



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:36 PM GMT

PDB ID : 2PQI  
Title : Crystal structure of active ribosome inactivating protein from maize (b-32)  
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Deposited on : 2007-05-02  
Resolution : 2.50 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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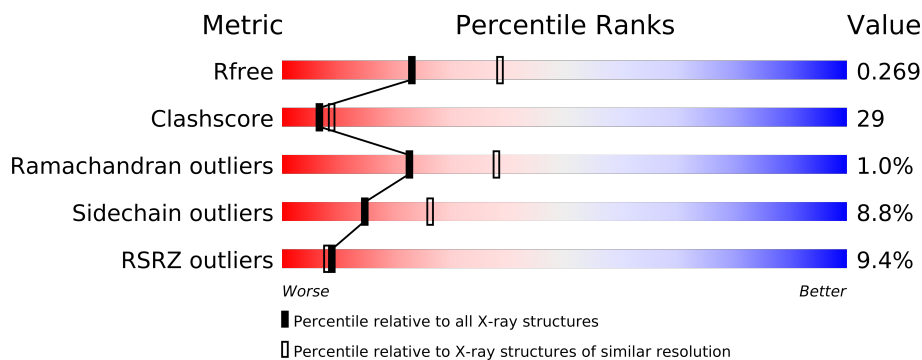
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	243	
1	B	243	
1	C	243	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5496 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 Ribosome-inactivatingprotein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1868	1193	329	338	8			
1	B	235	Total	C	N	O	S	0	0	0
			1857	1187	327	335	8			
1	C	227	Total	C	N	O	S	0	0	0
			1684	1073	295	309	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	EXPRESSION TAG	UNP P25891
A	165	LEU	-	LINKER	UNP P25891
A	166	GLU	-	LINKER	UNP P25891
B	21	MET	-	EXPRESSION TAG	UNP P25891
B	165	LEU	-	LINKER	UNP P25891
B	166	GLU	-	LINKER	UNP P25891
C	21	MET	-	EXPRESSION TAG	UNP P25891
C	165	LEU	-	LINKER	UNP P25891
C	166	GLU	-	LINKER	UNP P25891

- Molecule 2 is water.

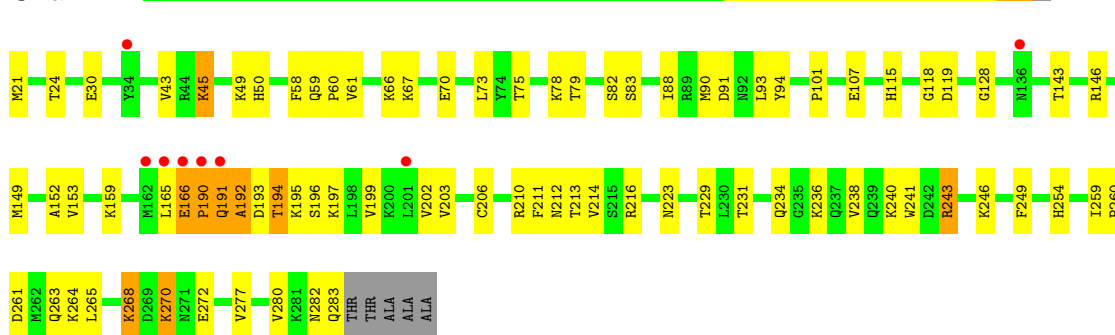
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	52	Total	O	0	0
			52	52		
2	B	20	Total	O	0	0
			20	20		
2	C	15	Total	O	0	0
			15	15		

### 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.

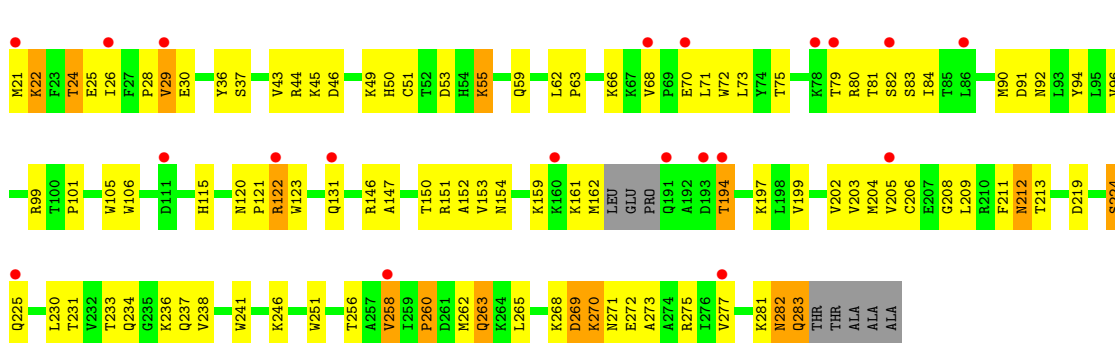
#### • Molecule 1: Ribosome-inactivatingprotein 3

Chain A:



