



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:23 pm GMT

PDB ID : 3DAE  
Title : Crystal structure of phosphorylated SNF1 kinase domain  
Authors : Zheng, L.-S.; Chen, L.; Jiao, Z.-H.; Wu, J.-W.  
Deposited on : 2008-05-29  
Resolution : 2.90 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

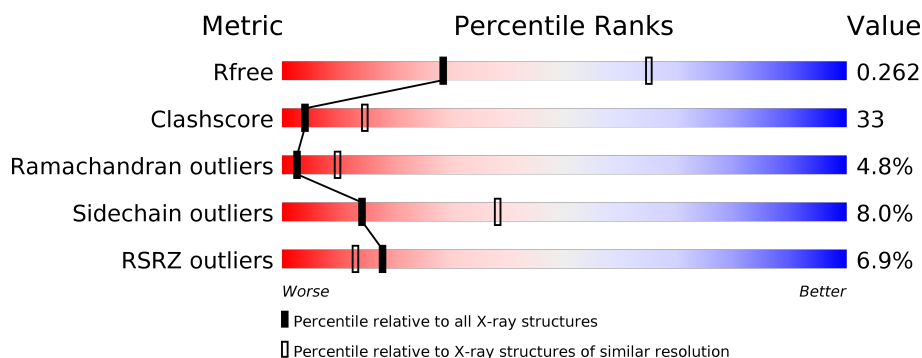
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	283	<div> <div>5%</div> <div> <div></div> <div>47%</div> <div>34%</div> <div>6%</div> <div>12%</div> </div> </div>
1	B	283	<div> <div>7%</div> <div> <div></div> <div>44%</div> <div>36%</div> <div>6%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4181 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 Carbon catabolite-derepressing protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			2003	1297	343	355	8			
1	B	246	Total	C	N	O	S	0	0	0
			1991	1291	341	351	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	INITIATING METHIONINE	UNP P06782
A	316	GLU	-	EXPRESSION TAG	UNP P06782
A	317	HIS	-	EXPRESSION TAG	UNP P06782
A	318	HIS	-	EXPRESSION TAG	UNP P06782
A	319	HIS	-	EXPRESSION TAG	UNP P06782
A	320	HIS	-	EXPRESSION TAG	UNP P06782
A	321	HIS	-	EXPRESSION TAG	UNP P06782
A	322	HIS	-	EXPRESSION TAG	UNP P06782
B	40	MET	-	INITIATING METHIONINE	UNP P06782
B	316	GLU	-	EXPRESSION TAG	UNP P06782
B	317	HIS	-	EXPRESSION TAG	UNP P06782
B	318	HIS	-	EXPRESSION TAG	UNP P06782
B	319	HIS	-	EXPRESSION TAG	UNP P06782
B	320	HIS	-	EXPRESSION TAG	UNP P06782
B	321	HIS	-	EXPRESSION TAG	UNP P06782
B	322	HIS	-	EXPRESSION TAG	UNP P06782

