



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:20 pm BST

PDB ID : 2PQI  
Title : Crystal structure of active ribosome inactivating protein from maize (b-32)  
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Wong, K.B.; Shaw, P.C.  
Deposited on : 2007-05-02  
Resolution : 2.50 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

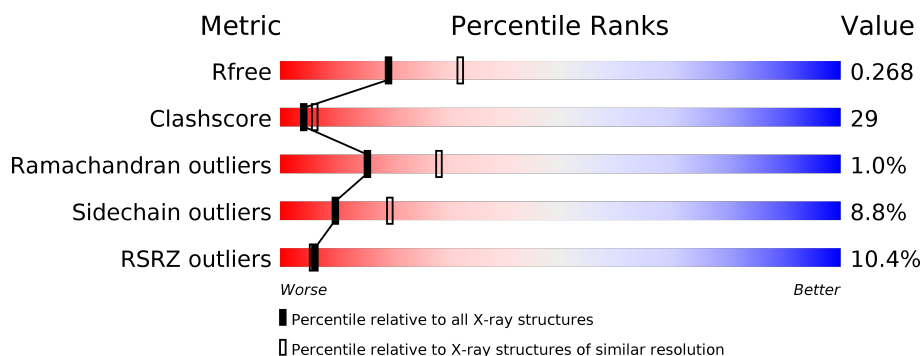
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	243	<div> <div>4%</div> <div>64%</div> <div>30%</div> <div>• •</div> </div>
1	B	243	<div> <div>11%</div> <div>54%</div> <div>36%</div> <div>6%</div> <div>•</div> </div>
1	C	243	<div> <div>15%</div> <div>49%</div> <div>39%</div> <div>5%</div> <div>7%</div> <div>•</div> </div>

## 2 Entry composition

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

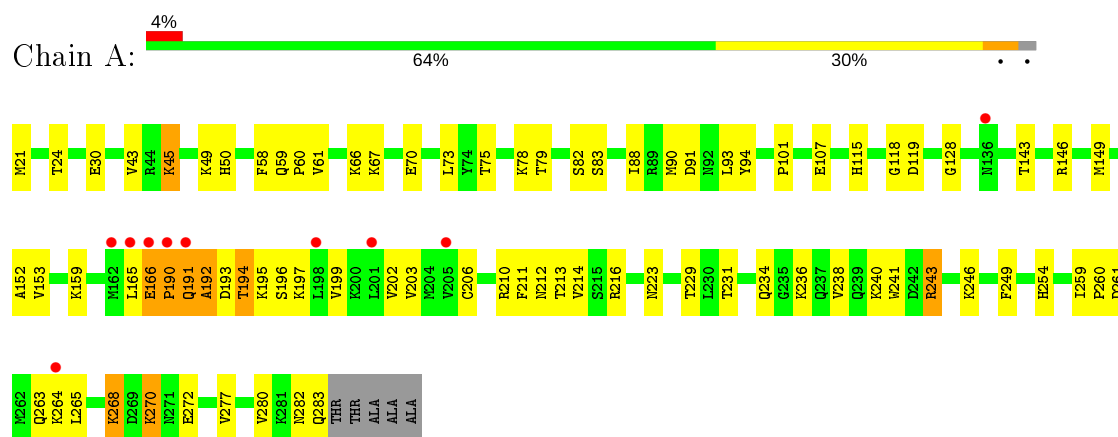
- Molecule 2 is water.

