



# Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 09:58 AM EDT

PDB ID : 3VUT / pdb\_00003vut  
Title : Crystal structures of non-phosphorylated MAP2K4  
Authors : Matsumoto, T.; Kinoshita, T.; Kirii, Y.; Tada, T.; Yamano, A.  
Deposited on : 2012-07-05  
Resolution : 3.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

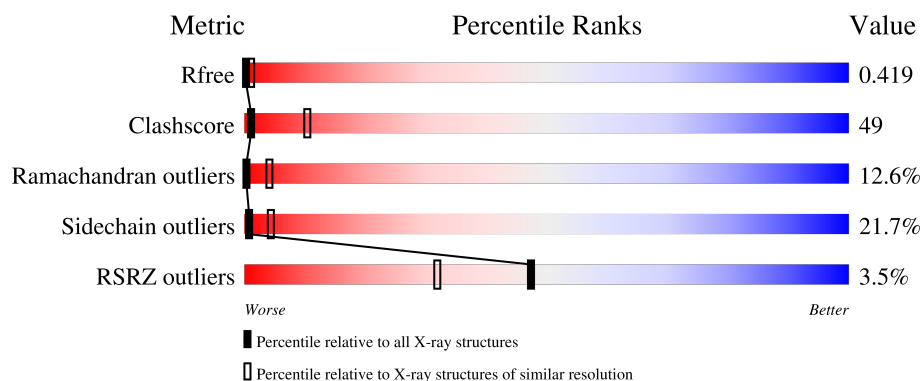
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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 of 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	327	<div> <div>4%</div> <div>24%</div> <div>25%</div> <div>9%</div> <div>•</div> <div>38%</div> </div>
1	B	327	<div> <div>4%</div> <div>28%</div> <div>34%</div> <div>14%</div> <div>•</div> <div>20%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3457 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 Dual specificity mitogen-activated protein kinase kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1563	1009	251	291	12			
1	B	260	Total	C	N	O	S	0	0	0
			1894	1197	309	376	12			

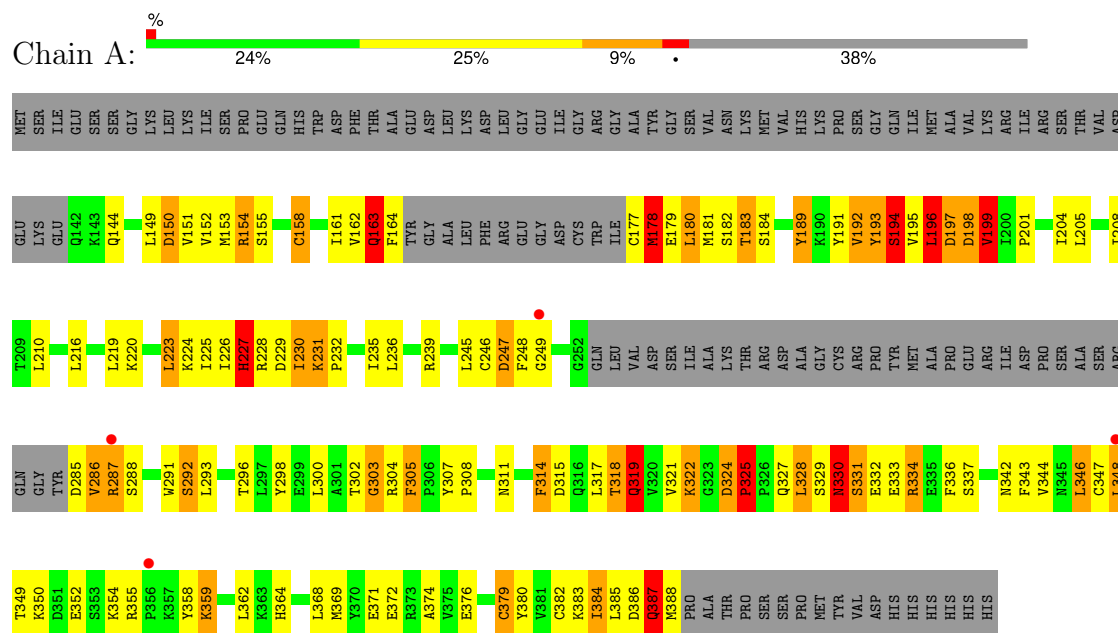
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	MET	-	expression tag	UNP P45985
A	400	HIS	-	expression tag	UNP P45985
A	401	HIS	-	expression tag	UNP P45985
A	402	HIS	-	expression tag	UNP P45985
A	403	HIS	-	expression tag	UNP P45985
A	404	HIS	-	expression tag	UNP P45985
A	405	HIS	-	expression tag	UNP P45985
B	79	MET	-	expression tag	UNP P45985
B	400	HIS	-	expression tag	UNP P45985
B	401	HIS	-	expression tag	UNP P45985
B	402	HIS	-	expression tag	UNP P45985
B	403	HIS	-	expression tag	UNP P45985
B	404	HIS	-	expression tag	UNP P45985
B	405	HIS	-	expression tag	UNP P45985

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Dual specificity mitogen-activated protein kinase kinase 4



K354	K355	K356	K357	Y358	K359	E360	L361	L362	K363	H364		L367	L368		E371	E372	K373	ALA	VAL	GLU	VAL	VAL	ALA	ALA	CYS	TYR	VAL	CYS	LYS	ILE	LEU	ASP	GLN	MET	PRO	ALA	ALA	THR	PRO	SER	SER	PRO	PRO	MET	TYR	VAL	ASP	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	--	------	------	--	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.77Å 87.36Å 118.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.50) 97.7 (20.00-3.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.34 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.331 , 0.407 0.331 , 0.419	Depositor DCC
$R_{free}$ test set	593 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 77.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	3457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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	0.74	0/1590	1.13	8/2153 (0.4%)
