



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:04 AM GMT

PDB ID : 1ZMV  
Title : Catalytic and ubiquitin-associated domains of MARK2/PAR-1: K82R mutant  
Authors : Panneerselvam, S.; Marx, A.; Mandelkow, E.-M.; Mandelkow, E.  
Deposited on : 2005-05-11  
Resolution : 3.10 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

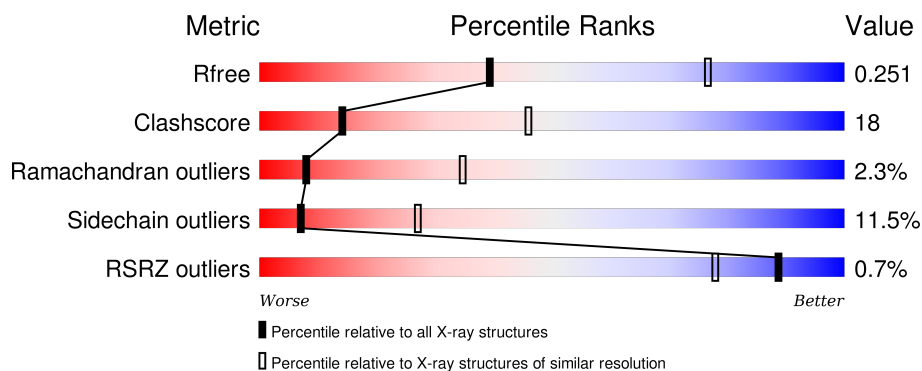
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	327	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 53%, yellow 30%, orange 6%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>53%</span> <span>30%</span> <span>6%</span> <span>10%</span> </div> </div>
1	B	327	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 57%, yellow 28%, orange 6%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>57%</span> <span>28%</span> <span>6%</span> <span>9%</span> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4667 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 MAP/Microtubule affinity regulating kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2321	1490	396	423	12			
1	B	296	Total	C	N	O	S	0	0	0
			2346	1507	401	426	12			

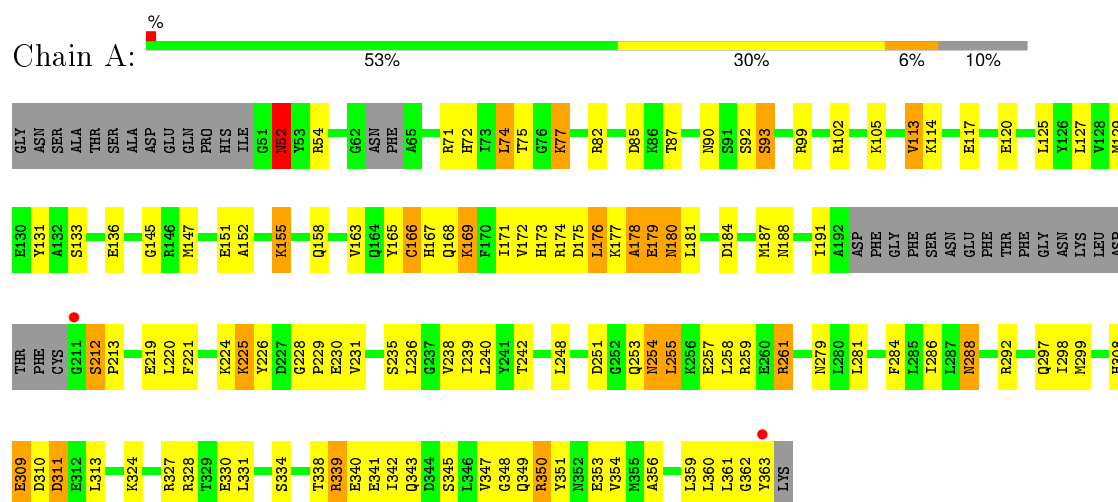
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLY	-	CLONING ARTIFACT	UNP O08679
A	82	ARG	LYS	ENGINEERED	UNP O08679
B	38	GLY	-	CLONING ARTIFACT	UNP O08679
B	82	ARG	LYS	ENGINEERED	UNP O08679

