



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 11:10 pm BST

PDB ID : 3DTZ
Title : Crystal structure of Putative Chlorite dismutase TA0507
Authors : Chang, C.; Xu, X.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-07-16
Resolution : 1.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

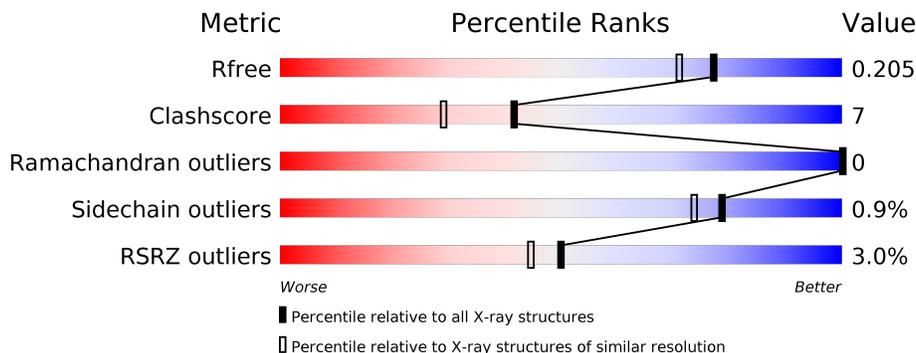
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 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	244	 7% 71% 16% 12%
1	B	244	 78% 12% 9%
1	C	244	 2% 81% 7% 12%
1	D	244	 2% 81% 11% 9%
1	E	244	 2% 80% 11% 9%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10178 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 Putative Chlorite dismutase TA0507.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	215	Total 1823	C 1172	N 305	O 338	Se 8	0	9	0
1	B	221	Total 1843	C 1187	N 306	O 342	Se 8	0	7	0
1	C	215	Total 1784	C 1150	N 299	O 327	Se 8	0	6	0
1	D	223	Total 1857	C 1198	N 309	O 341	Se 9	0	9	0
1	E	223	Total 1830	C 1179	N 302	O 340	Se 9	0	4	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP Q9HKT8
A	-18	GLY	-	expression tag	UNP Q9HKT8
A	-17	SER	-	expression tag	UNP Q9HKT8
A	-16	SER	-	expression tag	UNP Q9HKT8
A	-15	HIS	-	expression tag	UNP Q9HKT8
A	-14	HIS	-	expression tag	UNP Q9HKT8
A	-13	HIS	-	expression tag	UNP Q9HKT8
A	-12	HIS	-	expression tag	UNP Q9HKT8
A	-11	HIS	-	expression tag	UNP Q9HKT8
A	-10	HIS	-	expression tag	UNP Q9HKT8
A	-9	SER	-	expression tag	UNP Q9HKT8
A	-8	SER	-	expression tag	UNP Q9HKT8
A	-7	GLY	-	expression tag	UNP Q9HKT8
A	-6	LEU	-	expression tag	UNP Q9HKT8
A	-5	VAL	-	expression tag	UNP Q9HKT8
A	-4	PRO	-	expression tag	UNP Q9HKT8
A	-3	ARG	-	expression tag	UNP Q9HKT8
A	-2	GLY	-	expression tag	UNP Q9HKT8
A	-1	SER	-	expression tag	UNP Q9HKT8

