



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:34 am BST

PDB ID : 2NX9  
Title : Crystal structure of the carboxyltransferase domain of the oxaloacetate decarboxylase Na<sup>+</sup> pump from *Vibrio cholerae*  
Authors : Studer, R.; Dimroth, P.  
Deposited on : 2006-11-17  
Resolution : 1.70 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](mailto: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.

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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
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

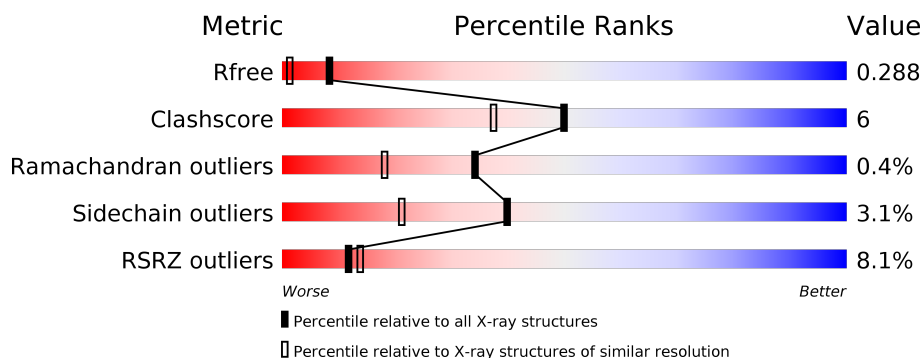
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	464	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	464	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7541 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 Oxaloacetate decarboxylase 2, subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	1	0
			3492	2202	608	661	21			
1	B	453	Total	C	N	O	S	0	1	0
			3508	2211	611	665	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	CLONING ARTIFACT	UNP Q6A1F6
A	458	GLU	-	CLONING ARTIFACT	UNP Q6A1F6
A	459	HIS	-	EXPRESSION TAG	UNP Q6A1F6
A	460	HIS	-	EXPRESSION TAG	UNP Q6A1F6
A	461	HIS	-	EXPRESSION TAG	UNP Q6A1F6
A	462	HIS	-	EXPRESSION TAG	UNP Q6A1F6
A	463	HIS	-	EXPRESSION TAG	UNP Q6A1F6
A	464	HIS	-	EXPRESSION TAG	UNP Q6A1F6
B	457	LEU	-	CLONING ARTIFACT	UNP Q6A1F6
B	458	GLU	-	CLONING ARTIFACT	UNP Q6A1F6
B	459	HIS	-	EXPRESSION TAG	UNP Q6A1F6
B	460	HIS	-	EXPRESSION TAG	UNP Q6A1F6
B	461	HIS	-	EXPRESSION TAG	UNP Q6A1F6
B	462	HIS	-	EXPRESSION TAG	UNP Q6A1F6
B	463	HIS	-	EXPRESSION TAG	UNP Q6A1F6
B	464	HIS	-	EXPRESSION TAG	UNP Q6A1F6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	315	Total 315	O 315	0	0
3	B	224	Total 224	O 224	0	0



- Molecule 1: Oxaloacetate decarboxylase 2, subunit alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.83Å 91.66Å 116.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 1.70 33.47 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.00-1.70) 98.5 (33.47-1.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.232 , 0.284 0.238 , 0.288	Depositor DCC
$R_{free}$ test set	5272 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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, 0.333 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	0.63	0/3551	0.79	0/4817
1	B	0.50	0/3567	0.67	0/4839
All	All	0.57	0/7118	0.73	0/9656

There are no bond length outliers.

There are no bond angle outliers.

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	3492	0	3533	45	0
1	B	3508	0	3548	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	315	0	0	0	0
3	B	224	0	0	0	0
All	All	7541	0	7081	82	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 6.

