



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 3, 2023 – 11:29 AM EDT

PDB ID : 3SPU
Title : apo NDM-1 Crystal Structure
Authors : Strynadka, N.C.J.; King, D.T.
Deposited on : 2011-07-03
Resolution : 2.10 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
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

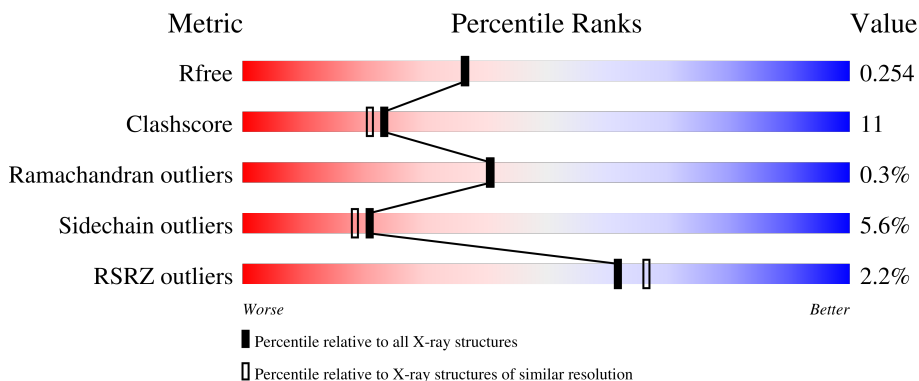
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	265	 2% 66% 20% 12%
1	B	265	 % 72% 14% 10%
1	C	265	 2% 69% 13% 5% 12%
1	D	265	 2% 67% 18% 13%
1	E	265	 3% 68% 15% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9130 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 Beta-lactamase NDM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	Total 1728	C 1089	N 307	O 324	S 8	0	4	0
1	B	238	Total 1769	C 1110	N 314	O 336	S 9	0	0	0
1	C	232	Total 1728	C 1089	N 307	O 324	S 8	0	4	0
1	D	231	Total 1721	C 1084	N 306	O 323	S 8	0	3	0
1	E	227	Total 1686	C 1061	N 298	O 319	S 8	0	0	0

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	LYS	-	expression tag	UNP C7C422
A	272	LEU	-	expression tag	UNP C7C422
A	273	VAL	-	expression tag	UNP C7C422
A	274	PRO	-	expression tag	UNP C7C422
A	275	ARG	-	expression tag	UNP C7C422
A	276	GLY	-	expression tag	UNP C7C422
A	277	SER	-	expression tag	UNP C7C422
A	278	ALA	-	expression tag	UNP C7C422
A	279	ALA	-	expression tag	UNP C7C422
A	280	ALA	-	expression tag	UNP C7C422
A	281	ALA	-	expression tag	UNP C7C422
A	282	LEU	-	expression tag	UNP C7C422
A	283	GLU	-	expression tag	UNP C7C422
A	284	HIS	-	expression tag	UNP C7C422
A	285	HIS	-	expression tag	UNP C7C422
A	286	HIS	-	expression tag	UNP C7C422
A	287	HIS	-	expression tag	UNP C7C422
A	288	HIS	-	expression tag	UNP C7C422
A	289	HIS	-	expression tag	UNP C7C422

