



wwPDB X-ray Structure Validation Summary Report

Feb 5, 2024 – 10:16 PM EST

PDB ID : 1YEW
Title : Crystal structure of particulate methane monooxygenase
Authors : Lieberman, R.L.; Rosenzweig, A.C.
Deposited on : 2004-12-28
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

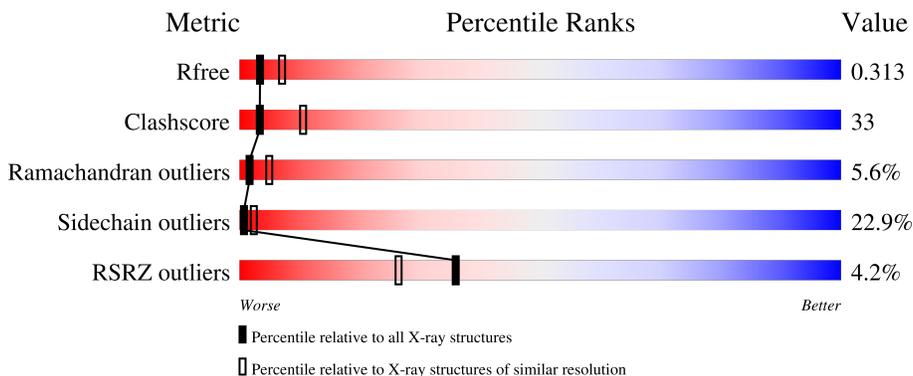
1 Overall quality at a glance

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.



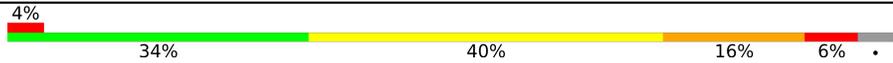
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	382	 2% 56% 31% 12% .
1	E	382	 3% 56% 30% 13% .
1	I	382	 3% 54% 34% 12% .
2	B	247	 5% 36% 37% 16% 7% .
2	F	247	 4% 34% 38% 19% 6% .

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Mol	Chain	Length	Quality of chain
2	J	247	
3	C	289	
3	G	289	
3	K	289	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 19772 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 particulate methane monooxygenase, B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	3018	1938	513	552	15	0	0	0
1	E	382	3018	1938	513	552	15	0	0	0
1	I	382	3018	1938	513	552	15	0	0	0

- Molecule 2 is a protein called particulate methane monooxygenase, A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	238	1955	1317	311	316	11	0	0	0
2	F	238	1955	1317	311	316	11	0	0	0
2	J	238	1955	1317	311	316	11	0	0	0

- Molecule 3 is a protein called particulate methane monooxygenase subunit C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	188	1612	1101	244	264	3	0	0	0
3	G	188	1612	1101	244	264	3	0	0	0
3	K	188	1612	1101	244	264	3	0	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

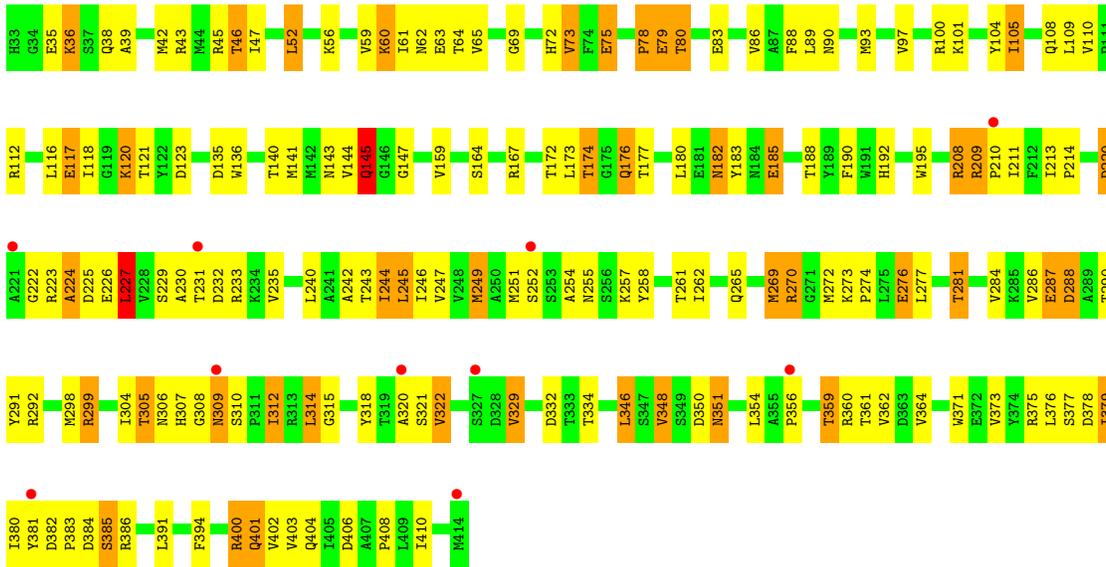
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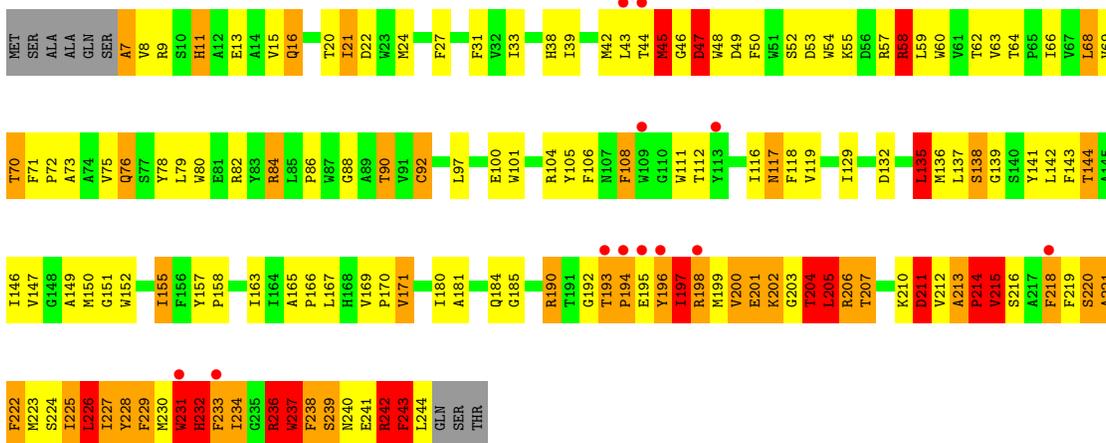
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Cu	0	0
			2	2		



