



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 03:28 am BST

PDB ID : 4JUE  
Title : Crystal structure of Plasmodium falciparum ubiquitin conjugating enzyme UBC9  
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Deposited on : 2013-03-24  
Resolution : 1.85 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](mailto: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.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

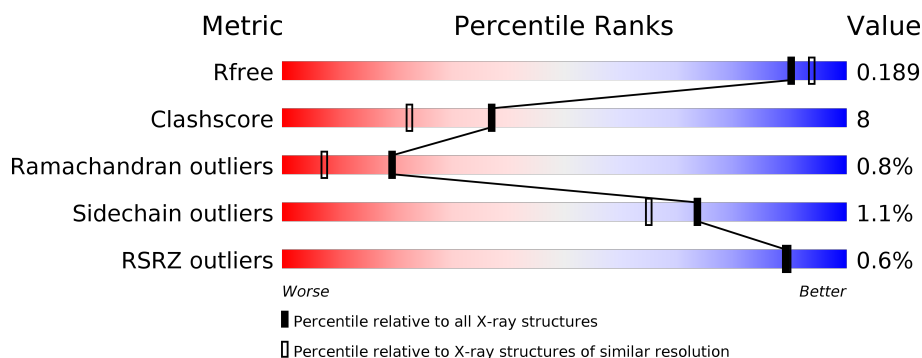
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 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	161	
1	B	161	
1	C	161	
1	D	161	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6378 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 Ubiquitin conjugating enzyme UBC9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	5	7	0
			1311	845	217	242	7			
1	B	159	Total	C	N	O	S	10	6	0
			1312	843	215	247	7			
1	C	159	Total	C	N	O	S	12	5	0
			1305	840	214	244	7			
1	D	159	Total	C	N	O	S	3	6	0
			1313	845	218	244	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q8I301
A	0	SER	-	EXPRESSION TAG	UNP Q8I301
B	-1	GLY	-	EXPRESSION TAG	UNP Q8I301
B	0	SER	-	EXPRESSION TAG	UNP Q8I301
C	-1	GLY	-	EXPRESSION TAG	UNP Q8I301
C	0	SER	-	EXPRESSION TAG	UNP Q8I301
D	-1	GLY	-	EXPRESSION TAG	UNP Q8I301
D	0	SER	-	EXPRESSION TAG	UNP Q8I301


- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	308	Total	O	0	0
			308	308		
2	B	256	Total	O	0	0
			256	256		
2	C	274	Total	O	0	0
			274	274		
2	D	299	Total	O	0	0
			299	299		

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

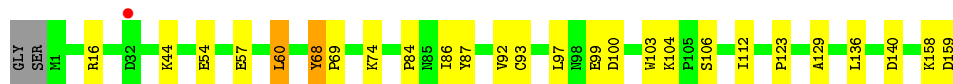
- Molecule 1: Ubiquitin conjugating enzyme UBC9

Chain A:  82% 16% ..




- Molecule 1: Ubiquitin conjugating enzyme UBC9

Chain B:  83% 15% ..




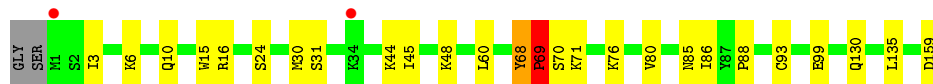
- Molecule 1: Ubiquitin conjugating enzyme UBC9

Chain C:  80% 19% ..



- Molecule 1: Ubiquitin conjugating enzyme UBC9

Chain D:  83% 15% ...



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	28.87Å 94.39Å 124.89Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	24.98 – 1.85 24.98 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.6 (24.98-1.85) 93.5 (24.98-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.146 , 0.188 0.149 , 0.189	Depositor DCC
$R_{free}$ test set	2709 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
Reported twinning fraction	0.490 for -h,-k,l	Depositor
Outliers	1 of 53373 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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 28.31 % 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 1.8841e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical 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](#)

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	0.33	0/1368	0.61	1/1848 (0.1%)
1	B	0.38	0/1366	0.68	1/1838 (0.1%)
1	C	0.35	0/1353	0.66	1/1824 (0.1%)
1	D	0.32	0/1364	0.80	3/1837 (0.2%)
All	All	0.35	0/5451	0.69	6/7347 (0.1%)

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	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	68	TYR	C-N-CD	-19.40	77.92	120.60
1	D	68	TYR	C-N-CA	10.29	165.23	122.00
1	B	68	TYR	C-N-CD	-9.82	98.99	120.60
1	C	68	TYR	C-N-CD	-9.81	99.01	120.60
1	A	68	TYR	C-N-CD	-7.33	104.48	120.60
1	D	69	PRO	CA-N-CD	-6.51	102.38	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	TYR	Peptide
1	B	158	LYS	Peptide
1	B	68	TYR	Peptide
1	C	68	TYR	Peptide
1	D	68	TYR	Peptide

