



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:21 AM GMT

PDB ID : 3I2D  
Title : Crystal Structure of S. Cerevisiae SUMO E3 Ligase SIZ1  
Authors : Lima, C.D.; Yunus, A.A.  
Deposited on : 2009-06-29  
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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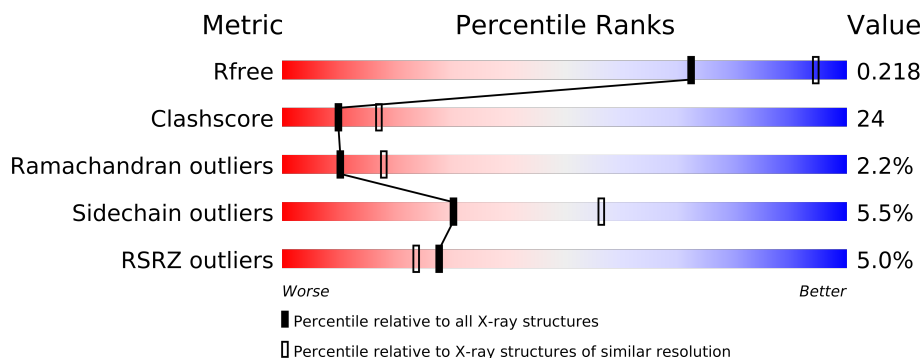
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	371	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2302 atoms, of which 0 are hydrogen and 0 are deuterium.

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 E3 SUMO-protein ligase SIZ1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2235	1430	376	415	14	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	SER	-	EXPRESSION TAG	UNP Q04195
A	111	LEU	-	EXPRESSION TAG	UNP Q04195
A	466	LEU	-	EXPRESSION TAG	UNP Q04195
A	467	GLY	-	EXPRESSION TAG	UNP Q04195
A	468	GLU	-	EXPRESSION TAG	UNP Q04195
A	469	GLY	-	EXPRESSION TAG	UNP Q04195
A	470	ALA	-	EXPRESSION TAG	UNP Q04195
A	471	ALA	-	EXPRESSION TAG	UNP Q04195
A	472	ALA	-	EXPRESSION TAG	UNP Q04195
A	473	LEU	-	EXPRESSION TAG	UNP Q04195
A	474	GLU	-	EXPRESSION TAG	UNP Q04195
A	475	HIS	-	EXPRESSION TAG	UNP Q04195
A	476	HIS	-	EXPRESSION TAG	UNP Q04195
A	477	HIS	-	EXPRESSION TAG	UNP Q04195
A	478	HIS	-	EXPRESSION TAG	UNP Q04195
A	479	HIS	-	EXPRESSION TAG	UNP Q04195
A	480	HIS	-	EXPRESSION TAG	UNP Q04195

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

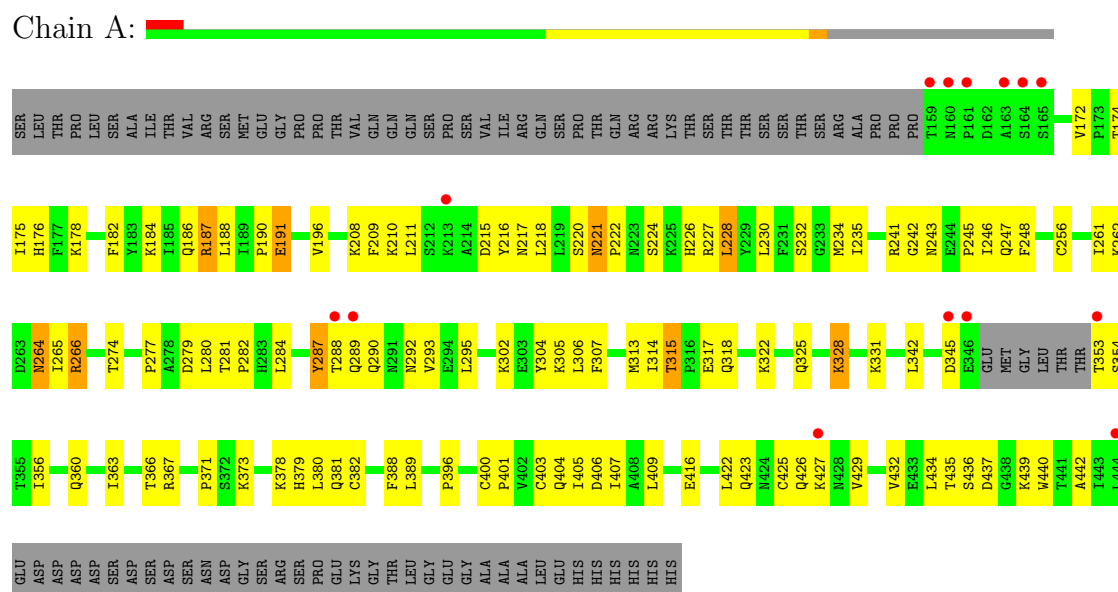
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total 66	O 66	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: E3 SUMO-protein ligase SIZ1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.49Å 88.98Å 105.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.02 – 2.60 34.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (34.02-2.60) 98.0 (34.02-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.211 , 0.259 0.215 , 0.218	Depositor DCC
$R_{free}$ test set	661 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 13193 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	A	0.43	0/2286	0.66	0/3097

