



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:35 AM UTC

PDB ID : 4AQN / pdb_00004aqn
Title : Crystal structure of pesticin from *Y. pestis*
Authors : Zeth, K.; Albrecht, R.
Deposited on : 2012-04-19
Resolution : 1.98 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

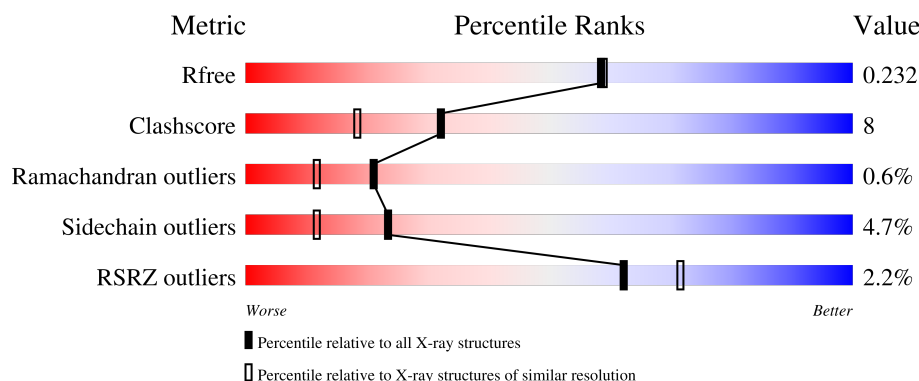
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	357	3% 74% 18% • 5%
1	B	357	2% 73% 20% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5802 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 PESTICIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	2	0
			2708	1707	468	527	6			
1	B	338	Total	C	N	O	S	0	3	0
			2708	1705	469	528	6			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

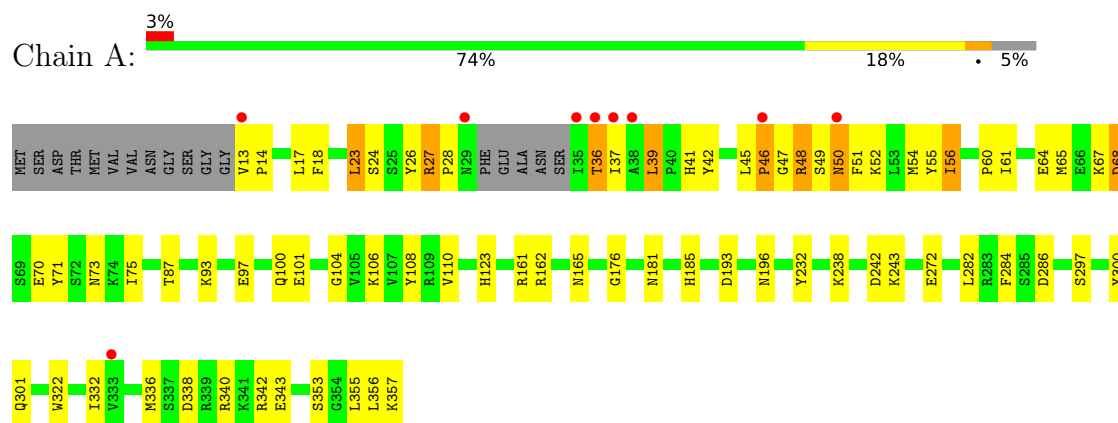
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	202	Total	O	0	0
			202	202		
3	B	183	Total	O	0	0
			183	183		