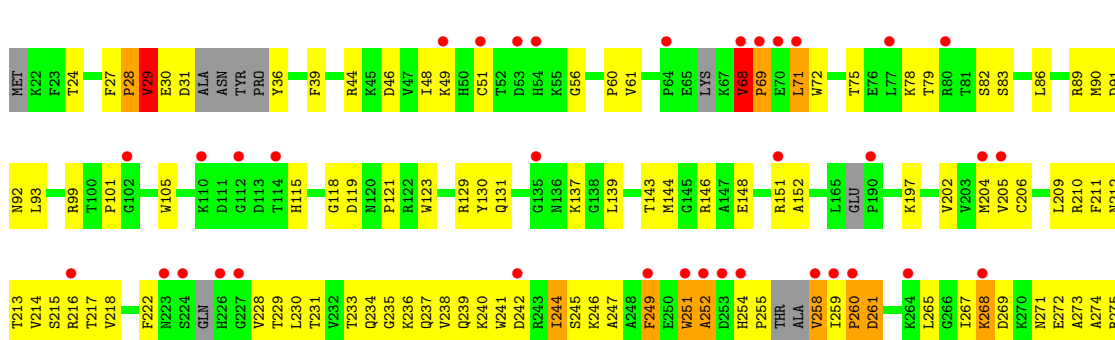
#### • Molecule 1: Ribosome-inactivatingprotein 3

Chain B:



#### • Molecule 1: Ribosome-inactivatingprotein 3

Chain C:



I276		
V277		
A278		
L279		
V280		
K281		
N282		
GLN		
THR		
THR		
ALA		
ALA		
ALA		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.19Å 115.19Å 45.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.9 (20.00-2.50) 93.9 (19.95-2.50)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.19 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.217 , 0.261 0.226 , 0.269	Depositor DCC
$R_{free}$ test set	1120 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.1	EDS
Estimated twinning fraction	0.033 for -h,-k,l 0.031 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 21753 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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

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	0.42	0/1910	0.62	0/2583
1	B	0.36	0/1897	0.60	0/2562
1	C	0.35	0/1714	0.60	1/2319 (0.0%)
All	All	0.38	0/5521	0.61	1/7464 (0.0%)

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	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	VAL	C-N-CD	-7.66	103.76	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	LEU	Peptide
1	A	192	ALA	Peptide
1	C	252	ALA	Peptide

## 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	1868	0	1881	94	0
1	B	1857	0	1882	104	0
1	C	1684	0	1620	130	0
2	A	52	0	0	1	0
2	B	20	0	0	1	0
2	C	15	0	0	0	0
All	All	5496	0	5383	318	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 29.