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		

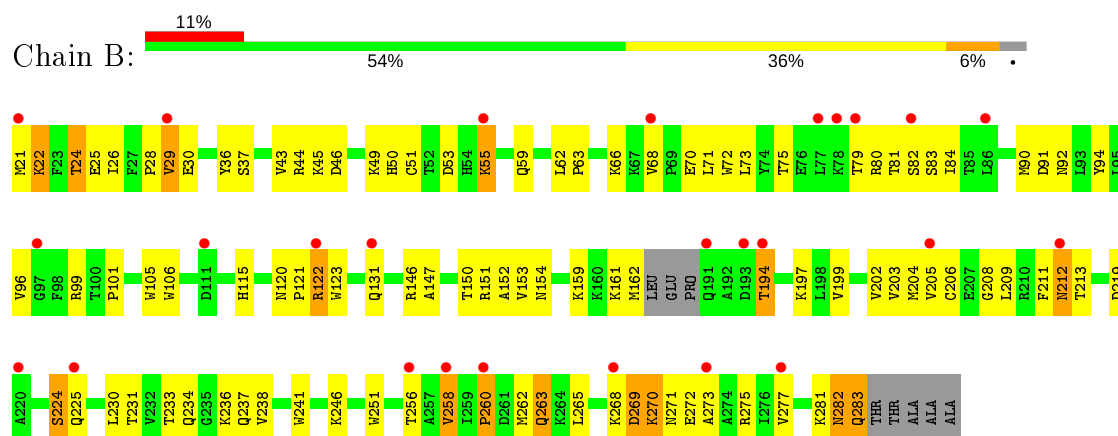
### 3 Residue-property plots [i](#)

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.

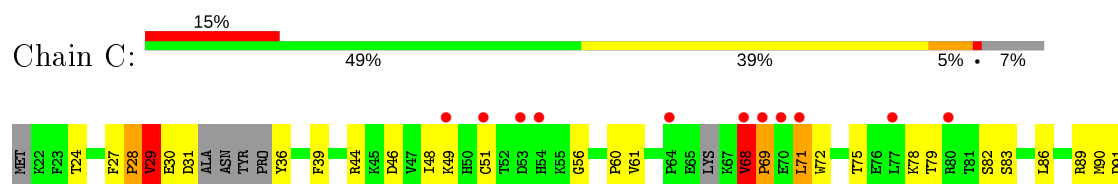
#### • Molecule 1: Ribosome-inactivating protein 3

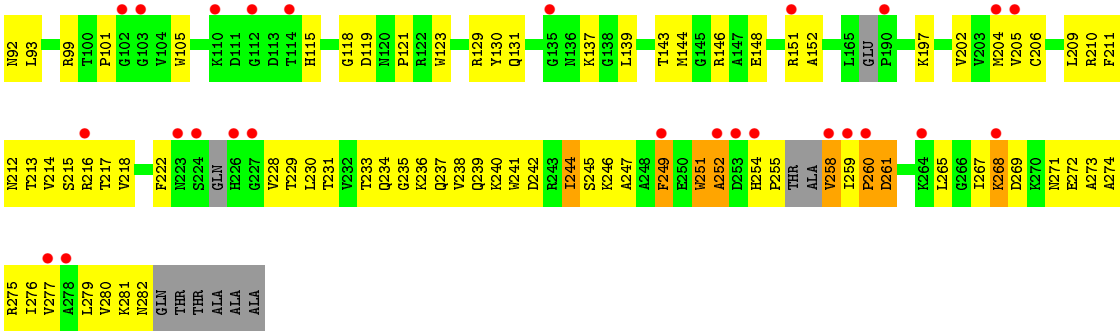


#### • Molecule 1: Ribosome-inactivating protein 3



#### • Molecule 1: Ribosome-inactivating protein 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.19 Å   115.19 Å   45.00 Å 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 2.50 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.217   ,   0.261 0.228   ,   0.268	Depositor DCC
$R_{free}$ test set	1120 reflections (5.15%)	wwPDB-VP
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> )	0.38 , 70.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l 0.031 for h,-h-k,-l 0.022 for -k,-h,-l	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.

<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

### 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 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	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

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 29.

