Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 09:16 PM EDT

PDB ID	:	6ZN4
Title	:	MaeB malic enzyme domain apoprotein
Authors	:	Lovering, A.L.; Harding, C.J.
Deposited on	:	2020-07-06
Resolution	:	1.68 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 (i) 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 (1)) were used in the production of this report:

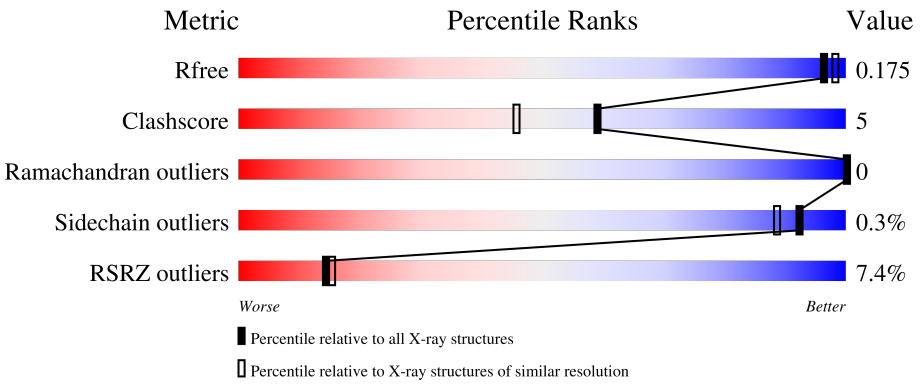
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 <=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	445	7%, 83%, 8%, 9%
1	B	445	7%, 82%, 10%, 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6800 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 NADP-dependent malate dehydrogenase,Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	406	3053	1933	525	578	17	0	1	0
1	B	408	3065	1941	527	580	17	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q6MM14
A	-9	GLY	-	expression tag	UNP Q6MM14
A	-8	SER	-	expression tag	UNP Q6MM14
A	-7	SER	-	expression tag	UNP Q6MM14
A	-6	HIS	-	expression tag	UNP Q6MM14
A	-5	HIS	-	expression tag	UNP Q6MM14
A	-4	HIS	-	expression tag	UNP Q6MM14
A	-3	HIS	-	expression tag	UNP Q6MM14
A	-2	HIS	-	expression tag	UNP Q6MM14
A	-1	HIS	-	expression tag	UNP Q6MM14
A	0	SER	-	expression tag	UNP Q6MM14
A	121	ASP	-	linker	UNP Q6MM14
A	122	ILE	-	linker	UNP Q6MM14
A	123	GLU	-	linker	UNP Q6MM14
A	124	VAL	-	linker	UNP Q6MM14
B	-10	MET	-	initiating methionine	UNP Q6MM14
B	-9	GLY	-	expression tag	UNP Q6MM14
B	-8	SER	-	expression tag	UNP Q6MM14
B	-7	SER	-	expression tag	UNP Q6MM14
B	-6	HIS	-	expression tag	UNP Q6MM14
B	-5	HIS	-	expression tag	UNP Q6MM14
B	-4	HIS	-	expression tag	UNP Q6MM14
B	-3	HIS	-	expression tag	UNP Q6MM14
B	-2	HIS	-	expression tag	UNP Q6MM14

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	expression tag	UNP Q6MM14
B	0	SER	-	expression tag	UNP Q6MM14
B	121	ASP	-	linker	UNP Q6MM14
B	122	ILE	-	linker	UNP Q6MM14
B	123	GLU	-	linker	UNP Q6MM14
B	124	VAL	-	linker	UNP Q6MM14

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

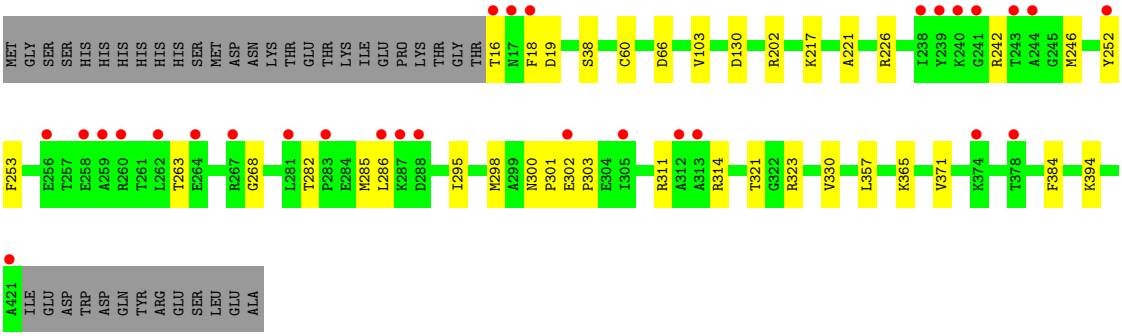
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	291	Total O 291 291	0	0
3	B	389	Total O 389 389	0	0

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.

