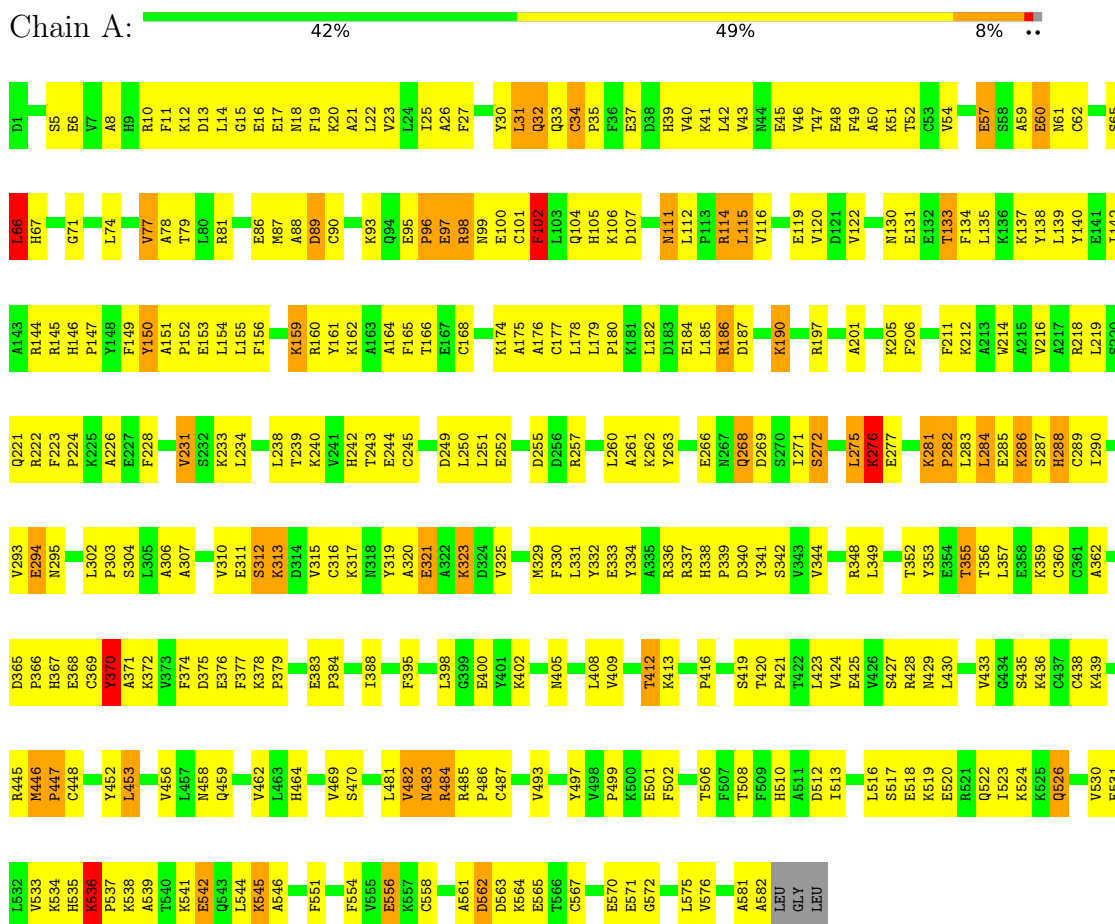


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	14	2	1		

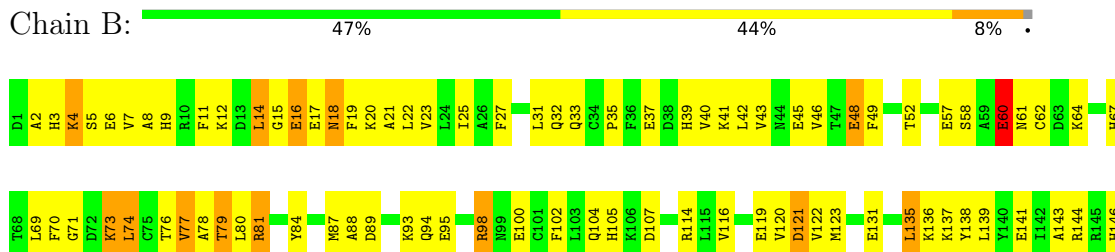
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