1	B	0.83	2/1919 (0.1%)	1.28	18/2597 (0.7%)
All	All	0.79	2/3509 (0.1%)	1.22	26/4750 (0.5%)

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	B	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	SER	N-CA	-5.56	1.39	1.46
1	B	261	THR	CA-C	5.04	1.58	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	CYS	CA-C-N	12.33	132.01	119.56
1	A	158	CYS	C-N-CA	12.33	132.01	119.56
1	B	118	LYS	N-CA-C	-10.32	95.07	110.24
1	B	257	SER	N-CA-C	-8.86	91.93	110.80
1	B	260	LYS	N-CA-C	7.54	120.30	110.43
1	B	313	VAL	N-CA-C	7.53	118.06	107.37
1	B	103	LYS	N-CA-C	-7.09	100.31	110.59
1	B	99	ALA	N-CA-C	-6.74	104.93	113.02
1	B	102	LEU	N-CA-C	-6.46	99.76	110.17
1	B	194	SER	N-CA-C	-6.35	104.44	111.36
1	B	104	ASP	N-CA-C	-6.31	97.35	110.80
1	A	343	PHE	N-CA-C	-5.93	105.04	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ASN	N-CA-C	-5.88	100.82	109.81
1	B	258	ILE	CB-CA-C	-5.75	100.11	111.60
1	B	124	SER	N-CA-C	-5.68	104.99	111.07
1	A	364	HIS	CA-C-N	5.49	126.70	119.84
1	A	364	HIS	C-N-CA	5.49	126.70	119.84
1	B	86	LYS	N-CA-C	5.47	117.59	110.43
1	A	325	PRO	N-CA-C	5.40	117.28	110.70
1	B	256	ASP	N-CA-C	-5.32	99.48	110.80
1	A	305	PHE	CA-C-N	5.30	126.47	119.84
1	A	305	PHE	C-N-CA	5.30	126.47	119.84
1	B	101	ASP	N-CA-C	-5.22	99.68	110.80
1	B	152	VAL	N-CA-C	5.21	115.98	110.72
1	B	120	VAL	N-CA-C	5.21	117.35	108.86
1	B	131	LYS	N-CA-C	5.18	117.83	111.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	GLU	Peptide
1	B	103	LYS	Peptide
1	B	105	LEU	Peptide
1	B	244	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	1563	0	1540	99	0
1	B	1894	0	1765	231	0
All	All	3457	0	3305	330	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 49.

All (330) 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:219:LEU:O	1:B:222:ASN:O	1.54	1.25
1:B:115:SER:O	1:B:131:LYS:O	1.53	1.24
1:B:133:ILE:CB	1:B:174:CYS:O	1.87	1.22
1:B:223:LEU:HG	1:B:224:LYS:CB	1.69	1.20
1:B:256:ASP:OD2	1:B:261:THR:HG23	1.47	1.13
1:B:98:THR:HB	1:B:100:GLU:HG2	1.20	1.12
1:A:154:ARG:HG2	1:A:154:ARG:HH11	0.99	1.11
1:B:85:GLY:HA2	1:B:126:GLN:HE22	1.13	1.10
1:B:102:LEU:HD12	1:B:103:LYS:O	1.52	1.10
1:B:234:ASN:HA	1:B:235:ILE:CB	1.89	1.03
1:B:85:GLY:HA2	1:B:126:GLN:NE2	1.73	1.03
1:B:314:PHE:CE1	1:B:315:ASP:CG	2.37	1.02
1:B:225:ILE:HD11	1:B:228:ARG:CB	1.94	0.97
1:B:133:ILE:CB	1:B:174:CYS:HB3	1.96	0.95
1:B:223:LEU:CG	1:B:224:LYS:CB	2.44	0.95
1:A:154:ARG:HG2	1:A:154:ARG:NH1	1.75	0.93
1:B:346:LEU:O	1:B:349:THR:OG1	1.86	0.93
1:A:314:PHE:HA	1:A:317:LEU:HB2	1.49	0.92
1:B:314:PHE:CE1	1:B:315:ASP:OD2	2.22	0.92
1:B:222:ASN:N	1:B:222:ASN:HD22	1.68	0.91
1:B:254:LEU:C	1:B:257:SER:OG	2.14	0.91
1:B:98:THR:CB	1:B:100:GLU:HG2	2.00	0.91
1:A:286:VAL:HG22	1:A:287:ARG:N	1.86	0.91