- Molecule 1: particulate methane monooxygenase, B subunit



- Molecule 2: particulate methane monooxygenase, A subunit



- Molecule 2: particulate methane monooxygenase, A subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	264.14Å 264.14Å 150.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.80 29.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.55-2.80) 91.2 (29.46-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.80Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.272 , 0.302 0.296 , 0.313	Depositor DCC
R_{free} test set	5932 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , -7.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	19772	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CU, CUA, 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	0.98	4/3100 (0.1%)	0.98	7/4215 (0.2%)
1	E	0.98	3/3100 (0.1%)	0.97	2/4215 (0.0%)
1	I	0.92	2/3100 (0.1%)	0.93	3/4215 (0.1%)
2	B	1.16	10/2031 (0.5%)	1.09	9/2780 (0.3%)
2	F	1.07	7/2031 (0.3%)	1.06	13/2780 (0.5%)
2	J	1.12	7/2031 (0.3%)	1.08	9/2780 (0.3%)
3	C	0.89	1/1680 (0.1%)	0.92	4/2302 (0.2%)
3	G	0.80	1/1680 (0.1%)	0.87	3/2302 (0.1%)
3	K	0.86	1/1680 (0.1%)	0.89	4/2302 (0.2%)
All	All	0.99	36/20433 (0.2%)	0.98	54/27891 (0.2%)

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	3
1	E	0	4
1	I	0	4
2	B	0	11
2	F	0	9
2	J	0	10
3	C	0	3
3	G	0	3
3	K	0	3
All	All	0	50

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	241	GLU	CG-CD	9.72	1.66	1.51
2	B	241	GLU	CG-CD	9.53	1.66	1.51
2	F	241	GLU	CG-CD	8.57	1.64	1.51
2	B	242	ARG	CB-CG	7.37	1.72	1.52
1	I	117	GLU	CG-CD	7.27	1.62	1.51

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	47	ASP	N-CA-C	8.38	133.62	111.00
2	J	47	ASP	N-CA-C	8.32	133.48	111.00
2	B	47	ASP	N-CA-C	7.97	132.53	111.00
2	F	135	LEU	CA-CB-CG	7.36	132.23	115.30
3	G	51	LEU	CA-CB-CG	6.82	130.98	115.30

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	VAL	Peptide
1	A	79	GLU	Peptide
1	A	80	THR	Peptide
2	B	46	GLY	Peptide
2	B	7	ALA	Peptide

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	3018	0	2980	142	1
1	E	3018	0	2980	138	1
1	I	3018	0	2980	148	0
2	B	1955	0	1916	207	2
2	F	1955	0	1916	209	0
2	J	1955	0	1916	218	0
3	C	1612	0	1541	135	0
3	G	1612	0	1541	137	0
3	K	1612	0	1541	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	E	3	0	0	0	0
5	G	1	0	0	0	0
5	K	1	0	0	0	0
6	A	2	0	0	0	0
6	E	2	0	0	0	0
6	I	2	0	0	0	0
All	All	19772	0	19311	1278	3

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 33.

