



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2017 – 01:29 AM EDT

PDB ID : 2HAK  
Title : Catalytic and ubiquitin-associated domains of MARK1/PAR-1  
Authors : Marx, A.; Nugoor, C.; Mueller, J.; Panneerselvam, S.; Mandelkow, E.-M.;  
Mandelkow, E.  
Deposited on : unknown  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

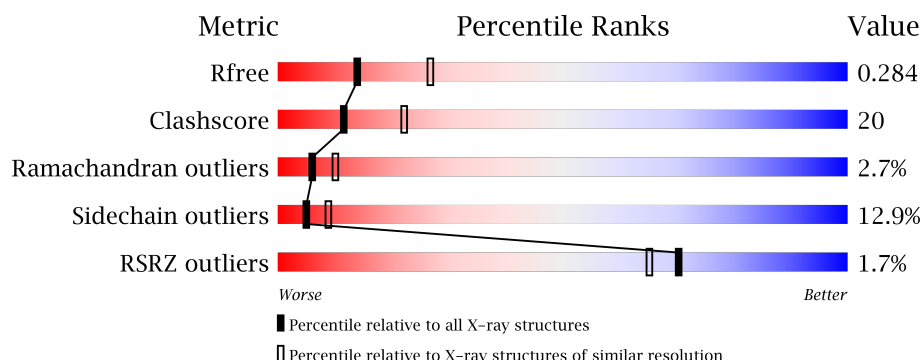
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	328	
1	B	328	
1	C	328	
1	D	328	
1	E	328	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	328	<p>3% 57% 32% 7% 4%</p>
1	G	328	<p>3% 42% 37% 10% 9%</p>
1	H	328	<p>5% 52% 29% 16% 3%</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19579 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 Serine/threonine-protein kinase MARK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2490	1599	426	453	12			
1	B	279	Total	C	N	O	S	0	0	0
			2231	1434	380	405	12			
1	C	310	Total	C	N	O	S	0	0	0
			2512	1612	432	456	12			
1	D	309	Total	C	N	O	S	0	0	0
			2503	1607	432	452	12			
1	E	318	Total	C	N	O	S	0	0	0
			2538	1627	437	461	13			
1	F	318	Total	C	N	O	S	0	0	0
			2562	1641	439	469	13			
1	G	297	Total	C	N	O	S	0	0	0
			2349	1506	402	429	12			
1	H	277	Total	C	N	O	S	0	0	0
			2184	1405	367	400	12			

There are 8 discrepancies between the modelled and reference sequences:

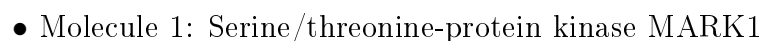
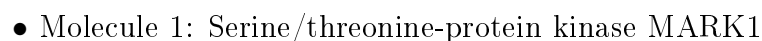
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	CLONING ARTIFACT	UNP Q9P0L2
B	37	GLY	-	CLONING ARTIFACT	UNP Q9P0L2
C	37	GLY	-	CLONING ARTIFACT	UNP Q9P0L2
D	37	GLY	-	CLONING ARTIFACT	UNP Q9P0L2
E	37	GLY	-	CLONING ARTIFACT	UNP Q9P0L2
F	37	GLY	-	CLONING ARTIFACT	UNP Q9P0L2
G	37	GLY	-	CLONING ARTIFACT	UNP Q9P0L2
H	37	GLY	-	CLONING ARTIFACT	UNP Q9P0L2