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2235	0	2246	107	0
2	A	1	0	0	0	0
3	A	66	0	0	7	0
All	All	2302	0	2246	107	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (107) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:ILE:HG22	1:A:279:ASP:HB2	1.56	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:MET:CE	1:A:302:LYS:HD3	2.10	0.82
1:A:211:LEU:HD11	1:A:284:LEU:HD13	1.65	0.78
1:A:234:MET:HE1	1:A:302:LYS:HD3	1.67	0.77
1:A:228:LEU:HD13	1:A:280:LEU:HD12	1.65	0.77
1:A:208:LYS:HG2	1:A:292:ASN:ND2	2.01	0.76
1:A:315:THR:HG22	1:A:318:GLN:H	1.52	0.75
1:A:184:LYS:HE3	1:A:314:ILE:HD11	1.70	0.74
1:A:227:ARG:HH21	1:A:281:THR:HB	1.54	0.73
1:A:315:THR:CG2	1:A:317:GLU:HG2	2.18	0.73
1:A:227:ARG:NH2	1:A:281:THR:HB	2.02	0.73
1:A:246:ILE:HD13	1:A:277:PRO:HD3	1.73	0.70
1:A:221:ASN:OD1	1:A:222:PRO:HD2	1.92	0.69
1:A:256:CYS:HB2	1:A:261:ILE:HD11	1.74	0.69
1:A:221:ASN:HB3	1:A:224:SER:HB3	1.74	0.69
1:A:287:TYR:CD2	1:A:288:THR:HG23	2.29	0.68
1:A:396:PRO:HB3	3:A:37:HOH:O	1.94	0.68
1:A:266:ARG:HH11	1:A:266:ARG:HB3	1.58	0.67
1:A:403:CYS:SG	1:A:405:ILE:HG23	2.35	0.67
1:A:210:LYS:HG2	1:A:290:GLN:HA	1.76	0.66
1:A:315:THR:HG22	1:A:318:GLN:HG3	1.79	0.65
1:A:328:LYS:HB3	1:A:328:LYS:NZ	2.12	0.65
1:A:245:PRO:HD2	3:A:28:HOH:O	1.96	0.65
1:A:210:LYS:HZ2	1:A:210:LYS:HB3	1.62	0.64
1:A:367:ARG:HD3	3:A:61:HOH:O	1.96	0.64
1:A:226:HIS:C	1:A:227:ARG:HG2	2.19	0.63
1:A:235:ILE:HD11	1:A:305:LYS:HB2	1.82	0.62
1:A:426:GLN:HB2	1:A:429:VAL:HG23	1.81	0.61
1:A:210:LYS:HB3	1:A:210:LYS:NZ	2.14	0.61
1:A:295:LEU:HD22	1:A:306:LEU:HD21	1.82	0.61
1:A:388:PHE:CZ	1:A:407:ILE:HD11	2.36	0.60
1:A:356:ILE:HD12	1:A:356:ILE:N	2.17	0.60
1:A:360:GLN:NE2	3:A:61:HOH:O	2.34	0.60
1:A:437:ASP:OD2	1:A:439:LYS:HD3	2.00	0.60
1:A:266:ARG:HH11	1:A:266:ARG:CB	2.15	0.60
1:A:262:LYS:HE2	1:A:264:ASN:HD22	1.66	0.60
1:A:287:TYR:HD2	1:A:288:THR:HG23	1.67	0.59
1:A:432:VAL:CG1	1:A:440:TRP:HB2	2.33	0.59
1:A:366:THR:HG22	1:A:367:ARG:N	2.16	0.58
1:A:429:VAL:HG11	1:A:442:ALA:HB1	1.84	0.58
1:A:373:LYS:HE3	3:A:64:HOH:O	2.03	0.58
1:A:187:ARG:HH11	1:A:187:ARG:HG2	1.70	0.57
1:A:209:PHE:HE2	1:A:293:VAL:HG23	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:353:THR:HG22	1:A:354:SER:N	2.20	0.57
1:A:325:GLN:O	1:A:325:GLN:HG2	2.04	0.57
1:A:328:LYS:HD3	1:A:416:GLU:HB2	1.88	0.56
1:A:234:MET:HE2	1:A:302:LYS:HD3	1.84	0.56
1:A:226:HIS:O	1:A:227:ARG:HG2	2.06	0.56
1:A:210:LYS:HE2	1:A:289:GLN:N	2.20	0.56
1:A:363:ILE:HD11	1:A:401:PRO:HG2	1.88	0.56
1:A:342:LEU:HD12	1:A:436:SER:HA	1.89	0.55
1:A:381:GLN:NE2	1:A:382:CYS:O	2.41	0.54