All (318) 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: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:B:122:ARG:HH21	1:B:122:ARG:HG3	1.26	0.97
1:C:68:VAL:O	1:C:68:VAL:HG22	1.63	0.97
1:A:59:GLN:HE21	1:A:277:VAL:HG23	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:A:24:THR:OG1	1:A:43:VAL:HG22	1.72	0.90
1:B:246:LYS:CE	1:B:283:GLN:HE21	1.83	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:B:251:TRP:CH2	1:B:262:MET:HG3	2.23	0.74
1:C:281:LYS:O	1:C:282:ASN:CB	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LYS:HE2	1:A:268:LYS:N	2.04	0.72
1:B:233:THR:O	1:B:237:GLN:HG3	1.89	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:A:231:THR:H	1:A:234:GLN:NE2	1.86	0.71
1:C:29:VAL:HG21	1:C:79:THR:CG2	2.20	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:B:258:VAL:O	1:B:258:VAL:CG2	2.40	0.70
1:C:68:VAL:O	1:C:68:VAL:CG2	2.36	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:A:264:LYS:CG	1:C:254:HIS:CE1	2.76	0.67
1:C:56:GLY:CA	1:C:252:ALA:HB1	2.16	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:224:SER:HA	2:B:304:HOH:O	1.97	0.64
1:B:246:LYS:CG	1:B:283:GLN:NE2	2.58	0.64
1:C:231:THR:HG23	1:C:234:GLN:NE2	2.14	0.63
1:C:29:VAL:CG2	1:C:79:THR:CA	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:92:ASN:HB3	1:B:281:LYS:HE2	1.84	0.60
1:C:68:VAL:O	1:C:69:PRO:C	2.40	0.60
1:B:199:VAL:O	1:B:203:VAL:HG23	2.01	0.60
1:B:268:LYS:HD3	1:B:269:ASP:OD2	2.00	0.60
1:C:211:PHE:HB3	1:C:213:THR:CG2	2.30	0.60
1:A:260:PRO:HB2	1:C:254:HIS:CE1	2.36	0.60
1:A:261:ASP:OD2	1:C:254:HIS:CD2	2.55	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:B:68:VAL:O	1:B:68:VAL:HG12	2.01	0.59
1:C:273:ALA:O	1:C:277:VAL:HG22	2.02	0.59
1:B:122:ARG:NH2	1:B:122:ARG:HG3	2.05	0.59
1:B:161:LYS:CG	1:B:162:MET:H	2.01	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:231:THR:H	1:B:234:GLN:HE21	1.50	0.58
1:B:268:LYS:HG3	1:B:272:GLU:HG3	1.86	0.58
1:B:83:SER:O	1:B:101:PRO:HG3	2.03	0.58
1:B:24:THR:CG2	1:B:43:VAL:HG22	2.25	0.58
1:C:129:ARG:HH12	1:C:131:GLN:NE2	2.01	0.58
1:C:29:VAL:HG22	1:C:78:LYS:C	2.24	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:A:199:VAL:O	1:A:203:VAL:HG23	2.04	0.57
1:C:130:TYR:CZ	1:C:139:LEU:HD21	2.39	0.57
1:C:78:LYS:HA	1:C:83:SER:CB	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:O	1:B:206:CYS:HB2	2.05	0.56
1:C:237:GLN:NE2	1:C:276:ILE:HD13	2.19	0.56
1:A:94:TYR:OH	1:A:128:GLY:O	2.24	0.56
1:B:90:MET:O	1:B:91:ASP:C	2.44	0.56
1:C:69:PRO:HD3	1:C:89:ARG:NH2	2.20	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:B:72:TRP:CH2	1:B:96:VAL:HG21	2.43	0.54
1:C:230:LEU:HD21	1:C:238:VAL:HG21	1.90	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:259:ILE:HG22	1:C:260:PRO:N	2.21	0.54
1:C:69:PRO:HG3	1:C:89:ARG:HH21	1.72	0.54
1:C:242:ASP:OD2	1:C:281:LYS:HD2	2.08	0.54
1:C:69:PRO:HD3	1:C:89:ARG:HH22	1.72	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:244:ILE:HD12	1:C:244:ILE:O	2.08	0.53
1:C:267:ILE:HG12	1:C:276:ILE:CD1	2.39	0.53
1:C:269:ASP:OD1	1:C:271:ASN:HB2	2.09	0.52
1:C:29:VAL:CG2	1:C:78:LYS:O	2.56	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:A:30:GLU:OE2	1:A:79:THR:HB	2.10	0.52
1:B:29:VAL:CG2	1:B:79:THR:HG22	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:213:THR:HG23	1:A:214:VAL:N	2.27	0.50