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	HIS	-	expression tag	UNP C7C422
A	291	HIS	-	expression tag	UNP C7C422
B	271	LYS	-	expression tag	UNP C7C422
B	272	LEU	-	expression tag	UNP C7C422
B	273	VAL	-	expression tag	UNP C7C422
B	274	PRO	-	expression tag	UNP C7C422
B	275	ARG	-	expression tag	UNP C7C422
B	276	GLY	-	expression tag	UNP C7C422
B	277	SER	-	expression tag	UNP C7C422
B	278	ALA	-	expression tag	UNP C7C422
B	279	ALA	-	expression tag	UNP C7C422
B	280	ALA	-	expression tag	UNP C7C422
B	281	ALA	-	expression tag	UNP C7C422
B	282	LEU	-	expression tag	UNP C7C422
B	283	GLU	-	expression tag	UNP C7C422
B	284	HIS	-	expression tag	UNP C7C422
B	285	HIS	-	expression tag	UNP C7C422
B	286	HIS	-	expression tag	UNP C7C422
B	287	HIS	-	expression tag	UNP C7C422
B	288	HIS	-	expression tag	UNP C7C422
B	289	HIS	-	expression tag	UNP C7C422
B	290	HIS	-	expression tag	UNP C7C422
B	291	HIS	-	expression tag	UNP C7C422
C	271	LYS	-	expression tag	UNP C7C422
C	272	LEU	-	expression tag	UNP C7C422
C	273	VAL	-	expression tag	UNP C7C422
C	274	PRO	-	expression tag	UNP C7C422
C	275	ARG	-	expression tag	UNP C7C422
C	276	GLY	-	expression tag	UNP C7C422
C	277	SER	-	expression tag	UNP C7C422
C	278	ALA	-	expression tag	UNP C7C422
C	279	ALA	-	expression tag	UNP C7C422
C	280	ALA	-	expression tag	UNP C7C422
C	281	ALA	-	expression tag	UNP C7C422
C	282	LEU	-	expression tag	UNP C7C422
C	283	GLU	-	expression tag	UNP C7C422
C	284	HIS	-	expression tag	UNP C7C422
C	285	HIS	-	expression tag	UNP C7C422
C	286	HIS	-	expression tag	UNP C7C422
C	287	HIS	-	expression tag	UNP C7C422
C	288	HIS	-	expression tag	UNP C7C422
C	289	HIS	-	expression tag	UNP C7C422

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	290	HIS	-	expression tag	UNP C7C422
C	291	HIS	-	expression tag	UNP C7C422
D	271	LYS	-	expression tag	UNP C7C422
D	272	LEU	-	expression tag	UNP C7C422
D	273	VAL	-	expression tag	UNP C7C422
D	274	PRO	-	expression tag	UNP C7C422
D	275	ARG	-	expression tag	UNP C7C422
D	276	GLY	-	expression tag	UNP C7C422
D	277	SER	-	expression tag	UNP C7C422
D	278	ALA	-	expression tag	UNP C7C422
D	279	ALA	-	expression tag	UNP C7C422
D	280	ALA	-	expression tag	UNP C7C422
D	281	ALA	-	expression tag	UNP C7C422
D	282	LEU	-	expression tag	UNP C7C422
D	283	GLU	-	expression tag	UNP C7C422
D	284	HIS	-	expression tag	UNP C7C422
D	285	HIS	-	expression tag	UNP C7C422
D	286	HIS	-	expression tag	UNP C7C422
D	287	HIS	-	expression tag	UNP C7C422
D	288	HIS	-	expression tag	UNP C7C422
D	289	HIS	-	expression tag	UNP C7C422
D	290	HIS	-	expression tag	UNP C7C422
D	291	HIS	-	expression tag	UNP C7C422
E	271	LYS	-	expression tag	UNP C7C422
E	272	LEU	-	expression tag	UNP C7C422
E	273	VAL	-	expression tag	UNP C7C422
E	274	PRO	-	expression tag	UNP C7C422
E	275	ARG	-	expression tag	UNP C7C422
E	276	GLY	-	expression tag	UNP C7C422
E	277	SER	-	expression tag	UNP C7C422
E	278	ALA	-	expression tag	UNP C7C422
E	279	ALA	-	expression tag	UNP C7C422
E	280	ALA	-	expression tag	UNP C7C422
E	281	ALA	-	expression tag	UNP C7C422
E	282	LEU	-	expression tag	UNP C7C422
E	283	GLU	-	expression tag	UNP C7C422
E	284	HIS	-	expression tag	UNP C7C422
E	285	HIS	-	expression tag	UNP C7C422
E	286	HIS	-	expression tag	UNP C7C422
E	287	HIS	-	expression tag	UNP C7C422
E	288	HIS	-	expression tag	UNP C7C422
E	289	HIS	-	expression tag	UNP C7C422

Continued on next page...