All (318) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:166:GLU:N	1:A:190:PRO:HD2	1.38	1.18
1:B:246:LYS:HE3	1:B:283:GLN:HE21	1.01	1.15
1:A:192:ALA:HB1	1:A:195:LYS:HG3	1.22	1.11
1:C:56:GLY:HA3	1:C:252:ALA:HB1	1.29	1.11
1:C:68:VAL:O	1:C:69:PRO:O	1.69	1.10
1:B:161:LYS:HG2	1:B:162:MET:H	1.13	1.10
1:C:69:PRO:HG2	1:C:72:TRP:CZ2	1.86	1.09
1:A:152:ALA:HA	1:A:197:LYS:HD2	1.34	1.09
1:C:71:LEU:HB2	1:C:90:MET:HE3	1.12	1.09
1:A:192:ALA:CB	1:A:195:LYS:HG3	1.85	1.05
1:B:29:VAL:HB	1:B:79:THR:HG22	1.38	1.05
1:B:246:LYS:HG3	1:B:283:GLN:NE2	1.71	1.05
1:C:29:VAL:CG2	1:C:79:THR:HA	1.87	1.04
1:A:166:GLU:H	1:A:190:PRO:CD	1.70	1.03
1:B:24:THR:HG21	1:B:43:VAL:HG22	1.40	1.03
1:C:71:LEU:CB	1:C:90:MET:HE3	1.89	1.03
1:A:246:LYS:HE2	1:A:283:GLN:NE2	1.75	1.02
1:B:161:LYS:HG2	1:B:162:MET:N	1.75	0.99
1:C:68:VAL:O	1:C:68:VAL:HG22	1.63	0.97
1:B:122:ARG:HH21	1:B:122:ARG:HG3	1.26	0.97
1:A:59:GLN:HE21	1:A:277:VAL:HG23	1.30	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:69:PRO:HG2	1:C:72:TRP:HZ2	1.29	0.95
1:B:246:LYS:HE3	1:B:283:GLN:NE2	1.81	0.94
1:A:190:PRO:O	1:A:191:GLN:HG3	1.68	0.94
1:A:231:THR:H	1:A:234:GLN:HE21	1.07	0.93
1:B:152:ALA:HA	1:B:197:LYS:HD2	1.49	0.92
1:A:246:LYS:HG2	1:A:283:GLN:NE2	1.84	0.92
1:A:166:GLU:N	1:A:190:PRO:CD	2.30	0.92
1:C:251:TRP:O	1:C:255:PRO:HB3	1.70	0.91
1:C:29:VAL:HG21	1:C:79:THR:HA	1.49	0.91
1:A:50:HIS:HB2	1:A:90:MET:HE1	1.53	0.90
1:B:246:LYS:CE	1:B:283:GLN:HE21	1.83	0.90
1:A:24:THR:OG1	1:A:43:VAL:HG22	1.72	0.90
1:B:258:VAL:O	1:B:258:VAL:HG22	1.71	0.89
1:C:211:PHE:HB3	1:C:213:THR:HG22	1.54	0.88
1:B:50:HIS:HB2	1:B:90:MET:HE1	1.57	0.86
1:B:59:GLN:HE21	1:B:277:VAL:HG13	1.40	0.85
1:A:246:LYS:HG2	1:A:283:GLN:CD	1.96	0.85
1:C:56:GLY:HA3	1:C:252:ALA:CB	2.08	0.84
1:A:192:ALA:HB1	1:A:195:LYS:CG	2.06	0.84
1:B:122:ARG:CG	1:B:122:ARG:HH21	1.90	0.84
1:A:212:ASN:O	1:A:216:ARG:HG2	1.78	0.83
1:C:71:LEU:HB2	1:C:90:MET:CE	2.04	0.83
1:A:24:THR:HG22	1:A:75:THR:HA	1.61	0.83
1:A:59:GLN:NE2	1:A:277:VAL:HG23	1.94	0.82
1:C:29:VAL:HG21	1:C:79:THR:CA	2.09	0.82
1:A:50:HIS:HB2	1:A:90:MET:CE	2.10	0.81
1:A:211:PHE:HB3	1:A:213:THR:HG22	1.62	0.81
1:B:59:GLN:NE2	1:B:277:VAL:HG13	1.95	0.80
1:A:264:LYS:HG3	1:C:254:HIS:CE1	2.17	0.80
1:A:192:ALA:HA	1:A:194:THR:HG23	1.64	0.79
1:C:29:VAL:HG22	1:C:78:LYS:O	1.83	0.79
1:B:29:VAL:CB	1:B:79:THR:HG22	2.12	0.78
1:B:273:ALA:O	1:B:277:VAL:HG12	1.82	0.78
1:C:69:PRO:CG	1:C:72:TRP:CZ2	2.66	0.77
1:C:281:LYS:O	1:C:282:ASN:CB	2.36	0.74
1:B:251:TRP:CH2	1:B:262:MET:HG3	2.23	0.74
1:C:251:TRP:O	1:C:255:PRO:CB	2.36	0.73
1:B:43:VAL:HG13	1:B:73:LEU:HD21	1.69	0.73
1:C:29:VAL:HG23	1:C:79:THR:HA	1.71	0.73
1:C:71:LEU:CB	1:C:90:MET:CE	2.65	0.73
1:A:152:ALA:CA	1:A:197:LYS:HD2	2.15	0.72
1:B:233:THR:O	1:B:237:GLN:HG3	1.89	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:268:LYS:HE2	1:A:268:LYS:N	2.04	0.72
1:C:152:ALA:HA	1:C:197:LYS:HD2	1.71	0.72
1:A:246:LYS:HE2	1:A:283:GLN:HE22	1.55	0.72
1:B:211:PHE:HB3	1:B:213:THR:HG22	1.71	0.72
1:C:268:LYS:HG3	1:C:272:GLU:OE1	1.90	0.71
1:C:237:GLN:HE22	1:C:276:ILE:HD13	1.56	0.71
1:A:246:LYS:HE2	1:A:283:GLN:HE21	1.55	0.71
1:C:29:VAL:HG21	1:C:79:THR:CG2	2.20	0.71
1:A:231:THR:H	1:A:234:GLN:NE2	1.86	0.71
1:B:43:VAL:CG1	1:B:73:LEU:HD21	2.21	0.70
1:A:93:LEU:HD12	1:A:210:ARG:HG2	1.72	0.70
1:A:24:THR:CG2	1:A:75:THR:HA	2.21	0.70
1:B:246:LYS:HG3	1:B:283:GLN:CD	2.12	0.70
1:C:68:VAL:O	1:C:68:VAL:CG2	2.36	0.70
1:B:258:VAL:O	1:B:258:VAL:CG2	2.40	0.70
1:B:24:THR:OG1	1:B:75:THR:HG22	1.92	0.69
1:A:50:HIS:CB	1:A:90:MET:HE1	2.20	0.69
1:C:240:LYS:O	1:C:244:ILE:HG22	1.92	0.69