1:B:248:PHE:N	1:B:249:GLY:HA3	1.86	0.90
1:B:223:LEU:CB	1:B:224:LYS:CB	2.50	0.90
1:A:150:ASP:H	1:A:154:ARG:NH2	1.68	0.90
1:B:228:ARG:HA	1:B:229:ASP:HB2	1.53	0.89
1:A:286:VAL:O	1:A:288:SER:N	2.05	0.89
1:A:154:ARG:HH11	1:A:154:ARG:CG	1.85	0.89
1:B:223:LEU:HB3	1:B:224:LYS:CB	2.02	0.89
1:A:164:PHE:CB	1:A:177:CYS:N	2.37	0.87
1:A:314:PHE:O	1:A:318:THR:HG22	1.75	0.86
1:B:254:LEU:O	1:B:257:SER:OG	1.90	0.86
1:A:178:MET:HG3	1:A:179:GLU:H	1.40	0.86
1:B:224:LYS:O	1:B:225:ILE:HG23	1.75	0.84
1:B:232:PRO:CB	1:B:233:SER:HA	2.08	0.84
1:B:256:ASP:HB3	1:B:260:LYS:HA	1.59	0.83
1:B:154:ARG:O	1:B:218:HIS:HE1	1.59	0.83
1:A:321:VAL:HA	1:A:350:LYS:HZ1	1.43	0.83
1:B:225:ILE:CD1	1:B:228:ARG:CB	2.56	0.83
1:B:98:THR:HB	1:B:100:GLU:CG	2.05	0.83
1:B:133:ILE:CB	1:B:174:CYS:CB	2.57	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LYS:HA	1:B:232:PRO:C	2.03	0.82
1:A:321:VAL:HA	1:A:350:LYS:NZ	1.96	0.81
1:B:104:ASP:O	1:B:105:LEU:CB	2.29	0.81
1:A:191:TYR:O	1:A:196:LEU:HD13	1.79	0.81
1:B:102:LEU:O	1:B:119:MET:HG2	1.79	0.81
1:A:383:LYS:O	1:A:387:GLN:NE2	2.14	0.81
1:B:121:HIS:C	1:B:123:PRO:HD2	2.06	0.80
1:B:314:PHE:HE1	1:B:315:ASP:OD2	1.60	0.80
1:B:225:ILE:HD11	1:B:228:ARG:N	1.96	0.80
1:B:255:VAL:C	1:B:257:SER:OG	2.24	0.79
1:A:151:VAL:C	1:A:154:ARG:HH12	1.89	0.79
1:A:230:ILE:HG22	1:A:292:SER:HB2	1.64	0.79
1:B:256:ASP:OD2	1:B:260:LYS:C	2.27	0.78
1:A:342:ASN:O	1:A:346:LEU:HD21	1.83	0.78
1:B:232:PRO:HB2	1:B:233:SER:HA	1.65	0.78
1:B:256:ASP:CG	1:B:259:ALA:O	2.27	0.78
1:B:228:ARG:CB	1:B:229:ASP:HB3	2.14	0.78
1:B:219:LEU:O	1:B:223:LEU:CD1	2.32	0.77
1:B:107:GLU:HA	1:B:116:VAL:CG2	2.14	0.77
1:A:181:MET:HG3	1:A:236:LEU:HB3	1.68	0.76
1:B:255:VAL:O	1:B:256:ASP:C	2.29	0.76
1:B:143:LYS:HG3	1:B:254:LEU:HD21	1.67	0.75
1:A:246:CYS:SG	1:A:247:ASP:N	2.59	0.75
1:B:100:GLU:CA	1:B:100:GLU:OE1	2.35	0.74
1:B:260:LYS:O	1:B:261:THR:HG22	1.88	0.74
1:B:100:GLU:OE1	1:B:100:GLU:HA	1.86	0.74
1:A:286:VAL:CG2	1:A:287:ARG:N	2.52	0.73
1:B:133:ILE:CB	1:B:174:CYS:C	2.60	0.73
1:B:255:VAL:O	1:B:256:ASP:O	2.06	0.73
1:B:192:VAL:HB	1:B:198:ASP:HA	1.70	0.72
1:B:256:ASP:CB	1:B:260:LYS:HA	2.19	0.71
1:B:228:ARG:HA	1:B:229:ASP:CB	2.19	0.71
1:B:256:ASP:OD2	1:B:260:LYS:HA	1.91	0.71
1:B:181:MET:SD	1:B:237:LEU:HG	2.30	0.71
1:B:219:LEU:C	1:B:222:ASN:O	2.34	0.71
1:B:165:TYR:HE2	1:B:178:MET:O	1.73	0.70
1:B:330:ASN:HB3	1:B:334:ARG:HG2	1.72	0.70
1:B:115:SER:O	1:B:131:LYS:C	2.32	0.70
1:B:228:ARG:CA	1:B:229:ASP:CB	2.68	0.70
1:B:219:LEU:O	1:B:223:LEU:HD13	1.91	0.70
1:A:239:ARG:HG2	1:A:382:CYS:SG	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:NH1	1:A:154:ARG:H	1.90	0.70
1:B:122:LYS:N	1:B:123:PRO:CD	2.55	0.70
1:B:164:PHE:CE1	1:B:178:MET:SD	2.84	0.70
1:B:255:VAL:O	1:B:257:SER:OG	2.09	0.70