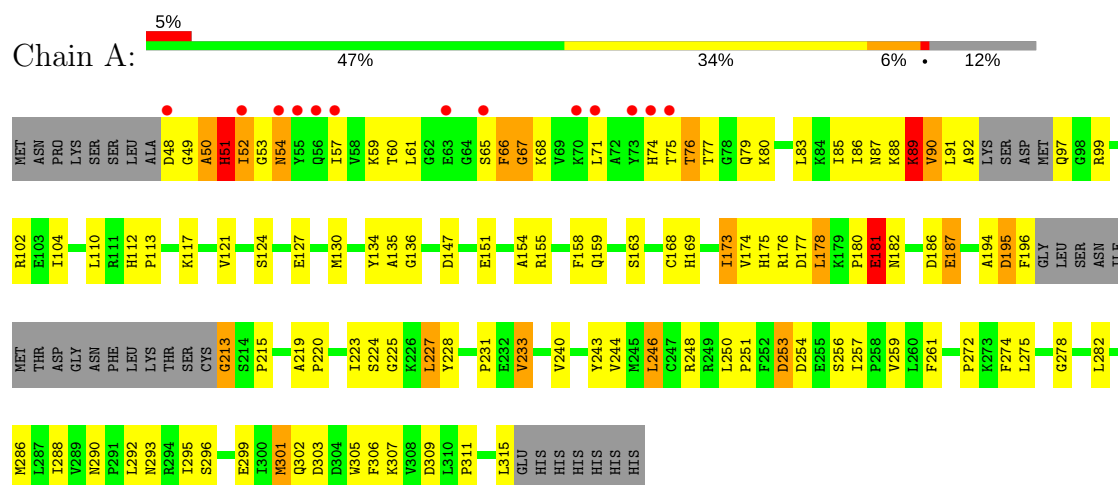
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	93	Total	O	0	0
			93	93		

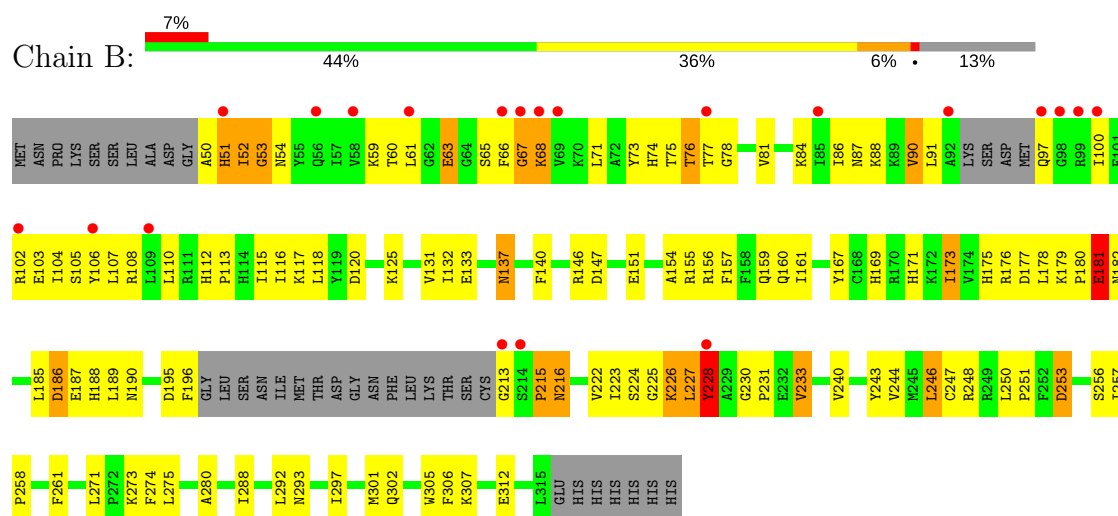
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Carbon catabolite-derepressing protein kinase



- Molecule 1: Carbon catabolite-derepressing protein kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.61Å 72.37Å 112.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 2.90 47.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.19-2.90) 99.9 (47.19-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.227 , 0.265 0.220 , 0.262	Depositor DCC
$R_{free}$ test set	706 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.4	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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	0.61	2/2045 (0.1%)	0.69	0/2762
1	B	0.57	0/2033	0.69	1/2746 (0.0%)
All	All	0.59	2/4078 (0.0%)	0.69	1/5508 (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	3
1	B	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	GLY	C-O	6.83	1.34	1.23
1	A	89	LYS	CD-CE	5.16	1.64	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	TYR	CA-CB-CG	-5.83	102.33	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	GLY	Peptide
1	A	48	ASP	Peptide
1	A	51	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	B	213	GLY	Peptide
1	B	227	LEU	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	2003	0	2046	130	0
1	B	1991	0	2039	142	0
2	A	94	0	0	30	0
2	B	93	0	0	34	0
All	All	4181	0	4085	266	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 33.