Continued from previous page...

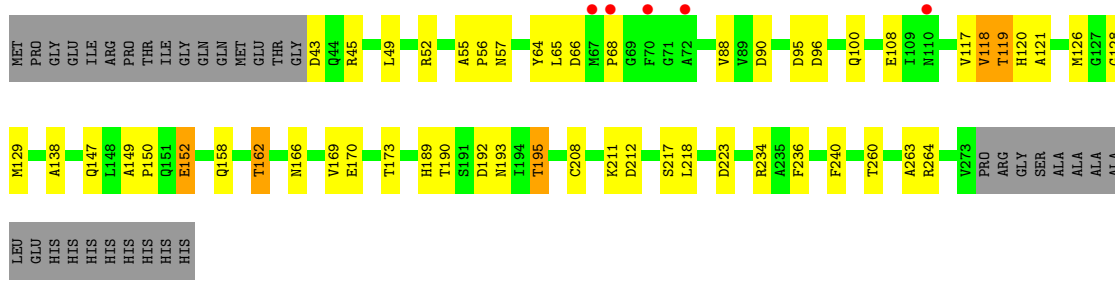
Chain	Residue	Modelled	Actual	Comment	Reference
E	290	HIS	-	expression tag	UNP C7C422
E	291	HIS	-	expression tag	UNP C7C422

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

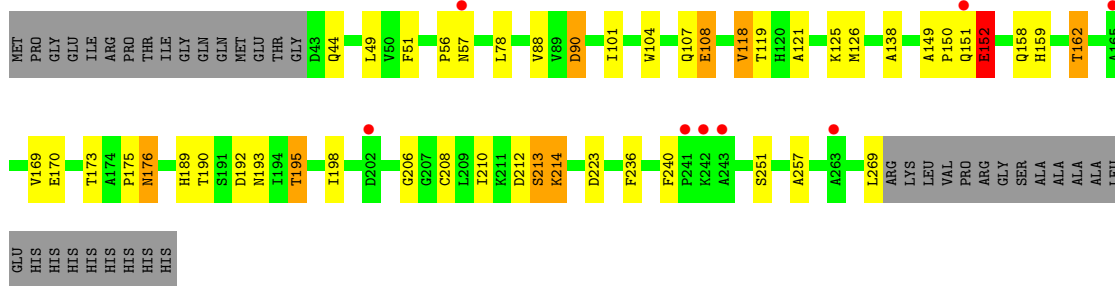
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total 101	O 101	0	0
3	B	105	Total 105	O 105	0	0
3	C	108	Total 108	O 108	0	0
3	D	102	Total 102	O 102	0	0
3	E	72	Total 72	O 72	0	0



• Molecule 1: Beta-lactamase NDM-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.54Å 73.90Å 77.41Å 70.32° 75.86° 65.30°	Depositor
Resolution (Å)	43.67 – 2.10 43.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.67-2.10) 96.0 (43.66-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.216 , 0.253 0.218 , 0.254	Depositor DCC
R_{free} test set	3563 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9130	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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:
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	1.13	9/1737 (0.5%)	0.87	2/2366 (0.1%)
1	B	1.26	11/1810 (0.6%)	0.89	6/2465 (0.2%)
1	C	1.22	10/1737 (0.6%)	0.90	6/2366 (0.3%)
1	D	1.12	9/1737 (0.5%)	0.83	1/2366 (0.0%)
1	E	1.15	9/1726 (0.5%)	0.91	5/2352 (0.2%)
All	All	1.18	48/8747 (0.5%)	0.88	20/11915 (0.2%)

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	GLU	CD-OE1	16.75	1.44	1.25
1	B	118	VAL	CB-CG2	-14.18	1.23	1.52
1	B	118	VAL	CB-CG1	-13.45	1.24	1.52
1	E	118	VAL	CB-CG2	-12.79	1.25	1.52
1	B	56	PRO	C-O	-11.47	1.00	1.23