1:B:254:LEU:O	1:B:257:SER:CB	2.40	0.69
1:A:178:MET:HG3	1:A:179:GLU:N	2.06	0.69
1:B:183:THR:O	1:B:236:LEU:N	2.26	0.69
1:A:192:VAL:O	1:A:193:TYR:HB2	1.91	0.69
1:B:367:ILE:HD12	1:B:368:LEU:N	2.09	0.68
1:A:191:TYR:O	1:A:196:LEU:CD1	2.40	0.68
1:A:162:VAL:HG23	1:A:179:GLU:OE1	1.94	0.68
1:B:122:LYS:N	1:B:123:PRO:HD2	2.09	0.67
1:B:131:LYS:HG3	1:B:178:MET:HE2	1.77	0.67
1:B:222:ASN:N	1:B:222:ASN:ND2	2.33	0.67
1:B:364:HIS:O	1:B:367:ILE:HG13	1.95	0.67
1:B:117:ASN:O	1:B:118:LYS:C	2.34	0.66
1:B:107:GLU:HA	1:B:116:VAL:HG22	1.77	0.66
1:B:256:ASP:OD2	1:B:261:THR:N	2.28	0.66
1:A:380:TYR:O	1:A:384:ILE:HG12	1.95	0.66
1:B:127:ILE:HG12	1:B:127:ILE:O	1.94	0.66
1:B:234:ASN:CA	1:B:235:ILE:CB	2.68	0.66
1:B:120:VAL:CG2	1:B:127:ILE:HA	2.25	0.65
1:B:256:ASP:CG	1:B:260:LYS:HA	2.22	0.65
1:B:232:PRO:CG	1:B:233:SER:HA	2.27	0.65
1:A:321:VAL:O	1:A:322:LYS:HB2	1.97	0.65
1:B:157:ASP:HB2	1:B:218:HIS:NE2	2.12	0.64
1:A:328:LEU:HD11	1:A:336:PHE:HE2	1.61	0.64
1:A:385:LEU:O	1:A:388:MET:HG3	1.97	0.64
1:A:304:ARG:HD2	1:A:305:PHE:H	1.62	0.64
1:B:85:GLY:CA	1:B:126:GLN:NE2	2.56	0.63
1:B:258:ILE:HG22	1:B:258:ILE:O	1.99	0.63
1:A:307:TYR:OH	1:A:324:ASP:O	2.11	0.63
1:B:133:ILE:CB	1:B:174:CYS:CA	2.78	0.62
1:A:315:ASP:O	1:A:319:GLN:NE2	2.33	0.62
1:B:256:ASP:OD2	1:B:261:THR:CG2	2.37	0.62
1:B:225:ILE:HD11	1:B:228:ARG:CA	2.29	0.62
1:B:120:VAL:HG23	1:B:127:ILE:HA	1.81	0.61
1:B:361:LEU:O	1:B:367:ILE:HG12	2.00	0.61
1:B:314:PHE:CE1	1:B:315:ASP:OD1	2.54	0.61
1:B:260:LYS:C	1:B:261:THR:CG2	2.74	0.61
1:B:264:ALA:O	1:B:265:GLY:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:HG12	1:A:348:LEU:HD11	1.83	0.60
1:B:193:TYR:H	1:B:196:LEU:HG	1.66	0.60
1:A:193:TYR:HA	1:A:198:ASP:HB3	1.83	0.60
1:B:160:TYR:HA	1:B:242:ASN:ND2	2.17	0.60
1:B:103:LYS:HA	1:B:119:MET:HG3	1.84	0.60
1:B:225:ILE:HG13	1:B:227:HIS:H	1.67	0.60
1:A:346:LEU:HD23	1:A:346:LEU:H	1.65	0.60
1:B:256:ASP:OD2	1:B:260:LYS:CA	2.50	0.59
1:B:134:ARG:O	1:B:135:SER:CB	2.51	0.59
1:B:248:PHE:N	1:B:249:GLY:CA	2.64	0.59
1:A:194:SER:OG	1:A:195:VAL:N	2.35	0.59
1:B:314:PHE:CD1	1:B:315:ASP:CG	2.81	0.58
1:B:238:ASP:CG	1:B:239:ARG:N	2.62	0.58
1:B:151:VAL:HG23	1:B:152:VAL:HG13	1.84	0.58
1:B:214:LYS:HE2	1:B:362:LEU:HD11	1.86	0.58
1:A:163:GLN:HA	1:A:178:MET:H	1.69	0.58
1:B:134:ARG:O	1:B:135:SER:HB2	2.04	0.58
1:B:232:PRO:HB2	1:B:233:SER:CA	2.31	0.58
1:B:368:LEU:HA	1:B:371:GLU:HB2	1.86	0.57
1:B:228:ARG:CB	1:B:229:ASP:CB	2.82	0.57
1:B:261:THR:O	1:B:262:ARG:CB	2.53	0.57
1:B:79:MET:SD	1:B:79:MET:N	2.78	0.57
1:B:85:GLY:CA	1:B:126:GLN:HE22	2.02	0.57
1:B:102:LEU:CD1	1:B:103:LYS:O	2.39	0.57
1:A:318:THR:O	1:A:321:VAL:N	2.38	0.56
1:B:321:VAL:O	1:B:323:GLY:N	2.38	0.56
1:A:154:ARG:NH1	1:A:154:ARG:N	2.53	0.56