All (266) 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:117:LYS:HE3	2:A:358:HOH:O	1.06	1.20
1:A:90:VAL:HG12	1:A:97:GLN:HG3	1.25	1.18
1:A:88:LYS:HB3	2:A:392:HOH:O	1.43	1.17
1:B:188:HIS:CD2	2:B:362:HOH:O	1.99	1.15
1:B:186:ASP:OD2	1:B:187:GLU:N	1.78	1.14
1:A:195:ASP:HA	2:A:383:HOH:O	1.45	1.12
1:A:147:ASP:HA	1:A:248:ARG:HH11	1.15	1.12
1:A:88:LYS:CD	2:A:392:HOH:O	2.00	1.07
1:B:106:TYR:HD2	2:B:350:HOH:O	1.36	1.06
1:B:312:GLU:HB3	2:B:336:HOH:O	1.57	1.03
1:A:92:ALA:HB3	2:A:384:HOH:O	1.57	1.01
1:B:90:VAL:HG12	1:B:97:GLN:HG3	1.45	0.99
1:A:88:LYS:HD2	2:A:392:HOH:O	1.62	0.98
1:A:50:ALA:O	1:A:51:HIS:HB3	1.59	0.98
1:B:302:GLN:HA	1:B:307:LYS:HE3	1.44	0.96
1:B:273:LYS:HG2	2:B:357:HOH:O	1.64	0.96
1:A:195:ASP:O	2:A:383:HOH:O	1.83	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:NH2	2:B:393:HOH:O	1.84	0.95
1:B:140:PHE:CE2	2:B:386:HOH:O	2.18	0.95
1:B:51:HIS:O	1:B:52:ILE:HG12	1.69	0.93
1:B:88:LYS:O	1:B:91:LEU:HG	1.70	0.90
1:A:147:ASP:HA	1:A:248:ARG:NH1	1.88	0.88
1:A:86:ILE:HG22	1:A:90:VAL:HG21	1.53	0.88
1:B:86:ILE:HG22	1:B:90:VAL:HG21	1.54	0.88
1:B:106:TYR:CD2	2:B:350:HOH:O	2.14	0.88
1:A:91:LEU:O	2:A:381:HOH:O	1.93	0.86
1:A:195:ASP:CA	2:A:383:HOH:O	2.11	0.86
1:A:74:HIS:HD2	1:A:77:THR:H	1.20	0.86
1:A:187:GLU:HG3	1:A:187:GLU:O	1.77	0.83
1:A:124:SER:O	2:A:388:HOH:O	1.97	0.81
1:B:216:ASN:HD22	1:B:216:ASN:H	1.29	0.81
1:B:51:HIS:O	1:B:52:ILE:CD1	2.30	0.79
1:B:105:SER:HA	2:B:395:HOH:O	1.82	0.79
1:A:50:ALA:O	1:A:51:HIS:CB	2.30	0.79
1:B:51:HIS:O	1:B:52:ILE:CG1	2.30	0.79
1:B:188:HIS:HD2	2:B:362:HOH:O	1.45	0.78
1:B:147:ASP:OD1	2:B:377:HOH:O	2.02	0.78
1:B:253:ASP:OD1	2:B:365:HOH:O	2.00	0.78
1:A:53:GLY:O	1:A:54:ASN:HB2	1.85	0.77
1:A:302:GLN:HA	1:A:307:LYS:HE3	1.65	0.76
1:B:110:LEU:HD11	1:B:173:ILE:HD13	1.66	0.75
1:B:175:HIS:HD2	1:B:177:ASP:H	1.32	0.75
1:A:227:LEU:O	2:A:347:HOH:O	2.05	0.75
1:B:74:HIS:HD2	1:B:77:THR:H	1.31	0.75
1:A:102:ARG:NH2	2:A:362:HOH:O	1.97	0.74
1:B:53:GLY:O	1:B:54:ASN:HB2	1.86	0.74
1:B:88:LYS:O	2:B:335:HOH:O	2.04	0.74
1:A:51:HIS:C	1:A:52:ILE:HG12	2.09	0.72
1:A:92:ALA:CB	2:A:361:HOH:O	2.37	0.72
1:A:315:LEU:O	2:A:390:HOH:O	2.08	0.72
1:B:112:HIS:CG	1:B:113:PRO:HD2	2.25	0.71
1:B:216:ASN:HD22	1:B:216:ASN:N	1.86	0.71
1:A:195:ASP:C	2:A:383:HOH:O	2.21	0.71
1:A:194:ALA:O	2:A:383:HOH:O	2.08	0.70