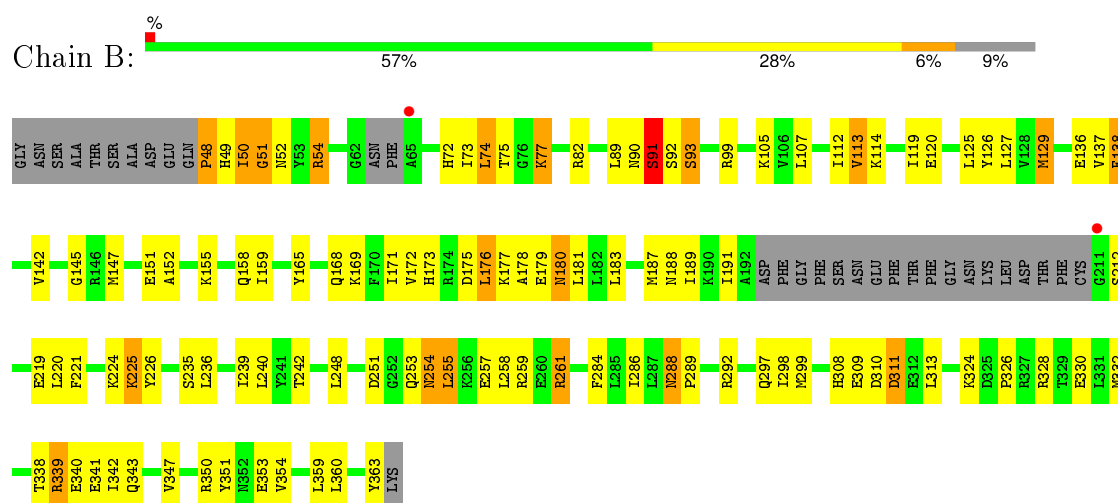
### 3 Residue-property plots

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: MAP/Microtubule affinity regulating kinase 2



- Molecule 1: MAP/Microtubule affinity regulating kinase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.19 Å 121.19 Å 99.66 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.78 – 3.10 51.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (51.78-3.10) 97.9 (51.78-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 3.13 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.200 , 0.251 0.199 , 0.251	Depositor DCC
$R_{free}$ test set	740 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.5	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.8	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 14813 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.03	3/2364 (0.1%)	0.98	2/3192 (0.1%)
1	B	1.00	1/2391 (0.0%)	0.93	1/3229 (0.0%)
All	All	1.01	4/4755 (0.1%)	0.95	3/6421 (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	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	GLU	CB-CG	6.49	1.64	1.52
1	A	309	GLU	CB-CG	6.48	1.64	1.52
1	A	166	CYS	CB-SG	-5.48	1.72	1.81
1	A	309	GLU	CG-CD	5.22	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	LEU	CA-CB-CG	7.11	131.66	115.30
1	B	258	LEU	CA-CB-CG	6.59	130.45	115.30
1	A	52	ASN	N-CA-C	6.04	127.32	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	ALA	Peptide
1	B	48	PRO	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	2321	0	2332	86	1
1	B	2346	0	2358	84	1
All	All	4667	0	4690	170	1