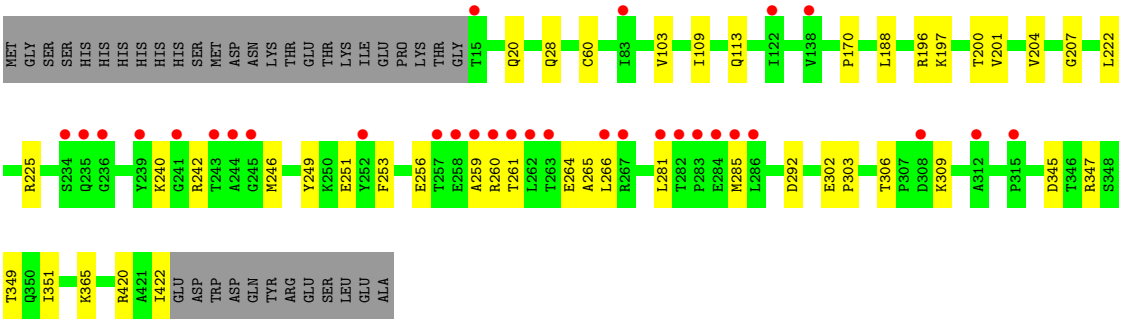
• Molecule 1: NADP-dependent malate dehydrogenase,Malate dehydrogenase

Chain A:



• Molecule 1: NADP-dependent malate dehydrogenase,Malate dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.03Å 92.65Å 96.96Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	48.02 – 1.68 43.36 – 1.66	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.02-1.68) 97.7 (43.36-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.66Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.170 , 0.204 0.175 , 0.175	Depositor DCC
R_{free} test set	4862 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.014 for -h,-l,-k 0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6800	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG

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	0/3110	0.50	0/4211
1	B	0.39	0/3119	0.56	0/4223
All	All	0.38	0/6229	0.53	0/8434

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 (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	3053	0	3099	24	0
1	B	3065	0	3112	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	291	0	0	3	1
3	B	389	0	0	19	1
All	All	6800	0	6211	58	1

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 5.

All (58) 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:265:ALA:O	3:B:901:HOH:O	1.77	0.99
1:A:130:ASP:OD2	3:A:901:HOH:O	1.88	0.92
1:B:420:ARG:NH1	3:B:906:HOH:O	2.07	0.79
1:B:207:GLY:O	3:B:903:HOH:O	2.02	0.78
1:B:196:ARG:NH2	1:B:292:ASP:O	2.17	0.77
1:B:281:LEU:O	3:B:904:HOH:O	2.03	0.75
1:A:286:LEU:HD21	1:A:295:ILE:HD11	1.67	0.74
1:B:200:THR:OG1	3:B:905:HOH:O	2.04	0.74
1:A:282:THR:H	1:A:285:MET:HE3	1.54	0.72
1:B:249:TYR:OH	3:B:908:HOH:O	2.09	0.70
1:B:253:PHE:O	3:B:907:HOH:O	2.08	0.69
1:B:201:VAL:O	3:B:909:HOH:O	2.09	0.69
1:A:301:PRO:O	1:A:323:ARG:NH1	2.26	0.67
1:B:261:THR:HG23	1:B:264:GLU:H	1.58	0.67
1:A:226:ARG:NH2	1:A:252:TYR:O	2.28	0.64
1:A:66:ASP:HB3	3:A:1116:HOH:O	1.99	0.62
1:B:285:MET:O	3:B:910:HOH:O	2.16	0.61
1:B:246:MET:HE2	1:B:251:GLU:HG2	1.82	0.60
1:B:225:ARG:HH11	1:B:225:ARG:HG3	1.67	0.58
1:A:394:LYS:NZ	3:A:908:HOH:O	2.38	0.57
1:B:306:THR:OG1	1:B:309:LYS:HG3	2.07	0.54
1:A:221:ALA:HB1	1:A:357:LEU:HD11	1.90	0.53
1:B:259:ALA:O	1:B:260:ARG:HD2	2.09	0.52
1:B:242:ARG:O	1:B:246:MET:HG3	2.10	0.51
1:B:28:GLN:NE2	3:B:917:HOH:O	2.30	0.51
1:A:298:MET:HE1	1:A:330:VAL:HG21	1.92	0.50
1:B:113:GLN:NE2	3:B:923:HOH:O	2.34	0.50
1:B:264:GLU:O	3:B:911:HOH:O	2.19	0.49
1:B:170:PRO:HB3	1:B:351:ILE:HG13	1.93	0.49
1:B:240:LYS:HE2	3:B:935:HOH:O	2.12	0.49
1:B:28:GLN:OE1	3:B:912:HOH:O	2.19	0.48
1:A:16:THR:HG22	1:A:19:ASP:H	1.78	0.47
1:B:246:MET:CE	1:B:251:GLU:HG2	2.45	0.47
1:B:197:LYS:N	1:B:197:LYS:HD2	2.30	0.46
1:B:256:GLU:N	3:B:935:HOH:O	2.48	0.46
1:A:302:GLU:HA	1:A:303:PRO:HD3	1.84	0.46
1:B:188:LEU:HD11	1:B:222:LEU:HD22	1.98	0.46
1:A:103:VAL:HG23	1:B:60:CYS:SG	2.56	0.46
1:B:20:GLN:NE2	3:B:902:HOH:O	2.02	0.45
1:A:38:SER:HB2	1:B:109:ILE:HD12	1.98	0.45
1:A:286:LEU:HD22	1:A:314:ARG:HG3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:HG22	1:A:18:PHE:H	1.82	0.44
1:A:371:VAL:HG21	1:A:384:PHE:HB2	1.99	0.44
1:A:217:LYS:HG3	1:A:253:PHE:HZ	1.81	0.44
1:A:242:ARG:O	1:A:246:MET:HG3	2.18	0.44
1:B:302:GLU:HA	1:B:303:PRO:HD3	1.91	0.44
1:A:60:CYS:SG	1:B:103:VAL:HG23	2.58	0.43
1:A:16:THR:HG22	1:A:18:PHE:N	2.33	0.43
1:A:300:ASN:HA	1:A:301:PRO:C	2.39	0.43
1:B:349:THR:OG1	3:B:913:HOH:O	2.21	0.43
1:B:365:LYS:HE3	1:B:365:LYS:HB3	1.79	0.43
1:B:204:VAL:HG21	1:B:266:LEU:HD12	2.02	0.42
1:A:202:ARG:HH21	1:A:268:GLY:C	2.23	0.42
1:B:347:ARG:NH1	3:B:925:HOH:O	2.38	0.42
1:A:263:THR:HA	1:A:285:MET:HG2	2.02	0.42
1:B:259:ALA:HB2	3:B:911:HOH:O	2.20	0.41
1:B:345:ASP:HB3	1:B:422:ILE:HD11	2.03	0.41
1:A:311:ARG:HA	1:A:314:ARG:O	2.21	0.40