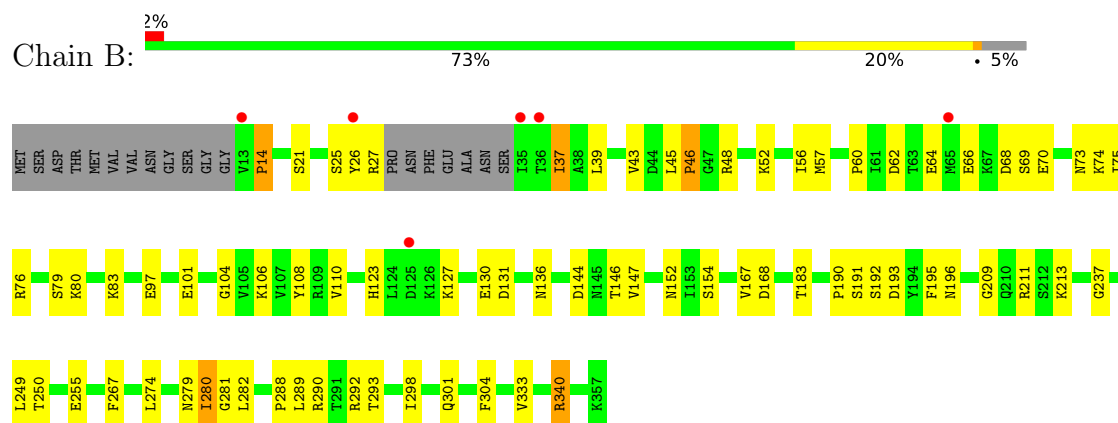
3 Residue-property plots [i](#)

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: PESTICIN



• Molecule 1: PESTICIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.55Å 86.78Å 122.27Å 90.00° 96.14° 90.00°	Depositor
Resolution (Å)	29.82 – 1.98 29.82 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.82-1.98) 99.7 (29.82-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.190 , 0.237 0.186 , 0.232	Depositor DCC
R_{free} test set	2640 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5802	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7364e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.50	0/2764	0.84	5/3731 (0.1%)
1	B	0.45	0/2760	0.86	3/3725 (0.1%)
All	All	0.48	0/5524	0.85	8/7456 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ILE	N-CA-C	-11.37	102.29	113.20
1	A	27	ARG	CA-C-N	9.89	129.70	120.21
1	A	27	ARG	C-N-CA	9.89	129.70	120.21
1	B	280	ILE	N-CA-C	9.48	125.72	112.35
1	B	282	LEU	N-CA-C	-6.87	98.86	109.24
1	A	45	LEU	CA-C-N	6.04	127.38	119.84
1	A	45	LEU	C-N-CA	6.04	127.38	119.84
1	A	48	ARG	N-CA-C	5.79	117.66	108.79

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	2708	0	2676	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2708	0	2673	44	1
2	B	1	0	0	0	0
3	A	202	0	0	4	2
3	B	183	0	0	7	1
All	All	5802	0	5349	86	2

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 8.