1:B:122:ARG:CG	1:B:122:ARG:NH2	2.60	0.50
1:C:118:GLY:O	1:C:119:ASP:HB2	2.12	0.50
1:C:28:PRO:O	1:C:29:VAL:C	2.50	0.50
1:C:258:VAL:O	1:C:258:VAL:HG12	2.10	0.50
1:C:272:GLU:C	1:C:274:ALA:H	2.14	0.50
1:A:143:THR:HA	1:A:229:THR:HG22	1.92	0.49
1:A:260:PRO:O	1:C:254:HIS:NE2	2.45	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:A:107:GLU:OE1	1:A:115:HIS:HD2	1.97	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: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:A:73:LEU:HB3	1:A:88:ILE:HB	1.95	0.47
1:C:230:LEU:HD23	1:C:235:GLY:HA2	1.96	0.47
1:C:61:VAL:HG22	1:C:280:VAL:CG2	2.44	0.47
1:C:27:PHE:O	1:C:29:VAL:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:58:PHE:HE1	1:A:270:LYS:HD2	1.81	0.46
1:C:247:ALA:O	1:C:251:TRP:N	2.49	0.46
1:C:36:TYR:O	1:C:39:PHE:HB3	2.15	0.46
1:B:82:SER:OG	1:B:83:SER:N	2.50	0.45
1:C:254:HIS:N	1:C:255:PRO:HD3	2.30	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:251:TRP:CG	1:B:270:LYS:HB3	2.51	0.45
1:B:29:VAL:HG21	1:B:79:THR:CG2	2.47	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:A:260:PRO:C	1:C:254:HIS:NE2	2.70	0.44
1:B:80:ARG:HG2	1:B:80:ARG:NH1	2.31	0.44
1:B:50:HIS:CB	1:B:90:MET:HE2	2.48	0.44
1:B:71:LEU:HD13	1:B:90:MET:HE3	1.98	0.44
1:C:211:PHE:CZ	1:C:241:TRP:HB2	2.52	0.44
1:A:231:THR:HG23	1:A:234:GLN:NE2	2.32	0.44
1:A:78:LYS:HB2	1:A:83:SER:HB3	2.00	0.44
1:A:50:HIS:CD2	1:A:90:MET:CE	3.01	0.44
1:C:83:SER:O	1:C:101:PRO:HG3	2.17	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:A:202:VAL:O	1:A:206:CYS:HB2	2.18	0.44
1:C:217:THR:HG22	1:C:228:VAL:CG2	2.48	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:B:55:LYS:HB2	1:B:55:LYS:NZ	2.33	0.43
1:C:271:ASN:O	1:C:274:ALA:HB3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:THR:N	1:A:234:GLN:HE21	1.92	0.43
1:B:91:ASP:OD1	1:B:92:ASN:N	2.51	0.43
1:C:213:THR:HB	1:C:276:ILE:HA	2.00	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
1:C:30:GLU:O	1:C:31:ASP:C	2.57	0.43
1:B:36:TYR:OH	1:B:204:MET:O	2.30	0.42
1:C:233:THR:O	1:C:236:LYS:HB2	2.19	0.42
1:C:205:VAL:O	1:C:209:LEU:HG	2.19	0.42
1:C:29:VAL:CG2	1:C:78:LYS:C	2.87	0.42
1:C:89:ARG:O	1:C:93:LEU:HA	2.19	0.42
1:B:115:HIS:CE1	1:B:123:TRP:CE2	3.08	0.42
1:B:59:GLN:HG2	1:B:277:VAL:O	2.20	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:B:53:ASP:C	1:B:53:ASP:OD2	2.58	0.42
1:C:115:HIS:CE1	1:C:123:TRP:CE2	3.08	0.42
1:B:251:TRP:CB	1:B:270:LYS:HB3	2.49	0.42
1:C:36:TYR:CE2	1:C:218:VAL:HB	2.54	0.42
1:C:259:ILE:CG2	1:C:261:ASP:HB3	2.50	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:37:SER:HB3	1:B:219:ASP:CG	2.39	0.42
1:B:241:TRP:CH2	1:B:281:LYS:HB2	2.55	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:A:118:GLY:O	1:A:119:ASP:HB2	2.20	0.41
1:B:99:ARG:HD2	1:B:105:TRP:NE1	2.35	0.41
1:C:44:ARG:HH22	1:C:212:ASN:HA	1.85	0.41
1:C:130:TYR:CD2	1:C:239:GLN:HG2	2.56	0.41
1:B:120:ASN:ND2	1:B:120:ASN:N	2.68	0.41
1:B:79:THR:O	1:B:80:ARG:C	2.59	0.41
1:C:214:VAL:C	1:C:216:ARG:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	19	35
1	B	231/243 (95%)	214 (93%)	16 (7%)	1 (0%)	34	54
1	C	215/243 (88%)	191 (89%)	20 (9%)	4 (2%)	8	13
All	All	682/729 (94%)	626 (92%)	49 (7%)	7 (1%)	15	28