1:A:110:LEU:HD11	1:A:173:ILE:HD13	1.74	0.70
1:B:151:GLU:OE2	2:B:366:HOH:O	2.09	0.70
1:A:92:ALA:HB2	2:A:361:HOH:O	1.91	0.70
1:A:51:HIS:CD2	1:A:52:ILE:N	2.61	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:VAL:HG23	1:B:233:VAL:HG21	1.74	0.69
1:B:248:ARG:HG3	2:B:343:HOH:O	1.92	0.69
1:B:177:ASP:OD1	1:B:179:LYS:HE3	1.93	0.69
1:A:50:ALA:HA	1:A:57:ILE:HB	1.75	0.68
1:A:86:ILE:HG22	1:A:90:VAL:CG2	2.22	0.68
1:B:108:ARG:HB2	2:B:395:HOH:O	1.93	0.68
1:B:106:TYR:HB3	2:B:350:HOH:O	1.93	0.68
1:B:186:ASP:OD2	1:B:188:HIS:N	2.26	0.68
1:A:228:TYR:OH	2:A:393:HOH:O	2.08	0.68
1:B:273:LYS:CD	2:B:357:HOH:O	2.42	0.68
1:B:273:LYS:CG	2:B:357:HOH:O	2.30	0.68
1:A:74:HIS:CD2	1:A:77:THR:H	2.07	0.68
1:A:278:GLY:O	2:A:344:HOH:O	2.11	0.67
1:B:186:ASP:C	1:B:186:ASP:OD2	2.29	0.67
1:A:51:HIS:HD2	1:A:52:ILE:H	1.43	0.66
1:A:250:LEU:HB2	1:A:253:ASP:HB2	1.76	0.66
1:B:86:ILE:CG2	1:B:90:VAL:HG21	2.23	0.66
1:B:222:VAL:HG23	1:B:233:VAL:CG2	2.26	0.66
1:A:180:PRO:O	1:A:181:GLU:HB3	1.95	0.66
1:B:195:ASP:O	1:B:196:PHE:HB2	1.96	0.66
1:B:51:HIS:C	1:B:52:ILE:HG12	2.15	0.65
1:A:49:GLY:O	1:A:51:HIS:N	2.29	0.65
1:B:125:LYS:NZ	2:B:387:HOH:O	2.06	0.65
1:B:256:SER:OG	1:B:258:PRO:HD2	1.95	0.65
1:A:151:GLU:OE2	2:A:351:HOH:O	2.14	0.65
1:B:146:ARG:O	1:B:248:ARG:NH1	2.31	0.64
1:A:77:THR:HG22	1:A:79:GLN:H	1.62	0.64
1:B:226:LYS:O	1:B:227:LEU:HB2	1.97	0.64
1:B:240:VAL:O	1:B:244:VAL:HG23	1.97	0.64
1:B:273:LYS:HD3	2:B:357:HOH:O	1.98	0.64
1:B:106:TYR:CB	2:B:350:HOH:O	2.47	0.63
1:B:157:PHE:O	1:B:161:ILE:HG13	1.99	0.63
1:B:167:TYR:O	1:B:171:HIS:HD2	1.81	0.63
1:A:175:HIS:CG	1:A:178:LEU:HD13	2.34	0.62
1:A:51:HIS:CD2	1:A:52:ILE:H	2.17	0.62
1:A:240:VAL:O	1:A:244:VAL:HG23	1.98	0.62
1:A:225:GLY:HA2	2:A:398:HOH:O	1.99	0.62
1:B:51:HIS:O	1:B:52:ILE:HD13	1.98	0.62
1:B:186:ASP:CG	1:B:187:GLU:H	1.96	0.62
1:A:88:LYS:O	1:A:91:LEU:HG	1.99	0.62
1:B:137:ASN:HB3	2:B:390:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:HD2	2:B:344:HOH:O	2.00	0.62
1:B:112:HIS:HB3	1:B:115:ILE:HG13	1.83	0.61
1:B:86:ILE:HG21	1:B:100:ILE:HD13	1.82	0.61
1:A:177:ASP:OD1	1:B:257:ILE:HB	2.01	0.61
1:B:147:ASP:HA	1:B:248:ARG:HH11	1.66	0.60
1:B:312:GLU:CG	2:B:336:HOH:O	2.47	0.60
1:B:196:PHE:HB3	2:B:350:HOH:O	2.00	0.60
1:B:257:ILE:HG23	1:B:261:PHE:CE2	2.36	0.60