1:B:232:PRO:HG2	1:B:233:SER:HA	1.87	0.56
1:A:232:PRO:HB3	1:A:300:LEU:HD21	1.88	0.56
1:B:115:SER:HB2	1:B:132:ARG:CB	2.36	0.56
1:B:120:VAL:CG2	1:B:127:ILE:HG22	2.35	0.56
1:A:205:LEU:HA	1:A:208:ILE:HD12	1.88	0.55
1:A:286:VAL:C	1:A:288:SER:N	2.58	0.55
1:B:165:TYR:CE2	1:B:178:MET:O	2.58	0.55
1:B:98:THR:CB	1:B:100:GLU:H	2.19	0.55
1:A:319:GLN:N	1:A:319:GLN:CD	2.65	0.55
1:B:149:LEU:O	1:B:150:ASP:O	2.24	0.55
1:B:154:ARG:O	1:B:218:HIS:CE1	2.50	0.55
1:B:182:SER:OG	1:B:237:LEU:HA	2.06	0.55
1:A:386:ASP:O	1:A:387:GLN:HB3	2.07	0.54
1:B:256:ASP:OD1	1:B:259:ALA:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PRO:HG2	1:B:124:SER:H	1.72	0.54
1:B:182:SER:HB2	1:B:236:LEU:O	2.08	0.54
1:A:302:THR:O	1:A:303:GLY:C	2.51	0.54
1:B:198:ASP:O	1:B:200:ILE:N	2.41	0.54
1:B:185:PHE:HA	1:B:188:PHE:HB3	1.89	0.54
1:A:372:GLU:O	1:A:372:GLU:HG3	2.07	0.54
1:B:98:THR:OG1	1:B:100:GLU:HB2	2.08	0.54
1:B:158:CYS:SG	1:B:215:ALA:HA	2.47	0.54
1:B:229:ASP:C	1:B:229:ASP:OD1	2.48	0.54
1:B:150:ASP:O	1:B:152:VAL:N	2.41	0.54
1:B:314:PHE:CD1	1:B:315:ASP:N	2.76	0.54
1:B:133:ILE:CA	1:B:174:CYS:O	2.56	0.53
1:B:205:LEU:HA	1:B:208:ILE:HD12	1.90	0.53
1:B:228:ARG:CA	1:B:229:ASP:HB2	2.29	0.53
1:B:260:LYS:C	1:B:261:THR:HG22	2.32	0.53
1:B:253:GLN:O	1:B:257:SER:OG	2.26	0.53
1:A:223:LEU:O	1:A:225:ILE:N	2.42	0.53
1:B:254:LEU:O	1:B:257:SER:HB2	2.07	0.53
1:B:165:TYR:OH	1:B:179:GLU:HA	2.09	0.53
1:A:178:MET:CG	1:A:179:GLU:H	2.19	0.53
1:B:222:ASN:HD22	1:B:222:ASN:H	1.52	0.52
1:B:327:GLN:O	1:B:328:LEU:HD12	2.10	0.52
1:A:286:VAL:O	1:A:287:ARG:C	2.51	0.52
1:B:226:ILE:O	1:B:227:HIS:CB	2.58	0.52
1:B:100:GLU:OE1	1:B:100:GLU:N	2.42	0.52
1:A:177:CYS:O	1:A:178:MET:HB3	2.09	0.52
1:B:360:GLU:CD	1:B:360:GLU:H	2.18	0.51
1:B:80:SER:HB3	1:B:95:TRP:HA	1.92	0.51
1:A:197:ASP:OD1	1:A:199:VAL:HG22	2.10	0.51
1:A:210:LEU:HD11	1:A:371:GLU:HA	1.91	0.51
1:B:150:ASP:OD1	1:B:150:ASP:N	2.43	0.51
1:A:349:THR:O	1:A:355:ARG:NH1	2.39	0.51
1:A:195:VAL:C	1:A:196:LEU:HG	2.36	0.51
1:B:232:PRO:CB	1:B:233:SER:CA	2.86	0.51
1:B:330:ASN:HD22	1:B:334:ARG:HA	1.75	0.51
1:A:180:LEU:HD23	1:A:180:LEU:O	2.11	0.50
1:A:342:ASN:C	1:A:346:LEU:HD21	2.36	0.50
1:A:286:VAL:C	1:A:288:SER:H	2.19	0.50
1:B:158:CYS:SG	1:B:161:ILE:HG13	2.52	0.50
1:B:156:SER:O	1:B:157:ASP:C	2.54	0.50
1:B:184:SER:HA	1:B:235:ILE:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ILE:HG21	1:A:285:ASP:O	2.12	0.49
1:B:185:PHE:O	1:B:186:ASP:C	2.55	0.49
1:A:164:PHE:H	1:A:177:CYS:N	2.10	0.49
1:A:232:PRO:HA	1:A:235:ILE:HD12	1.93	0.49
1:A:330:ASN:HB2	1:A:334:ARG:HA	1.95	0.49
1:A:291:TRP:HA	1:A:347:CYS:O	2.12	0.49
1:B:120:VAL:CG2	1:B:127:ILE:CA	2.90	0.49
1:B:151:VAL:HG23	1:B:152:VAL:H	1.78	0.49
1:A:371:GLU:O	1:A:372:GLU:HB3	2.12	0.49
