Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2023 – 12:16 pm GMT

PDB ID	:	7ZG8
Title	:	Crystal structure of A. baumannii penicillin-binding protein 2
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Deposited on	:	2022-04-02
Resolution	:	2.65 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:

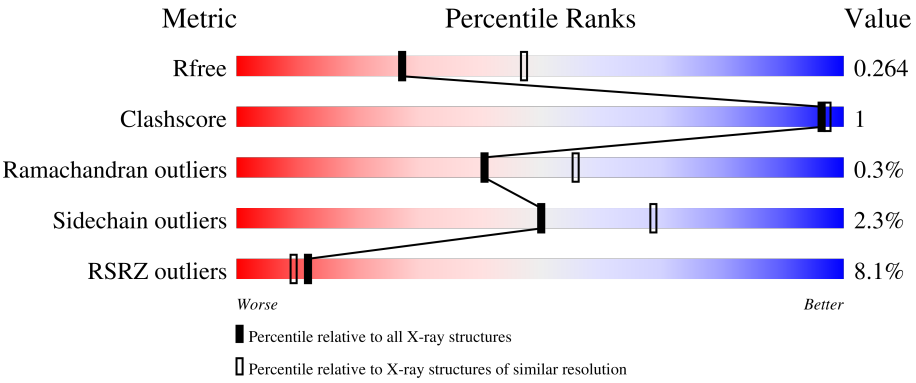
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	AAA	642	4% 77% · 18%
1	BBB	642	9% 75% · 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8194 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 Peptidoglycan D,D-transpeptidase MrdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	525	Total	C	N	O	S	0	1	0
			4128	2625	725	763	15			
1	BBB	504	Total	C	N	O	S	0	0	0
			3951	2515	690	732	14			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	31	MET	-	initiating methionine	UNP G1C6X4
AAA	32	ALA	-	expression tag	UNP G1C6X4
AAA	33	HIS	-	expression tag	UNP G1C6X4
AAA	34	HIS	-	expression tag	UNP G1C6X4
AAA	35	HIS	-	expression tag	UNP G1C6X4
AAA	36	HIS	-	expression tag	UNP G1C6X4
AAA	37	HIS	-	expression tag	UNP G1C6X4
AAA	38	HIS	-	expression tag	UNP G1C6X4
AAA	39	SER	-	expression tag	UNP G1C6X4
AAA	40	ALA	-	expression tag	UNP G1C6X4
AAA	41	ALA	-	expression tag	UNP G1C6X4
AAA	42	LEU	-	expression tag	UNP G1C6X4
AAA	43	GLU	-	expression tag	UNP G1C6X4
AAA	44	VAL	-	expression tag	UNP G1C6X4
AAA	45	LEU	-	expression tag	UNP G1C6X4
AAA	46	PHE	-	expression tag	UNP G1C6X4
AAA	47	GLN	-	expression tag	UNP G1C6X4
AAA	48	GLY	-	expression tag	UNP G1C6X4
AAA	49	PRO	-	expression tag	UNP G1C6X4
AAA	50	GLY	-	expression tag	UNP G1C6X4
AAA	51	TYR	-	expression tag	UNP G1C6X4
AAA	52	GLN	-	expression tag	UNP G1C6X4
BBB	31	MET	-	initiating methionine	UNP G1C6X4
BBB	32	ALA	-	expression tag	UNP G1C6X4
BBB	33	HIS	-	expression tag	UNP G1C6X4