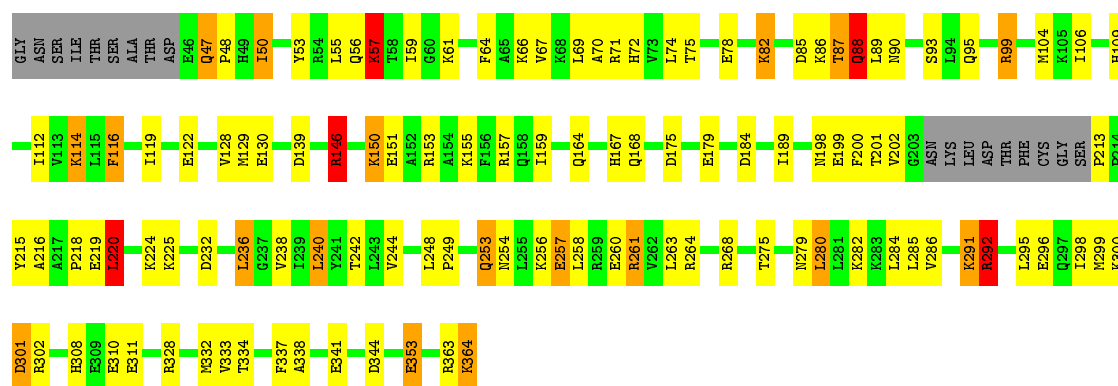
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total 27	O 27	0	0
2	B	17	Total 17	O 17	0	0
2	C	47	Total 47	O 47	0	0
2	D	24	Total 24	O 24	0	0
2	E	35	Total 35	O 35	0	0
2	F	37	Total 37	O 37	0	0
2	G	14	Total 14	O 14	0	0
2	H	9	Total 9	O 9	0	0