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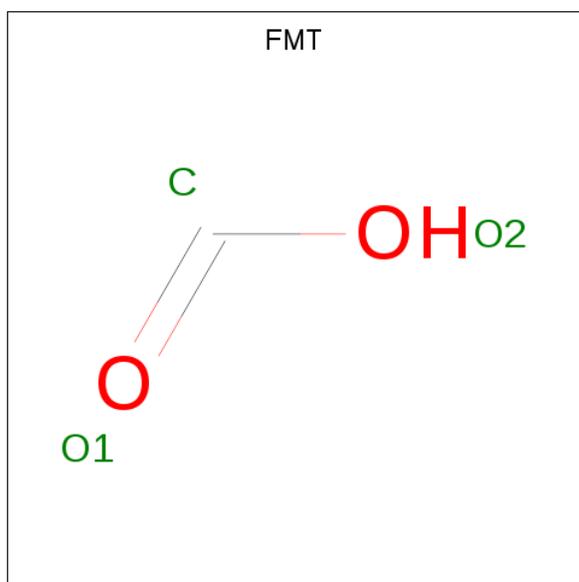
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q9HKT8
B	-19	MSE	-	expression tag	UNP Q9HKT8
B	-18	GLY	-	expression tag	UNP Q9HKT8
B	-17	SER	-	expression tag	UNP Q9HKT8
B	-16	SER	-	expression tag	UNP Q9HKT8
B	-15	HIS	-	expression tag	UNP Q9HKT8
B	-14	HIS	-	expression tag	UNP Q9HKT8
B	-13	HIS	-	expression tag	UNP Q9HKT8
B	-12	HIS	-	expression tag	UNP Q9HKT8
B	-11	HIS	-	expression tag	UNP Q9HKT8
B	-10	HIS	-	expression tag	UNP Q9HKT8
B	-9	SER	-	expression tag	UNP Q9HKT8
B	-8	SER	-	expression tag	UNP Q9HKT8
B	-7	GLY	-	expression tag	UNP Q9HKT8
B	-6	LEU	-	expression tag	UNP Q9HKT8
B	-5	VAL	-	expression tag	UNP Q9HKT8
B	-4	PRO	-	expression tag	UNP Q9HKT8
B	-3	ARG	-	expression tag	UNP Q9HKT8
B	-2	GLY	-	expression tag	UNP Q9HKT8
B	-1	SER	-	expression tag	UNP Q9HKT8
B	0	HIS	-	expression tag	UNP Q9HKT8
C	-19	MSE	-	expression tag	UNP Q9HKT8
C	-18	GLY	-	expression tag	UNP Q9HKT8
C	-17	SER	-	expression tag	UNP Q9HKT8
C	-16	SER	-	expression tag	UNP Q9HKT8
C	-15	HIS	-	expression tag	UNP Q9HKT8
C	-14	HIS	-	expression tag	UNP Q9HKT8
C	-13	HIS	-	expression tag	UNP Q9HKT8
C	-12	HIS	-	expression tag	UNP Q9HKT8
C	-11	HIS	-	expression tag	UNP Q9HKT8
C	-10	HIS	-	expression tag	UNP Q9HKT8
C	-9	SER	-	expression tag	UNP Q9HKT8
C	-8	SER	-	expression tag	UNP Q9HKT8
C	-7	GLY	-	expression tag	UNP Q9HKT8
C	-6	LEU	-	expression tag	UNP Q9HKT8
C	-5	VAL	-	expression tag	UNP Q9HKT8
C	-4	PRO	-	expression tag	UNP Q9HKT8
C	-3	ARG	-	expression tag	UNP Q9HKT8
C	-2	GLY	-	expression tag	UNP Q9HKT8
C	-1	SER	-	expression tag	UNP Q9HKT8
C	0	HIS	-	expression tag	UNP Q9HKT8
D	-19	MSE	-	expression tag	UNP Q9HKT8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	GLY	-	expression tag	UNP Q9HKT8
D	-17	SER	-	expression tag	UNP Q9HKT8
D	-16	SER	-	expression tag	UNP Q9HKT8
D	-15	HIS	-	expression tag	UNP Q9HKT8
D	-14	HIS	-	expression tag	UNP Q9HKT8
D	-13	HIS	-	expression tag	UNP Q9HKT8
D	-12	HIS	-	expression tag	UNP Q9HKT8
D	-11	HIS	-	expression tag	UNP Q9HKT8
D	-10	HIS	-	expression tag	UNP Q9HKT8
D	-9	SER	-	expression tag	UNP Q9HKT8
D	-8	SER	-	expression tag	UNP Q9HKT8
D	-7	GLY	-	expression tag	UNP Q9HKT8
D	-6	LEU	-	expression tag	UNP Q9HKT8
D	-5	VAL	-	expression tag	UNP Q9HKT8
D	-4	PRO	-	expression tag	UNP Q9HKT8
D	-3	ARG	-	expression tag	UNP Q9HKT8
D	-2	GLY	-	expression tag	UNP Q9HKT8
D	-1	SER	-	expression tag	UNP Q9HKT8
D	0	HIS	-	expression tag	UNP Q9HKT8
E	-19	MSE	-	expression tag	UNP Q9HKT8
E	-18	GLY	-	expression tag	UNP Q9HKT8
E	-17	SER	-	expression tag	UNP Q9HKT8
E	-16	SER	-	expression tag	UNP Q9HKT8
E	-15	HIS	-	expression tag	UNP Q9HKT8
E	-14	HIS	-	expression tag	UNP Q9HKT8
E	-13	HIS	-	expression tag	UNP Q9HKT8
E	-12	HIS	-	expression tag	UNP Q9HKT8
E	-11	HIS	-	expression tag	UNP Q9HKT8
E	-10	HIS	-	expression tag	UNP Q9HKT8
E	-9	SER	-	expression tag	UNP Q9HKT8
E	-8	SER	-	expression tag	UNP Q9HKT8
E	-7	GLY	-	expression tag	UNP Q9HKT8
E	-6	LEU	-	expression tag	UNP Q9HKT8
E	-5	VAL	-	expression tag	UNP Q9HKT8
E	-4	PRO	-	expression tag	UNP Q9HKT8
E	-3	ARG	-	expression tag	UNP Q9HKT8
E	-2	GLY	-	expression tag	UNP Q9HKT8
E	-1	SER	-	expression tag	UNP Q9HKT8
E	0	HIS	-	expression tag	UNP Q9HKT8