1:A:74:HIS:CD2	1:A:77:THR:HB	2.37	0.59
1:B:223:ILE:HD12	1:B:261:PHE:CE1	2.38	0.59
1:A:74:HIS:HD2	1:A:77:THR:N	1.97	0.59
1:A:282:LEU:O	1:A:286:MET:HE2	2.02	0.59
1:A:110:LEU:HD11	1:A:173:ILE:CD1	2.32	0.59
1:A:61:LEU:HD11	1:A:71:LEU:HB2	1.84	0.59
1:B:312:GLU:CB	2:B:336:HOH:O	2.31	0.59
1:A:215:PRO:HG3	1:B:215:PRO:HG3	1.84	0.59
1:B:88:LYS:HA	2:B:335:HOH:O	2.03	0.58
1:B:154:ALA:HB3	1:B:246:LEU:HD13	1.86	0.58
1:B:110:LEU:HD11	1:B:173:ILE:CD1	2.33	0.58
1:A:88:LYS:CB	2:A:392:HOH:O	2.16	0.58
1:B:61:LEU:HD11	1:B:71:LEU:HB2	1.85	0.58
1:A:244:VAL:CG2	1:A:250:LEU:HD23	2.33	0.58
1:A:136:GLY:N	2:A:355:HOH:O	1.93	0.57
1:B:180:PRO:O	1:B:181:GLU:HB3	2.03	0.57
1:B:91:LEU:HD23	1:B:97:GLN:NE2	2.19	0.57
1:A:174:VAL:HG12	1:A:176:ARG:HG3	1.86	0.57
1:B:175:HIS:O	1:B:176:ARG:HB2	2.05	0.56
1:B:74:HIS:CD2	1:B:76:THR:HG23	2.41	0.56
1:A:244:VAL:HG21	1:A:250:LEU:HD23	1.87	0.56
1:B:120:ASP:H	1:B:131:VAL:HB	1.70	0.56
1:B:67:GLY:O	1:B:68:LYS:O	2.23	0.56
1:A:87:ASN:HD21	1:A:89:LYS:HG3	1.71	0.56
1:B:154:ALA:CB	1:B:246:LEU:HD13	2.36	0.55
1:B:222:VAL:CG2	1:B:233:VAL:HG21	2.37	0.55
1:A:175:HIS:CD2	1:A:178:LEU:HD13	2.41	0.55
1:B:216:ASN:HB3	2:B:323:HOH:O	2.06	0.55
1:A:112:HIS:ND1	1:A:113:PRO:HD2	2.21	0.55
1:B:155:ARG:O	1:B:159:GLN:HG3	2.06	0.55
1:A:177:ASP:O	1:A:182:ASN:ND2	2.40	0.55
1:A:296:SER:OG	1:A:299:GLU:HG3	2.06	0.55
1:B:112:HIS:CD2	1:B:113:PRO:HD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:HIS:CD2	1:B:77:THR:H	2.19	0.54
1:B:253:ASP:HA	2:B:365:HOH:O	2.07	0.54
1:B:73:TYR:HD1	1:B:78:GLY:HA2	1.73	0.54
1:B:107:LEU:HB3	1:B:118:LEU:HB2	1.89	0.54
1:A:195:ASP:O	1:A:196:PHE:HB2	2.08	0.53
1:A:309:ASP:O	1:A:311:PRO:HD3	2.08	0.53
1:A:92:ALA:CB	2:A:384:HOH:O	2.32	0.53
1:B:54:ASN:HA	1:B:75:THR:HG22	1.89	0.53
1:A:155:ARG:HD3	1:A:305:TRP:O	2.08	0.52
1:B:195:ASP:O	1:B:196:PHE:CB	2.56	0.52
1:A:49:GLY:O	1:A:50:ALA:C	2.47	0.52
1:B:54:ASN:O	1:B:75:THR:N	2.40	0.52
1:B:155:ARG:HB2	1:B:305:TRP:CH2	2.45	0.52
1:A:231:PRO:C	1:A:233:VAL:H	2.12	0.51
1:A:180:PRO:O	1:A:181:GLU:CB	2.59	0.51
1:B:186:ASP:OD1	1:B:190:ASN:HB2	2.10	0.51
1:A:90:VAL:CG1	1:A:97:GLN:HG3	2.18	0.51
1:A:175:HIS:HD2	1:A:177:ASP:H	1.59	0.51
1:B:244:VAL:CG2	1:B:250:LEU:HD23	2.41	0.50
1:A:186:ASP:C	1:A:186:ASP:OD2	2.49	0.50
1:A:92:ALA:C	2:A:384:HOH:O	2.49	0.50
