



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 07:39 am GMT

PDB ID : 2CBG
Title : Crystal structure of the PMSF-inhibited thioesterase domain of the fengycin biosynthesis cluster
Authors : Samel, S.; Marahiel, M.A.; Essen, L.-O.
Deposited on : 2006-01-03
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.4, 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

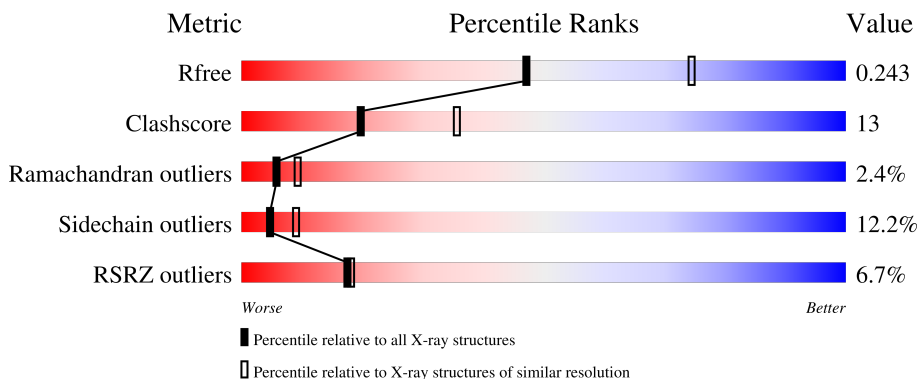
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	244	

2 Entry composition [i](#)

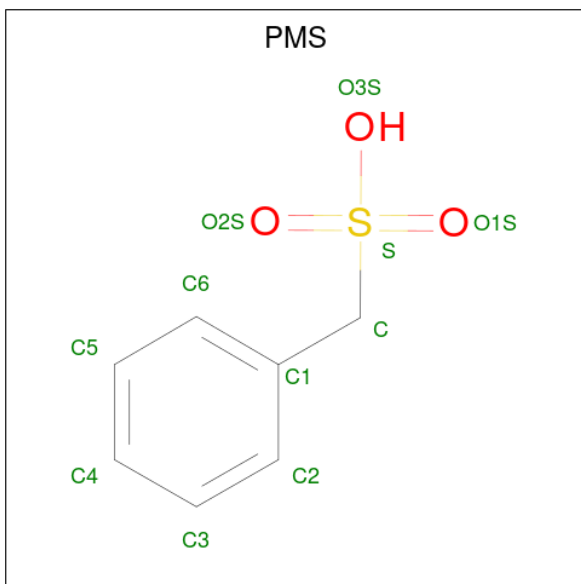
There are 3 unique types of molecules in this entry. The entry contains 1750 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FENGYCIN SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	1665	1063	275	321	6	0	0	0

- Molecule 2 is phenylmethanesulfonic acid (three-letter code: PMS) (formula: C₇H₈O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	10	7	2	1	0	0

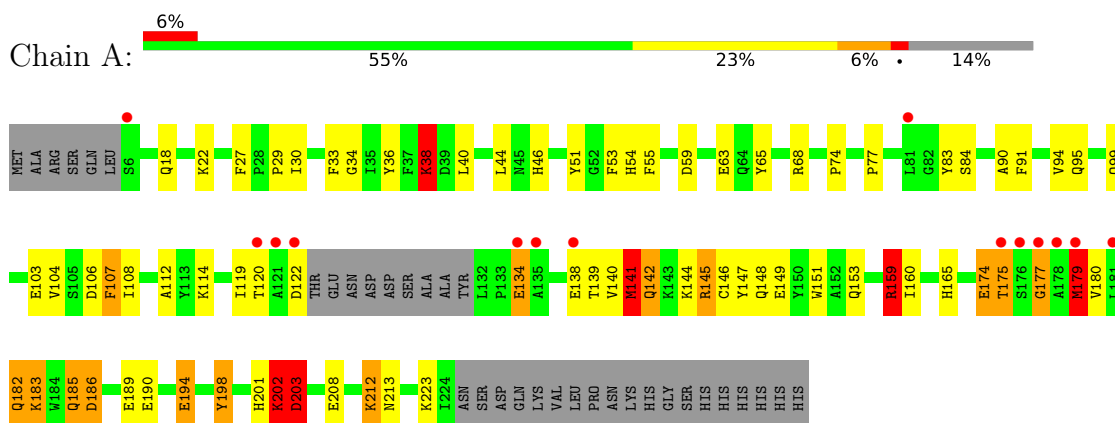
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	75	75	75	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: FENGYCIN SYNTHETASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	72.35Å 72.35Å 96.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.00 – 2.50 24.02 – 2.49	Depositor EDS
% Data completeness (in resolution range)	92.2 (24.00-2.50) 91.8 (24.02-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.50Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.162 , 0.237 0.170 , 0.243	Depositor DCC
R_{free} test set	489 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtrriage
Anisotropy	0.216	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.082 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1750	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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: PMS

