



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 09:42 AM EDT

PDB ID : 2PRS
Title : Structure and metal binding properties of ZnuA, a periplasmic zinc transporter from Escherichia coli
Authors : Yatsunyk, L.A.; Kim, L.R.; Vorontsov, I.I.; Rosenzweig, A.C.
Deposited on : 2007-05-04
Resolution : 1.70 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 : 2022.3.0, CSD as543be (2022)
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

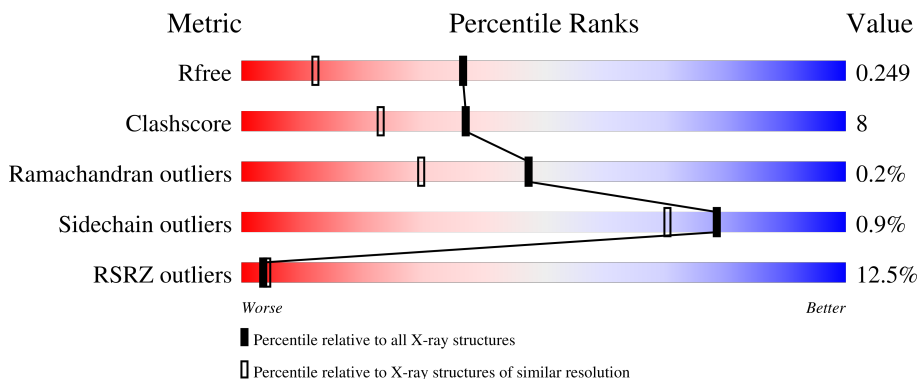
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	284	
1	B	284	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4608 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.

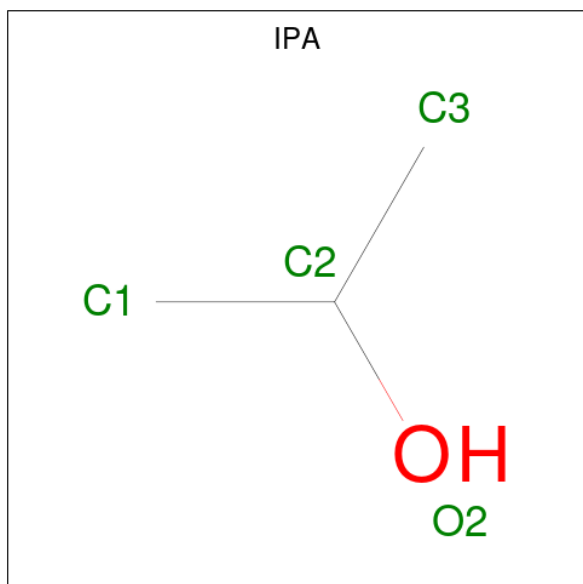
- Molecule 1 is a protein called High-affinity zinc uptake system protein znuA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	Total 2063	C 1320	N 348	O 386	S 9	0	7	0
1	B	264	Total 2097	C 1337	N 356	O 395	S 9	0	8	0

- 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	1	Total 1	Zn 1	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		

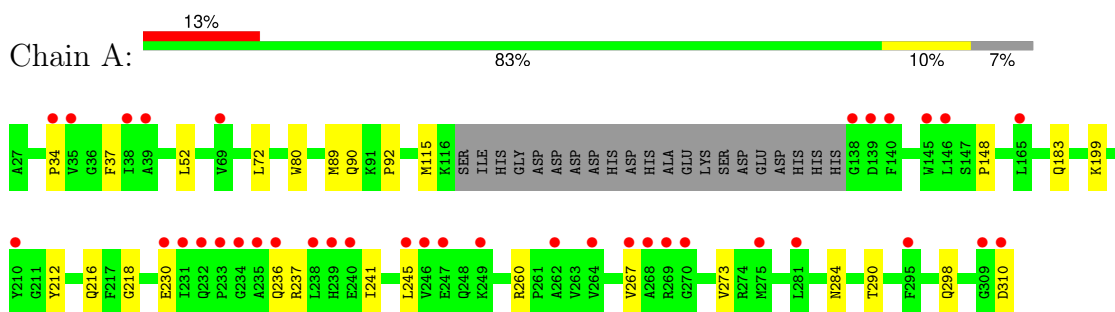
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total	O	0	0
			213	213		
4	B	228	Total	O	0	0
			228	228		