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	ASP	CB-CG-OD2	5.93	123.63	118.30
1	E	152	GLU	O-C-N	-5.91	113.15	123.20
1	B	118	VAL	CG1-CB-CG2	-5.88	101.49	110.90
1	B	56	PRO	O-C-N	-5.87	113.31	122.70
1	C	124	ASP	CB-CG-OD2	5.81	123.53	118.30

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	1728	0	1687	56	0
1	B	1769	0	1715	30	0
1	C	1728	0	1687	47	0
1	D	1721	0	1680	31	0
1	E	1686	0	1633	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	101	0	0	3	0
3	B	105	0	0	2	0
3	C	108	0	0	6	0
3	D	102	0	0	2	0
3	E	72	0	0	0	0
All	All	9130	0	8402	193	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 11.

The worst 5 of 193 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:118:VAL:HG11	1:A:126:MET:HG2	1.40	0.99
1:E:176:ASN:OD1	1:E:176:ASN:N	1.99	0.93
1:B:162:THR:HG22	1:B:170:GLU:HG3	1.48	0.93
1:E:162:THR:HG22	1:E:170:GLU:HG3	1.51	0.91
1:D:162:THR:HG22	1:D:170:GLU:HG3	1.52	0.91

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	230/265 (87%)	224 (97%)	6 (3%)	0	100	100
1	B	236/265 (89%)	231 (98%)	5 (2%)	0	100	100
1	C	230/265 (87%)	223 (97%)	6 (3%)	1 (0%)	34	32
1	D	229/265 (86%)	225 (98%)	4 (2%)	0	100	100
1	E	225/265 (85%)	212 (94%)	11 (5%)	2 (1%)	17	12
All	All	1150/1325 (87%)	1115 (97%)	32 (3%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	71	GLY
1	E	213	SER
1	E	90	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	171/200 (86%)	162 (95%)	9 (5%)	22	20
1	B	179/200 (90%)	167 (93%)	12 (7%)	16	13
1	C	171/200 (86%)	160 (94%)	11 (6%)	17	14
1	D	171/200 (86%)	163 (95%)	8 (5%)	26	25
1	E	170/200 (85%)	162 (95%)	8 (5%)	26	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	862/1000 (86%)	814 (94%)	48 (6%)	21	18

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	166	ASN
1	D	108	GLU
1	C	190	THR
1	D	45	ARG
1	D	162	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	193	ASN
1	D	158	GLN
1	D	151	GLN
1	D	193	ASN
1	B	123	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 10 ligands modelled in this entry, 10 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	232/265 (87%)	0.22	4 (1%) 70 74	16, 25, 43, 61	0
1	B	238/265 (89%)	0.01	2 (0%) 86 88	16, 25, 44, 61	0
1	C	232/265 (87%)	0.17	6 (2%) 56 61	16, 25, 46, 61	0
1	D	231/265 (87%)	0.08	5 (2%) 62 66	16, 25, 44, 61	0
1	E	227/265 (85%)	0.21	8 (3%) 44 50	17, 25, 49, 61	0
All	All	1160/1325 (87%)	0.14	25 (2%) 62 66	16, 25, 46, 61	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	PRO	5.8
1	C	69	GLY	5.1
1	C	70	PHE	5.0
1	D	70	PHE	4.9
1	C	72	ALA	3.8

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	ZN	A	301	1/1	0.99	0.11	24,24,24,24	0
2	ZN	B	302	1/1	0.99	0.08	34,34,34,34	0
2	ZN	D	302	1/1	0.99	0.07	33,33,33,33	0
2	ZN	E	1001	1/1	0.99	0.08	33,33,33,33	0
2	ZN	E	1002	1/1	0.99	0.03	37,37,37,37	0
2	ZN	C	302	1/1	1.00	0.05	30,30,30,30	0
2	ZN	D	301	1/1	1.00	0.08	24,24,24,24	0
2	ZN	B	301	1/1	1.00	0.12	25,25,25,25	0
2	ZN	A	302	1/1	1.00	0.04	32,32,32,32	0
2	ZN	C	301	1/1	1.00	0.09	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.