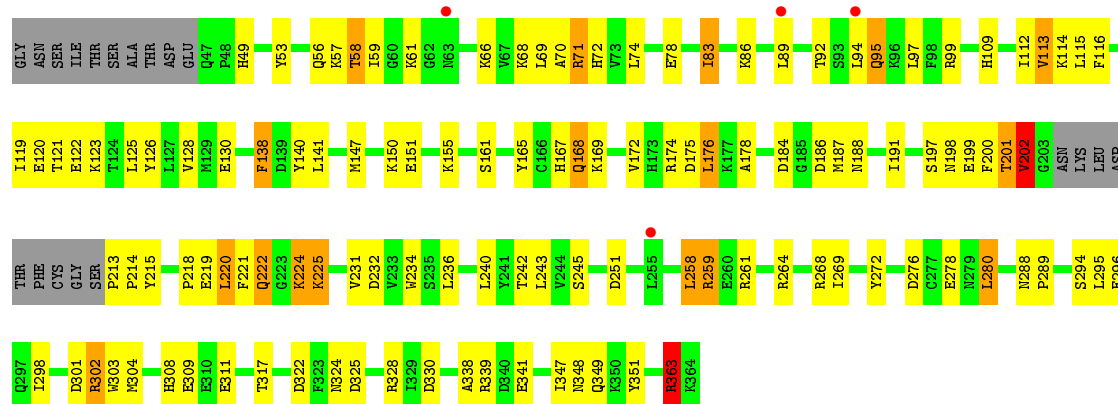


- Molecule 1: Serine/threonine-protein kinase MARK1

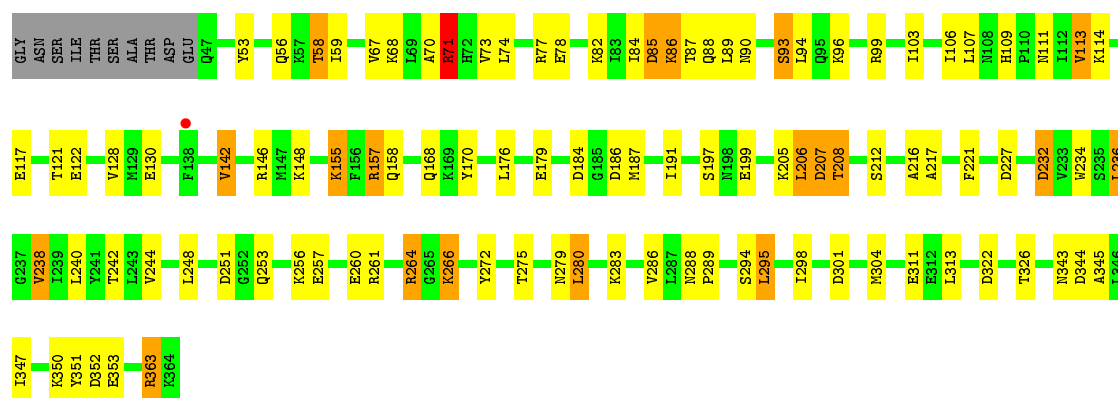




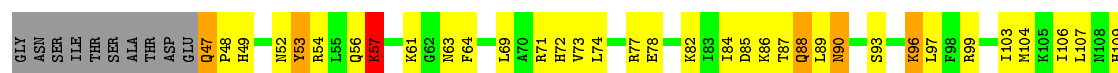
• Molecule 1: Serine/threonine-protein kinase MARK1

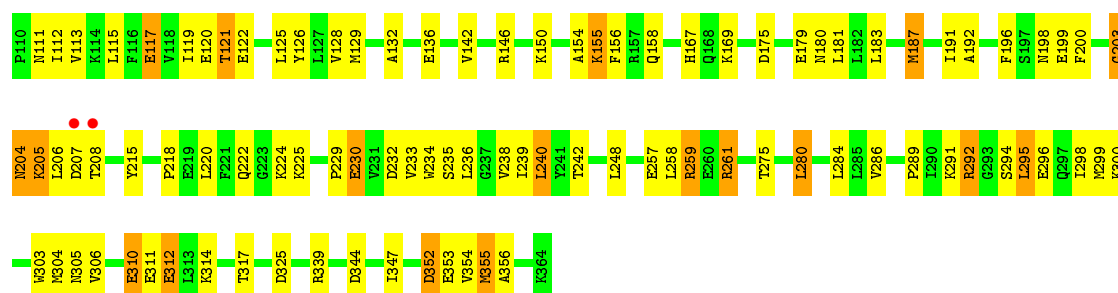


• Molecule 1: Serine/threonine-protein kinase MARK1

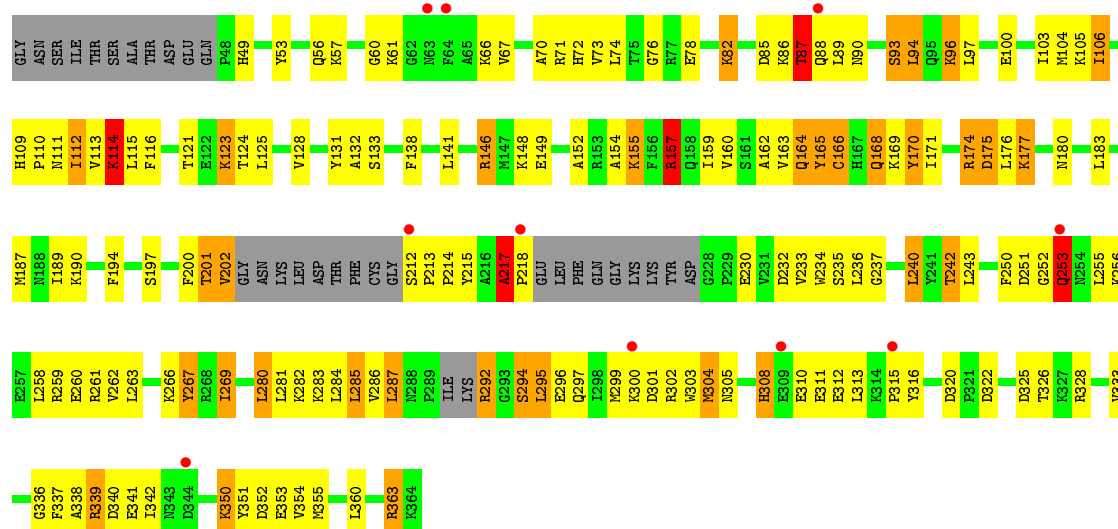
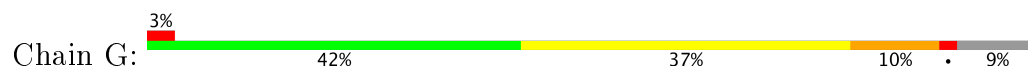