1:A:198:ASP:OD1	1:A:198:ASP:N	2.45	0.48
1:B:288:SER:O	1:B:289:ASP:C	2.55	0.48
1:A:386:ASP:C	1:A:387:GLN:NE2	2.71	0.48
1:B:147:MET:SD	1:B:147:MET:C	2.97	0.48
1:B:256:ASP:C	1:B:257:SER:OG	2.53	0.48
1:B:142:GLN:O	1:B:146:LEU:HD22	2.14	0.48
1:A:152:VAL:N	1:A:154:ARG:HH12	2.12	0.48
1:B:99:ALA:C	1:B:100:GLU:OE1	2.57	0.48
1:B:185:PHE:CZ	1:B:236:LEU:HD23	2.48	0.48
1:B:237:LEU:HD12	1:B:239:ARG:O	2.14	0.48
1:B:326:PRO:C	1:B:328:LEU:H	2.20	0.48
1:A:386:ASP:N	1:A:387:GLN:HE22	2.11	0.47
1:B:298:TYR:O	1:B:302:THR:HG22	2.13	0.47
1:B:357:LYS:HB2	1:B:360:GLU:OE2	2.13	0.47
1:B:98:THR:CG2	1:B:100:GLU:HG2	2.44	0.47
1:B:121:HIS:O	1:B:125:GLY:N	2.41	0.47
1:B:84:SER:OG	1:B:89:ILE:HG13	2.15	0.47
1:B:124:SER:OG	1:B:125:GLY:N	2.48	0.47
1:B:120:VAL:HG22	1:B:127:ILE:HA	1.96	0.47
1:B:289:ASP:O	1:B:292:SER:OG	2.30	0.47
1:A:325:PRO:HB2	1:A:327:GLN:HG2	1.97	0.47
1:B:120:VAL:HG13	1:B:121:HIS:N	2.29	0.47
1:B:246:CYS:C	1:B:247:ASP:CG	2.81	0.47
1:A:216:LEU:HD21	1:A:230:ILE:HD13	1.97	0.47
1:A:286:VAL:HG22	1:A:287:ARG:H	1.72	0.46
1:B:182:SER:H	1:B:237:LEU:HA	1.80	0.46
1:A:181:MET:HG3	1:A:236:LEU:CB	2.42	0.46
1:B:116:VAL:HA	1:B:130:VAL:O	2.15	0.46
1:B:160:TYR:CD1	1:B:211:ALA:HA	2.50	0.46
1:B:95:TRP:CD1	1:B:95:TRP:H	2.33	0.46
1:B:299:GLU:HG3	1:B:305:PHE:HA	1.97	0.46
1:B:120:VAL:HG23	1:B:127:ILE:CA	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ARG:N	1:B:173:ASP:O	2.48	0.46
1:A:162:VAL:N	1:A:179:GLU:OE1	2.48	0.46
1:A:164:PHE:N	1:A:177:CYS:N	2.65	0.46
1:B:223:LEU:HA	1:B:223:LEU:HD12	1.21	0.46
1:B:326:PRO:O	1:B:328:LEU:N	2.42	0.46
1:B:193:TYR:CB	1:B:198:ASP:CB	2.94	0.45
1:B:290:VAL:HA	1:B:293:LEU:HB3	1.97	0.45
1:A:298:TYR:HE1	1:A:328:LEU:HA	1.81	0.45
1:B:84:SER:OG	1:B:84:SER:O	2.32	0.45
1:A:346:LEU:HD23	1:A:346:LEU:N	2.29	0.45
1:A:226:ILE:O	1:A:227:HIS:ND1	2.50	0.45
1:B:89:ILE:HG12	1:B:89:ILE:O	2.16	0.45
1:B:349:THR:HG21	1:B:354:LYS:O	2.17	0.45
1:B:226:ILE:HG21	1:B:264:ALA:O	2.16	0.45
1:B:238:ASP:CG	1:B:239:ARG:H	2.25	0.45
1:A:178:MET:O	1:A:179:GLU:HB3	2.17	0.44
1:A:331:SER:O	1:A:332:GLU:HG2	2.17	0.44
1:A:229:ASP:O	1:A:248:PHE:HZ	2.00	0.44
1:A:329:SER:O	1:A:331:SER:N	2.51	0.44
1:B:123:PRO:HG2	1:B:124:SER:N	2.32	0.44
1:B:123:PRO:CG	1:B:124:SER:H	2.30	0.44
1:B:193:TYR:N	1:B:196:LEU:HG	2.32	0.44
1:B:219:LEU:O	1:B:223:LEU:HD12	2.13	0.44
1:A:376:GLU:HG3	1:A:379:CYS:HB3	1.99	0.44
1:B:225:ILE:HD11	1:B:228:ARG:H	1.79	0.44
1:A:314:PHE:C	1:A:317:LEU:H	2.26	0.44
1:A:319:GLN:NE2	1:A:319:GLN:N	2.66	0.44
1:A:321:VAL:HA	1:A:350:LYS:HZ3	1.81	0.44
1:B:81:ILE:HD12	1:B:97:PHE:CB	2.47	0.44
1:A:163:GLN:HE21	1:A:163:GLN:HB3	1.56	0.44
1:A:319:GLN:NE2	1:A:319:GLN:H	2.16	0.44
1:B:143:LYS:HG2	1:B:144:GLN:N	2.33	0.44