1:B:84:ILE:HG12	1:B:153:VAL:HG13	1.74	0.69
1:B:26:ILE:O	1:B:28:PRO:HD3	1.93	0.69
1:C:234:GLN:O	1:C:238:VAL:HG23	1.93	0.69
1:B:50:HIS:HB2	1:B:90:MET:CE	2.23	0.68
1:C:56:GLY:CA	1:C:252:ALA:HB1	2.16	0.67
1:A:264:LYS:CG	1:C:254:HIS:CE1	2.76	0.67
1:A:24:THR:HG21	1:A:75:THR:HG22	1.77	0.67
1:C:29:VAL:HG21	1:C:79:THR:HG22	1.76	0.67
1:C:251:TRP:O	1:C:255:PRO:CA	2.44	0.66
1:A:240:LYS:HG3	1:A:265:LEU:HD11	1.77	0.65
1:C:92:ASN:HB3	1:C:281:LYS:HE2	1.78	0.64
1:B:50:HIS:CB	1:B:90:MET:HE1	2.28	0.64
1:A:190:PRO:C	1:A:191:GLN:HG3	2.16	0.64
1:A:264:LYS:CG	1:C:254:HIS:HE1	2.10	0.64
1:B:246:LYS:CG	1:B:283:GLN:NE2	2.58	0.64
1:B:224:SER:HA	2:B:304:HOH:O	1.97	0.64
1:C:29:VAL:CG2	1:C:79:THR:CA	2.69	0.63
1:C:231:THR:HG23	1:C:234:GLN:NE2	2.14	0.63
1:C:202:VAL:O	1:C:206:CYS:HB2	2.00	0.62
1:A:246:LYS:CE	1:A:283:GLN:NE2	2.58	0.62
1:B:62:LEU:O	1:B:282:ASN:ND2	2.30	0.62
1:B:106:TRP:HH2	1:B:161:LYS:HA	1.65	0.61
1:A:66:LYS:NZ	1:A:70:GLU:OE1	2.33	0.61
1:C:233:THR:HA	1:C:236:LYS:HD3	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:LEU:HD12	1:A:210:ARG:CG	2.31	0.61
1:C:231:THR:OG1	1:C:234:GLN:HB2	2.00	0.61
1:C:68:VAL:O	1:C:69:PRO:C	2.40	0.60
1:B:92:ASN:HB3	1:B:281:LYS:HE2	1.84	0.60
1:C:211:PHE:HB3	1:C:213:THR:CG2	2.30	0.60
1:B:268:LYS:HD3	1:B:269:ASP:OD2	2.00	0.60
1:B:199:VAL:O	1:B:203:VAL:HG23	2.01	0.60
1:A:261:ASP:OD2	1:C:254:HIS:CD2	2.55	0.60
1:A:260:PRO:HB2	1:C:254:HIS:CE1	2.36	0.60
1:C:231:THR:H	1:C:234:GLN:HE21	1.50	0.60
1:C:129:ARG:NH1	1:C:131:GLN:HE21	1.99	0.60
1:C:273:ALA:O	1:C:277:VAL:HG22	2.02	0.59
1:B:68:VAL:O	1:B:68:VAL:HG12	2.01	0.59
1:B:161:LYS:CG	1:B:162:MET:H	2.01	0.59
1:B:122:ARG:NH2	1:B:122:ARG:HG3	2.05	0.59
1:B:50:HIS:CB	1:B:90:MET:CE	2.80	0.59
1:B:71:LEU:HD13	1:B:90:MET:CE	2.33	0.59
1:C:129:ARG:NH1	1:C:131:GLN:NE2	2.50	0.59
1:A:264:LYS:HG2	1:C:254:HIS:HE1	1.67	0.59
1:A:261:ASP:OD2	1:C:254:HIS:HD2	1.86	0.58
1:B:79:THR:O	1:B:81:THR:N	2.36	0.58
1:B:268:LYS:HG3	1:B:272:GLU:HG3	1.86	0.58
1:B:231:THR:H	1:B:234:GLN:HE21	1.50	0.58
1:B:24:THR:CG2	1:B:43:VAL:HG22	2.25	0.58
1:B:83:SER:O	1:B:101:PRO:HG3	2.03	0.58
1:C:29:VAL:HG22	1:C:78:LYS:C	2.24	0.58
1:C:129:ARG:HH12	1:C:131:GLN:NE2	2.01	0.58
1:A:246:LYS:CG	1:A:283:GLN:NE2	2.62	0.57
1:B:115:HIS:CD2	1:B:121:PRO:HG2	2.39	0.57
1:C:78:LYS:HA	1:C:83:SER:CB	2.34	0.57
1:C:130:TYR:CZ	1:C:139:LEU:HD21	2.39	0.57
1:A:199:VAL:O	1:A:203:VAL:HG23	2.04	0.57
1:B:147:ALA:HB1	1:B:151:ARG:HH12	1.70	0.57
1:C:240:LYS:HG3	1:C:265:LEU:HD11	1.86	0.57
1:C:82:SER:OG	1:C:101:PRO:HG2	2.05	0.57
1:C:115:HIS:CD2	1:C:121:PRO:HG2	2.39	0.56
1:A:211:PHE:CZ	1:A:238:VAL:HA	2.41	0.56
1:C:212:ASN:HA	1:C:215:SER:OG	2.04	0.56
1:C:92:ASN:O	1:C:210:ARG:NH2	2.36	0.56
1:C:237:GLN:NE2	1:C:276:ILE:HD13	2.19	0.56
1:B:202:VAL:O	1:B:206:CYS:HB2	2.05	0.56
1:A:94:TYR:OH	1:A:128:GLY:O	2.24	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:69:PRO:HD3	1:C:89:ARG:NH2	2.20	0.56
1:B:90:MET:O	1:B:91:ASP:C	2.44	0.56
1:A:24:THR:CG2	1:A:75:THR:HG22	2.36	0.55
1:C:29:VAL:O	1:C:146:ARG:NH2	2.40	0.55
1:B:231:THR:H	1:B:234:GLN:NE2	2.05	0.55
1:C:251:TRP:O	1:C:255:PRO:HA	2.06	0.54
1:C:144:MET:HB3	1:C:204:MET:SD	2.46	0.54
1:C:230:LEU:HD21	1:C:238:VAL:HG21	1.90	0.54
1:B:72:TRP:CH2	1:B:96:VAL:HG21	2.43	0.54
1:C:259:ILE:HG22	1:C:261:ASP:H	1.72	0.54
1:B:159:LYS:HE3	1:B:194:THR:OG1	2.08	0.54
1:C:69:PRO:HG3	1:C:89:ARG:HH21	1.72	0.54
1:C:259:ILE:HG22	1:C:260:PRO:N	2.21	0.54
1:C:69:PRO:HD3	1:C:89:ARG:HH22	1.72	0.54
1:C:242:ASP:OD2	1:C:281:LYS:HD2	2.08	0.54
1:A:61:VAL:HG22	1:A:280:VAL:HG23	1.90	0.54
1:B:29:VAL:O	1:B:146:ARG:NH2	2.35	0.54
1:C:272:GLU:O	1:C:275:ARG:HG2	2.07	0.53