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	1.88	33/1698 (1.9%)	1.34	10/2290 (0.4%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	LYS	CE-NZ	14.42	1.85	1.49
1	A	63	GLU	CD-OE1	9.32	1.35	1.25
1	A	212	LYS	CE-NZ	8.36	1.70	1.49
1	A	149	GLU	CD-OE1	6.96	1.33	1.25
1	A	179	MET	SD-CE	6.95	2.16	1.77
1	A	65	TYR	CE2-CZ	6.95	1.47	1.38
1	A	149	GLU	CD-OE2	6.85	1.33	1.25
1	A	91	PHE	CE1-CZ	6.76	1.50	1.37
1	A	99	GLN	CG-CD	6.67	1.66	1.51
1	A	141	MET	SD-CE	6.31	2.13	1.77
1	A	63	GLU	CG-CD	6.25	1.61	1.51
1	A	55	PHE	CG-CD1	6.25	1.48	1.38
1	A	91	PHE	CG-CD2	6.25	1.48	1.38
1	A	27	PHE	CG-CD2	6.22	1.48	1.38
1	A	53	PHE	CE2-CZ	6.21	1.49	1.37
1	A	27	PHE	CE2-CZ	6.16	1.49	1.37
1	A	142	GLN	CB-CG	-6.07	1.36	1.52
1	A	55	PHE	CE1-CZ	6.01	1.48	1.37
1	A	38	LYS	CG-CD	5.79	1.72	1.52
1	A	194	GLU	CD-OE2	5.77	1.31	1.25
1	A	107	PHE	CE2-CZ	5.76	1.48	1.37
1	A	108	ILE	CA-CB	5.55	1.67	1.54
1	A	189	GLU	CD-OE2	5.54	1.31	1.25
1	A	212	LYS	CD-CE	5.51	1.65	1.51
1	A	33	PHE	CG-CD1	5.49	1.47	1.38
1	A	63	GLU	CD-OE2	5.42	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	LYS	CD-CE	5.27	1.64	1.51
1	A	145	ARG	NE-CZ	5.25	1.39	1.33
1	A	51	TYR	CG-CD2	5.21	1.46	1.39
1	A	186	ASP	CB-CG	5.16	1.62	1.51
1	A	107	PHE	CD1-CE1	5.13	1.49	1.39
1	A	134	GLU	CG-CD	5.10	1.59	1.51
1	A	198	TYR	CE2-CZ	5.05	1.45	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	A	159	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	A	183	LYS	CD-CE-NZ	9.23	132.93	111.70
1	A	145	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	A	203	ASP	CB-CA-C	-6.14	98.12	110.40
1	A	186	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	177	GLY	N-CA-C	5.24	126.20	113.10
1	A	122	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	159	ARG	CD-NE-CZ	5.04	130.65	123.60
1	A	59	ASP	CB-CG-OD1	-5.01	113.79	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	1665	0	1614	42	0
2	A	10	0	7	2	0
3	A	75	0	0	10	0
All	All	1750	0	1621	42	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 13.