1:A:230:ILE:CG2	1:A:292:SER:HB2	2.43	0.43
1:A:342:ASN:O	1:A:342:ASN:CG	2.61	0.43
1:B:226:ILE:O	1:B:226:ILE:HG12	2.12	0.43
1:B:115:SER:C	1:B:116:VAL:CG1	2.90	0.43
1:A:195:VAL:H	1:A:196:LEU:HG	1.83	0.43
1:B:230:ILE:HD13	1:B:296:THR:OG1	2.19	0.43
1:A:150:ASP:HB3	1:A:163:GLN:HE22	1.83	0.43
1:B:230:ILE:C	1:B:230:ILE:HD12	2.43	0.43
1:B:247:ASP:C	1:B:249:GLY:HA3	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LYS:HG3	1:B:254:LEU:CD2	2.45	0.43
1:B:341:ILE:HG12	1:B:345:ASN:HD21	1.84	0.43
1:B:360:GLU:CD	1:B:360:GLU:N	2.76	0.43
1:B:79:MET:O	1:B:97:PHE:CB	2.67	0.43
1:B:237:LEU:HD13	1:B:238:ASP:OD2	2.19	0.43
1:B:295:ILE:O	1:B:296:THR:C	2.62	0.43
1:A:227:HIS:HD2	1:A:248:PHE:CZ	2.37	0.42
1:B:123:PRO:CG	1:B:124:SER:N	2.83	0.42
1:B:181:MET:SD	1:B:237:LEU:CG	3.05	0.42
1:A:352:GLU:C	1:A:354:LYS:H	2.27	0.42
1:B:152:VAL:HB	1:B:164:PHE:HD2	1.84	0.42
1:A:183:THR:HG23	1:A:184:SER:O	2.20	0.42
1:A:189:TYR:O	1:A:193:TYR:HD2	2.03	0.42
1:B:130:VAL:O	1:B:130:VAL:CG2	2.66	0.42
1:B:214:LYS:HD3	1:B:362:LEU:HD21	2.02	0.42
1:A:358:TYR:O	1:A:362:LEU:HB2	2.19	0.42
1:B:158:CYS:HA	1:B:159:PRO:HD3	1.81	0.42
1:B:120:VAL:HG23	1:B:127:ILE:CB	2.50	0.41
1:B:247:ASP:HB2	1:B:250:ILE:HG22	2.01	0.41
1:A:219:LEU:O	1:A:223:LEU:O	2.38	0.41
1:B:149:LEU:HB3	1:B:150:ASP:H	1.58	0.41
1:B:349:THR:HG21	1:B:354:LYS:C	2.46	0.41
1:A:231:LYS:O	1:A:235:ILE:HG13	2.20	0.41
1:B:151:VAL:HG23	1:B:152:VAL:N	2.36	0.41
1:B:158:CYS:HB2	1:B:218:HIS:CG	2.56	0.41
1:B:182:SER:CB	1:B:236:LEU:O	2.68	0.41
1:B:230:ILE:CG1	1:B:292:SER:HB2	2.50	0.41
1:B:224:LYS:O	1:B:225:ILE:CG2	2.58	0.41
1:B:117:ASN:C	1:B:118:LYS:O	2.51	0.41
1:B:250:ILE:HD13	1:B:250:ILE:C	2.46	0.41
1:B:352:GLU:C	1:B:354:LYS:H	2.29	0.41
1:B:158:CYS:SG	1:B:160:TYR:HB2	2.61	0.41
1:B:229:ASP:OD1	1:B:230:ILE:N	2.54	0.40
1:B:327:GLN:O	1:B:328:LEU:CD1	2.69	0.40
1:B:191:TYR:O	1:B:196:LEU:HD11	2.22	0.40
1:B:245:LEU:HA	1:B:245:LEU:HD12	1.80	0.40
1:B:253:GLN:O	1:B:257:SER:CB	2.70	0.40
1:A:201:PRO:HB2	1:A:204:ILE:H	1.86	0.40
1:B:131:LYS:O	1:B:132:ARG:CB	2.68	0.40
1:B:226:ILE:HG21	1:B:265:GLY:C	2.47	0.40
1:B:253:GLN:HE21	1:B:253:GLN:HB2	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:CG	1:B:315:ASP:N	2.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	197/327 (60%)	142 (72%)	26 (13%)	29 (15%)	0	3
1	B	248/327 (76%)	169 (68%)	52 (21%)	27 (11%)	0	5
All	All	445/654 (68%)	311 (70%)	78 (18%)	56 (13%)	0	4

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	MET
1	A	247	ASP
1	A	287	ARG
1	A	330	ASN
1	A	334	ARG
1	A	387	GLN
1	B	89	ILE
1	B	105	LEU
1	B	150	ASP
1	B	151	VAL
1	B	227	HIS
1	B	229	ASP
1	B	231	LYS
1	B	232	PRO
1	B	235	ILE
1	B	322	LYS
1	A	150	ASP

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Mol	Chain	Res	Type
