



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:20 PM GMT

PDB ID : 1JWO  
Title : Crystal Structure Analysis of the SH2 Domain of the Csk Homologous Kinase CHK  
Authors : Murthy, T.V.S.; Webster, G.D.  
Deposited on : 2001-09-04  
Resolution : 2.50 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  
<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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

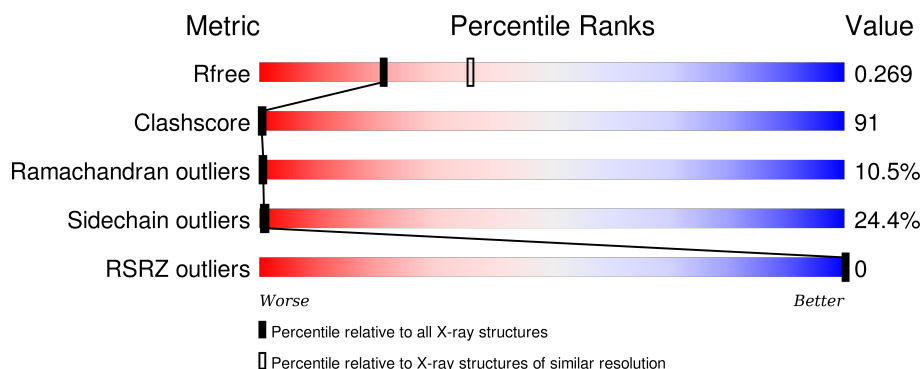
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	97	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 833 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 Csk Homologous Kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	21	0	0
			785	501	142	136	6			

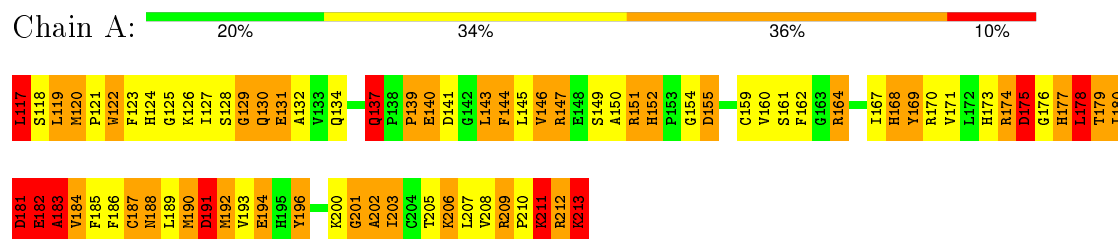
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total	O	0	0
			48	48		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: Csk Homologous Kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.15Å 58.70Å 28.82Å 90.00° 115.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 29.35 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-2.50) 94.3 (29.35-2.49)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.191 , 0.257 0.202 , 0.269	Depositor DCC
$R_{free}$ test set	140 reflections (4.55%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 105.7	EDS
Estimated twinning fraction	0.000 for k+l,h+l,-l 0.031 for -k+l,-h-l,-l 0.056 for -h-2*l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 3237 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 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	2.87	25/805 (3.1%)	2.98	43/1085 (4.0%)