## 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	1311	0	1328	22	0
1	B	1312	0	1314	20	1
1	C	1305	0	1309	23	2
1	D	1313	0	1325	18	2
2	A	308	0	0	15	1
2	B	256	0	0	8	1
2	C	274	0	0	11	3
2	D	299	0	0	15	3
All	All	6378	0	5276	81	8

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 (81) 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:C:159[A]:ASP:OD2	2:C:227:HOH:O	1.99	0.79
1:A:19:HIS:CE1	1:B:159[A]:ASP:HA	2.20	0.76
1:C:2:SER:O	1:C:4:ALA:N	2.22	0.73
1:A:70[A]:SER:OG	2:A:291:HOH:O	2.08	0.72
1:D:85:ASN:O	2:D:485:HOH:O	2.09	0.71
1:A:74:LYS:NZ	2:A:407:HOH:O	2.25	0.70
1:C:93:CYS:SG	2:C:428:HOH:O	2.51	0.68
1:C:2:SER:O	2:C:233:HOH:O	2.13	0.66
1:B:60:LEU:HB3	2:B:432:HOH:O	1.95	0.65
1:A:51:GLY:O	2:A:279:HOH:O	2.14	0.65
1:B:140:ASP:OD2	2:B:349:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:SER:HA	1:B:159[C]:ASP:OD1	1.97	0.64
1:C:2:SER:OG	1:C:66:GLU:OE1	2.14	0.61
1:D:6:LYS:NZ	2:D:445:HOH:O	2.33	0.60
1:C:130:GLN:OE1	2:C:326:HOH:O	2.16	0.60
1:A:6:LYS:NZ	2:A:393:HOH:O	2.35	0.59
1:A:145:GLU:OE2	2:A:436:HOH:O	2.17	0.58
1:C:99:GLU:OE1	2:C:409:HOH:O	2.17	0.58
1:D:93:CYS:N	2:D:485:HOH:O	2.35	0.58
1:A:74:LYS:NZ	2:A:453:HOH:O	2.37	0.57
1:A:11:GLU:OE1	2:A:491:HOH:O	2.17	0.56
1:D:48:LYS:HD2	2:D:470:HOH:O	2.05	0.56
1:A:1:MET:N	2:A:498:HOH:O	2.39	0.55
1:D:60:LEU:HB3	2:D:469:HOH:O	2.06	0.55
1:B:97:LEU:HD21	1:B:112:ILE:HG23	1.90	0.54
1:D:10[B]:GLN:HG3	2:D:474:HOH:O	2.09	0.53
1:C:121:ASP:OD2	2:C:221:HOH:O	2.19	0.52
1:C:57[B]:GLU:CD	1:C:157:PRO:HG3	2.30	0.52
1:B:99:GLU:OE2	2:B:357:HOH:O	2.19	0.52
1:D:69:PRO:HD2	1:D:70:SER:H	1.76	0.51
1:D:76[B]:LYS:HD2	2:D:293:HOH:O	2.12	0.49
1:B:100:ASP:OD2	2:B:232:HOH:O	2.19	0.49
1:D:16:ARG:HD2	2:D:437:HOH:O	2.12	0.49
1:B:44:LYS:HE3	2:B:409:HOH:O	2.14	0.48
1:A:30[A]:MET:HG3	1:A:37:ASP:HB2	1.96	0.47
1:A:93:CYS:SG	2:A:446:HOH:O	2.60	0.47
1:C:26:LYS:NZ	2:C:366:HOH:O	2.47	0.47
1:D:45:ILE:HG13	2:D:469:HOH:O	2.14	0.47
1:B:16:ARG:NH1	2:B:446:HOH:O	2.48	0.47
1:D:86:ILE:O	1:D:130:GLN:HB2	2.15	0.46
1:B:87:TYR:CE2	1:B:93[B]:CYS:SG	3.08	0.46
1:B:54:GLU:OE1	2:B:375:HOH:O	2.21	0.46
1:C:124:ASN:HB2	2:C:321:HOH:O	2.15	0.46
1:A:142:ASP:OD2	1:A:146[B]:LYS:HE3	2.16	0.46
1:B:136:LEU:HD22	1:B:140:ASP:HB3	1.99	0.45
1:B:44:LYS:HD3	1:B:57[A]:GLU:OE1	2.16	0.45
1:C:16:ARG:NH1	2:C:308:HOH:O	2.49	0.45
1:D:71:LYS:HG2	1:D:99:GLU:OE1	2.16	0.45
1:B:93[B]:CYS:SG	1:B:129:ALA:HB2	2.57	0.45
1:C:99:GLU:HA	1:C:103:TRP:HB3	1.99	0.45
1:D:44:LYS:NZ	2:D:457:HOH:O	2.23	0.45
1:D:30:MET:O	2:D:497:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:HB3	1:A:121:ASP:OD2	2.18	0.44
1:C:2:SER:C	1:C:4:ALA:H	2.17	0.44
1:B:74:LYS:HD2	2:D:461:HOH:O	2.18	0.44
1:A:42:ILE:HG21	2:A:372:HOH:O	2.17	0.44
1:A:72:PRO:HB3	1:A:103:TRP:CD2	2.53	0.43
1:A:14:GLU:HG2	2:A:487:HOH:O	2.17	0.43
1:C:98:ASN:HB3	1:C:101:GLU:HB2	1.99	0.43
1:C:149:LYS:O	1:C:153[B]:ILE:HG12	2.19	0.43
1:A:124:ASN:HB2	2:A:257:HOH:O	2.18	0.42
1:A:25:ALA:N	1:B:159[C]:ASP:OD2	2.38	0.42
1:D:80:VAL:HG21	1:D:88:PRO:O	2.20	0.42
1:C:85:ASN:ND2	1:C:127:SER:O	2.45	0.42
1:C:5:LYS:HG2	1:C:39[B]:MET:HE3	2.01	0.42
1:C:57[A]:GLU:OE2	1:C:157:PRO:HG3	2.20	0.42
1:B:86:ILE:HD12	1:B:92:VAL:HG22	2.01	0.41
1:C:64:PHE:CD2	1:C:73:PRO:HB3	2.55	0.41
1:D:159[A]:ASP:OD2	2:D:397:HOH:O	2.22	0.41
1:A:27:TYR:HB2	1:A:36:LEU:HB3	2.03	0.41
1:A:30[B]:MET:HG2	2:A:481:HOH:O	2.21	0.41
1:B:104:LYS:NZ	2:B:220:HOH:O	2.54	0.41
1:B:99:GLU:HA	1:B:103:TRP:HB3	2.03	0.41
1:C:86:ILE:O	1:C:130:GLN:HB2	2.21	0.41
1:C:153[B]:ILE:HD13	2:C:275:HOH:O	2.21	0.41
1:D:135:LEU:HD23	2:D:473:HOH:O	2.20	0.40
1:A:127:SER:HA	2:A:425:HOH:O	2.21	0.40
1:D:93:CYS:SG	2:D:471:HOH:O	2.51	0.40
1:B:84:PRO:HG2	1:B:123:PRO:HB3	2.04	0.40
1:C:122:ASN:ND2	2:C:436:HOH:O	2.38	0.40