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 18.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ARG:HH11	1:B:261:ARG:HG2	1.21	1.06
1:A:261:ARG:HH11	1:A:261:ARG:HG2	1.22	1.01
1:A:330:GLU:HA	1:A:330:GLU:OE1	1.71	0.87
1:B:49:HIS:HE1	1:B:73:ILE:HD11	1.42	0.84
1:B:311:ASP:O	1:B:311:ASP:OD1	1.98	0.81
1:B:49:HIS:CE1	1:B:73:ILE:HD11	2.15	0.80
1:A:324:LYS:HE2	1:A:343:GLN:HE22	1.49	0.77
1:A:343:GLN:O	1:A:347:VAL:HG23	1.84	0.77
1:B:220:LEU:HB2	1:B:226:TYR:CE2	2.20	0.76
1:A:219:GLU:HB2	1:A:224:LYS:HB2	1.68	0.76
1:A:220:LEU:HB2	1:A:226:TYR:CE2	2.22	0.74
1:A:77:LYS:HE2	1:A:363:TYR:HB2	1.69	0.74
1:A:169:LYS:HB2	1:A:171:ILE:HD12	1.69	0.74
1:B:219:GLU:HB2	1:B:224:LYS:HB2	1.70	0.71
1:A:261:ARG:HG2	1:A:261:ARG:NH1	2.01	0.71
1:B:169:LYS:HB2	1:B:171:ILE:HD12	1.72	0.70
1:B:261:ARG:HH11	1:B:261:ARG:CG	2.02	0.70
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.57	0.70
1:A:330:GLU:OE1	1:A:330:GLU:CA	2.36	0.69
1:B:77:LYS:HD3	1:B:360:LEU:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LYS:HE2	1:B:363:TYR:HB2	1.74	0.69
1:A:147:MET:HG2	1:A:151:GLU:OE1	1.93	0.68
1:B:286:ILE:O	1:B:292:ARG:NH1	2.24	0.68
1:B:225:LYS:H	1:B:225:LYS:HD3	1.59	0.68
1:A:131:TYR:CE2	1:A:133:SER:HB3	2.29	0.67
1:B:120:GLU:HG2	1:B:125:LEU:CD1	2.25	0.67
1:B:330:GLU:HA	1:B:330:GLU:OE1	1.94	0.67
1:B:49:HIS:HE1	1:B:73:ILE:CD1	2.09	0.66
1:B:311:ASP:OD1	1:B:311:ASP:C	2.34	0.65
1:A:311:ASP:O	1:A:311:ASP:OD1	2.14	0.65
1:B:48:PRO:HD2	1:B:54:ARG:CZ	2.26	0.64
1:B:261:ARG:HG2	1:B:261:ARG:NH1	2.01	0.63
1:B:324:LYS:HE2	1:B:343:GLN:HE22	1.62	0.62
1:A:261:ARG:CG	1:A:261:ARG:HH11	2.05	0.62
1:A:175:ASP:OD1	1:A:177:LYS:HE2	1.99	0.62
1:A:105:LYS:HG2	1:A:351:TYR:CD2	2.35	0.62
1:B:136:GLU:OE1	1:B:179:GLU:HA	1.99	0.62
1:A:288:ASN:HD22	1:A:288:ASN:C	2.02	0.61
1:B:90:ASN:ND2	1:B:93:SER:OG	2.33	0.61
1:A:228:GLY:HA3	1:A:230:GLU:OE2	2.00	0.60
1:A:77:LYS:HE2	1:A:363:TYR:CB	2.31	0.60
1:B:175:ASP:OD1	1:B:177:LYS:HE2	2.00	0.60
1:B:175:ASP:O	1:B:175:ASP:OD1	2.20	0.59
1:A:331:LEU:O	1:A:334:SER:HB2	2.02	0.59
1:A:308:HIS:HB3	1:A:311:ASP:O	2.03	0.58
1:A:324:LYS:HE2	1:A:343:GLN:NE2	2.19	0.58
1:A:311:ASP:OD1	1:A:311:ASP:C	2.42	0.58
1:A:72:HIS:CE1	1:A:75:THR:HG23	2.38	0.58
1:B:338:THR:O	1:B:342:ILE:HD12	2.03	0.58
1:A:286:ILE:O	1:A:292:ARG:NH1	2.36	0.58
1:B:225:LYS:HD3	1:B:225:LYS:N	2.19	0.57
1:A:288:ASN:C	1:A:288:ASN:ND2	2.58	0.57
1:A:299:MET:HG2	1:A:313:LEU:HD23	1.86	0.57
1:A:75:THR:OG1	1:A:77:LYS:HG3	2.05	0.57
1:A:105:LYS:HG2	1:A:351:TYR:CE2	2.40	0.56