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	1	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	ALA	CA-CB	46.85	2.50	1.52
1	A	181	ASP	C-N	-20.72	0.86	1.34
1	A	212	ARG	CG-CD	18.75	1.98	1.51
1	A	146	VAL	CB-CG1	15.73	1.85	1.52
1	A	169	TYR	CE1-CZ	-9.47	1.26	1.38
1	A	164	ARG	CD-NE	9.30	1.62	1.46
1	A	169	TYR	CB-CG	8.09	1.63	1.51
1	A	144	PHE	CE1-CZ	-7.37	1.23	1.37
1	A	150	ALA	CA-CB	-7.33	1.37	1.52
1	A	122	TRP	CE3-CZ3	-7.21	1.26	1.38
1	A	160	VAL	CB-CG2	-6.62	1.39	1.52
1	A	169	TYR	CD1-CE1	6.58	1.49	1.39
1	A	184	VAL	CA-CB	-6.54	1.41	1.54
1	A	211	LYS	CD-CE	6.47	1.67	1.51
1	A	168	HIS	CB-CG	-6.10	1.39	1.50
1	A	146	VAL	CA-CB	-6.07	1.42	1.54
1	A	130	GLN	CB-CG	-5.87	1.36	1.52
1	A	161	SER	CB-OG	-5.87	1.34	1.42
1	A	120	MET	CB-CG	5.70	1.69	1.51
1	A	186	PHE	CB-CG	5.63	1.60	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	HIS	C-O	-5.40	1.13	1.23
1	A	160	VAL	CB-CG1	5.33	1.64	1.52
1	A	180	ILE	CA-C	5.25	1.66	1.52
1	A	177	HIS	C-O	-5.21	1.13	1.23
1	A	196	TYR	CB-CG	5.00	1.59	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASP	O-C-N	-54.05	36.22	122.70
1	A	119	LEU	CB-CG-CD1	-27.32	64.56	111.00
1	A	202	ALA	N-CA-CB	-16.60	86.86	110.10
1	A	169	TYR	CB-CG-CD1	12.66	128.59	121.00
1	A	182	GLU	O-C-N	12.57	142.82	122.70
1	A	182	GLU	C-N-CA	-11.61	92.67	121.70
1	A	212	ARG	CG-CD-NE	11.44	135.81	111.80
1	A	206	LYS	CA-CB-CG	10.49	136.47	113.40
1	A	191	ASP	CB-CG-OD2	10.26	127.54	118.30
1	A	182	GLU	CA-C-N	-9.70	95.86	117.20
1	A	150	ALA	CB-CA-C	9.40	124.20	110.10
1	A	213	LYS	N-CA-C	-9.01	86.67	111.00
1	A	181	ASP	CA-C-N	-8.87	97.68	117.20
1	A	175	ASP	CB-CG-OD2	8.80	126.22	118.30
1	A	164	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	A	181	ASP	CB-CG-OD2	8.42	125.88	118.30
1	A	209	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	177	HIS	N-CA-CB	-8.09	96.04	110.60
1	A	150	ALA	N-CA-CB	7.66	120.82	110.10
1	A	191	ASP	OD1-CG-OD2	-7.61	108.84	123.30
1	A	192	MET	CB-CG-SD	-7.48	89.97	112.40
1	A	187	CYS	CA-CB-SG	-7.38	100.72	114.00
1	A	194	GLU	CB-CA-C	-7.27	95.85	110.40
1	A	181	ASP	C-N-CA	-7.04	104.09	121.70
1	A	117	LEU	CA-CB-CG	-6.83	99.58	115.30
1	A	147	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	137	GLN	N-CA-C	6.49	128.52	111.00
1	A	119	LEU	CB-CG-CD2	-6.39	100.14	111.00
1	A	183	ALA	N-CA-C	6.37	128.19	111.00
1	A	213	LYS	N-CA-CB	6.30	121.94	110.60
1	A	141	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	129	GLY	CA-C-N	-6.07	103.84	117.20
1	A	159	CYS	CA-CB-SG	-5.68	103.77	114.00

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LYS	CD-CE-NZ	5.68	124.76	111.70
1	A	178	LEU	N-CA-CB	-5.67	99.07	110.40
1	A	177	HIS	CB-CA-C	-5.60	99.19	110.40
1	A	191	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	194	GLU	CB-CG-CD	-5.43	99.54	114.20
1	A	179	THR	CA-CB-CG2	5.43	120.00	112.40
1	A	131	GLU	CB-CA-C	-5.27	99.86	110.40
1	A	164	ARG	CB-CA-C	5.27	120.94	110.40
1	A	180	ILE	CG1-CB-CG2	-5.27	99.81	111.40
1	A	169	TYR	CB-CG-CD2	-5.08	117.95	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	183	ALA	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ASP	Mainchain

## 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	785	0	779	138	10
2	A	48	0	0	29	3
All	All	833	0	779	138	12

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 91.