• Molecule 1: Serine/threonine-protein kinase MARK1

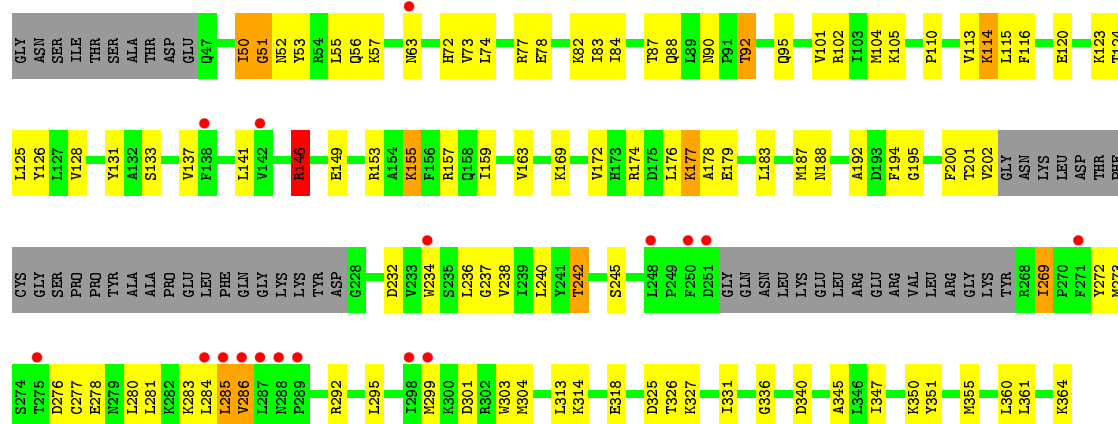




• Molecule 1: Serine/threonine-protein kinase MARK1



• Molecule 1: Serine/threonine-protein kinase MARK1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.68Å 116.47Å 285.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 49.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (10.00-2.60) 99.3 (49.68-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.212 , 0.290 0.209 , 0.284	Depositor DCC
$R_{free}$ test set	2786 reflections (2.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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	1.30	9/2539 (0.4%)	1.17	11/3421 (0.3%)
1	B	1.31	6/2269 (0.3%)	1.27	17/3055 (0.6%)
1	C	1.41	11/2561 (0.4%)	1.25	10/3448 (0.3%)
1	D	1.33	11/2552 (0.4%)	1.16	10/3436 (0.3%)
1	E	1.33	8/2589 (0.3%)	1.22	10/3496 (0.3%)
1	F	1.36	12/2613 (0.5%)	1.20	14/3524 (0.4%)
1	G	1.11	2/2394 (0.1%)	1.06	2/3232 (0.1%)
1	H	1.08	0/2225	1.01	4/3007 (0.1%)
All	All	1.29	59/19742 (0.3%)	1.17	78/26619 (0.3%)

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
1	E	0	1
1	F	0	1
1	G	0	3
All	All	0	7

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	353	GLU	CG-CD	11.27	1.68	1.51
1	C	353	GLU	CB-CG	9.91	1.71	1.52
1	B	312	GLU	CG-CD	9.07	1.65	1.51
1	B	363	ARG	CG-CD	-8.25	1.31	1.51
1	A	224	LYS	CE-NZ	7.63	1.68	1.49

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	A	363	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	A	77	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	B	153	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	77	ARG	NE-CZ-NH2	-8.05	116.27	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	ARG	Peptide
1	B	90	ASN	Peptide
1	E	363	ARG	Peptide
1	F	203	GLY	Peptide
1	G	114	LYS	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	2490	0	2520	77	0
1	B	2231	0	2248	142	1
1	C	2512	0	2551	79	1
1	D	2503	0	2547	77	0
1	E	2538	0	2541	74	0
1	F	2562	0	2579	89	0
1	G	2349	0	2332	171	0
1	H	2184	0	2166	64	0
2	A	27	0	0	2	0
2	B	17	0	0	2	0
2	C	47	0	0	8	0
2	D	24	0	0	2	0
2	E	35	0	0	3	0
2	F	37	0	0	3	0
2	G	14	0	0	11	0
2	H	9	0	0	2	0
All	All	19579	0	19484	761	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 20.