All (86) 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:79:SER:OG	3:B:2019:HOH:O	2.01	0.78
1:B:279[B]:ASN:OD1	3:B:2139:HOH:O	2.03	0.75
1:A:300:TYR:OH	3:A:2108:HOH:O	2.06	0.74
1:B:168:ASP:H	1:B:293[B]:THR:HG22	1.51	0.73
1:A:55:TYR:OH	3:A:2004:HOH:O	2.07	0.72
1:A:13:VAL:HB	1:A:100:GLN:HG3	1.74	0.70
1:B:66:GLU:O	1:B:74:LYS:NZ	2.24	0.69
1:A:301:GLN:OE1	1:A:340:ARG:NH2	2.27	0.68
1:B:255:GLU:OE1	3:B:2115:HOH:O	2.11	0.67
1:B:64:GLU:HB2	1:B:106:LYS:HB2	1.74	0.67
1:A:26:TYR:CZ	1:A:28:PRO:HB3	2.30	0.66
1:A:356:LEU:O	3:A:2199:HOH:O	2.14	0.66
1:B:101:GLU:HB2	1:B:106:LYS:HG2	1.79	0.65
1:B:168:ASP:H	1:B:293[B]:THR:CG2	2.09	0.65
1:A:68:ASP:OD1	1:A:68:ASP:N	2.28	0.63
1:B:45:LEU:HD23	1:B:48:ARG:HG3	1.79	0.63
1:B:56:ILE:HG22	1:B:57:MET:HG2	1.81	0.63
1:A:282:LEU:HD12	1:A:286:ASP:HB2	1.80	0.62
1:A:46:PRO:O	1:A:48:ARG:N	2.33	0.62
1:B:60:PRO:HG2	1:B:110:VAL:HB	1.83	0.61
1:A:322:TRP:HD1	1:A:357:LYS:HD3	1.66	0.60
1:B:25:SER:N	3:B:2004:HOH:O	2.33	0.59
1:B:301:GLN:OE1	1:B:340:ARG:NH2	2.35	0.58
1:B:195:PHE:O	1:B:237:GLY:HA2	2.04	0.57
1:A:238:LYS:NZ	1:A:242:ASP:OD2	2.37	0.57
1:A:336:MET:SD	1:B:193:ASP:HB3	2.46	0.56
1:A:97:GLU:HB3	1:A:108:TYR:HB3	1.88	0.56
1:B:289:LEU:O	1:B:293[B]:THR:HG23	2.05	0.55
1:B:281:GLY:HA2	3:B:2141:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:TRP:CD1	1:A:357:LYS:HD3	2.42	0.54
1:A:60:PRO:HG2	1:A:110:VAL:HB	1.90	0.53
1:B:68:ASP:OD1	1:B:69:SER:N	2.42	0.53
1:B:290:ARG:O	1:B:293[B]:THR:OG1	2.26	0.52
1:B:152:ASN:OD1	1:B:154:SER:OG	2.26	0.52
1:A:37:ILE:HB	1:A:39:LEU:HD22	1.92	0.51
1:A:181:ASN:HB3	1:A:185:HIS:CE1	2.46	0.51
1:B:211:ARG:NH2	3:B:2100:HOH:O	2.44	0.51
1:A:24:SER:O	1:A:27:ARG:NH1	2.44	0.50
1:A:23:LEU:HD12	1:A:123:HIS:HB2	1.93	0.50
1:A:87:THR:HG22	1:A:162:ARG:HB3	1.94	0.49
1:A:353[B]:SER:OG	1:A:355:LEU:HG	2.12	0.49
1:A:272:GLU:HG3	1:A:284:PHE:HB3	1.93	0.49
1:A:14:PRO:HB2	1:A:17:LEU:HD13	1.95	0.49
1:A:101:GLU:HB2	1:A:106:LYS:HG2	1.95	0.49
1:B:52:LYS:N	1:B:73:ASN:OD1	2.32	0.49
1:B:101:GLU:OE1	1:B:108:TYR:OH	2.14	0.48
1:A:37:ILE:HG13	1:A:41:HIS:CE1	2.49	0.48
1:A:297:SER:OG	1:A:343:GLU:OE2	2.24	0.47
1:B:190:PRO:HA	1:B:195:PHE:CG	2.49	0.47
1:A:52:LYS:N	1:A:73:ASN:OD1	2.38	0.47
1:B:62:ASP:CG	1:B:76:ARG:HH12	2.22	0.47
1:B:127:LYS:HA	1:B:130:GLU:HG3	1.97	0.46
1:A:176:GLY:O	1:A:342:ARG:NE	2.39	0.46
1:A:18:PHE:CZ	1:A:56:ILE:HD11	2.50	0.46
1:B:298:ILE:HD12	1:B:340:ARG:HD2	1.99	0.45
1:B:183:THR:HA	1:B:250:THR:HA	1.99	0.45
1:A:161:ARG:HA	1:A:161:ARG:HD2	1.82	0.45
1:B:45:LEU:HD12	1:B:46:PRO:HD2	1.98	0.45
1:B:167:VAL:HB	1:B:293[B]:THR:HG22	1.98	0.45
1:B:14:PRO:HA	1:B:136:ASN:OD1	2.18	0.44
1:A:42:TYR:CD1	1:A:71:TYR:HB3	2.53	0.44
1:A:37:ILE:HG13	1:A:41:HIS:HE1	1.80	0.44
1:A:232:TYR:CE1	1:A:243:LYS:HE2	2.53	0.43
1:B:21[A]:SER:HB3	1:B:123:HIS:CE1	2.53	0.43
1:B:62:ASP:OD2	1:B:76:ARG:NH1	2.51	0.43
1:B:97:GLU:HB3	1:B:108:TYR:HB3	2.00	0.43
1:B:209:GLY:HA3	3:B:2093:HOH:O	2.17	0.43
1:B:74:LYS:HD3	1:B:74:LYS:HA	1.72	0.43
1:B:21[A]:SER:HB3	1:B:123:HIS:HE1	1.83	0.43
1:A:54:MET:O	1:A:61:ILE:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:O	1:A:36:THR:OG1	2.36	0.43
1:A:49:SER:HA	1:A:50:ASN:HA	1.80	0.42
1:A:193:ASP:CG	1:B:301:GLN:HE21	2.28	0.42
1:B:144:ASP:OD1	1:B:146:THR:OG1	2.36	0.42
1:B:267:PHE:CZ	1:B:304:PHE:HB3	2.55	0.42
1:A:65:MET:HA	1:A:104:GLY:O	2.20	0.41
1:A:161:ARG:HE	1:A:165:ASN:HD21	1.67	0.41
1:A:49:SER:HA	1:A:51:PHE:H	1.86	0.41
1:A:340:ARG:HA	1:A:340:ARG:HD3	1.86	0.41
1:B:26:TYR:CD2	1:B:27:ARG:HG3	2.56	0.41
1:B:288:PRO:O	1:B:292:ARG:HG3	2.21	0.40
1:B:66:GLU:HB2	1:B:104:GLY:HA3	2.03	0.40
1:A:46:PRO:C	1:A:48:ARG:H	2.28	0.40
1:A:51:PHE:N	3:A:2008:HOH:O	2.48	0.40
1:A:64:GLU:HB3	1:A:75:ILE:HD13	2.02	0.40
1:B:80:LYS:HD3	1:B:80:LYS:HA	1.90	0.40

