



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:13 am BST

PDB ID : 2WTT  
Title : Structure of the human p73 tetramerization domain (crystal form II)  
Authors : Joerger, A.C.  
Deposited on : 2009-09-21  
Resolution : 2.30 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

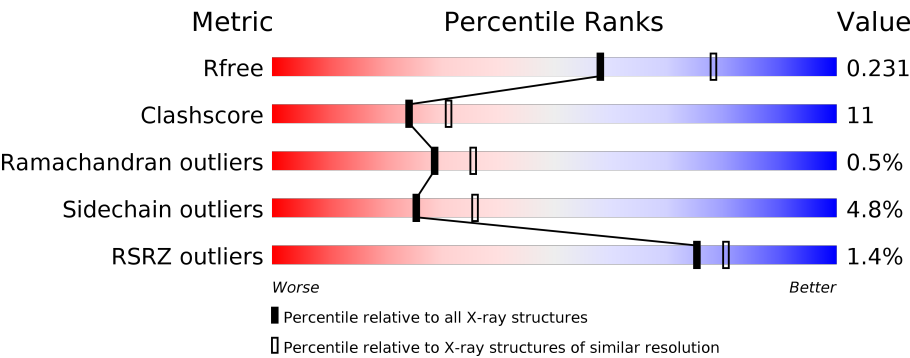
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	51	<div><div></div><div><div>73%</div><div>8%</div><div>•</div><div>18%</div></div></div>
1	B	51	<div><div></div><div><div>69%</div><div>16%</div><div></div><div>16%</div></div></div>
1	C	51	<div><div></div><div><div>55%</div><div>27%</div><div></div><div>18%</div></div></div>
1	D	51	<div><div></div><div><div>73%</div><div>18%</div><div>•</div><div>8%</div></div></div>
1	E	51	<div><div></div><div><div>69%</div><div>12%</div><div>•</div><div>18%</div></div></div>
1	F	51	<div><div>2%</div><div><div>61%</div><div>20%</div><div>•</div><div>18%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	51	
1	H	51	
1	I	51	
1	J	51	
1	K	51	
1	L	51	
1	M	51	
1	N	51	
1	O	51	
1	P	51	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5778 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 TUMOR PROTEIN P73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	42	Total	C	N	O	Se	0	0	0
			350	223	55	70	2			
1	B	43	Total	C	N	O	Se	0	0	0
			355	227	57	69	2			
1	C	42	Total	C	N	O	Se	0	0	0
			355	227	57	69	2			
1	D	47	Total	C	N	O	Se	0	0	0
			403	256	69	76	2			
1	E	42	Total	C	N	O	Se	0	0	0
			353	225	56	70	2			
1	F	42	Total	C	N	O	Se	0	0	0
			351	226	58	65	2			
1	G	43	Total	C	N	O	Se	0	0	0
			359	230	60	67	2			
1	H	45	Total	C	N	O	Se	0	0	0
			373	240	62	69	2			
1	I	44	Total	C	N	O	Se	0	0	0
			363	231	58	72	2			
1	J	45	Total	C	N	O	Se	0	0	0
			384	246	66	70	2			
1	K	42	Total	C	N	O	Se	0	0	0
			354	226	57	69	2			
1	L	46	Total	C	N	O	Se	0	0	0
			389	248	65	74	2			
1	M	29	Total	C	N	O	Se	0	0	0
			241	155	39	45	2			
1	N	42	Total	C	N	O	Se	0	0	0
			359	230	60	67	2			
1	O	41	Total	C	N	O	Se	0	0	0
			324	206	50	66	2			
1	P	43	Total	C	N	O	Se	0	0	0
			358	229	62	65	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	12	Total O 12 12	0	0
2	C	7	Total O 7 7	0	0
2	D	9	Total O 9 9	0	0
2	E	9	Total O 9 9	0	0
2	F	8	Total O 8 8	0	0
2	G	5	Total O 5 5	0	0
2	H	4	Total O 4 4	0	0
2	I	2	Total O 2 2	0	0
2	J	12	Total O 12 12	0	0
2	K	7	Total O 7 7	0	0
2	L	7	Total O 7 7	0	0
2	N	4	Total O 4 4	0	0
2	O	2	Total O 2 2	0	0
2	P	2	Total O 2 2	0	0