1:B:339:ARG:HG2	1:B:339:ARG:NH1	2.19	0.56
1:B:177:LYS:HE3	1:B:180:ASN:OD1	2.05	0.56
1:B:127:LEU:HB3	1:B:129:MET:HE1	1.88	0.56
1:A:178:ALA:C	1:A:180:ASN:H	2.09	0.55
1:B:308:HIS:HB3	1:B:311:ASP:O	2.07	0.55
1:B:147:MET:HG2	1:B:151:GLU:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LYS:HG2	1:B:351:TYR:CE2	2.42	0.54
1:B:220:LEU:HB2	1:B:226:TYR:HE2	1.72	0.54
1:A:220:LEU:HB2	1:A:226:TYR:HE2	1.67	0.53
1:A:175:ASP:O	1:A:175:ASP:OD1	2.26	0.52
1:A:147:MET:HE3	1:A:155:LYS:HD3	1.92	0.52
1:A:178:ALA:C	1:A:180:ASN:N	2.62	0.52
1:B:120:GLU:HG2	1:B:125:LEU:HD11	1.91	0.52
1:A:339:ARG:H	1:A:339:ARG:HD2	1.75	0.51
1:B:288:ASN:C	1:B:288:ASN:HD22	2.14	0.51
1:A:235:SER:O	1:A:239:ILE:HG13	2.11	0.51
1:A:221:PHE:CG	1:A:259:ARG:HG3	2.46	0.51
1:A:345:SER:HA	1:A:350:ARG:HG3	1.93	0.50
1:B:297:GLN:O	1:B:298:ILE:C	2.50	0.50
1:B:343:GLN:O	1:B:347:VAL:HG23	2.11	0.50
1:B:178:ALA:C	1:B:180:ASN:H	2.15	0.49
1:B:165:TYR:HA	1:B:168:GLN:HG3	1.94	0.49
1:A:177:LYS:HE3	1:A:180:ASN:OD1	2.11	0.49
1:A:136:GLU:OE1	1:A:179:GLU:HA	2.13	0.48
1:A:120:GLU:HG2	1:A:125:LEU:CD1	2.43	0.48
1:B:178:ALA:C	1:B:180:ASN:N	2.66	0.48
1:A:173:HIS:CG	1:A:176:LEU:HD13	2.48	0.48
1:A:254:ASN:HD21	1:A:257:GLU:HB2	1.78	0.48
1:A:360:LEU:C	1:A:362:GLY:H	2.17	0.48
1:B:288:ASN:C	1:B:288:ASN:ND2	2.67	0.48
1:A:212:SER:N	1:A:213:PRO:CD	2.77	0.47
1:B:254:ASN:HD21	1:B:257:GLU:HB2	1.79	0.47
1:B:77:LYS:CE	1:B:363:TYR:HB2	2.44	0.47
1:A:339:ARG:HH11	1:A:339:ARG:HG2	1.80	0.47
1:B:113:VAL:HG13	1:B:191:ILE:O	2.15	0.47
1:B:242:THR:CG2	1:B:248:LEU:HD23	2.44	0.47
1:B:286:ILE:HB	1:B:292:ARG:HG2	1.95	0.47
1:B:328:ARG:O	1:B:332:MET:HG3	2.14	0.47
1:B:119:ILE:HB	1:B:126:TYR:HB2	1.96	0.47
1:A:338:THR:O	1:A:342:ILE:HD12	2.15	0.47
1:A:284:PHE:CZ	1:A:298:ILE:HG21	2.49	0.47
1:A:253:GLN:O	1:A:254:ASN:HB3	2.15	0.46
1:B:52:ASN:ND2	1:B:74:LEU:HD11	2.30	0.46
1:A:163:VAL:O	1:A:166:CYS:HB2	2.14	0.46
1:B:172:VAL:O	1:B:172:VAL:HG23	2.15	0.46
1:B:49:HIS:CE1	1:B:73:ILE:CD1	2.90	0.46
1:B:326:PRO:O	1:B:330:GLU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:SER:O	1:B:239:ILE:HG13	2.16	0.46
1:A:113:VAL:HG13	1:A:191:ILE:O	2.16	0.46
1:A:226:TYR:CE1	1:A:231:VAL:HG11	2.51	0.46
1:A:120:GLU:HG2	1:A:125:LEU:HD11	1.98	0.46
1:A:242:THR:HG22	1:A:248:LEU:HA	1.97	0.46
1:B:48:PRO:HD2	1:B:54:ARG:NE	2.29	0.46
1:B:284:PHE:CZ	1:B:298:ILE:HG21	2.51	0.46
1:A:338:THR:O	1:A:341:GLU:HG2	2.16	0.46
1:A:225:LYS:HD3	1:A:225:LYS:H	1.81	0.46
1:A:127:LEU:HB3	1:A:129:MET:HE1	1.98	0.46