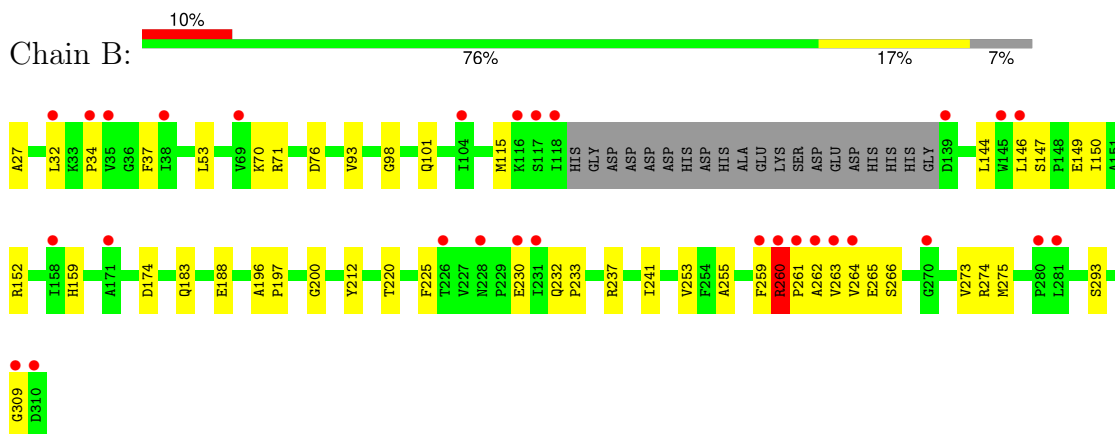
3 Residue-property plots [i](#)

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: High-affinity zinc uptake system protein znuA



- Molecule 1: High-affinity zinc uptake system protein znuA



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.38Å 78.07Å 86.37Å 90.00° 91.37° 90.00°	Depositor
Resolution (Å)	28.80 – 1.70 28.78 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.80-1.70) 97.0 (28.78-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.250 0.210 , 0.249	Depositor DCC
R_{free} test set	3254 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtrriage
Anisotropy	0.035	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4608	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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, IPA

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	0.47	0/2117	0.56	0/2868
1	B	0.46	0/2142	0.59	0/2903
All	All	0.47	0/4259	0.58	0/5771

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	260	ARG	Peptide

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	2063	0	2092	19	0
1	B	2097	0	2109	46	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	8	0	0
4	A	213	0	0	2	0
4	B	228	0	0	1	0
All	All	4608	0	4209	65	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 8.