1:A:92:ALA:N	2:A:361:HOH:O	2.45	0.50
1:A:66:PHE:O	1:A:67:GLY:C	2.49	0.50
1:B:216:ASN:ND2	1:B:216:ASN:N	2.52	0.50
1:A:288:ILE:HG21	1:A:293:ASN:HB2	1.93	0.50
1:B:173:ILE:HG12	1:B:173:ILE:O	2.11	0.49
1:B:180:PRO:O	1:B:181:GLU:CB	2.59	0.49
1:B:288:ILE:HG21	1:B:293:ASN:HB2	1.94	0.49
1:A:154:ALA:O	1:A:158:PHE:HB2	2.13	0.49
1:B:175:HIS:HD2	1:B:177:ASP:N	2.07	0.49
1:B:50:ALA:O	1:B:51:HIS:O	2.30	0.49
1:A:80:LYS:HE2	1:A:134:TYR:CD2	2.48	0.49
1:A:51:HIS:CD2	1:A:51:HIS:C	2.87	0.49
1:A:49:GLY:C	1:A:51:HIS:H	2.17	0.48
1:A:83:LEU:HA	1:A:130:MET:O	2.13	0.48
1:B:250:LEU:HB2	1:B:253:ASP:HB2	1.94	0.48
1:A:86:ILE:O	1:A:127:GLU:HA	2.13	0.48
1:A:220:PRO:HA	1:A:223:ILE:HG12	1.94	0.48
1:A:290:ASN:OD1	1:A:292:LEU:HB2	2.13	0.48
1:B:173:ILE:HD11	1:B:196:PHE:CE2	2.48	0.48
1:B:195:ASP:O	1:B:196:PHE:HD1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASN:ND2	1:A:89:LYS:HG3	2.29	0.48
1:B:225:GLY:O	1:B:227:LEU:N	2.46	0.48
1:B:228:TYR:CE2	1:B:230:GLY:HA2	2.49	0.48
1:B:240:VAL:HG13	1:B:251:PRO:HG2	1.96	0.48
1:A:169:HIS:CE1	1:A:231:PRO:HB3	2.49	0.47
1:B:171:HIS:O	1:B:173:ILE:HG22	2.14	0.47
1:A:272:PRO:CB	1:A:274:PHE:CE2	2.97	0.47
1:B:84:LYS:HG3	1:B:132:ILE:HD12	1.96	0.47
1:A:240:VAL:HG13	1:A:251:PRO:CD	2.45	0.47
1:B:271:LEU:HD13	1:B:280:ALA:HB1	1.97	0.47
1:A:49:GLY:C	1:A:51:HIS:N	2.67	0.47
1:B:195:ASP:O	1:B:196:PHE:CD1	2.68	0.47
1:B:154:ALA:HB3	1:B:246:LEU:CD1	2.45	0.46
1:A:175:HIS:O	1:A:176:ARG:HB2	2.16	0.46
1:B:117:LYS:H	1:B:133:GLU:HB3	1.79	0.46
1:B:50:ALA:O	1:B:51:HIS:C	2.54	0.46
1:B:88:LYS:C	2:B:335:HOH:O	2.51	0.46
1:A:92:ALA:CA	2:A:384:HOH:O	2.62	0.46
1:A:87:ASN:O	1:A:90:VAL:HG23	2.16	0.46
1:A:74:HIS:CD2	1:A:76:THR:HG23	2.51	0.46
1:B:84:LYS:HG3	1:B:132:ILE:CD1	2.46	0.46
1:B:274:PHE:C	1:B:274:PHE:CD1	2.90	0.46
1:B:312:GLU:HG2	2:B:336:HOH:O	2.11	0.46
1:A:223:ILE:HD12	1:B:224:SER:O	2.16	0.45
1:A:243:TYR:CG	1:A:251:PRO:HG3	2.51	0.45
1:B:182:ASN:ND2	1:B:195:ASP:HB2	2.32	0.45
1:B:118:LEU:HD12	1:B:131:VAL:O	2.17	0.45
1:A:104:ILE:HD13	1:A:121:VAL:HG11	1.98	0.45
1:A:85:ILE:C	1:A:86:ILE:HG13	2.35	0.45
1:A:85:ILE:C	1:A:86:ILE:CG1	2.85	0.45
1:B:297:ILE:O	1:B:301:MET:HG3	2.16	0.45
1:B:302:GLN:CA	1:B:307:LYS:HE3	2.31	0.45
1:A:176:ARG:O	1:B:258:PRO:HG3	2.17	0.45
1:A:88:LYS:HD3	2:A:392:HOH:O	1.93	0.44
1:A:219:ALA:HB1	1:A:220:PRO:HD2	1.99	0.44