1:B:254:ASN:ND2	1:B:257:GLU:HB2	2.30	0.45
1:A:254:ASN:ND2	1:A:257:GLU:HB2	2.32	0.45
1:A:172:VAL:O	1:A:172:VAL:HG23	2.16	0.45
1:A:353:GLU:HG3	1:A:354:VAL:N	2.31	0.45
1:B:173:HIS:CG	1:B:176:LEU:HD13	2.52	0.45
1:A:117:GLU:HB2	1:A:356:ALA:HB2	1.98	0.45
1:B:338:THR:O	1:B:341:GLU:HG2	2.17	0.44
1:A:297:GLN:O	1:A:298:ILE:C	2.54	0.44
1:B:330:GLU:OE1	1:B:330:GLU:CA	2.59	0.44
1:B:221:PHE:CG	1:B:259:ARG:HG3	2.53	0.44
1:A:165:TYR:HA	1:A:168:GLN:HG3	1.98	0.44
1:B:50:ILE:O	1:B:51:GLY:C	2.55	0.44
1:A:261:ARG:HD3	1:A:261:ARG:HA	1.77	0.44
1:B:72:HIS:CE1	1:B:74:LEU:HD12	2.53	0.43
1:B:242:THR:HG21	1:B:248:LEU:HD23	1.99	0.43
1:B:72:HIS:CE1	1:B:75:THR:HG23	2.52	0.43
1:A:286:ILE:HB	1:A:292:ARG:HG2	1.99	0.43
1:B:181:LEU:HD11	1:B:239:ILE:HD13	1.99	0.43
1:B:77:LYS:HE2	1:B:363:TYR:CB	2.44	0.43
1:B:75:THR:OG1	1:B:77:LYS:HG3	2.19	0.43
1:A:129:MET:HB3	1:A:129:MET:HE2	1.64	0.43
1:A:181:LEU:HD11	1:A:239:ILE:HD13	1.99	0.43
1:B:151:GLU:O	1:B:152:ALA:C	2.57	0.43
1:A:167:HIS:CE1	1:A:229:PRO:HB3	2.54	0.43
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.80	0.43
1:B:299:MET:HG2	1:B:313:LEU:HD23	2.01	0.42
1:B:147:MET:HE1	1:B:152:ALA:HA	2.01	0.42
1:A:238:VAL:HG23	1:A:238:VAL:H	1.52	0.42
1:B:255:LEU:HD12	1:B:255:LEU:HA	1.85	0.42
1:A:281:LEU:HA	1:A:281:LEU:HD23	1.75	0.42
1:B:137:VAL:O	1:B:138:PHE:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HA	1:A:255:LEU:HD12	1.85	0.42
1:B:253:GLN:O	1:B:254:ASN:HB3	2.19	0.42
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.79	0.42
1:B:339:ARG:CG	1:B:339:ARG:NH1	2.83	0.42
1:A:151:GLU:O	1:A:152:ALA:C	2.54	0.42
1:A:74:LEU:H	1:A:74:LEU:HG	1.69	0.42
1:A:72:HIS:CE1	1:A:74:LEU:HD12	2.55	0.41
1:A:327:ARG:O	1:A:331:LEU:HG	2.19	0.41
1:B:107:LEU:HD13	1:B:112:ILE:HG21	2.02	0.41
1:A:184:ASP:OD2	1:A:188:ASN:HB2	2.20	0.41
1:B:183:LEU:HA	1:B:188:ASN:O	2.20	0.41
1:B:359:LEU:HA	1:B:359:LEU:HD23	1.79	0.41
1:B:90:ASN:O	1:B:91:SER:C	2.59	0.41
1:B:353:GLU:HG3	1:B:354:VAL:N	2.35	0.41
1:A:90:ASN:ND2	1:A:93:SER:OG	2.54	0.41
1:B:288:ASN:HA	1:B:289:PRO:HD3	1.93	0.41
1:B:332:MET:HE2	1:B:332:MET:HB3	1.98	0.41
1:A:173:HIS:C	1:A:175:ASP:H	2.24	0.41
1:B:159:ILE:HG13	1:B:189:ILE:HG13	2.03	0.41
1:B:120:GLU:HG2	1:B:125:LEU:HD12	2.01	0.40
1:A:348:GLY:O	1:A:349:GLN:HB2	2.22	0.40
1:A:77:LYS:CE	1:A:363:TYR:HB2	2.44	0.40
1:A:52:ASN:ND2	1:A:74:LEU:HD11	2.36	0.40
1:A:99:ARG:HA	1:A:102:ARG:NH2	2.36	0.40
1:A:360:LEU:C	1:A:362:GLY:N	2.75	0.40
1:A:328:ARG:HD3	1:A:361:LEU:O	2.22	0.40
1:A:85:ASP:OD1	1:A:87:THR:HG23	2.21	0.40