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



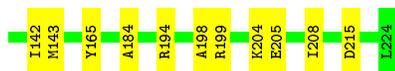
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 3 1 2	0	0
2	B	1	Total C O 3 1 2	0	0
2	C	1	Total C O 3 1 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	208	Total O 208 208	0	0
3	B	238	Total O 238 238	0	0
3	C	188	Total O 188 188	0	0
3	D	208	Total O 208 208	0	0
3	E	190	Total O 190 190	0	0



● Molecule 1: Putative Chlorite dismutase TA0507



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.40Å 135.73Å 74.15Å 90.00° 110.33° 90.00°	Depositor
Resolution (Å)	50.00 – 1.81 43.79 – 1.81	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-1.81) 98.7 (43.79-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.167 , 0.206 0.167 , 0.205	Depositor DCC
R_{free} test set	5538 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10178	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: FMT

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	0/1868	0.64	0/2513
1	B	0.68	0/1903	0.69	0/2564
1	C	0.69	0/1836	0.73	2/2474 (0.1%)
1	D	0.68	0/1923	0.71	1/2591 (0.0%)
1	E	0.64	0/1881	0.63	0/2538
All	All	0.66	0/9411	0.68	3/12680 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	212	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	182	ASP	CB-CG-OD1	5.43	123.19	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1823	0	1785	31	0
1	B	1843	0	1820	36	0
1	C	1784	0	1751	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1857	0	1842	25	0
1	E	1830	0	1783	26	0
2	A	3	0	1	0	0
2	B	3	0	1	1	0
2	C	3	0	1	0	0
3	A	208	0	0	1	0
3	B	238	0	0	10	0
3	C	188	0	0	5	0
3	D	208	0	0	1	0
3	E	190	0	0	8	0
All	All	10178	0	8984	126	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 7.

The worst 5 of 126 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:D:104[A]:MSE:CE	1:D:106[A]:LYS:HE2	1.13	1.55
1:D:104[A]:MSE:CE	1:D:106[A]:LYS:CE	2.05	1.33
1:B:30:MSE:HE3	1:B:34:ILE:HD12	1.31	1.12
1:D:104[A]:MSE:HE2	1:D:106[A]:LYS:HE2	1.16	1.08
1:D:104[A]:MSE:HE1	1:D:106[A]:LYS:HE2	1.31	1.08

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	220/244 (90%)	218 (99%)	2 (1%)	0	100	100
1	B	224/244 (92%)	222 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	217/244 (89%)	214 (99%)	3 (1%)	0	100	100
1	D	230/244 (94%)	230 (100%)	0	0	100	100
1	E	225/244 (92%)	223 (99%)	2 (1%)	0	100	100
All	All	1116/1220 (92%)	1107 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	197/208 (95%)	193 (98%)	4 (2%)	55	43
1	B	202/208 (97%)	200 (99%)	2 (1%)	76	70
1	C	192/208 (92%)	190 (99%)	2 (1%)	76	70
1	D	203/208 (98%)	202 (100%)	1 (0%)	88	87
1	E	197/208 (95%)	197 (100%)	0	100	100
All	All	991/1040 (95%)	982 (99%)	9 (1%)	78	74

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	LYS
1	D	79	GLN
1	C	145	GLU
1	A	130	ASP
1	B	30	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	144	HIS
1	C	146	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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	FMT	B	301	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	A	301	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C	301	-	0,2,2	0.00	-	0,1,1	0.00	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	FMT	1	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	207/244 (84%)	0.06	17 (8%) 11 9	14, 21, 40, 52	0
1	B	213/244 (87%)	-0.41	1 (0%) 91 89	12, 18, 28, 36	0
1	C	208/244 (85%)	-0.13	5 (2%) 59 54	12, 18, 31, 36	0
1	D	215/244 (88%)	-0.09	4 (1%) 66 63	9, 18, 34, 39	0
1	E	215/244 (88%)	-0.09	5 (2%) 60 56	15, 21, 33, 47	0
All	All	1058/1220 (86%)	-0.13	32 (3%) 50 44	9, 19, 33, 52	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	103	ALA	6.2
1	A	137	ASP	5.9
1	A	136	PHE	5.5
1	A	144	HIS	5.4
1	A	103	ALA	5.2

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(Å ²)	Q<0.9
2	FMT	A	301	3/3	0.71	0.25	65,65,65,65	0
2	FMT	C	301	3/3	0.81	0.23	39,39,40,40	0
2	FMT	B	301	3/3	0.92	0.20	32,32,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.