All (2) 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)
1:B:280:ILE:O	3:A:2147:HOH:O[2_556]	2.04	0.16
3:A:2061:HOH:O	3:B:2162:HOH:O[2_546]	2.09	0.11

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	338/357 (95%)	328 (97%)	8 (2%)	2 (1%)	21	12
1	B	337/357 (94%)	321 (95%)	14 (4%)	2 (1%)	21	12
All	All	675/714 (94%)	649 (96%)	22 (3%)	4 (1%)	21	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO
1	A	47	GLY
1	B	46	PRO
1	B	14	PRO

5.3.2 Protein sidechains ⓘ

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	303/315 (96%)	291 (96%)	12 (4%)	28	17
1	B	303/315 (96%)	287 (95%)	16 (5%)	20	9
All	All	606/630 (96%)	578 (95%)	28 (5%)	23	12

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	36	THR
1	A	39	LEU
1	A	50	ASN
1	A	56	ILE
1	A	67	LYS
1	A	68	ASP
1	A	70	GLU
1	A	93	LYS
1	A	196	ASN
1	A	332	ILE
1	A	338	ASP
1	B	37	ILE
1	B	39	LEU
1	B	43	VAL
1	B	70	GLU
1	B	75	ILE
1	B	83	LYS
1	B	131	ASP

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Mol	Chain	Res	Type
1	B	147	VAL
1	B	191	SER
1	B	192	SER
1	B	196	ASN
1	B	213	LYS
1	B	249	LEU
1	B	274	LEU
1	B	333	VAL
1	B	340	ARG

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	123	HIS
1	A	149	ASN
1	A	165	ASN
1	B	123	HIS
1	B	189	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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	340/357 (95%)	-0.03	9 (2%) 57 67	20, 41, 80, 112	2 (0%)
1	B	338/357 (94%)	0.07	6 (1%) 67 76	12, 44, 89, 140	3 (0%)
All	All	678/714 (94%)	0.02	15 (2%) 62 71	12, 42, 85, 140	5 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	ILE	4.3
1	B	36	THR	3.7
1	A	35	ILE	3.4
1	A	13	VAL	3.2
1	A	37	ILE	3.1
1	B	65	MET	3.0
1	B	13	VAL	2.8
1	A	46	PRO	2.7
1	B	26	TYR	2.5
1	A	333	VAL	2.4
1	A	38	ALA	2.4
1	A	50	ASN	2.2
1	B	125	ASP	2.1
1	A	36	THR	2.1
1	A	29	ASN	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 oligosaccharides in this entry.

6.4 Ligands

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($\text{\AA}^2$)	Q<0.9
2	MG	B	1358	1/1	0.88	0.13	61,61,61,61	0

6.5 Other polymers

There are no such residues in this entry.