1:A:211:LEU:CD1	1:A:284:LEU:HD13	2.37	0.54
1:A:322:LYS:NZ	1:A:322:LYS:HB3	2.23	0.54
1:A:315:THR:HG23	1:A:317:GLU:HG2	1.86	0.54
1:A:426:GLN:HB2	1:A:429:VAL:CG2	2.38	0.53
1:A:306:LEU:N	1:A:306:LEU:HD12	2.23	0.53
1:A:371:PRO:HG3	1:A:422:LEU:CD2	2.39	0.52
1:A:315:THR:HG21	1:A:317:GLU:HG2	1.92	0.52
1:A:187:ARG:NH2	1:A:218:LEU:HD11	2.24	0.52
1:A:217:ASN:ND2	3:A:34:HOH:O	2.43	0.52
1:A:208:LYS:HE3	1:A:292:ASN:HD21	1.75	0.51
1:A:366:THR:CG2	1:A:367:ARG:N	2.74	0.50
1:A:187:ARG:NH1	1:A:215:ASP:OD1	2.44	0.49
1:A:211:LEU:HD11	1:A:284:LEU:CD1	2.39	0.49
1:A:208:LYS:HE3	1:A:292:ASN:ND2	2.28	0.49
1:A:315:THR:CG2	1:A:318:GLN:HG3	2.42	0.48
1:A:328:LYS:HZ3	1:A:328:LYS:HB3	1.78	0.48
1:A:175:ILE:HG13	1:A:241:ARG:NH2	2.29	0.48
1:A:196:VAL:HB	1:A:304:TYR:HB2	1.96	0.48
1:A:227:ARG:HH21	1:A:281:THR:CB	2.24	0.48
1:A:262:LYS:HE2	1:A:264:ASN:ND2	2.29	0.47
1:A:315:THR:HG22	1:A:318:GLN:N	2.26	0.47
1:A:371:PRO:HG3	1:A:422:LEU:HD22	1.97	0.46
1:A:218:LEU:HB3	1:A:226:HIS:CG	2.50	0.46
1:A:182:PHE:HB3	1:A:266:ARG:HH22	1.79	0.46
1:A:331:LYS:HG3	1:A:416:GLU:OE1	2.15	0.46
1:A:230:LEU:HD12	1:A:307:PHE:O	2.15	0.46
1:A:322:LYS:HZ1	1:A:322:LYS:HB3	1.81	0.46
1:A:184:LYS:CE	1:A:314:ILE:HD11	2.43	0.45
1:A:247:GLN:CD	3:A:29:HOH:O	2.56	0.44
1:A:265:ILE:HD13	1:A:277:PRO:O	2.16	0.44
1:A:217:ASN:N	1:A:217:ASN:ND2	2.66	0.44
1:A:426:GLN:O	1:A:429:VAL:HG23	2.19	0.43
1:A:315:THR:HB	1:A:318:GLN:HE21	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:LYS:HB3	1:A:328:LYS:HZ2	1.84	0.42
1:A:232:SER:HB3	1:A:248:PHE:CD1	2.54	0.42
1:A:178:LYS:HG2	1:A:243:ASN:ND2	2.34	0.42
1:A:389:LEU:HD21	1:A:409:LEU:HD21	2.01	0.42
1:A:227:ARG:NH2	1:A:282:PRO:HD3	2.34	0.42
1:A:190:PRO:HG2	1:A:191:GLU:HG2	2.02	0.42
1:A:378:LYS:O	1:A:379:HIS:HB3	2.20	0.42
1:A:217:ASN:N	1:A:217:ASN:HD22	2.16	0.42
1:A:210:LYS:HE2	1:A:289:GLN:H	1.85	0.41
1:A:210:LYS:HZ1	1:A:288:THR:HA	1.85	0.41
1:A:435:THR:C	1:A:437:ASP:N	2.73	0.41
1:A:313:MET:HA	1:A:313:MET:CE	2.50	0.41
1:A:315:THR:HG23	1:A:317:GLU:H	1.85	0.41
1:A:400:CYS:O	1:A:404:GLN:HA	2.19	0.41
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.92	0.41
1:A:354:SER:HB2	1:A:434:LEU:O	2.21	0.41
1:A:184:LYS:HB2	1:A:184:LYS:HE3	1.88	0.40
1:A:191:GLU:HB2	1:A:209:PHE:HB3	2.03	0.40
1:A:353:THR:CG2	1:A:354:SER:N	2.84	0.40
1:A:425:CYS:SG	1:A:429:VAL:HB	2.61	0.40
1:A:247:GLN:HA	1:A:274:THR:O	2.21	0.40
1:A:176:HIS:HB3	1:A:242:GLY:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	276/371 (74%)	238 (86%)	32 (12%)	6 (2%)	10 18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	TYR