The worst 5 of 1278 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)
2:B:70:THR:CG2	2:B:227:ILE:HD11	1.47	1.42
2:J:70:THR:CG2	2:J:227:ILE:HD11	1.54	1.34
2:B:70:THR:HG22	2:B:227:ILE:CD1	1.57	1.33
2:F:195:GLU:HG2	3:G:160:HIS:CE1	1.65	1.30
2:F:70:THR:CG2	2:F:227:ILE:HD11	1.61	1.29

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:HIS:CE1	2:B:11:HIS:NE2[7_556]	2.03	0.17
2:B:11:HIS:NE2	2:B:11:HIS:NE2[7_556]	2.14	0.06
1:A:60:LYS:NZ	1:E:338:GLU:OE2[4_455]	2.17	0.03

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	380/382 (100%)	334 (88%)	34 (9%)	12 (3%)	4	13
1	E	380/382 (100%)	336 (88%)	33 (9%)	11 (3%)	4	15
1	I	380/382 (100%)	327 (86%)	42 (11%)	11 (3%)	4	15
2	B	236/247 (96%)	173 (73%)	42 (18%)	21 (9%)	1	1
2	F	236/247 (96%)	168 (71%)	44 (19%)	24 (10%)	0	1
2	J	236/247 (96%)	166 (70%)	48 (20%)	22 (9%)	0	1
3	C	184/289 (64%)	147 (80%)	25 (14%)	12 (6%)	1	3
3	G	184/289 (64%)	146 (79%)	27 (15%)	11 (6%)	1	4
3	K	184/289 (64%)	145 (79%)	28 (15%)	11 (6%)	1	4
All	All	2400/2754 (87%)	1942 (81%)	323 (14%)	135 (6%)	2	5

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	220	ASP
1	A	224	ALA
1	A	225	ASP
1	A	288	ASP

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	323/323 (100%)	256 (79%)	67 (21%)	1	3
1	E	323/323 (100%)	251 (78%)	72 (22%)	1	2
1	I	323/323 (100%)	257 (80%)	66 (20%)	1	4
2	B	203/210 (97%)	157 (77%)	46 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	203/210 (97%)	155 (76%)	48 (24%)	1	2
2	J	203/210 (97%)	156 (77%)	47 (23%)	1	2
3	C	161/237 (68%)	118 (73%)	43 (27%)	0	1
3	G	161/237 (68%)	119 (74%)	42 (26%)	0	1
3	K	161/237 (68%)	120 (74%)	41 (26%)	0	1
All	All	2061/2310 (89%)	1589 (77%)	472 (23%)	1	2

5 of 472 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	21	ILE
3	K	118	ASN
3	G	113	LYS
3	K	103	THR
2	J	116	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	62	ASN
1	I	309	ASN
1	I	143	ASN
1	I	192	HIS
1	I	401	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
6	CUA	I	600	1	0,1,1	-	-	-		
6	CUA	A	3	1	0,1,1	-	-	-		
6	CUA	E	500	1	0,1,1	-	-	-		

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 [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	382/382 (100%)	-0.09	8 (2%) 63 54	65, 70, 73, 76	0
1	E	382/382 (100%)	-0.02	10 (2%) 56 46	66, 70, 73, 76	0
1	I	382/382 (100%)	-0.09	10 (2%) 56 46	66, 70, 73, 76	0
2	B	238/247 (96%)	0.26	12 (5%) 28 19	66, 70, 74, 78	0
2	F	238/247 (96%)	0.20	9 (3%) 40 30	66, 70, 74, 78	0
2	J	238/247 (96%)	0.15	10 (4%) 36 26	66, 70, 74, 78	0
3	C	188/289 (65%)	0.15	10 (5%) 26 17	67, 70, 72, 73	0
3	G	188/289 (65%)	0.35	15 (7%) 12 6	67, 70, 72, 73	0
3	K	188/289 (65%)	0.23	17 (9%) 9 5	67, 70, 72, 73	0
All	All	2424/2754 (88%)	0.08	101 (4%) 36 26	65, 70, 73, 78	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	194	PRO	11.8
2	B	194	PRO	8.1
2	J	194	PRO	7.2
2	J	237	TRP	5.0
3	C	117	ARG	5.0

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 monosaccharides 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
6	CUA	A	3	2/2	0.88	0.14	74,74,74,82	0
5	ZN	E	702	1/1	0.91	0.22	213,213,213,213	0
6	CUA	E	500	2/2	0.91	0.06	75,75,75,82	0
5	ZN	E	701	1/1	0.92	0.11	55,55,55,55	1
5	ZN	C	661	1/1	0.95	0.04	73,73,73,73	0
5	ZN	C	700	1/1	0.95	0.04	46,46,46,46	1
6	CUA	I	600	2/2	0.96	0.09	76,76,76,82	0
5	ZN	E	900	1/1	0.97	0.05	76,76,76,76	0
5	ZN	A	800	1/1	0.98	0.03	77,77,77,77	0
4	CU	A	4	1/1	0.98	0.04	61,61,61,61	0
4	CU	E	501	1/1	0.98	0.06	61,61,61,61	0
4	CU	I	601	1/1	0.99	0.04	61,61,61,61	0
5	ZN	G	662	1/1	0.99	0.13	46,46,46,46	0
5	ZN	K	663	1/1	0.99	0.02	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.