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	34	HIS	-	expression tag	UNP G1C6X4
BBB	35	HIS	-	expression tag	UNP G1C6X4
BBB	36	HIS	-	expression tag	UNP G1C6X4
BBB	37	HIS	-	expression tag	UNP G1C6X4
BBB	38	HIS	-	expression tag	UNP G1C6X4
BBB	39	SER	-	expression tag	UNP G1C6X4
BBB	40	ALA	-	expression tag	UNP G1C6X4
BBB	41	ALA	-	expression tag	UNP G1C6X4
BBB	42	LEU	-	expression tag	UNP G1C6X4
BBB	43	GLU	-	expression tag	UNP G1C6X4
BBB	44	VAL	-	expression tag	UNP G1C6X4
BBB	45	LEU	-	expression tag	UNP G1C6X4
BBB	46	PHE	-	expression tag	UNP G1C6X4
BBB	47	GLN	-	expression tag	UNP G1C6X4
BBB	48	GLY	-	expression tag	UNP G1C6X4
BBB	49	PRO	-	expression tag	UNP G1C6X4
BBB	50	GLY	-	expression tag	UNP G1C6X4
BBB	51	TYR	-	expression tag	UNP G1C6X4
BBB	52	GLN	-	expression tag	UNP G1C6X4

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Zn 1 1	0	0
2	BBB	1	Total Zn 1 1	0	0

- Molecule 3 is water.

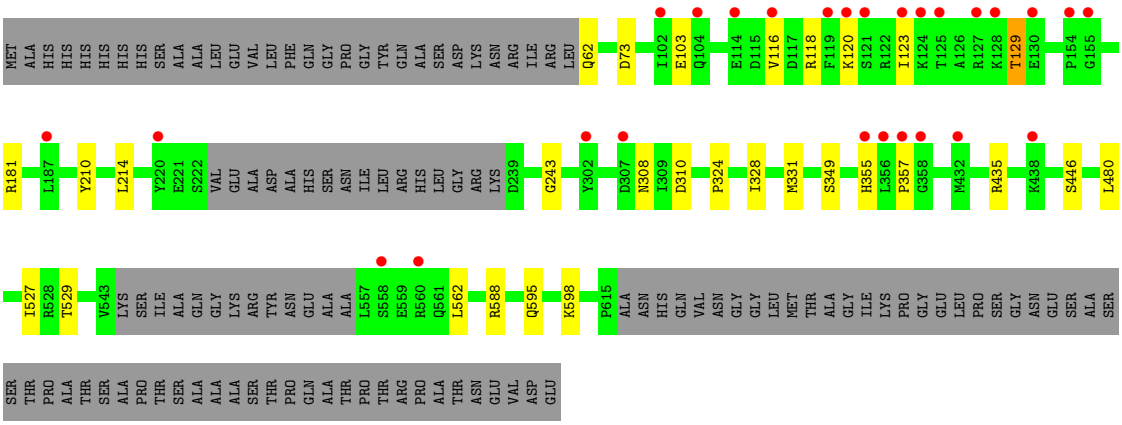
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	67	Total O 67 67	0	0
3	BBB	46	Total O 46 46	0	0

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.

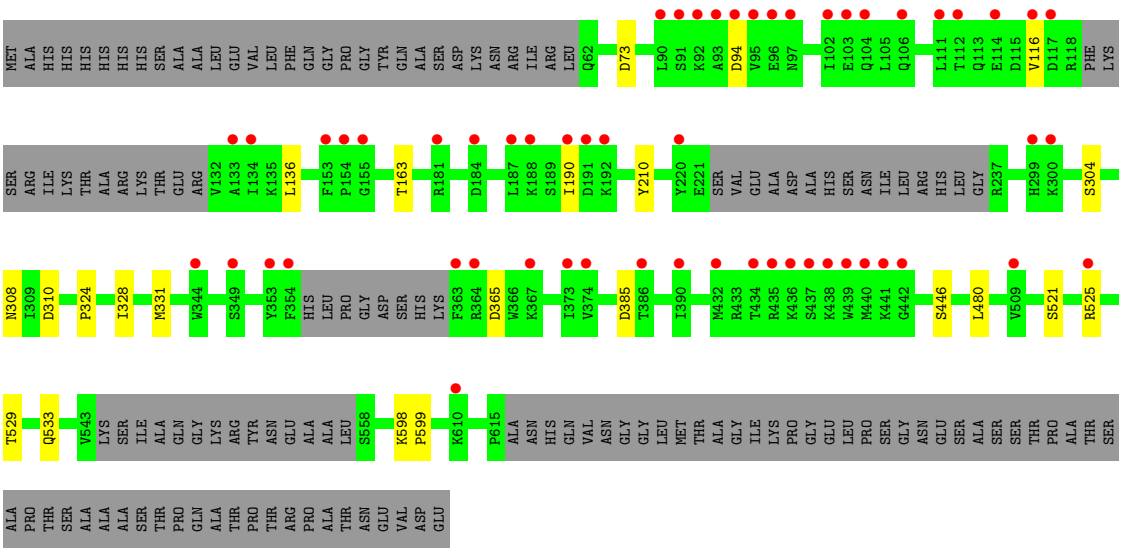
• Molecule 1: Peptidoglycan D,D-transpeptidase MrdA