### 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: TUMOR PROTEIN P73

Chain A: 



#### • Molecule 1: TUMOR PROTEIN P73

Chain B: 



#### • Molecule 1: TUMOR PROTEIN P73

Chain C: 



#### • Molecule 1: TUMOR PROTEIN P73

Chain D: 



#### • Molecule 1: TUMOR PROTEIN P73

Chain E: 



#### • Molecule 1: TUMOR PROTEIN P73

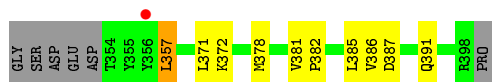
Chain F: 



- Molecule 1: TUMOR PROTEIN P73



- Molecule 1: TUMOR PROTEIN P73



- Molecule 1: TUMOR PROTEIN P73



- Molecule 1: TUMOR PROTEIN P73



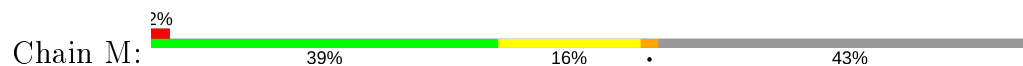
- Molecule 1: TUMOR PROTEIN P73

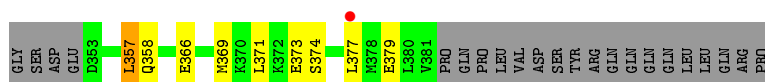


- Molecule 1: TUMOR PROTEIN P73



- Molecule 1: TUMOR PROTEIN P73

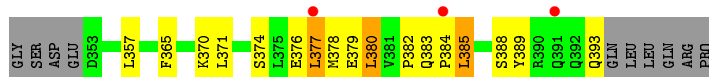




• Molecule 1: TUMOR PROTEIN P73



• Molecule 1: TUMOR PROTEIN P73



• Molecule 1: TUMOR PROTEIN P73





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.12Å 84.00Å 169.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.79 – 2.30 59.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.79-2.30) 99.9 (59.71-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.230 , 0.287 0.229 , 0.231	Depositor DCC
$R_{free}$ test set	1853 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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 [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.50	0/353	0.62	0/473
1	B	0.50	0/358	0.60	0/479
1	C	0.45	0/358	0.56	0/478
1	D	0.46	0/407	0.54	0/543
1	E	0.47	0/356	0.59	0/476
1	F	0.50	0/354	0.56	0/473
1	G	0.45	0/362	0.53	0/484
1	H	0.47	0/376	0.58	0/503
1	I	0.40	0/365	0.55	0/490
1	J	0.50	0/387	0.66	0/516
1	K	0.48	0/357	0.52	0/477
1	L	0.47	0/392	0.63	0/524
1	M	0.43	0/240	0.61	0/318
1	N	0.41	0/362	0.52	0/483
1	O	0.30	0/326	0.47	0/439
1	P	0.37	0/360	0.51	0/480
All	All	0.45	0/5713	0.57	0/7636

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	350	0	334	6	0
1	B	355	0	346	10	0
1	C	355	0	352	16	0
1	D	403	0	409	10	0
1	E	353	0	346	8	0
1	F	351	0	354	10	0
1	G	359	0	360	12	0
1	H	373	0	375	7	0
1	I	363	0	345	12	0
1	J	384	0	394	8	0
1	K	354	0	350	19	0
1	L	389	0	391	14	0
1	M	241	0	236	12	0
1	N	359	0	366	18	0
1	O	324	0	302	16	0
1	P	358	0	367	9	0
2	A	17	0	0	0	0
2	B	12	0	0	0	0
2	C	7	0	0	1	0
2	D	9	0	0	0	0
2	E	9	0	0	0	0
2	F	8	0	0	0	0
2	G	5	0	0	0	0
2	H	4	0	0	0	0
2	I	2	0	0	0	0
2	J	12	0	0	0	0
2	K	7	0	0	0	0
2	L	7	0	0	1	0
2	N	4	0	0	1	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
All	All	5778	0	5627	124	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 11.