All (65) 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:263:VAL:CG1	1:B:263:VAL:O	2.25	0.84
1:B:255:ALA:HB1	1:B:260:ARG:HB2	1.62	0.80
1:B:263:VAL:O	1:B:263:VAL:HG12	1.82	0.78
1:A:245:LEU:HG	1:A:273[A]:VAL:HG21	1.66	0.76
1:B:200:GLY:H	1:B:220[B]:THR:HG21	1.51	0.76
1:B:200:GLY:H	1:B:220[B]:THR:CG2	1.98	0.75
1:B:183[B]:GLN:HG3	1:B:293:SER:OG	1.87	0.73
1:A:199:LYS:HD2	1:A:218:GLY:O	1.96	0.65
1:B:263:VAL:HA	1:B:264:VAL:HB	1.78	0.65
1:B:253[A]:VAL:HG13	1:B:275[A]:MET:SD	2.43	0.59
1:B:261:PRO:HD2	1:B:263:VAL:HB	1.85	0.58
1:B:253[B]:VAL:HG23	1:B:273:VAL:HG11	1.86	0.57
1:B:274:ARG:NH1	1:B:309:GLY:O	2.38	0.57
1:B:259:PHE:O	1:B:260:ARG:HB2	2.04	0.57
1:B:230:GLU:C	1:B:263:VAL:HG11	2.25	0.56
1:B:263:VAL:N	1:B:264:VAL:HA	2.20	0.56
1:B:264:VAL:HG22	1:B:265:GLU:HG2	1.87	0.55
1:B:98:GLY:HA2	1:B:101[B]:GLN:HE21	1.72	0.54
1:B:253[A]:VAL:CG1	1:B:275[A]:MET:SD	2.96	0.54
1:B:147:SER:HB2	1:B:212:TYR:HB3	1.89	0.54
1:B:261:PRO:HG2	1:B:263:VAL:HB	1.90	0.54
1:B:265:GLU:HB2	1:B:275[B]:MET:SD	2.48	0.53
1:B:200:GLY:N	1:B:220[B]:THR:HG21	2.21	0.53
1:B:27:ALA:N	1:B:76:ASP:OD2	2.42	0.52
1:B:264:VAL:HG22	1:B:265:GLU:N	2.25	0.52
1:B:263:VAL:O	1:B:263:VAL:HG13	2.10	0.51
1:A:310:ASP:N	1:A:310:ASP:OD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:VAL:HG13	1:B:266:SER:OG	2.10	0.50
1:A:230:GLU:HG3	4:A:697:HOH:O	2.10	0.49
1:B:159:HIS:HD2	4:B:527:HOH:O	1.95	0.49
1:A:241:ILE:O	1:A:245:LEU:HB2	2.12	0.49
1:B:232:GLN:HG3	1:B:263:VAL:HG22	1.95	0.48
1:A:115:MET:HG2	1:A:212:TYR:CZ	2.48	0.48
1:B:32:LEU:HD22	1:B:53:LEU:HD22	1.96	0.48
1:A:90:GLN:NE2	4:A:748:HOH:O	2.46	0.47
1:B:260:ARG:HG2	1:B:262:ALA:HA	1.95	0.47
1:B:261:PRO:CD	1:B:263:VAL:HB	2.45	0.46
1:A:52:LEU:HD11	1:A:72:LEU:HD21	1.97	0.46
1:A:236:GLN:HG3	1:A:237:ARG:H	1.81	0.46
1:B:144:LEU:HB3	1:B:150:ILE:HG21	1.98	0.45
1:B:93:VAL:CG1	1:B:101[A]:GLN:HE22	2.29	0.45
1:A:148:PRO:HD2	1:A:216:GLN:OE1	2.16	0.45
1:B:34:PRO:HA	1:B:37:PHE:CD2	2.52	0.45
1:B:196:ALA:N	1:B:197:PRO:HD2	2.31	0.45
1:B:261:PRO:HD2	1:B:263:VAL:N	2.32	0.45
1:B:233:PRO:HD2	1:B:264:VAL:HG12	2.00	0.44
1:B:152[A]:ARG:HH22	1:B:188:GLU:CD	2.19	0.44
1:B:115:MET:HG3	1:B:212:TYR:CE2	2.53	0.43
1:B:159:HIS:HE1	1:B:174:ASP:OD1	2.00	0.43
1:B:232:GLN:HG2	1:B:264:VAL:HB	2.00	0.43
1:A:34:PRO:HA	1:A:37:PHE:CD2	2.53	0.43
1:A:183:GLN:OE1	1:A:290:THR:HA	2.18	0.43
1:A:284[B]:ASN:OD1	1:A:298:GLN:NE2	2.51	0.43
1:B:261:PRO:CG	1:B:263:VAL:HB	2.48	0.42
1:B:149:GLU:OE2	1:B:152[A]:ARG:NH2	2.53	0.42
1:B:225:PHE:CE2	1:B:241:ILE:HG23	2.55	0.42
1:A:245:LEU:HD21	1:A:273[B]:VAL:HG11	2.02	0.41
1:A:72:LEU:HD13	1:A:92:PRO:HB2	2.02	0.41
1:B:146:LEU:HD23	1:B:146:LEU:HA	1.91	0.41
1:A:260:ARG:NE	1:A:260:ARG:HA	2.35	0.41
1:B:260:ARG:HG2	1:B:262:ALA:CA	2.51	0.41
1:A:115:MET:HG2	1:A:212:TYR:CE2	2.56	0.41
1:B:262:ALA:C	1:B:264:VAL:HA	2.42	0.41
1:A:236:GLN:HG3	1:A:237:ARG:N	2.35	0.40
1:A:80:TRP:CE3	1:A:89:MET:HB2	2.56	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	266/284 (94%)	264 (99%)	2 (1%)	0	100	100
1	B	268/284 (94%)	260 (97%)	7 (3%)	1 (0%)	34	18
All	All	534/568 (94%)	524 (98%)	9 (2%)	1 (0%)	47	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	ARG