1	A	155	SER
1	A	224	LYS
1	A	231	LYS
1	A	249	GLY
1	A	303	GLY
1	A	308	PRO
1	A	311	ASN
1	A	319	GLN
1	A	322	LYS
1	A	325	PRO
1	B	101	ASP
1	B	149	LEU
1	B	225	ILE
1	B	262	ARG
1	B	327	GLN
1	B	330	ASN
1	A	194	SER
1	A	196	LEU
1	A	227	HIS
1	A	228	ARG
1	A	328	LEU
1	A	374	ALA
1	B	87	LEU
1	B	134	ARG
1	B	157	ASP
1	B	224	LYS
1	A	197	ASP
1	A	359	LYS
1	B	240	SER
1	B	312	SER
1	B	357	LYS
1	A	163	GLN
1	A	193	TYR
1	A	337	SER
1	B	104	ASP
1	B	132	ARG
1	B	199	VAL
1	A	199	VAL
1	B	241	GLY

### 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	172/296 (58%)	130 (76%)	42 (24%)	0	3
1	B	196/296 (66%)	158 (81%)	38 (19%)	1	6
All	All	368/592 (62%)	288 (78%)	80 (22%)	1	4

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	149	LEU
1	A	153	MET
1	A	154	ARG
1	A	158	CYS
1	A	161	ILE
1	A	163	GLN
1	A	178	MET
1	A	180	LEU
1	A	182	SER
1	A	183	THR
1	A	189	TYR
1	A	192	VAL
1	A	194	SER
1	A	196	LEU
1	A	198	ASP
1	A	199	VAL
1	A	220	LYS
1	A	223	LEU
1	A	227	HIS
1	A	230	ILE
1	A	245	LEU
1	A	286	VAL
1	A	292	SER
1	A	293	LEU
1	A	296	THR
1	A	314	PHE

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Mol	Chain	Res	Type
1	A	318	THR
1	A	319	GLN
1	A	324	ASP
1	A	325	PRO
1	A	330	ASN
1	A	331	SER
1	A	333	GLU
1	A	346	LEU
1	A	348	LEU
1	A	359	LYS
1	A	368	LEU
1	A	369	MET
1	A	379	CYS
1	A	384	ILE
1	A	387	GLN
1	B	79	MET
1	B	87	LEU
1	B	88	LYS
1	B	100	GLU
1	B	101	ASP
1	B	102	LEU
1	B	116	VAL
1	B	119	MET
1	B	120	VAL
1	B	127	ILE
1	B	130	VAL
1	B	146	LEU
1	B	162	VAL
1	B	171	GLU
1	B	195	VAL
1	B	204	ILE
1	B	212	THR
1	B	222	ASN
1	B	223	LEU
1	B	226	ILE
1	B	234	ASN
1	B	236	LEU
1	B	240	SER
1	B	246	CYS
1	B	247	ASP
1	B	250	ILE
1	B	253	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	257	SER
1	B	258	ILE
1	B	261	THR
1	B	286	VAL
1	B	290	VAL
1	B	296	THR
1	B	328	LEU
1	B	359	LYS
1	B	360	GLU
1	B	368	LEU
1	B	372	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	163	GLN
1	A	342	ASN
1	B	126	GLN
1	B	218	HIS
1	B	222	ASN
1	B	242	ASN
1	B	253	GLN
1	B	345	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 oligosaccharides 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	203/327 (62%)	0.29	4 (1%) 64 45	64, 98, 143, 166	0
1	B	260/327 (79%)	0.44	12 (4%) 38 27	58, 99, 134, 171	0
All	All	463/654 (70%)	0.37	16 (3%) 47 32	58, 99, 137, 171	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ASP	5.2
1	B	173	ASP	4.1
1	B	227	HIS	3.4
1	B	303	GLY	3.0
1	A	249	GLY	2.9
1	B	265	GLY	2.8
1	B	186	ASP	2.5
1	B	305	PHE	2.5
1	B	226	ILE	2.4
1	B	356	PRO	2.4
1	A	287	ARG	2.4
1	A	348	LEU	2.4
1	A	356	PRO	2.2
1	B	232	PRO	2.1
1	B	310	TRP	2.1
1	B	156	SER	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 monosaccharides 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.