Chain AAA:



• Molecule 1: Peptidoglycan D,D-transpeptidase MrdA

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	121.25Å 151.03Å 177.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.33 – 2.65 43.46 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.33-2.65) 98.4 (43.46-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.252 0.224 , 0.264	Depositor DCC
R_{free} test set	2395 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8194	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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

5.1 Standard geometry

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	AAA	0.68	0/4227	0.90	0/5731
1	BBB	0.67	0/4044	0.89	0/5484
All	All	0.67	0/8271	0.90	0/11215

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

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	AAA	4128	0	4099	10	0
1	BBB	3951	0	3914	6	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
3	AAA	67	0	0	0	0
3	BBB	46	0	0	0	0
All	All	8194	0	8013	16	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 1.

All (16) 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:BBB:365:ASP:HA	1:BBB:385:ASP:HB2	1.95	0.49
1:AAA:62:GLN:HA	1:AAA:129:THR:HB	1.95	0.49
1:AAA:120:LYS:HA	1:AAA:123:ILE:HG22	1.98	0.45
1:AAA:529:THR:HG22	1:AAA:598:LYS:CE	2.45	0.45
1:AAA:562:LEU:HD13	1:AAA:588:ARG:HD2	1.99	0.45
1:BBB:308:ASN:OD1	1:BBB:310:ASP:N	2.49	0.44
1:AAA:324:PRO:HB2	1:AAA:328:ILE:HG23	1.99	0.44
1:BBB:324:PRO:HB2	1:BBB:328:ILE:HG23	1.99	0.43
1:AAA:210:TYR:CE1	1:AAA:480:LEU:HD22	2.53	0.43
1:AAA:308:ASN:OD1	1:AAA:310:ASP:N	2.46	0.42
1:BBB:210:TYR:CE1	1:BBB:480:LEU:HD22	2.54	0.42
1:BBB:521:SER:HA	1:BBB:525:ARG:HD3	2.01	0.42
1:AAA:118:ARG:HH11	1:AAA:181:ARG:HB2	1.83	0.42
1:BBB:598:LYS:N	1:BBB:599:PRO:CD	2.84	0.41
1:AAA:529:THR:HG22	1:AAA:598:LYS:HE3	2.04	0.40
1:AAA:214:LEU:O	1:AAA:243:GLY:HA3	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	AAA	520/642 (81%)	494 (95%)	24 (5%)	2 (0%)	34	48
1	BBB	494/642 (77%)	474 (96%)	19 (4%)	1 (0%)	47	64
All	All	1014/1284 (79%)	968 (96%)	43 (4%)	3 (0%)	41	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	116	VAL

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Mol	Chain	Res	Type
1	BBB	116	VAL
1	AAA	357	PRO