All (82) 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:316:ASN:HB2	1:B:317:ALA:HA	1.19	1.09
1:B:148:CYS:SG	1:B:178:LYS:NZ	2.41	0.94
1:A:246:THR:O	1:A:250:VAL:HG23	1.73	0.89
1:B:316:ASN:HB2	1:B:317:ALA:CA	2.03	0.88
1:B:394:ALA:H	1:B:395:GLY:HA2	1.43	0.84
1:A:425:GLN:HE21	1:A:425:GLN:HA	1.43	0.81
1:B:316:ASN:CB	1:B:317:ALA:HA	2.05	0.76
1:B:122:ALA:O	1:B:339:PRO:HG2	1.86	0.76
1:B:108:ARG:HD3	1:B:435:ASP:OD1	1.91	0.70
1:B:12:ASP:HB2	1:B:44:TYR:CE1	2.26	0.69
1:A:74:LYS:HE2	1:A:113:GLY:O	1.94	0.68
1:B:394:ALA:N	1:B:395:GLY:HA2	2.08	0.68
1:A:175:ILE:HD12	1:A:202:VAL:HG21	1.75	0.67
1:B:330:ARG:HB3	1:B:361:ARG:HH22	1.60	0.67
1:A:107:GLU:O	1:A:111:LYS:HG2	1.95	0.67
1:A:338:LEU:HD22	1:A:344:THR:CG2	2.25	0.66
1:B:175:ILE:HD12	1:B:202:VAL:HG21	1.79	0.65
1:A:148:CYS:SG	1:A:178:LYS:NZ	2.70	0.64
1:B:108:ARG:HD2	1:B:434:ILE:HG23	1.80	0.63
1:A:215:ALA:O	1:A:219:LEU:HD13	1.97	0.63
1:A:288:MET:CE	1:A:292:ASP:HB2	2.30	0.61
1:B:29:ILE:HD13	1:B:69:ARG:HG3	1.84	0.60
1:B:157:LEU:O	1:B:161:VAL:HG23	2.02	0.59
1:A:132:ALA:O	1:A:136:VAL:HG23	2.04	0.58
1:A:338:LEU:HD22	1:A:344:THR:HG23	1.86	0.57
1:A:288:MET:HG3	1:A:288:MET:O	2.06	0.56
1:B:97:TYR:OH	1:B:442:LEU:HA	2.06	0.55
1:A:200:VAL:HG12	1:A:202:VAL:HG22	1.88	0.55
1:A:15:LEU:O	1:A:19:HIS:HE1	1.90	0.55
1:B:328:ILE:HB	1:B:329:PRO:HD3	1.87	0.55
1:A:19:HIS:HD2	1:A:25:THR:HA	1.71	0.55
1:B:108:ARG:HD2	1:B:434:ILE:CG2	2.36	0.55
1:B:132:ALA:O	1:B:136:VAL:HG23	2.06	0.54
1:A:425:GLN:NE2	1:A:425:GLN:HA	2.19	0.54
1:A:288:MET:HE2	1:A:292:ASP:HB2	1.91	0.53
1:A:10:VAL:O	1:A:45:TRP:N	2.36	0.52
1:A:349:GLY:O	1:A:353:VAL:HG23	2.10	0.52
1:B:156:ASN:OD1	1:B:158:GLN:HG2	2.10	0.52
1:B:276:ASP:O	1:B:279:LYS:HB2	2.10	0.51
1:A:288:MET:HE1	1:A:292:ASP:HB2	1.93	0.51
1:A:336:GLY:O	1:A:381:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG13	1:A:35:ILE:O	2.11	0.51
1:A:87:ARG:CG	1:A:87:ARG:O	2.58	0.51
1:B:230:VAL:HG21	1:B:249:LEU:CD2	2.42	0.50
1:A:87:ARG:HG2	1:A:87:ARG:O	2.12	0.50
1:A:133:LEU:CD2	1:A:143:ALA:HB1	2.42	0.49
1:A:29:ILE:HD13	1:A:69:ARG:HG3	1.93	0.49
1:A:65:ASP:HB3	1:A:68:GLN:HB3	1.95	0.49
1:B:8:VAL:HG23	1:B:258:TYR:HB3	1.95	0.49
1:A:338:LEU:HD22	1:A:344:THR:HG21	1.94	0.48
1:A:133:LEU:HD23	1:A:143:ALA:HB1	1.96	0.48
1:B:163:VAL:HA	1:B:166:GLN:HE21	1.77	0.48
1:B:223:ILE:HA	1:B:227:VAL:HG12	1.96	0.47
1:A:219:LEU:HD22	1:A:244:PRO:HG2	1.97	0.47
1:B:223:ILE:HD13	1:B:253:LEU:HD11	1.96	0.47
1:B:393:LEU:HB3	1:B:396:ALA:H	1.80	0.46
1:A:11:THR:HA	1:A:46:SER:O	2.15	0.46
1:B:23:PHE:HB2	1:B:284:PHE:HB2	1.99	0.45
1:B:35:ILE:HD11	1:B:270:ILE:HA	1.97	0.45
1:B:386:THR:HA	1:B:387:GLU:HA	1.69	0.45
1:A:187:TYR:CD2	1:B:256:THR:HG21	2.52	0.45
1:A:296:LEU:HA	1:A:296:LEU:HD23	1.78	0.45
1:A:347:ILE:HG12	1:A:368:GLU:HB3	2.00	0.44
1:B:35:ILE:HD13	1:B:273:TYR:CG	2.53	0.44
1:B:387:GLU:HB2	1:B:390:ALA:HB3	1.98	0.44
1:A:311:GLN:HE22	1:A:350:THR:HA	1.83	0.44
1:A:37:GLN:O	1:A:41:GLN:HG2	2.18	0.42
1:A:137:LYS:HB3	1:A:137:LYS:HE3	1.83	0.42
1:A:18:ALA:O	1:A:22:LEU:HG	2.20	0.42
1:B:394:ALA:N	1:B:395:GLY:CA	2.80	0.42
1:A:18:ALA:O	1:A:22:LEU:HB2	2.20	0.42
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.87	0.42
1:B:258:TYR:O	1:B:259:ASP:C	2.59	0.42
1:A:223:ILE:HD13	1:A:253:LEU:HD11	2.01	0.41
1:A:23:PHE:HB2	1:A:284:PHE:HB2	2.02	0.41
1:A:308:MET:CE	1:A:328:ILE:HD11	2.50	0.41
1:B:219:LEU:HD22	1:B:244:PRO:HG2	2.02	0.41
1:A:308:MET:HE1	1:A:328:ILE:HD11	2.02	0.41
1:A:65:ASP:OD1	1:A:67:TRP:HB2	2.21	0.41
1:B:347:ILE:HG12	1:B:368:GLU:HB3	2.02	0.41
1:B:312:LEU:O	1:B:316:ASN:HA	2.21	0.41
1:B:197:LYS:HD2	1:B:197:LYS:HA	1.89	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	450/464 (97%)	431 (96%)	16 (4%)	3 (1%)	22	8
1	B	452/464 (97%)	435 (96%)	16 (4%)	1 (0%)	47	30
All	All	902/928 (97%)	866 (96%)	32 (4%)	4 (0%)	34	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ALA
1	B	394	ALA
1	A	259	ASP
1	A	316	ASN