1:B:161:LYS:CG	1:B:162:MET:N	2.58	0.53
1:C:69:PRO:HB2	1:C:72:TRP:NE1	2.23	0.53
1:A:45:LYS:O	1:A:49:LYS:HG3	2.07	0.53
1:C:267:ILE:HG12	1:C:276:ILE:CD1	2.39	0.53
1:C:244:ILE:HD12	1:C:244:ILE:O	2.08	0.53
1:C:29:VAL:CG2	1:C:78:LYS:O	2.56	0.52
1:C:269:ASP:OD1	1:C:271:ASN:HB2	2.09	0.52
1:C:46:ASP:O	1:C:49:LYS:HB2	2.08	0.52
1:A:24:THR:HG1	1:A:43:VAL:HG22	1.74	0.52
1:B:29:VAL:CG2	1:B:79:THR:HG22	2.39	0.52
1:A:30:GLU:OE2	1:A:79:THR:HB	2.10	0.52
1:B:50:HIS:CG	1:B:90:MET:HE2	2.44	0.52
1:B:79:THR:OG1	1:B:154:ASN:ND2	2.41	0.52
1:C:60:PRO:HB2	1:C:279:LEU:HD23	1.92	0.52
1:C:48:ILE:HA	1:C:51:CYS:SG	2.50	0.51
1:A:268:LYS:HB2	1:A:272:GLU:OE1	2.10	0.51
1:C:272:GLU:HA	1:C:275:ARG:HG2	1.92	0.51
1:B:79:THR:HG21	1:B:150:THR:HA	1.93	0.51
1:A:146:ARG:NE	1:A:223:ASN:OD1	2.33	0.51
1:B:230:LEU:HA	1:B:234:GLN:NE2	2.26	0.51
1:B:50:HIS:O	1:B:63:PRO:HG3	2.11	0.51
1:B:106:TRP:CH2	1:B:161:LYS:HA	2.44	0.50
1:B:90:MET:O	1:B:92:ASN:N	2.44	0.50
1:B:122:ARG:CG	1:B:122:ARG:NH2	2.60	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:213:THR:HG23	1:A:214:VAL:N	2.27	0.50
1:C:28:PRO:O	1:C:29:VAL:C	2.50	0.50
1:C:118:GLY:O	1:C:119:ASP:HB2	2.12	0.50
1:C:258:VAL:HG12	1:C:258:VAL:O	2.10	0.50
1:C:272:GLU:C	1:C:274:ALA:H	2.14	0.50
1:A:260:PRO:O	1:C:254:HIS:NE2	2.45	0.49
1:A:143:THR:HA	1:A:229:THR:HG22	1.92	0.49
1:A:61:VAL:HG22	1:A:280:VAL:CG2	2.42	0.49
1:B:260:PRO:HA	1:B:263:GLN:HG3	1.94	0.49
1:B:212:ASN:ND2	1:B:275:ARG:O	2.45	0.49
1:C:245:SER:O	1:C:249:PHE:HB2	2.13	0.49
1:C:143:THR:HA	1:C:229:THR:HG22	1.95	0.49
1:C:258:VAL:CG1	1:C:258:VAL:O	2.59	0.49
1:C:75:THR:HG23	1:C:86:LEU:HB2	1.94	0.49
1:C:69:PRO:HG3	1:C:89:ARG:NH2	2.27	0.48
1:B:205:VAL:O	1:B:209:LEU:HG	2.13	0.48
1:A:211:PHE:CZ	1:A:241:TRP:HB2	2.49	0.48
1:A:190:PRO:C	1:A:191:GLN:CG	2.81	0.48
1:B:44:ARG:NH2	1:B:208:GLY:O	2.46	0.48
1:B:99:ARG:HB2	1:B:105:TRP:CE2	2.48	0.48
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.78	0.48
1:C:211:PHE:CZ	1:C:238:VAL:HA	2.49	0.48
1:A:107:GLU:OE1	1:A:115:HIS:HD2	1.97	0.48
1:A:166:GLU:H	1:A:190:PRO:HD2	0.73	0.48
1:A:93:LEU:CD1	1:A:210:ARG:HG3	2.44	0.48
1:A:260:PRO:O	1:C:254:HIS:CE1	2.67	0.47
1:C:71:LEU:HB3	1:C:90:MET:CE	2.43	0.47
1:C:56:GLY:CA	1:C:252:ALA:CB	2.86	0.47
1:C:69:PRO:HB2	1:C:72:TRP:HE1	1.78	0.47
1:A:192:ALA:CB	1:A:195:LYS:CG	2.73	0.47
1:C:27:PHE:O	1:C:29:VAL:N	2.48	0.47
1:C:230:LEU:HD23	1:C:235:GLY:HA2	1.96	0.47
1:A:73:LEU:HB3	1:A:88:ILE:HB	1.95	0.47
1:C:61:VAL:HG22	1:C:280:VAL:CG2	2.44	0.47
1:C:230:LEU:HG	1:C:234:GLN:HB3	1.97	0.47
1:A:24:THR:HG21	1:A:75:THR:CG2	2.45	0.47
1:A:91:ASP:HB3	2:A:290:HOH:O	2.14	0.46
1:B:120:ASN:HD22	1:B:120:ASN:N	2.12	0.46
1:A:93:LEU:HD13	1:A:210:ARG:HG3	1.98	0.46
1:B:46:ASP:O	1:B:49:LYS:HB2	2.15	0.46
1:A:59:GLN:HG2	1:A:277:VAL:O	2.16	0.46
1:A:50:HIS:HD2	1:A:90:MET:HE3	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211:PHE:CZ	1:B:238:VAL:HA	2.50	0.46
1:C:78:LYS:HA	1:C:83:SER:HB2	1.97	0.46
1:C:247:ALA:O	1:C:251:TRP:N	2.49	0.46
1:A:58:PHE:HE1	1:A:270:LYS:HD2	1.81	0.46
1:C:36:TYR:O	1:C:39:PHE:HB3	2.15	0.46
1:C:254:HIS:N	1:C:255:PRO:HD3	2.30	0.45
1:B:82:SER:OG	1:B:83:SER:N	2.50	0.45
1:B:29:VAL:CG2	1:B:79:THR:CG2	2.94	0.45
1:B:59:GLN:NE2	1:B:277:VAL:CG1	2.74	0.45
1:C:218:VAL:O	1:C:222:PHE:HB2	2.17	0.45
1:B:29:VAL:HG21	1:B:79:THR:CG2	2.47	0.45
1:B:251:TRP:CG	1:B:270:LYS:HB3	2.51	0.45
1:C:272:GLU:C	1:C:274:ALA:N	2.70	0.45
1:C:213:THR:HG22	1:C:276:ILE:O	2.17	0.45
1:B:80:ARG:HG2	1:B:80:ARG:NH1	2.31	0.44
1:A:260:PRO:C	1:C:254:HIS:NE2	2.70	0.44
1:B:50:HIS:CB	1:B:90:MET:HE2	2.48	0.44
1:C:211:PHE:CZ	1:C:241:TRP:HB2	2.52	0.44