All (124) 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:371:LEU:HD11	1:C:371:LEU:HD11	1.23	1.13
1:A:372:LYS:HD2	1:B:357:LEU:HD21	1.44	0.98
1:F:371:LEU:HD11	1:G:371:LEU:HD11	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:363:GLU:CD	1:K:363:GLU:H	1.72	0.90
1:J:397:GLN:HG2	1:K:357:LEU:HA	1.54	0.88
1:N:371:LEU:HD11	1:O:371:LEU:HD11	1.56	0.88
1:M:371:LEU:HD22	1:O:371:LEU:HD22	1.55	0.85
1:L:363:GLU:HG2	2:L:2001:HOH:O	1.80	0.80
1:A:372:LYS:HD2	1:B:357:LEU:CD2	2.12	0.78
1:A:372:LYS:CD	1:B:357:LEU:HD21	2.15	0.76
1:I:371:LEU:HD11	1:L:371:LEU:HD11	1.68	0.76
1:C:358:GLN:O	1:D:372:LYS:HE3	1.87	0.74
1:M:357:LEU:CD2	1:N:357:LEU:HB3	2.17	0.74
1:L:359:VAL:HG21	1:L:368:LEU:HD12	1.68	0.73
1:E:373:GLU:HG3	1:G:389:TYR:HE2	1.53	0.73
1:N:394:GLN:C	1:N:395:LEU:HD23	2.09	0.73
1:J:371:LEU:HD11	1:K:371:LEU:HD11	1.69	0.73
1:B:371:LEU:CD1	1:C:371:LEU:HD11	2.13	0.73
1:C:394:GLN:OE1	1:G:394:GLN:HG3	1.90	0.71
1:F:371:LEU:CD1	1:G:371:LEU:HD11	2.21	0.70
1:E:358:GLN:HB3	1:F:356:TYR:CE2	2.28	0.69
1:M:371:LEU:HD11	1:P:371:LEU:HD11	1.74	0.69
1:C:391:GLN:NE2	1:G:391:GLN:HB3	2.07	0.69
1:E:362:ARG:NH2	1:E:366:GLU:OE1	2.25	0.69
1:F:357:LEU:HD23	1:F:358:GLN:N	2.10	0.66
1:O:382:PRO:HD2	1:O:385:LEU:HD23	1.78	0.66
1:B:371:LEU:HD11	1:C:371:LEU:CD1	2.14	0.66
1:F:357:LEU:HD23	1:F:357:LEU:C	2.17	0.65
1:M:357:LEU:HD23	1:N:357:LEU:HB3	1.78	0.65
1:H:387:ASP:O	1:H:391:GLN:HG2	1.98	0.63
1:M:377:LEU:HD12	1:O:378:MSE:HE3	1.81	0.63
1:C:372:LYS:HD3	1:D:357:LEU:HD21	1.81	0.62
1:E:373:GLU:HG3	1:G:389:TYR:CE2	2.35	0.61
1:H:382:PRO:HD2	1:H:385:LEU:HD12	1.81	0.61
1:G:389:TYR:O	1:G:393:GLN:HG2	2.01	0.60
1:I:370:LYS:NZ	1:K:378:MSE:HE1	2.16	0.60
1:F:371:LEU:HD22	1:H:371:LEU:HD22	1.83	0.60
1:L:357:LEU:HD21	1:L:359:VAL:CG2	2.32	0.60
1:O:380:LEU:N	1:O:380:LEU:HD23	2.17	0.59
1:K:357:LEU:HG	1:L:357:LEU:HD22	1.84	0.59
1:N:361:GLY:HA3	2:N:2002:HOH:O	2.03	0.59
1:O:357:LEU:HD22	1:P:357:LEU:HD22	1.84	0.58
1:E:371:LEU:HD11	1:H:371:LEU:HD11	1.84	0.58
1:A:371:LEU:HD11	1:D:371:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:369:MSE:SE	1:N:357:LEU:CD1	3.01	0.58
1:K:369:MSE:HE2	1:L:357:LEU:HD12	1.85	0.58
1:I:371:LEU:CD1	1:L:371:LEU:HD11	2.33	0.58
1:P:357:LEU:HD23	1:P:357:LEU:O	2.03	0.58
1:G:369:MSE:SE	1:H:357:LEU:HD13	2.54	0.57
1:M:357:LEU:HD21	1:N:357:LEU:HD23	1.87	0.56
1:F:363:GLU:O	1:F:367:ILE:HG13	2.06	0.56
1:N:394:GLN:O	1:N:395:LEU:HD23	2.06	0.56
1:I:362:ARG:HD3	1:J:355:TYR:OH	2.06	0.55
1:L:357:LEU:C	1:L:357:LEU:HD23	2.27	0.55
1:M:357:LEU:HD21	1:N:357:LEU:HB3	1.86	0.55
1:M:373:GLU:HG3	1:O:389:TYR:CE2	2.42	0.55
1:M:373:GLU:HG3	1:O:389:TYR:HE2	1.72	0.55
1:B:357:LEU:HD23	1:B:358:GLN:N	2.22	0.54
1:I:378:MSE:SE	1:K:377:LEU:HD12	2.58	0.54
1:K:369:MSE:CE	1:L:357:LEU:HD12	2.38	0.54
1:I:378:MSE:HE2	1:K:374:SER:CB	2.39	0.53
1:O:376:GLU:O	1:O:379:GLU:HG2	2.08	0.53
1:N:363:GLU:O	1:N:367:ILE:HG13	2.08	0.53
1:K:357:LEU:HD13	1:L:372:LYS:HD2	1.92	0.52
1:N:390:ARG:O	1:N:393:GLN:HB2	2.09	0.52
1:L:357:LEU:HD23	1:L:357:LEU:O	2.10	0.52
1:G:362:ARG:O	1:G:366:GLU:HG3	2.10	0.51
1:O:370:LYS:O	1:O:374:SER:HB2	2.10	0.51
1:O:376:GLU:O	1:O:378:MSE:N	2.39	0.51
1:C:389:TYR:O	1:C:393:GLN:HG2	2.11	0.51