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Mol	Chain	Res	Type
1	A	427	LYS
1	A	220	SER
1	A	221	ASN
1	A	216	TYR
1	A	172	VAL

### 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	256/338 (76%)	242 (94%)	14 (6%)	30 56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	THR
1	A	186	GLN
1	A	187	ARG
1	A	188	LEU
1	A	191	GLU
1	A	228	LEU
1	A	264	ASN
1	A	266	ARG
1	A	315	THR
1	A	328	LYS
1	A	345	ASP
1	A	380	LEU
1	A	406	ASP
1	A	423	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	223	ASN
1	A	243	ASN

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Mol	Chain	Res	Type
1	A	260	GLN
1	A	264	ASN
1	A	289	GLN
1	A	292	ASN
1	A	318	GLN
1	A	399	GLN
1	A	411	ASN
1	A	424	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	280/371 (75%)	0.19	14 (5%) 28 24	39, 61, 106, 135	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	ASN	5.7
1	A	164	SER	5.6
1	A	346	GLU	5.2
1	A	163	ALA	4.7
1	A	288	THR	4.2
1	A	345	ASP	4.1
1	A	213	LYS	3.8
1	A	165	SER	3.7
1	A	161	PRO	3.4
1	A	289	GLN	2.9
1	A	159	THR	2.5
1	A	353	THR	2.4
1	A	427	LYS	2.3
1	A	444	LEU	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	1	1/1	0.12	-0.48	57,57,57,57	0

## 6.5 Other polymers

There are no such residues in this entry.