All (8) 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:C:159[B]:ASP:OD2	1:D:24:SER:OG[1_556]	1.98	0.22
2:C:258:HOH:O	2:C:447:HOH:O[1_455]	2.05	0.15
2:D:282:HOH:O	2:D:468:HOH:O[1_455]	2.12	0.08
1:C:16:ARG:NH2	2:D:467:HOH:O[1_656]	2.12	0.08
2:D:226:HOH:O	2:D:249:HOH:O[1_455]	2.16	0.04
1:B:106[B]:SER:OG	2:B:277:HOH:O[1_455]	2.17	0.03
2:A:342:HOH:O	2:C:383:HOH:O[1_455]	2.17	0.03
1:D:15:TRP:NE1	2:C:466:HOH:O[1_554]	2.18	0.02

## 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	164/161 (102%)	161 (98%)	2 (1%)	1 (1%)	25	12
1	B	162/161 (101%)	159 (98%)	2 (1%)	1 (1%)	25	12
1	C	161/161 (100%)	156 (97%)	3 (2%)	2 (1%)	13	3
1	D	162/161 (101%)	158 (98%)	3 (2%)	1 (1%)	25	12
All	All	649/644 (101%)	634 (98%)	10 (2%)	5 (1%)	19	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	PRO
1	B	69	PRO
1	C	3	ILE
1	C	69	PRO
1	D	69	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	147/142 (104%)	145 (99%)	2 (1%)	67	55
1	B	147/142 (104%)	146 (99%)	1 (1%)	84	79
1	C	145/142 (102%)	143 (99%)	2 (1%)	67	55
1	D	146/142 (103%)	144 (99%)	2 (1%)	67	55
All	All	585/568 (103%)	578 (99%)	7 (1%)	73	62

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70[A]	SER
1	A	70[B]	SER
1	B	60	LEU
1	C	30	MET
1	C	142	ASP
1	D	3	ILE
1	D	31	SER

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

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

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, 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	159/161 (98%)	-0.79	0	100   100	12, 21, 38, 69	3 (1%)
1	B	159/161 (98%)	-0.73	1 (0%)	89   89	13, 22, 40, 78	6 (3%)
1	C	159/161 (98%)	-0.74	1 (0%)	89   89	12, 22, 42, 77	8 (5%)
1	D	159/161 (98%)	-0.78	2 (1%)	77   78	13, 21, 43, 77	3 (1%)
All	All	636/644 (98%)	-0.76	4 (0%)	89   89	12, 22, 42, 78	20 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	ASP	2.7
1	D	34	LYS	2.4
1	C	31	SER	2.3
1	D	1	MET	2.2

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.