1:C:361:GLY:HA3	2:C:2002:HOH:O	2.11	0.50
1:P:389:TYR:CE1	1:P:393:GLN:NE2	2.79	0.50
1:N:359:VAL:HG22	1:N:360:ARG:N	2.26	0.50
1:J:397:GLN:OE1	1:L:372:LYS:HE2	2.11	0.49
1:C:372:LYS:HD2	1:D:358:GLN:O	2.12	0.48
1:K:363:GLU:N	1:K:363:GLU:OE1	2.46	0.48
1:F:388:SER:O	1:F:392:GLN:HG3	2.14	0.47
1:E:389:TYR:OH	1:G:376:GLU:OE1	2.29	0.47
1:I:378:MSE:HE2	1:K:374:SER:HB2	1.97	0.47
1:K:355:TYR:CE1	1:L:362:ARG:NH2	2.83	0.47
1:D:357:LEU:C	1:D:357:LEU:HD23	2.36	0.46
1:P:372:LYS:O	1:P:376:GLU:HG3	2.15	0.46
1:O:377:LEU:HG	1:O:377:LEU:O	2.15	0.46
1:A:357:LEU:HD23	1:B:357:LEU:HB3	1.97	0.46
1:I:389:TYR:HE2	1:K:373:GLU:HG3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:363:GLU:O	1:K:367:ILE:HG12	2.16	0.46
1:M:369:MSE:SE	1:N:357:LEU:HD13	2.66	0.46
1:F:377:LEU:HD13	1:H:386:VAL:HG22	1.97	0.45
1:K:369:MSE:HE2	1:L:357:LEU:CD1	2.47	0.45
1:I:392:GLN:O	1:I:393:GLN:C	2.55	0.45
1:N:371:LEU:CD1	1:O:371:LEU:HD11	2.36	0.45
1:F:357:LEU:CD2	1:F:357:LEU:C	2.83	0.44
1:J:383:GLN:NE2	1:J:387:ASP:OD1	2.48	0.44
1:B:363:GLU:O	1:B:367:ILE:HG13	2.17	0.44
1:N:359:VAL:CG2	1:N:360:ARG:N	2.80	0.44
1:G:383:GLN:HB3	1:G:384:PRO:HD3	1.99	0.44
1:E:362:ARG:O	1:E:366:GLU:HG3	2.18	0.43
1:I:389:TYR:CE2	1:K:373:GLU:HG3	2.53	0.43
1:C:357:LEU:HD13	1:D:369:MSE:SE	2.68	0.43
1:B:380:LEU:HA	1:B:380:LEU:HD23	1.78	0.43
1:A:388:SER:O	1:A:392:GLN:HG3	2.19	0.43
1:D:357:LEU:HD23	1:D:358:GLN:N	2.34	0.43
1:O:383:GLN:N	1:O:384:PRO:CD	2.81	0.43
1:C:356:TYR:N	1:C:356:TYR:CD2	2.87	0.42
1:O:379:GLU:H	1:O:379:GLU:HG2	1.66	0.42
1:N:371:LEU:HD22	1:P:371:LEU:HD22	2.01	0.42
1:D:370:LYS:HE3	1:E:363:GLU:OE1	2.19	0.42
1:C:362:ARG:HD3	1:D:355:TYR:OH	2.19	0.42
1:M:358:GLN:O	1:N:372:LYS:HD2	2.19	0.42
1:P:377:LEU:HD23	1:P:377:LEU:HA	1.94	0.42
1:H:378:MSE:HA	1:H:381:VAL:HG23	2.01	0.41
1:P:378:MSE:HA	1:P:381:VAL:HG23	2.01	0.41
1:N:388:SER:O	1:N:392:GLN:HB3	2.20	0.41
1:G:371:LEU:HA	1:G:371:LEU:HD23	1.83	0.41
1:I:357:LEU:HD11	1:J:357:LEU:HG	2.03	0.41
1:K:389:TYR:O	1:K:393:GLN:HG2	2.21	0.41
1:O:393:GLN:OE1	1:O:393:GLN:HA	2.21	0.41
1:C:390:ARG:O	1:C:394:GLN:HG2	2.21	0.41
1:C:357:LEU:HD12	1:C:358:GLN:N	2.36	0.41
1:C:359:VAL:HG21	1:C:368:LEU:CD1	2.50	0.41
1:D:359:VAL:HG21	1:D:368:LEU:HD12	2.03	0.41
1:P:389:TYR:O	1:P:393:GLN:HG2	2.20	0.41
1:I:359:VAL:HG13	1:J:355:TYR:HB2	2.03	0.40
1:J:397:GLN:OE1	1:K:358:GLN:N	2.50	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	40/51 (78%)	40 (100%)	0	0	100	100
1	B	41/51 (80%)	37 (90%)	3 (7%)	1 (2%)	6	4
1	C	40/51 (78%)	40 (100%)	0	0	100	100
1	D	45/51 (88%)	45 (100%)	0	0	100	100
1	E	40/51 (78%)	40 (100%)	0	0	100	100
1	F	40/51 (78%)	39 (98%)	0	1 (2%)	5	4
1	G	41/51 (80%)	41 (100%)	0	0	100	100
1	H	43/51 (84%)	43 (100%)	0	0	100	100
1	I	42/51 (82%)	40 (95%)	2 (5%)	0	100	100
1	J	43/51 (84%)	43 (100%)	0	0	100	100
1	K	40/51 (78%)	40 (100%)	0	0	100	100
1	L	44/51 (86%)	44 (100%)	0	0	100	100
1	M	27/51 (53%)	26 (96%)	1 (4%)	0	100	100
1	N	40/51 (78%)	39 (98%)	1 (2%)	0	100	100
1	O	39/51 (76%)	28 (72%)	10 (26%)	1 (3%)	5	4
1	P	41/51 (80%)	40 (98%)	1 (2%)	0	100	100
All	All	646/816 (79%)	625 (97%)	18 (3%)	3 (0%)	29	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	394	GLN
1	O	377	LEU
1	B	391	GLN