1:B:71:LEU:HD13	1:B:90:MET:HE3	1.98	0.44
1:C:83:SER:O	1:C:101:PRO:HG3	2.17	0.44
1:A:231:THR:HG23	1:A:234:GLN:NE2	2.32	0.44
1:A:50:HIS:CD2	1:A:90:MET:CE	3.01	0.44
1:A:78:LYS:HB2	1:A:83:SER:HB3	2.00	0.44
1:A:149:MET:O	1:A:153:VAL:HG23	2.17	0.44
1:A:249:PHE:HZ	1:A:282:ASN:HD22	1.66	0.44
1:C:217:THR:HG22	1:C:228:VAL:CG2	2.48	0.44
1:A:202:VAL:O	1:A:206:CYS:HB2	2.18	0.44
1:A:58:PHE:CE1	1:A:270:LYS:HD2	2.53	0.43
1:C:217:THR:HG22	1:C:228:VAL:HG21	2.00	0.43
1:C:271:ASN:O	1:C:274:ALA:HB3	2.18	0.43
1:B:55:LYS:NZ	1:B:55:LYS:HB2	2.33	0.43
1:A:246:LYS:CE	1:A:283:GLN:HE21	2.27	0.43
1:A:93:LEU:CD1	1:A:210:ARG:CG	2.95	0.43
1:C:75:THR:CG2	1:C:86:LEU:HB2	2.48	0.43
1:B:269:ASP:OD1	1:B:271:ASN:HB2	2.18	0.43
1:A:192:ALA:HA	1:A:194:THR:H	1.84	0.43
1:A:231:THR:N	1:A:234:GLN:HE21	1.92	0.43
1:C:213:THR:HB	1:C:276:ILE:HA	2.00	0.43
1:B:91:ASP:OD1	1:B:92:ASN:N	2.51	0.43
1:A:59:GLN:HA	1:A:60:PRO:HD3	1.90	0.43
1:B:231:THR:OG1	1:B:234:GLN:HG3	2.19	0.43
1:C:99:ARG:HB2	1:C:105:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:30:GLU:O	1:C:31:ASP:C	2.57	0.43
1:C:233:THR:O	1:C:236:LYS:HB2	2.19	0.42
1:B:36:TYR:OH	1:B:204:MET:O	2.30	0.42
1:C:89:ARG:O	1:C:93:LEU:HA	2.19	0.42
1:C:29:VAL:CG2	1:C:78:LYS:C	2.87	0.42
1:C:205:VAL:O	1:C:209:LEU:HG	2.19	0.42
1:B:59:GLN:HG2	1:B:277:VAL:O	2.20	0.42
1:B:115:HIS:CE1	1:B:123:TRP:CE2	3.08	0.42
1:C:259:ILE:HG21	1:C:261:ASP:HB3	2.01	0.42
1:B:30:GLU:HG3	1:B:79:THR:HB	2.01	0.42
1:B:51:CYS:SG	1:B:62:LEU:HD23	2.59	0.42
1:C:115:HIS:CE1	1:C:123:TRP:CE2	3.08	0.42
1:B:53:ASP:C	1:B:53:ASP:OD2	2.58	0.42
1:B:251:TRP:CB	1:B:270:LYS:HB3	2.49	0.42
1:C:259:ILE:CG2	1:C:261:ASP:HB3	2.50	0.42
1:C:36:TYR:CE2	1:C:218:VAL:HB	2.54	0.42
1:B:28:PRO:O	1:B:29:VAL:C	2.58	0.42
1:A:50:HIS:CD2	1:A:90:MET:HE3	2.54	0.42
1:A:259:ILE:HA	1:A:260:PRO:HD2	1.86	0.42
1:B:22:LYS:HD2	1:B:22:LYS:HA	1.82	0.42
1:B:241:TRP:CH2	1:B:281:LYS:HB2	2.55	0.42
1:B:37:SER:HB3	1:B:219:ASP:CG	2.39	0.42
1:A:94:TYR:HH	1:A:128:GLY:C	2.23	0.41
1:B:120:ASN:HD22	1:B:120:ASN:H	1.68	0.41
1:A:24:THR:HG21	1:A:75:THR:CB	2.50	0.41
1:A:82:SER:OG	1:A:101:PRO:HG2	2.20	0.41
1:C:267:ILE:HG12	1:C:276:ILE:HD12	2.01	0.41
1:B:268:LYS:HB2	1:B:268:LYS:HE2	1.89	0.41
1:C:44:ARG:HH22	1:C:212:ASN:HA	1.85	0.41
1:B:99:ARG:HD2	1:B:105:TRP:NE1	2.35	0.41
1:A:118:GLY:O	1:A:119:ASP:HB2	2.20	0.41
1:C:130:TYR:CD2	1:C:239:GLN:HG2	2.56	0.41
1:B:79:THR:O	1:B:80:ARG:C	2.59	0.41
1:B:120:ASN:ND2	1:B:120:ASN:N	2.68	0.41
1:C:214:VAL:C	1:C:216:ARG:H	2.24	0.41
1:C:212:ASN:O	1:C:216:ARG:HG3	2.21	0.41
1:B:94:TYR:C	1:B:94:TYR:CD2	2.93	0.41
1:A:243:ARG:HD2	1:A:261:ASP:HB3	2.02	0.41
1:C:242:ASP:O	1:C:246:LYS:HG3	2.20	0.41
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.86	0.40
1:A:166:GLU:O	1:A:190:PRO:O	2.39	0.40
1:B:115:HIS:CE1	1:B:123:TRP:NE1	2.90	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:148:GLU:CD	1:C:151:ARG:HH21	2.23	0.40
1:B:152:ALA:CA	1:B:197:LYS:HD2	2.34	0.40
1:A:211:PHE:HZ	1:A:241:TRP:HB2	1.85	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	236/243 (97%)	221 (94%)	13 (6%)	2 (1%)	27	46
1	B	231/243 (95%)	214 (93%)	16 (7%)	1 (0%)	43	66
1	C	215/243 (88%)	191 (89%)	20 (9%)	4 (2%)	12	19
All	All	682/729 (94%)	626 (92%)	49 (7%)	7 (1%)	22	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	PRO
1	C	69	PRO
1	C	28	PRO
1	A	166	GLU
1	C	260	PRO
1	C	29	VAL
1	B	29	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	199/206 (97%)	185 (93%)	14 (7%)	21	38
1	B	199/206 (97%)	175 (88%)	24 (12%)	7	13
1	C	168/206 (82%)	156 (93%)	12 (7%)	21	37
All	All	566/618 (92%)	516 (91%)	50 (9%)	14	26