All (42) 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:212:LYS:CE	1:A:212:LYS:NZ	1.70	1.53
1:A:183:LYS:CE	1:A:183:LYS:NZ	1.85	1.38
1:A:141:MET:CE	1:A:141:MET:SD	2.13	1.36
1:A:179:MET:CE	1:A:179:MET:SD	2.16	1.33
1:A:34:GLY:H	1:A:54:HIS:HD2	1.15	0.92
1:A:185:GLN:HG3	3:A:2059:HOH:O	1.76	0.85
1:A:74:PRO:HD2	3:A:2027:HOH:O	1.79	0.82
1:A:34:GLY:H	1:A:54:HIS:CD2	2.02	0.76
1:A:144:LYS:O	1:A:148:GLN:HG3	1.87	0.74
1:A:139:THR:O	1:A:142:GLN:HG2	1.90	0.71
1:A:142:GLN:O	1:A:146:CYS:HB2	1.91	0.70
1:A:34:GLY:N	1:A:54:HIS:HD2	1.89	0.68
1:A:141:MET:CE	1:A:141:MET:HA	2.23	0.68
1:A:202:LYS:HG3	1:A:203:ASP:OD1	1.94	0.67
1:A:106:ASP:OD1	1:A:165:HIS:HE1	1.81	0.63
1:A:140:VAL:HG12	1:A:141:MET:HE2	1.80	0.62
1:A:151:TRP:CE2	2:A:1225:PMS:H4	2.39	0.58
1:A:185:GLN:CG	3:A:2059:HOH:O	2.45	0.57
1:A:198:TYR:H	1:A:213:ASN:HD21	1.52	0.57
1:A:151:TRP:CD2	2:A:1225:PMS:H4	2.41	0.56
1:A:38:LYS:O	1:A:38:LYS:HD3	2.07	0.55
1:A:179:MET:O	1:A:182:GLN:HB2	2.08	0.53
1:A:29:PRO:HG3	1:A:83:TYR:HD2	1.75	0.52
1:A:179:MET:O	1:A:182:GLN:N	2.35	0.52
1:A:183:LYS:HE3	3:A:2056:HOH:O	2.08	0.52
1:A:77:PRO:HA	1:A:103:GLU:O	2.11	0.51
1:A:68:ARG:HD2	3:A:2026:HOH:O	2.10	0.51
1:A:159:ARG:HD3	1:A:186:ASP:O	2.12	0.48
1:A:36:TYR:OH	3:A:2014:HOH:O	2.17	0.48
1:A:40:LEU:HD11	1:A:44:LEU:HD11	1.94	0.48
1:A:90:ALA:HB3	1:A:107:PHE:CE1	2.51	0.46
1:A:94:VAL:HG13	1:A:104:VAL:HG21	1.98	0.46
1:A:186:ASP:HA	3:A:2061:HOH:O	2.16	0.45
1:A:84:SER:O	1:A:112:ALA:HB2	2.18	0.43
1:A:175:THR:HG22	3:A:2058:HOH:O	2.18	0.43
1:A:18:GLN:HG3	1:A:46:HIS:CE1	2.53	0.43
1:A:95:GLN:HG3	1:A:160:ILE:HG22	2.00	0.42
1:A:30:ILE:HG23	1:A:144:LYS:HE3	2.01	0.42
1:A:114:LYS:O	1:A:182:GLN:HG3	2.19	0.42
1:A:180:VAL:CG2	3:A:2058:HOH:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HG3	1:A:83:TYR:CD2	2.54	0.40
1:A:180:VAL:HG21	3:A:2058:HOH:O	2.21	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	206/244 (84%)	192 (93%)	9 (4%)	5 (2%)	6 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	GLU
1	A	175	THR
1	A	177	GLY
1	A	201	HIS
1	A	202	LYS

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	172/202 (85%)	151 (88%)	21 (12%)	5 9

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	38	LYS
1	A	119	ILE
1	A	120	THR
1	A	134	GLU
1	A	138	GLU
1	A	141	MET
1	A	145	ARG
1	A	147	TYR
1	A	153	GLN
1	A	159	ARG
1	A	174	GLU
1	A	179	MET
1	A	182	GLN
1	A	185	GLN
1	A	190	GLU
1	A	194	GLU
1	A	202	LYS
1	A	203	ASP
1	A	208	GLU
1	A	223	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	153	GLN
1	A	165	HIS
1	A	182	GLN
1	A	213	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PMS	A	1225	1	7,10,11	1.54	2 (28%)	11,12,15	1.51	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PMS	A	1225	1	-	1/4/4/5	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1225	PMS	C5-C6	2.48	1.44	1.38
2	A	1225	PMS	C3-C2	2.19	1.43	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1225	PMS	O2S-S-C	3.39	111.06	105.56
2	A	1225	PMS	C6-C1-C2	2.13	121.51	118.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1225	PMS	C1-C-S-O1S

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1225	PMS	2	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	210/244 (86%)	0.02	14 (6%) 17 18	21, 31, 76, 89	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	ASP	5.8
1	A	178	ALA	5.6
1	A	177	GLY	5.0
1	A	181	LEU	4.9
1	A	121	ALA	4.7
1	A	176	SER	4.1
1	A	138	GLU	3.4
1	A	134	GLU	3.3
1	A	175	THR	3.3
1	A	120	THR	3.2
1	A	135	ALA	3.2
1	A	179	MET	2.6
1	A	81	LEU	2.6
1	A	6	SER	2.5

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(\AA^2)	Q<0.9
2	PMS	A	1225	10/11	0.99	0.09	26,28,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.