The worst 5 of 761 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:224:LYS:NZ	1:A:224:LYS:CE	1.68	1.55
1:D:347:ILE:CG1	1:D:347:ILE:CD1	1.78	1.54
1:G:164:GLN:NE2	1:G:315:PRO:HB3	1.37	1.37
1:B:125:LEU:HD12	1:B:126:TYR:N	1.56	1.21
1:A:290:ILE:O	1:A:290:ILE:HD12	1.51	1.11

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:B:327:LYS:NZ	1:C:364:LYS:O[4_455]	2.11	0.09

## 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	305/328 (93%)	290 (95%)	12 (4%)	3 (1%)	18	37
1	B	269/328 (82%)	230 (86%)	20 (7%)	19 (7%)	1	1
1	C	306/328 (93%)	290 (95%)	12 (4%)	4 (1%)	14	29
1	D	305/328 (93%)	279 (92%)	22 (7%)	4 (1%)	14	29
1	E	316/328 (96%)	294 (93%)	18 (6%)	4 (1%)	14	29
1	F	316/328 (96%)	293 (93%)	17 (5%)	6 (2%)	9	18
1	G	289/328 (88%)	241 (83%)	33 (11%)	15 (5%)	2	2
1	H	271/328 (83%)	237 (88%)	25 (9%)	9 (3%)	4	7
All	All	2377/2624 (91%)	2154 (91%)	159 (7%)	64 (3%)	6	10

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	93	SER
1	B	94	LEU
1	B	301	ASP
1	B	306	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	269/290 (93%)	237 (88%)	32 (12%)	6	11
1	B	240/290 (83%)	203 (85%)	37 (15%)	3	5
1	C	272/290 (94%)	238 (88%)	34 (12%)	5	10
1	D	271/290 (93%)	231 (85%)	40 (15%)	3	6
1	E	271/290 (93%)	244 (90%)	27 (10%)	9	17
1	F	277/290 (96%)	247 (89%)	30 (11%)	7	14
1	G	249/290 (86%)	208 (84%)	41 (16%)	2	4
1	H	232/290 (80%)	205 (88%)	27 (12%)	6	11
All	All	2081/2320 (90%)	1813 (87%)	268 (13%)	5	9

5 of 268 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	197	SER
1	E	114	LYS
1	H	114	LYS
1	D	201	THR
1	D	264	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	167	HIS
1	E	279	ASN
1	G	180	ASN
1	E	63	ASN
1	E	308	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	309/328 (94%)	-0.15	0 100 100	25, 42, 77, 89	0
1	B	279/328 (85%)	0.04	7 (2%) 58 50	25, 52, 81, 93	0
1	C	310/328 (94%)	-0.21	0 100 100	20, 36, 62, 73	0
1	D	309/328 (94%)	-0.12	4 (1%) 77 73	26, 43, 72, 84	0
1	E	318/328 (96%)	-0.22	1 (0%) 93 93	23, 40, 59, 72	0
1	F	318/328 (96%)	-0.18	2 (0%) 89 88	20, 39, 64, 75	0
1	G	297/328 (90%)	0.14	10 (3%) 46 38	38, 62, 95, 101	0
1	H	277/328 (84%)	0.14	17 (6%) 22 16	34, 60, 87, 94	0
All	All	2417/2624 (92%)	-0.08	41 (1%) 70 65	20, 46, 81, 101	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	286	VAL	6.1
1	H	250	PHE	5.3
1	H	284	LEU	4.6
1	H	285	LEU	4.3
1	G	63	ASN	4.3

### 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.