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	45	LYS
1	A	67	LYS
1	A	159	LYS
1	A	191	GLN
1	A	193	ASP
1	A	194	THR
1	A	196	SER
1	A	236	LYS
1	A	243	ARG
1	A	254	HIS
1	A	263	GLN
1	A	268	LYS
1	A	270	LYS
1	B	21	MET
1	B	22	LYS
1	B	24	THR
1	B	25	GLU
1	B	45	LYS
1	B	55	LYS
1	B	66	LYS
1	B	70	GLU
1	B	122	ARG
1	B	131	GLN
1	B	194	THR
1	B	212	ASN
1	B	224	SER
1	B	225	GLN
1	B	236	LYS
1	B	256	THR
1	B	258	VAL
1	B	260	PRO
1	B	263	GLN
1	B	265	LEU

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Mol	Chain	Res	Type
1	B	269	ASP
1	B	270	LYS
1	B	282	ASN
1	B	283	GLN
1	C	24	THR
1	C	29	VAL
1	C	68	VAL
1	C	71	LEU
1	C	91	ASP
1	C	137	LYS
1	C	244	ILE
1	C	249	PHE
1	C	251	TRP
1	C	258	VAL
1	C	261	ASP
1	C	268	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	115	HIS
1	A	120	ASN
1	A	154	ASN
1	A	234	GLN
1	A	282	ASN
1	A	283	GLN
1	B	54	HIS
1	B	115	HIS
1	B	154	ASN
1	B	212	ASN
1	B	225	GLN
1	B	234	GLN
1	B	283	GLN
1	C	50	HIS
1	C	115	HIS
1	C	120	ASN
1	C	131	GLN
1	C	154	ASN
1	C	212	ASN
1	C	234	GLN
1	C	237	GLN