### 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	38/47 (81%)	37 (97%)	1 (3%)	46	63
1	B	39/47 (83%)	38 (97%)	1 (3%)	46	63
1	C	40/47 (85%)	40 (100%)	0	100	100
1	D	46/47 (98%)	44 (96%)	2 (4%)	29	40
1	E	40/47 (85%)	39 (98%)	1 (2%)	47	65
1	F	39/47 (83%)	37 (95%)	2 (5%)	24	33
1	G	40/47 (85%)	40 (100%)	0	100	100
1	H	41/47 (87%)	39 (95%)	2 (5%)	25	35
1	I	39/47 (83%)	38 (97%)	1 (3%)	46	63
1	J	43/47 (92%)	42 (98%)	1 (2%)	50	67
1	K	40/47 (85%)	36 (90%)	4 (10%)	7	9
1	L	44/47 (94%)	42 (96%)	2 (4%)	27	39
1	M	25/47 (53%)	21 (84%)	4 (16%)	2	2
1	N	41/47 (87%)	38 (93%)	3 (7%)	14	18
1	O	35/47 (74%)	31 (89%)	4 (11%)	5	6
1	P	40/47 (85%)	38 (95%)	2 (5%)	24	34
All	All	630/752 (84%)	600 (95%)	30 (5%)	25	36