All (1) 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:A:71:ARG:NH2	1:B:341:GLU:OE1[3_665]	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	287/327 (88%)	256 (89%)	25 (9%)	6 (2%)	9	37
1	B	290/327 (89%)	258 (89%)	25 (9%)	7 (2%)	7	33
All	All	577/654 (88%)	514 (89%)	50 (9%)	13 (2%)	8	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	145	GLY
1	A	340	GLU
1	B	50	ILE
1	B	145	GLY
1	B	340	GLU
1	B	91	SER
1	B	138	PHE
1	A	179	GLU
1	A	309	GLU
1	A	174	ARG
1	B	51	GLY
1	B	142	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	247/289 (86%)	219 (89%)	28 (11%)	7	28
1	B	250/289 (86%)	221 (88%)	29 (12%)	7	27
All	All	497/578 (86%)	440 (88%)	57 (12%)	7	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	74	LEU
1	A	77	LYS
1	A	82	ARG
1	A	92	SER
1	A	93	SER
1	A	113	VAL
1	A	114	LYS
1	A	155	LYS
1	A	158	GLN
1	A	169	LYS
1	A	176	LEU
1	A	180	ASN
1	A	187	MET
1	A	212	SER
1	A	225	LYS
1	A	236	LEU
1	A	240	LEU
1	A	251	ASP
1	A	254	ASN
1	A	255	LEU
1	A	261	ARG
1	A	279	ASN
1	A	288	ASN
1	A	310	ASP
1	A	311	ASP
1	A	339	ARG
1	A	350	ARG
1	B	54	ARG
1	B	74	LEU
1	B	77	LYS
1	B	82	ARG
1	B	91	SER
1	B	92	SER
1	B	93	SER
1	B	99	ARG
1	B	113	VAL
1	B	114	LYS
1	B	129	MET
1	B	155	LYS
1	B	158	GLN
1	B	176	LEU
1	B	180	ASN

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Mol	Chain	Res	Type
1	B	187	MET
1	B	212	SER
1	B	225	LYS
1	B	236	LEU
1	B	240	LEU
1	B	251	ASP
1	B	254	ASN
1	B	255	LEU
1	B	261	ARG
1	B	288	ASN
1	B	310	ASP
1	B	311	ASP
1	B	339	ARG
1	B	350	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	88	GLN
1	A	90	ASN
1	A	254	ASN
1	A	288	ASN
1	B	52	ASN
1	B	88	GLN
1	B	90	ASN
1	B	254	ASN
1	B	288	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [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	293/327 (89%)	-0.27	2 (0%) 89 78	68, 68, 68, 68	0
1	B	296/327 (90%)	-0.32	2 (0%) 89 78	68, 68, 68, 68	0
All	All	589/654 (90%)	-0.30	4 (0%) 89 78	68, 68, 68, 68	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	ALA	3.6
1	A	363	TYR	2.3
1	A	211	GLY	2.1
1	B	211	GLY	2.1

### 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.