



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:40 PM UTC

PDB ID : 1QLJ / pdb_00001qlj
Title : HORSE LIVER ALCOHOL DEHYDROGENASE APO ENZYME DOUBLE
MUTANT OF GLY 293 ALA AND PRO 295 THR
Authors : Ramaswamy, S.; Plapp, B.V.
Deposited on : 1999-09-01
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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

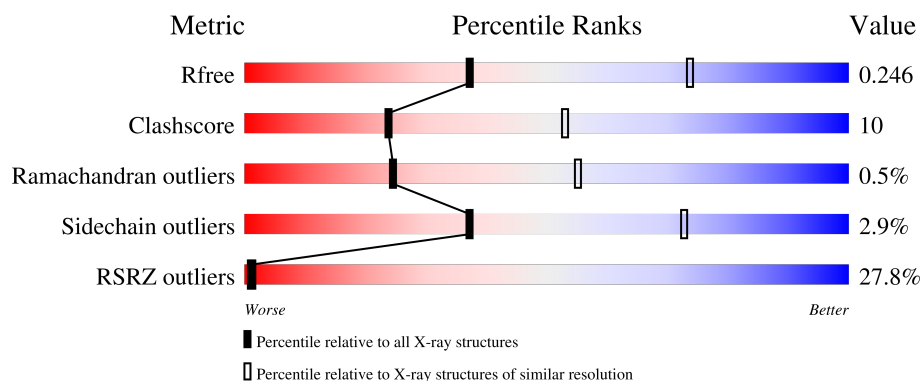
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	374	28% 75% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2874 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 ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	ALA	GLY	engineered mutation	UNP P00327
A	295	THR	PRO	engineered mutation	UNP P00327

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

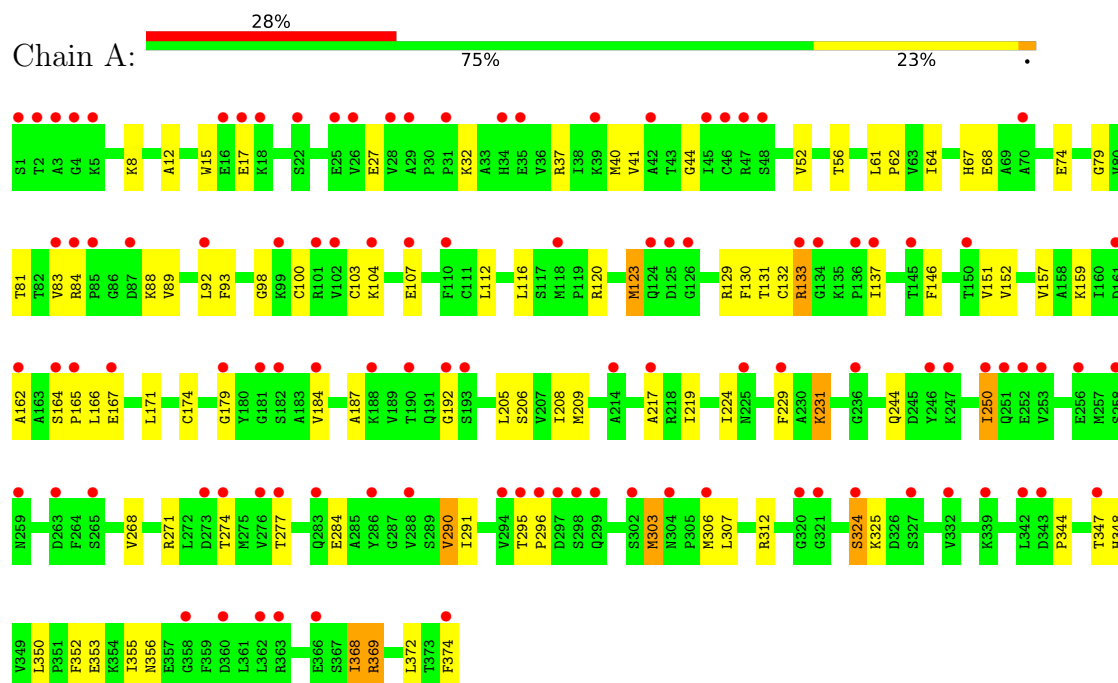
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		

3 Residue-property plots [i](#)

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: ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.14Å 72.92Å 180.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.80) 93.7 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.80Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.226 , 0.257 0.218 , 0.246	Depositor DCC
R_{free} test set	898 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.49	EDS
Total number of atoms	2874	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.1769e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN

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	0.47	0/2836	1.00	11/3834 (0.3%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	THR	CA-C-N	7.77	128.48	119.47
1	A	295	THR	C-N-CA	7.77	128.48	119.47
1	A	368	ILE	N-CA-C	-6.78	105.15	111.45
1	A	250	ILE	N-CA-C	6.37	117.12	110.62
1	A	123	MET	N-CA-C	-6.30	102.40	110.53
1	A	184	VAL	N-CA-C	6.06	116.22	110.53
1	A	284	GLU	N-CA-C	5.98	118.59	111.71
1	A	120	ARG	N-CA-C	-5.61	106.98	113.88
1	A	290	VAL	N-CA-C	5.38	115.70	108.17
1	A	229	PHE	N-CA-C	5.27	117.11	111.36
1	A	52	VAL	N-CA-C	-5.20	105.64	110.53

There are no chirality outliers.