1:A:86:ILE:CG2	1:A:90:VAL:HG21	2.36	0.44
1:B:244:VAL:HG22	1:B:250:LEU:HD23	1.99	0.44
1:B:257:ILE:N	1:B:258:PRO:CD	2.80	0.44
1:B:243:TYR:CG	1:B:251:PRO:HG3	2.53	0.44
1:A:173:ILE:HD11	1:A:196:PHE:CE2	2.53	0.44
1:A:261:PHE:CE2	1:B:223:ILE:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:CYS:HB3	1:A:173:ILE:O	2.18	0.44
1:A:303:ASP:HB3	1:A:306:PHE:HB3	1.99	0.44
1:A:240:VAL:HG13	1:A:251:PRO:HD2	2.00	0.43
1:A:301:MET:HA	1:A:306:PHE:CE2	2.53	0.43
1:A:51:HIS:C	1:A:52:ILE:CG1	2.83	0.43
1:B:106:TYR:CD2	1:B:173:ILE:HD12	2.53	0.43
1:B:54:ASN:HA	1:B:75:THR:CG2	2.47	0.43
1:A:75:THR:HG23	1:A:76:THR:N	2.34	0.43
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.77	0.43
1:B:54:ASN:O	1:B:74:HIS:HA	2.19	0.43
1:A:256:SER:HB3	1:A:259:VAL:HB	2.02	0.42
1:B:100:ILE:O	1:B:104:ILE:HG13	2.18	0.42
1:B:120:ASP:HB3	1:B:131:VAL:HG21	2.01	0.42
1:A:223:ILE:O	1:B:223:ILE:HG22	2.19	0.42
1:B:140:PHE:HE2	2:B:386:HOH:O	1.77	0.42
1:B:222:VAL:CG2	1:B:233:VAL:CG2	2.96	0.42
1:A:175:HIS:CD2	1:A:177:ASP:H	2.36	0.42
1:A:282:LEU:HD13	1:A:303:ASP:CG	2.40	0.42
1:B:169:HIS:CE1	1:B:231:PRO:HB3	2.55	0.42
1:B:189:LEU:HD23	2:B:367:HOH:O	2.20	0.42
1:B:102:ARG:O	1:B:106:TYR:HB2	2.20	0.41
1:B:185:LEU:HD23	1:B:190:ASN:O	2.20	0.41
1:B:301:MET:HA	1:B:306:PHE:CD2	2.55	0.41
1:A:135:ALA:HA	2:A:355:HOH:O	2.21	0.41
1:A:231:PRO:C	1:A:233:VAL:N	2.73	0.41
1:A:53:GLY:O	1:A:54:ASN:CB	2.60	0.41
1:A:243:TYR:CD2	1:A:243:TYR:C	2.94	0.41
1:A:66:PHE:HD1	1:A:67:GLY:N	2.18	0.41
1:B:112:HIS:CG	1:B:113:PRO:CD	3.01	0.41
1:A:66:PHE:HD1	1:A:67:GLY:H	1.69	0.41
1:B:160:GLN:HG3	2:B:347:HOH:O	2.21	0.41
1:B:61:LEU:CD1	1:B:71:LEU:HB2	2.51	0.41
1:A:86:ILE:CG2	1:A:90:VAL:CG2	2.96	0.41
1:B:52:ILE:O	1:B:53:GLY:C	2.58	0.41
1:A:272:PRO:HB3	1:A:274:PHE:CE2	2.56	0.41
1:A:257:ILE:HG23	1:A:261:PHE:CE2	2.55	0.41
1:B:116:ILE:HA	1:B:116:ILE:HD12	1.83	0.41
1:B:247:CYS:O	1:B:248:ARG:HB2	2.20	0.41
1:A:159:GLN:O	1:A:163:SER:HB2	2.22	0.40
1:A:295:ILE:HG13	1:A:299:GLU:HB2	2.02	0.40
1:A:99:ARG:NH1	2:A:391:HOH:O	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:O	1:A:75:THR:N	2.41	0.40
1:B:87:ASN:HB2	1:B:88:LYS:H	1.61	0.40
1:A:175:HIS:CE1	1:A:196:PHE:H	2.39	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	242/283 (86%)	208 (86%)	23 (10%)	11 (4%)	3	11