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%)	15	29
1	B	199/206 (97%)	175 (88%)	24 (12%)	5	9
1	C	168/206 (82%)	156 (93%)	12 (7%)	14	28
All	All	566/618 (92%)	516 (91%)	50 (9%)	10	19

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	C	254	HIS

### 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

### 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%)	0.22	10 (4%) 36 39	17, 34, 53, 88	0
1	B	235/243 (96%)	0.69	26 (11%) 5 5	22, 47, 74, 90	0
1	C	227/243 (93%)	0.96	37 (16%) 1 1	32, 60, 86, 98	0
All	All	700/729 (96%)	0.62	73 (10%) 6 6	17, 46, 81, 98	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	HIS	8.8
1	A	165	LEU	7.6
1	C	264	LYS	6.2
1	B	21	MET	5.9
1	C	268	LYS	5.3
1	A	166	GLU	5.3
1	C	224	SER	5.1
1	C	112	GLY	5.1
1	B	191	GLN	4.8
1	C	249	PHE	4.5
1	C	253	ASP	4.0
1	B	258	VAL	3.8
1	C	190	PRO	3.8
1	B	225	GLN	3.8
1	C	260	PRO	3.8
1	C	205	VAL	3.7
1	A	162	MET	3.7
1	C	252	ALA	3.7
1	C	70	GLU	3.6
1	B	131	GLN	3.6
1	B	193	ASP	3.5
1	C	54	HIS	3.5
1	C	68	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	77	LEU	3.5
1	B	82	SER	3.4
1	C	254	HIS	3.2
1	C	135	GLY	3.2
1	A	190	PRO	3.2
1	C	102	GLY	3.1
1	B	68	VAL	3.1
1	C	110	LYS	3.1
1	C	259	ILE	3.0
1	B	122	ARG	3.0
1	C	51	CYS	2.9
1	C	114	THR	2.9
1	A	136	ASN	2.9
1	B	111	ASP	2.8
1	C	258	VAL	2.8
1	B	79	THR	2.7
1	B	29	VAL	2.7
1	C	278	ALA	2.7
1	C	204	MET	2.5
1	C	80	ARG	2.5
1	B	277	VAL	2.5
1	A	191	GLN	2.4
1	C	216	ARG	2.4
1	B	205	VAL	2.4
1	C	64	PRO	2.4
1	C	49	LYS	2.3
1	A	205	VAL	2.3
1	C	69	PRO	2.3
1	A	201	LEU	2.3
1	B	194	THR	2.2
1	B	220	ALA	2.2
1	C	227	GLY	2.2
1	B	256	THR	2.2
1	A	198	LEU	2.2
1	B	268	LYS	2.2
1	C	71	LEU	2.2
1	C	223	ASN	2.2
1	B	55	LYS	2.2
1	C	53	ASP	2.2
1	C	103	GLY	2.2
1	B	86	LEU	2.2
1	A	264	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	97	GLY	2.1
1	C	151	ARG	2.1
1	B	260	PRO	2.1
1	B	77	LEU	2.1
1	B	273	ALA	2.1
1	B	212	ASN	2.1
1	C	277	VAL	2.0
1	B	78	LYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.