There are no planarity outliers.

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	2785	0	2850	57	0
2	A	2	0	0	0	0
3	A	87	0	0	4	0
All	All	2874	0	2850	57	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 10.

All (57) 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:347:THR:HG21	1:A:368:ILE:H	1.31	0.93
1:A:347:THR:HG22	1:A:369:ARG:H	1.53	0.73
1:A:8:LYS:HD3	1:A:27:GLU:HG2	1.71	0.73
1:A:79:GLY:O	1:A:81:THR:HG23	1.92	0.70
1:A:123:MET:HA	1:A:123:MET:HE2	1.73	0.69
1:A:56:THR:HG22	1:A:296:PRO:HB2	1.78	0.65
1:A:347:THR:HG23	1:A:348:HIS:ND1	2.14	0.62
1:A:132:CYS:O	1:A:133:ARG:HB2	2.00	0.61
1:A:205:LEU:O	1:A:209:MET:HG3	2.02	0.59
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.84	0.59
1:A:12:ALA:HB3	1:A:146:PHE:HB3	1.87	0.57
1:A:291:ILE:HG23	3:A:2071:HOH:O	2.03	0.57
1:A:37:ARG:HD2	1:A:74:GLU:OE2	2.04	0.57
1:A:15:TRP:HA	1:A:62:PRO:HB3	1.88	0.55
1:A:100:CYS:O	1:A:104:LYS:HG3	2.06	0.55
1:A:167:GLU:H	1:A:167:GLU:CD	2.15	0.54
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.10	0.52
1:A:208:ILE:HG23	1:A:219:ILE:HG21	1.92	0.52
1:A:347:THR:CG2	1:A:369:ARG:H	2.21	0.51
1:A:32:LYS:HD2	1:A:129:ARG:NH2	2.25	0.51
1:A:83:VAL:HG12	1:A:159:LYS:HB2	1.93	0.50
1:A:130:PHE:HB3	1:A:137:ILE:HB	1.93	0.50
1:A:179:GLY:HA3	1:A:206:SER:HB2	1.92	0.50
1:A:192:GLY:HA2	1:A:217:ALA:HB2	1.95	0.48
1:A:231:LYS:HB2	3:A:2054:HOH:O	2.13	0.48
1:A:187:ALA:HB2	1:A:290:VAL:HG21	1.97	0.47
1:A:88:LYS:HE2	1:A:162:ALA:O	2.15	0.47
1:A:347:THR:HG21	1:A:368:ILE:N	2.14	0.47
1:A:64:ILE:HG13	1:A:137:ILE:HG21	1.97	0.46
1:A:352:PHE:HA	1:A:372:LEU:HB3	1.96	0.46
1:A:157:VAL:O	1:A:325:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:MET:SD	1:A:303:MET:C	3.00	0.45
1:A:84:ARG:HH11	1:A:84:ARG:HG2	1.82	0.45
1:A:307:LEU:O	1:A:312:ARG:HD2	2.17	0.44
1:A:350:LEU:O	1:A:372:LEU:HA	2.17	0.44
1:A:92:LEU:HD22	1:A:324:SER:HB2	1.98	0.44
1:A:98:GLY:HA2	1:A:103:CYS:HB3	1.99	0.44
1:A:40:MET:HB3	1:A:374:PHE:CE1	2.53	0.43
1:A:164:SER:HA	1:A:165:PRO:HD3	1.82	0.43
1:A:41:VAL:HG21	1:A:166:LEU:HD12	2.00	0.43
1:A:231:LYS:HE3	1:A:344:PRO:O	2.18	0.43
1:A:44:GLY:HA3	1:A:68:GLU:OE1	2.19	0.43
1:A:92:LEU:HA	3:A:2046:HOH:O	2.17	0.43
1:A:268:VAL:O	1:A:268:VAL:HG12	2.19	0.43
1:A:171:LEU:HD21	1:A:369:ARG:HG3	2.01	0.42
1:A:37:ARG:HG3	1:A:151:VAL:HG22	2.01	0.42
1:A:123:MET:HE1	1:A:152:VAL:HA	2.00	0.42
1:A:17:GLU:HG2	1:A:61:LEU:HD11	2.02	0.42
1:A:67:HIS:HB2	1:A:93:PHE:HB3	2.02	0.42
1:A:37:ARG:HD2	1:A:74:GLU:CD	2.45	0.41
1:A:103:CYS:HA	3:A:2027:HOH:O	2.19	0.41
1:A:61:LEU:HA	1:A:62:PRO:C	2.45	0.41
1:A:224:ILE:HG22	1:A:244:GLN:HG3	2.02	0.41
1:A:355:ILE:HG23	1:A:356:ASN:N	2.35	0.41
1:A:84:ARG:HG2	1:A:84:ARG:NH1	2.35	0.41
1:A:89:VAL:HG12	1:A:159:LYS:HA	2.02	0.40
1:A:250:ILE:CG2	1:A:277:THR:HG21	2.51	0.40