### 5.3.2 Protein sidechains [i](#)

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	374/386 (97%)	362 (97%)	12 (3%)	39	20
1	B	376/386 (97%)	365 (97%)	11 (3%)	42	23
All	All	750/772 (97%)	727 (97%)	23 (3%)	40	21

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	50	TRP
1	A	70	LEU
1	A	151	THR
1	A	152	SER
1	A	202	VAL
1	A	227	VAL
1	A	288	MET
1	A	338	LEU
1	A	386	THR
1	A	425	GLN
1	A	454	ARG
1	B	2	THR
1	B	25	THR
1	B	30	ASP
1	B	50	TRP
1	B	134	GLN
1	B	138	LYS
1	B	158	GLN
1	B	288	MET
1	B	338	LEU
1	B	391	ARG
1	B	397	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	130	GLN
1	A	134	GLN
1	A	307	ASN
1	A	311	GLN
1	A	425	GLN
1	B	19	HIS
1	B	166	GLN
1	B	314	GLN
1	B	346	GLN

### 5.3.3 RNA ⓘ

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](#)

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, 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	451/464 (97%)	0.44	20 (4%) 34 38	3, 16, 37, 57	0
1	B	453/464 (97%)	0.78	53 (11%) 4 5	5, 19, 39, 49	0
All	All	904/928 (97%)	0.61	73 (8%) 12 14	3, 17, 38, 57	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	ALA	11.3
1	B	362	TYR	6.8
1	B	420	GLN	6.2
1	A	318	LEU	6.1
1	A	317	ALA	5.4
1	B	323	LEU	5.4
1	B	386	THR	5.2
1	A	358	LEU	4.9
1	B	390	ALA	4.9
1	B	387	GLU	4.8
1	B	357	VAL	4.7
1	B	356	VAL	4.5
1	B	365	ILE	4.4
1	A	312	LEU	4.0
1	B	358	LEU	3.8
1	B	419	LEU	3.8
1	A	414	LEU	3.6
1	A	316	ASN	3.5
1	B	367	LYS	3.5
1	A	357	VAL	3.5
1	B	388	LEU	3.4
1	A	364	THR	3.4
1	B	394	ALA	3.4
1	B	158	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	392	VAL	3.3
1	B	318	LEU	3.3
1	B	424	GLU	3.3
1	B	414	LEU	3.2
1	B	423	LYS	3.0
1	B	354	ILE	2.9
1	A	323	LEU	2.9
1	A	341	VAL	2.9
1	B	94	TYR	2.9
1	B	416	ASP	2.8
1	A	320	LYS	2.8
1	B	413	THR	2.8
1	B	317	ALA	2.8
1	B	417	ARG	2.8
1	B	364	THR	2.7
1	B	361	ARG	2.7
1	B	401	CYS	2.7
1	B	230	VAL	2.6
1	A	428	THR	2.6
1	B	393	LEU	2.6
1	B	407	ILE	2.5
1	B	2	THR	2.4
1	B	377	TYR	2.3
1	B	312	LEU	2.3
1	B	409	ALA	2.3
1	B	451	LEU	2.3
1	B	426	HIS	2.3
1	B	335	LEU	2.3
1	B	76	ALA	2.3
1	B	430	ALA	2.2
1	A	342	THR	2.2
1	B	85	LEU	2.2
1	A	322	ASP	2.2
1	B	363	LYS	2.2
1	B	170	LEU	2.1
1	A	354	ILE	2.1
1	B	360	GLU	2.1
1	B	119	VAL	2.1
1	B	324	VAL	2.1
1	B	316	ASN	2.1
1	B	418	VAL	2.1
1	B	148	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	395	GLY	2.0
1	B	395	GLY	2.0
1	A	392	VAL	2.0
1	A	393	LEU	2.0
1	B	342	THR	2.0
1	B	383	PRO	2.0
1	A	315	GLN	2.0

## 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	602	1/1	0.98	0.07	36,36,36,36	0
2	ZN	A	601	1/1	0.99	0.04	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.