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Mol	Chain	Res	Type
1	C	254	HIS

### 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 ⓘ

There are no ligands in this entry.

### 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	238/243 (97%)	0.21	8 (3%) 43 44	17, 34, 53, 88	0
1	B	235/243 (96%)	0.68	20 (8%) 11 10	22, 47, 74, 90	0
1	C	227/243 (93%)	0.94	38 (16%) 2 2	32, 60, 86, 98	0
All	All	700/729 (96%)	0.60	66 (9%) 9 8	17, 46, 81, 98	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	HIS	7.6
1	A	165	LEU	7.3
1	B	21	MET	5.7
1	C	224	SER	5.5
1	B	191	GLN	5.1
1	C	268	LYS	4.7
1	C	112	GLY	4.7
1	C	264	LYS	4.6
1	A	166	GLU	4.6
1	C	249	PHE	4.4
1	B	82	SER	3.9
1	C	54	HIS	3.6
1	B	68	VAL	3.5
1	C	70	GLU	3.5
1	C	254	HIS	3.4
1	B	131	GLN	3.4
1	A	162	MET	3.4
1	C	205	VAL	3.3
1	C	190	PRO	3.3
1	C	253	ASP	3.3
1	B	225	GLN	3.2
1	C	51	CYS	3.1
1	B	193	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	260	PRO	3.1
1	C	252	ALA	3.0
1	B	258	VAL	3.0
1	C	114	THR	3.0
1	B	122	ARG	2.9
1	A	190	PRO	2.9
1	C	110	LYS	2.8
1	C	77	LEU	2.8
1	C	258	VAL	2.7
1	C	68	VAL	2.7
1	C	278	ALA	2.6
1	B	78	LYS	2.6
1	C	135	GLY	2.6
1	B	79	THR	2.6
1	C	49	LYS	2.6
1	A	136	ASN	2.6
1	B	29	VAL	2.6
1	C	204	MET	2.5
1	C	259	ILE	2.5
1	C	102	GLY	2.5
1	C	53	ASP	2.5
1	C	71	LEU	2.5
1	C	223	ASN	2.5
1	B	111	ASP	2.4
1	B	194	THR	2.4
1	C	80	ARG	2.4
1	B	277	VAL	2.3
1	C	227	GLY	2.3
1	A	34	TYR	2.2
1	C	216	ARG	2.2
1	C	279	LEU	2.1
1	B	205	VAL	2.1
1	C	64	PRO	2.1
1	C	69	PRO	2.1
1	A	201	LEU	2.1
1	C	251	TRP	2.1
1	B	70	GLU	2.1
1	B	26	ILE	2.1
1	B	86	LEU	2.1
1	B	160	LYS	2.0
1	C	151	ARG	2.0
1	C	242	ASP	2.0

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	191	GLN	2.0

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.