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	372/374 (100%)	352 (95%)	18 (5%)	2 (0%)	24 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	CYS
1	A	324	SER

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	308/308 (100%)	299 (97%)	9 (3%)	37 73

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	116	LEU
1	A	131	THR
1	A	133	ARG
1	A	231	LYS
1	A	303	MET
1	A	306	MET
1	A	353	GLU
1	A	369	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	225	ASN
1	A	300	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	374/374 (100%)	1.56	104 (27%) 1 1	9, 21, 35, 52	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	GLU	5.4
1	A	298	SER	4.9
1	A	101	ARG	4.7
1	A	34	HIS	4.6
1	A	259	ASN	4.5
1	A	339	LYS	3.9
1	A	1	SER	3.8
1	A	22	SER	3.8
1	A	133	ARG	3.7
1	A	297	ASP	3.7
1	A	47	ARG	3.7
1	A	274	THR	3.6
1	A	294	VAL	3.4
1	A	4	GLY	3.3
1	A	39	LYS	3.2
1	A	125	ASP	3.2
1	A	304	ASN	3.2
1	A	179	GLY	3.2
1	A	29	ALA	3.1
1	A	5	LYS	3.1
1	A	165	PRO	3.0
1	A	286	TYR	3.0
1	A	3	ALA	2.9
1	A	283	GLN	2.9
1	A	17	GLU	2.9
1	A	110	PHE	2.9
1	A	16	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	332	VAL	2.8
1	A	87	ASP	2.8
1	A	251	GLN	2.8
1	A	84	ARG	2.8
1	A	134	GLY	2.8
1	A	162	ALA	2.7
1	A	2	THR	2.7
1	A	277	THR	2.7
1	A	299	GLN	2.7
1	A	347	THR	2.6
1	A	28	VAL	2.6
1	A	118	MET	2.6
1	A	161	ASP	2.6
1	A	252	GLU	2.6
1	A	306	MET	2.6
1	A	360	ASP	2.5
1	A	296	PRO	2.5
1	A	48	SER	2.5
1	A	236	GLY	2.4
1	A	137	ILE	2.4
1	A	85	PRO	2.4
1	A	253	VAL	2.4
1	A	104	LYS	2.3
1	A	167	GLU	2.3
1	A	217	ALA	2.3
1	A	190	THR	2.3
1	A	83	VAL	2.3
1	A	273	ASP	2.3
1	A	42	ALA	2.3
1	A	18	LYS	2.3
1	A	102	VAL	2.3
1	A	265	SER	2.3
1	A	35	GLU	2.3
1	A	124	GLN	2.3
1	A	31	PRO	2.3
1	A	99	LYS	2.2
1	A	263	ASP	2.2
1	A	276	VAL	2.2
1	A	246	TYR	2.2
1	A	70	ALA	2.2
1	A	188	LYS	2.2
1	A	247	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	342	LEU	2.2
1	A	288	VAL	2.2
1	A	321	GLY	2.2
1	A	358	GLY	2.2
1	A	320	GLY	2.2
1	A	229	PHE	2.2
1	A	374	PHE	2.2
1	A	25	GLU	2.2
1	A	366	GLU	2.2
1	A	250	ILE	2.2
1	A	225	ASN	2.2
1	A	46	CYS	2.2
1	A	324	SER	2.2
1	A	184	VAL	2.1
1	A	193	SER	2.1
1	A	363	ARG	2.1
1	A	45	ILE	2.1
1	A	258	SER	2.1
1	A	302	SER	2.1
1	A	136	PRO	2.1
1	A	327	SER	2.1
1	A	192	GLY	2.1
1	A	145	THR	2.1
1	A	182	SER	2.0
1	A	26	VAL	2.0
1	A	150	THR	2.0
1	A	214	ALA	2.0
1	A	107	GLU	2.0
1	A	164	SER	2.0
1	A	92	LEU	2.0
1	A	362	LEU	2.0
1	A	126	GLY	2.0
1	A	181	GLY	2.0
1	A	295	THR	2.0
1	A	343	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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($\text{\AA}^2$)	Q<0.9
2	ZN	A	375	1/1	0.93	0.07	32,32,32,32	0
2	ZN	A	376	1/1	0.93	0.06	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.