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	AAA	439/527 (83%)	429 (98%)	10 (2%)	50 68
1	BBB	419/527 (80%)	409 (98%)	10 (2%)	49 67
All	All	858/1054 (81%)	838 (98%)	20 (2%)	50 68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	73	ASP
1	AAA	103	GLU
1	AAA	129	THR
1	AAA	331	MET
1	AAA	349	SER
1	AAA	355	HIS
1	AAA	435	ARG
1	AAA	446	SER
1	AAA	527	ILE
1	AAA	595	GLN
1	BBB	73	ASP
1	BBB	94	ASP
1	BBB	136	LEU
1	BBB	163	THR
1	BBB	190	ILE
1	BBB	304	SER
1	BBB	331	MET
1	BBB	446	SER
1	BBB	529	THR
1	BBB	533	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	AAA	525/642 (81%)	0.14	27 (5%) 28 25	30, 52, 110, 147	0
1	BBB	504/642 (78%)	0.42	56 (11%) 5 3	31, 61, 125, 166	0
All	All	1029/1284 (80%)	0.28	83 (8%) 12 9	30, 56, 118, 166	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	363	PHE	5.2
1	BBB	134	ILE	5.0
1	BBB	90	LEU	4.5
1	BBB	93	ALA	4.5
1	AAA	356	LEU	4.2
1	BBB	354	PHE	4.1
1	AAA	432	MET	4.0
1	AAA	355	HIS	3.9
1	AAA	120	LYS	3.9
1	BBB	441	LYS	3.8
1	BBB	102	ILE	3.8
1	AAA	127	ARG	3.8
1	BBB	114	GLU	3.7
1	BBB	187	LEU	3.7
1	BBB	154	PRO	3.6
1	BBB	184	ASP	3.5
1	BBB	92	LYS	3.5
1	BBB	112	THR	3.5
1	AAA	155	GLY	3.5
1	BBB	116	VAL	3.5
1	BBB	94	ASP	3.4
1	BBB	438	LYS	3.4
1	AAA	220	TYR	3.4
1	AAA	102	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	192	LYS	3.3
1	AAA	121	SER	3.2
1	BBB	386	THR	3.2
1	BBB	390	ILE	3.2
1	BBB	103	GLU	3.2
1	BBB	106	GLN	3.1
1	BBB	133	ALA	3.1
1	BBB	525	ARG	3.1
1	BBB	437	SER	3.1
1	BBB	91	SER	3.1
1	BBB	95	VAL	3.1
1	BBB	373	ILE	3.0
1	BBB	299	HIS	2.9
1	BBB	111	LEU	2.9
1	AAA	357	PRO	2.9
1	BBB	97	ASN	2.9
1	BBB	435	ARG	2.9
1	AAA	187	LEU	2.9
1	AAA	128	LYS	2.8
1	AAA	123	ILE	2.8
1	AAA	358	GLY	2.8
1	AAA	125	THR	2.7
1	BBB	353	TYR	2.7
1	BBB	432	MET	2.6
1	AAA	302	TYR	2.6
1	BBB	191	ASP	2.6
1	AAA	558	SER	2.6
1	BBB	364	ARG	2.6
1	BBB	344	TRP	2.6
1	BBB	610	LYS	2.6
1	AAA	104	GLN	2.6
1	BBB	96	GLU	2.5
1	AAA	116	VAL	2.5
1	AAA	130	GLU	2.5
1	AAA	154	PRO	2.5
1	BBB	220	TYR	2.5
1	AAA	119	PHE	2.5
1	BBB	434	THR	2.4
1	BBB	153	PHE	2.4
1	BBB	181	ARG	2.4
1	BBB	440	MET	2.4
1	BBB	436	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	438	LYS	2.3
1	BBB	439	TRP	2.3
1	AAA	307	ASP	2.3
1	AAA	124	LYS	2.3
1	BBB	190	ILE	2.3
1	BBB	104	GLN	2.2
1	BBB	509	VAL	2.2
1	BBB	300	LYS	2.2
1	AAA	114	GLU	2.2
1	AAA	560	ARG	2.2
1	BBB	374	VAL	2.2
1	BBB	188	LYS	2.2
1	BBB	155	GLY	2.1
1	BBB	442	GLY	2.1
1	BBB	117	ASP	2.0
1	BBB	349	SER	2.0
1	BBB	367	LYS	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, 95^{th} 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	ZN	BBB	700	1/1	0.86	0.04	118,118,118,118	0
2	ZN	AAA	700	1/1	0.99	0.09	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.