All (1) 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)
3:A:1013:HOH:O	3:B:1153:HOH:O[1_655]	2.15	0.05

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	405/445 (91%)	393 (97%)	12 (3%)	0	100	100
1	B	406/445 (91%)	390 (96%)	16 (4%)	0	100	100
All	All	811/890 (91%)	783 (96%)	28 (4%)	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	319/354 (90%)	317 (99%)	2 (1%)	86	79
1	B	320/354 (90%)	320 (100%)	0	100	100
All	All	639/708 (90%)	637 (100%)	2 (0%)	92	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	THR
1	A	365	LYS

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

Mol	Chain	Res	Type
1	B	228	ASN
1	B	235	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 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 (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	406/445 (91%)	0.33	29 (7%)	16	17	14, 35, 70, 83	0
1	B	408/445 (91%)	0.31	31 (7%)	13	15	12, 28, 72, 90	0
All	All	814/890 (91%)	0.32	60 (7%)	14	15	12, 31, 71, 90	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	ALA	6.0
1	B	262	LEU	5.5
1	B	282	THR	5.4
1	B	261	THR	5.1
1	B	234	SER	5.1
1	B	283	PRO	5.1
1	A	252	TYR	4.8
1	A	239	TYR	4.7
1	A	17	ASN	4.5
1	A	241	GLY	4.5
1	B	286	LEU	4.2
1	B	266	LEU	3.9
1	B	243	THR	3.8
1	B	235	GLN	3.8
1	A	18	PHE	3.7
1	B	239	TYR	3.7
1	A	286	LEU	3.6
1	B	312	ALA	3.5
1	A	283	PRO	3.4
1	A	240	LYS	3.3
1	B	236	GLY	3.2
1	A	421	ALA	3.1
1	A	244	ALA	3.0
1	B	315	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	241	GLY	3.0
1	B	245	GLY	3.0
1	A	259	ALA	2.9
1	B	15	THR	2.9
1	B	122	ILE	2.9
1	B	281	LEU	2.9
1	A	16	THR	2.9
1	B	285	MET	2.8
1	B	263	THR	2.8
1	A	287	LYS	2.8
1	A	258	GLU	2.7
1	B	252	TYR	2.7
1	A	267	ARG	2.6
1	A	264	GLU	2.5
1	B	244	ALA	2.5
1	A	243	THR	2.5
1	A	312	ALA	2.4
1	A	262	LEU	2.4
1	A	281	LEU	2.4
1	A	305	ILE	2.4
1	B	260	ARG	2.3
1	B	83	ILE	2.3
1	B	284	GLU	2.3
1	A	378	THR	2.3
1	B	267	ARG	2.3
1	B	258	GLU	2.2
1	A	238	ILE	2.2
1	A	313	ALA	2.1
1	B	257	THR	2.1
1	A	260	ARG	2.1
1	A	374	LYS	2.1
1	A	256	GLU	2.0
1	B	308	ASP	2.0
1	A	302	GLU	2.0
1	B	138	VAL	2.0
1	A	288	ASP	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 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
2	MG	A	801	1/1	0.98	0.03	27,27,27,27	0
2	MG	B	801	1/1	0.99	0.04	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.