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	224/236 (95%)	223 (100%)	1 (0%)	91	87
1	B	227/236 (96%)	224 (99%)	3 (1%)	69	56
All	All	451/472 (96%)	447 (99%)	4 (1%)	78	70

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	VAL
1	B	70	LYS
1	B	71	ARG
1	B	237	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	106	GLN
1	A	159	HIS
1	A	190	GLN
1	B	90	GLN
1	B	106	GLN
1	B	159	HIS
1	B	236	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
3	IPA	A	601	-	3,3,3	0.54	0	3,3,3	0.33	0

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	263/284 (92%)	0.72	37 (14%) 2 3	18, 29, 54, 60	1 (0%)
1	B	264/284 (92%)	0.67	29 (10%) 5 6	21, 31, 44, 52	0
All	All	527/568 (92%)	0.70	66 (12%) 3 4	18, 30, 52, 60	1 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	VAL	10.4
1	B	118	ILE	8.8
1	A	138	GLY	7.8
1	B	261	PRO	7.3
1	A	231	ILE	6.5
1	B	310	ASP	6.1
1	A	270	GLY	5.9
1	B	117	SER	5.6
1	A	309	GLY	5.2
1	A	234	GLY	5.1
1	A	269	ARG	4.7
1	B	309	GLY	4.5
1	B	262	ALA	4.2
1	A	236	GLN	4.2
1	B	264	VAL	4.0
1	A	275[A]	MET	4.0
1	A	239	HIS	3.9
1	A	267	VAL	3.8
1	A	310	ASP	3.8
1	A	249	LYS	3.8
1	B	231	ILE	3.7
1	B	139	ASP	3.6
1	B	226	THR	3.5
1	A	246	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	145	TRP	3.3
1	B	260	ARG	3.1
1	A	165	LEU	3.1
1	B	69	VAL	3.1
1	A	139	ASP	3.0
1	B	171	ALA	3.0
1	B	116	LYS	3.0
1	B	230	GLU	2.9
1	A	233	PRO	2.9
1	B	35	VAL	2.8
1	A	268	ALA	2.8
1	A	262	ALA	2.6
1	A	230	GLU	2.6
1	B	38	ILE	2.6
1	B	158	ILE	2.6
1	A	69[A]	VAL	2.6
1	A	140	PHE	2.5
1	A	235	ALA	2.5
1	B	270	GLY	2.5
1	A	38	ILE	2.5
1	B	281	LEU	2.5
1	A	281	LEU	2.5
1	A	146	LEU	2.4
1	B	104	ILE	2.3
1	B	146	LEU	2.3
1	B	280	PRO	2.3
1	A	34	PRO	2.2
1	A	35	VAL	2.2
1	A	210	TYR	2.2
1	A	232	GLN	2.2
1	A	145	TRP	2.2
1	A	240	GLU	2.2
1	A	39	ALA	2.2
1	B	259	PHE	2.1
1	B	32	LEU	2.1
1	B	34	PRO	2.1
1	A	247	GLU	2.1
1	A	245	LEU	2.1
1	A	295	PHE	2.1
1	B	228	ASN	2.0
1	A	264	VAL	2.0
1	A	238	LEU	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	ZN	A	503	1/1	0.93	0.30	38,38,38,38	1
3	IPA	A	601	4/4	0.93	0.08	29,29,30,31	0
2	ZN	B	502	1/1	1.00	0.07	24,24,24,24	0
2	ZN	A	501	1/1	1.00	0.09	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.