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	LEU
1	B	354	THR
1	D	358	GLN
1	D	362	ARG
1	E	358	GLN
1	F	358	GLN
1	F	378	MSE
1	H	357	LEU

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Mol	Chain	Res	Type
1	H	372	LYS
1	I	378	MSE
1	J	397	GLN
1	K	353	ASP
1	K	359	VAL
1	K	363	GLU
1	K	392	GLN
1	L	353	ASP
1	L	357	LEU
1	M	357	LEU
1	M	366	GLU
1	M	374	SER
1	M	379	GLU
1	N	389	TYR
1	N	392	GLN
1	N	395	LEU
1	O	365	PHE
1	O	380	LEU
1	O	385	LEU
1	O	388	SER
1	P	357	LEU
1	P	372	LYS

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

### 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 [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	40/51 (78%)	-0.22	0 100 100	24, 29, 51, 52	0
1	B	41/51 (80%)	-0.04	0 100 100	24, 34, 58, 63	0
1	C	40/51 (78%)	-0.02	0 100 100	27, 37, 52, 53	0
1	D	45/51 (88%)	-0.06	0 100 100	25, 34, 50, 52	0
1	E	40/51 (78%)	-0.10	0 100 100	22, 32, 54, 60	0
1	F	40/51 (78%)	-0.05	1 (2%) 57 64	24, 32, 46, 52	0
1	G	41/51 (80%)	0.09	1 (2%) 59 66	31, 39, 53, 55	0
1	H	43/51 (84%)	-0.13	1 (2%) 60 67	26, 32, 45, 49	0
1	I	42/51 (82%)	-0.09	0 100 100	27, 34, 54, 59	0
1	J	43/51 (84%)	-0.22	0 100 100	25, 34, 42, 44	0
1	K	40/51 (78%)	0.04	0 100 100	25, 35, 54, 61	0
1	L	44/51 (86%)	-0.09	0 100 100	23, 31, 41, 44	0
1	M	27/51 (52%)	0.58	1 (3%) 41 48	34, 47, 69, 70	0
1	N	40/51 (78%)	-0.05	0 100 100	27, 40, 59, 63	0
1	O	39/51 (76%)	0.54	3 (7%) 13 17	58, 67, 74, 77	0
1	P	41/51 (80%)	0.21	2 (4%) 29 36	29, 41, 67, 75	0
All	All	646/816 (79%)	0.01	9 (1%) 75 80	22, 36, 66, 77	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	384	PRO	4.2
1	M	377	LEU	3.3
1	O	391	GLN	3.1
1	P	356	TYR	2.9
1	O	377	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	395	LEU	2.3
1	P	357	LEU	2.3
1	G	394	GLN	2.2
1	H	356	TYR	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.