1	B	240/283 (85%)	209 (87%)	19 (8%)	12 (5%)	2	8
All	All	482/566 (85%)	417 (86%)	42 (9%)	23 (5%)	2	10

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ILE
1	A	65	SER
1	B	52	ILE
1	B	68	LYS
1	B	226	LYS
1	A	51	HIS
1	A	67	GLY
1	A	68	LYS
1	A	90	VAL
1	A	181	GLU
1	B	67	GLY
1	B	186	ASP
1	B	253	ASP
1	A	50	ALA
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	253	ASP
1	B	228	TYR
1	B	53	GLY
1	B	181	GLU
1	B	215	PRO
1	A	224	SER
1	B	63	GLU
1	B	90	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	219/252 (87%)	202 (92%)	17 (8%)	15	39
1	B	218/252 (86%)	200 (92%)	18 (8%)	13	36
All	All	437/504 (87%)	402 (92%)	35 (8%)	14	38

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	59	LYS
1	A	60	THR
1	A	66	PHE
1	A	76	THR
1	A	89	LYS
1	A	173	ILE
1	A	178	LEU
1	A	181	GLU
1	A	187	GLU
1	A	195	ASP
1	A	227	LEU
1	A	233	VAL
1	A	246	LEU
1	A	254	ASP

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Mol	Chain	Res	Type
1	A	275	LEU
1	A	301	MET
1	B	51	HIS
1	B	59	LYS
1	B	60	THR
1	B	63	GLU
1	B	65	SER
1	B	66	PHE
1	B	76	THR
1	B	81	VAL
1	B	103	GLU
1	B	137	ASN
1	B	173	ILE
1	B	178	LEU
1	B	181	GLU
1	B	216	ASN
1	B	233	VAL
1	B	246	LEU
1	B	275	LEU
1	B	292	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	56	GLN
1	A	74	HIS
1	A	175	HIS
1	A	216	ASN
1	A	266	ASN
1	B	74	HIS
1	B	97	GLN
1	B	171	HIS
1	B	175	HIS
1	B	182	ASN
1	B	188	HIS
1	B	216	ASN

### 5.3.3 RNA ⓘ

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	248/283 (87%)	0.13	13 (5%) 28 23	16, 44, 98, 182	0
1	B	246/283 (86%)	0.19	21 (8%) 11 8	18, 48, 120, 177	0
All	All	494/566 (87%)	0.16	34 (6%) 18 13	16, 46, 113, 182	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	GLY	4.0
1	A	55	TYR	4.0
1	B	61	LEU	3.7
1	B	100	ILE	3.6
1	A	56	GLN	3.5
1	A	65	SER	3.3
1	B	97	GLN	3.2
1	A	63	GLU	3.2
1	B	56	GLN	3.1
1	B	68	LYS	3.0
1	B	106	TYR	3.0
1	B	228	TYR	2.8
1	B	77	THR	2.8
1	A	57	ILE	2.7
1	A	71	LEU	2.7
1	A	48	ASP	2.7
1	B	85	ILE	2.6
1	B	67	GLY	2.5
1	A	73	TYR	2.5
1	B	109	LEU	2.5
1	A	75	THR	2.4
1	B	214	SER	2.3
1	B	58	VAL	2.3
1	B	99	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	52	ILE	2.3
1	B	51	HIS	2.3
1	B	213	GLY	2.2
1	B	69	VAL	2.2
1	B	66	PHE	2.2
1	A	54	ASN	2.2
1	A	70	LYS	2.2
1	A	74	HIS	2.1
1	B	92	ALA	2.0
1	B	102	ARG	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.