F149 Y150 A151 P152 E153 L154 L155 F156 F157 K158 R159 R160 Y161 K162 F165 A175 A176 C177 L178 L179 P180 K190 K195 K199 C200 A201 S202 L203 Q204 K205 F211 W214 A215 V216 A217 R218 R222 F223 P224 K225 A226 E227 F228 K233 L234 V235 T239 T243
D249 L250 L251 E252 R257 A258 K262 E266 N267 I271 S272 S273 K274 L275 K276 E277 P282 L283 K286 S287 H288 C289 I290 V293 E294 N295 D296 E297 W298 P299 L302 P303 S304 L305 A306 A307 D308 F309 V310 E311 S312 K313 D314 V315 C316 K317 W318 Y319 A320 E321 A322
K323 D324 V325 F326 L327 G328 M329 F330 E333 Y334 A335 R336 R337 H338 P339 D340 Y341 S342 V343 V344 R348 Y353 E354 T355 T356 L357 E358 K359 C360 C361 A362 A364 D365 P366 H367 Y370 A371 K372 V373 F374 D375 E376 F377 K378 P379 E383 P384 Q385 N386 L387 I388 L398 G399
E400 Y401 K402 F403 Q404 L408 T412 V415 P416 Q417 V418 S419 T420 P421 T422 L423 G431 K432 V433 G434 S435 K436 C437 C438 K439 K444 R445 M446 P447 C448 A449 E450 D451 Y452 L453 V456 L457 N458 Q459 L460 C461 V462 L463 H464 E465 V469 S470 D471 R472 K475 E479
S480 L481 V482 N483 R484 R485 P486 E492 V493 Y497 V498 P499 A500 E501 F502 N503 A504 F509 H510 A511 D512 I513 G514 T515 L516 S517 E518 K519 E520 R521 Q522 I523 K524 K525 Q526 V530 H535 K536 P537 K538 A539 T540 Q543 V547 N548 F551 F554 V555 E556 K557 C558
A561 D562 D563 K564 E565 T566 G567 F568 A569 E570 E571 K574 L575 A581 A582 LEU GLY LEU

4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.268 0.213 , 0.263	Depositor DCC
R_{free} test set	1054 reflections (5.13%)	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)	0.29 , 98.6	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	0.37	2/4721 (0.0%)	0.75	11/6368 (0.2%)
1	B	0.28	0/4721	0.73	4/6368 (0.1%)
All	All	0.33	2/9442 (0.0%)	0.74	15/12736 (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
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	11.11	1.48	1.32
1	A	182	LEU	C-N	-8.78	1.21	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	GLU	N-CA-C	-8.15	102.38	113.30
1	A	184	GLU	N-CA-C	-8.06	102.58	111.36
1	A	111	ASN	O-C-N	-7.95	112.12	122.61
1	B	565	GLU	N-CA-C	-7.04	104.84	113.50
1	B	18	ASN	N-CA-C	-6.09	105.89	113.38

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 [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	4631	0	4552	302	0
1	B	4631	0	4552	272	0
2	A	17	0	22	5	0
All	All	9279	0	9126	564	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 31.

The worst 5 of 564 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 [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	580/585 (99%)	468 (81%)	86 (15%)	26 (4%)	2	13
1	B	580/585 (99%)	459 (79%)	94 (16%)	27 (5%)	2	12
All	All	1160/1170 (99%)	927 (80%)	180 (16%)	53 (5%)	2	13

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%)	471 (92%)	38 (8%)	12	38
1	B	509/511 (100%)	469 (92%)	40 (8%)	11	36
All	All	1018/1022 (100%)	940 (92%)	78 (8%)	12	37

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	239	THR
1	B	479	GLU
1	B	276	LYS
1	B	388	ILE
1	B	547	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	HIS

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Mol	Chain	Res	Type
1	B	417	GLN
1	B	204	GLN
1	B	295	ASN
1	B	464	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	6.56	9 (52%)	22,22,22	1.55	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	14.19	1.60	1.40
2	A	586	LQZ	CAP-CAN	11.07	1.56	1.40
2	A	586	LQZ	CAF-CAG	10.82	1.57	1.38
2	A	586	LQZ	CAF-CAH	10.74	1.57	1.38
2	A	586	LQZ	CAG-CAN	8.25	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	4.37	122.32	114.23
2	A	586	LQZ	O-C-NAL	-2.34	119.45	123.64
2	A	586	LQZ	CAH-CAO-CAP	2.26	120.90	117.76
2	A	586	LQZ	CAN-CAP-NAL	2.16	122.21	118.99

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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	586	LQZ	5	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%)	-0.78	0 100 100	75, 135, 213, 291	0
1	B	582/585 (99%)	-0.78	0 100 100	78, 140, 213, 306	0
All	All	1164/1170 (99%)	-0.78	0 100 100	75, 137, 213, 306	0

There are no RSRZ outliers to report.

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 oligosaccharides 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(Å ²)	Q<0.9
2	LQZ	A	586	17/17	0.92	0.09	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.