All (138) 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:169:TYR:CE2	1:A:203:ILE:HG22	1.41	1.54

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:CG1	1:A:146:VAL:CB	1.85	1.52
1:A:152:HIS:CG	1:A:170:ARG:NH2	1.86	1.41
1:A:176:GLY:HA2	2:A:322:HOH:O	1.22	1.38
1:A:169:TYR:CE2	1:A:203:ILE:CG2	2.09	1.33
1:A:173:HIS:CD2	2:A:348:HOH:O	1.89	1.24
1:A:130:GLN:O	2:A:317:HOH:O	1.54	1.21
1:A:176:GLY:HA3	2:A:327:HOH:O	1.43	1.17
1:A:152:HIS:CG	1:A:170:ARG:HH21	1.56	1.16
1:A:181:ASP:C	1:A:183:ALA:N	1.97	1.16
1:A:152:HIS:ND1	1:A:170:ARG:NH2	1.87	1.15
1:A:200:LYS:C	2:A:335:HOH:O	1.81	1.15
1:A:201:GLY:N	2:A:335:HOH:O	1.76	1.13
1:A:180:ILE:HD11	1:A:184:VAL:HG23	1.08	1.08
1:A:205:THR:HG23	2:A:310:HOH:O	0.92	1.08
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.23	1.03
1:A:180:ILE:O	1:A:181:ASP:C	1.95	1.00
1:A:169:TYR:CZ	1:A:203:ILE:HG22	1.98	0.98
1:A:169:TYR:CD1	2:A:309:HOH:O	2.17	0.97
1:A:174:ARG:HH11	1:A:174:ARG:HG2	1.27	0.96
1:A:181:ASP:C	1:A:183:ALA:H	1.50	0.93
1:A:180:ILE:HD11	1:A:184:VAL:CG2	1.98	0.93
1:A:173:HIS:NE2	2:A:348:HOH:O	1.94	0.92
1:A:169:TYR:HE2	1:A:203:ILE:HG22	1.24	0.91
1:A:152:HIS:CB	1:A:170:ARG:HH21	1.84	0.90
1:A:180:ILE:CD1	1:A:184:VAL:HG23	2.00	0.89
1:A:152:HIS:CB	1:A:170:ARG:NH2	2.36	0.89
1:A:169:TYR:CD2	1:A:203:ILE:CG2	2.56	0.88
1:A:137:GLN:OE1	1:A:139:PRO:HD3	1.74	0.87
1:A:169:TYR:CE1	2:A:309:HOH:O	2.26	0.87
1:A:137:GLN:O	1:A:139:PRO:HD3	1.73	0.87
1:A:200:LYS:CG	1:A:201:GLY:N	2.38	0.87
1:A:137:GLN:O	1:A:139:PRO:CD	2.24	0.86
1:A:212:ARG:O	1:A:213:LYS:HD2	1.77	0.84
1:A:167:ILE:HG21	1:A:169:TYR:CZ	2.13	0.84
1:A:162:PHE:CD2	1:A:205:THR:OG1	2.30	0.83
1:A:155:ASP:HA	2:A:348:HOH:O	1.78	0.83
1:A:180:ILE:O	1:A:183:ALA:N	2.14	0.80
1:A:194:GLU:HA	1:A:194:GLU:OE1	1.80	0.80
1:A:140:GLU:OE2	1:A:209:ARG:NE	2.13	0.80
1:A:196:TYR:CD1	1:A:203:ILE:HD11	2.17	0.79
1:A:178:LEU:HD11	1:A:180:ILE:C	2.02	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:HG3	1:A:201:GLY:N	1.96	0.79
1:A:146:VAL:CG1	1:A:146:VAL:CA	2.60	0.79
1:A:146:VAL:CG2	1:A:146:VAL:CG1	2.64	0.75
1:A:180:ILE:O	1:A:180:ILE:HG13	1.87	0.74
1:A:152:HIS:HB2	1:A:170:ARG:HH21	1.50	0.74
1:A:152:HIS:HB2	1:A:170:ARG:NH2	2.02	0.72
1:A:154:GLY:O	2:A:348:HOH:O	2.10	0.70
1:A:201:GLY:CA	2:A:335:HOH:O	2.30	0.70
1:A:137:GLN:OE1	1:A:137:GLN:O	2.10	0.69
1:A:167:ILE:HG22	1:A:168:HIS:N	2.06	0.69
1:A:140:GLU:O	1:A:143:LEU:HB2	1.93	0.69
1:A:174:ARG:HH11	1:A:174:ARG:CG	2.05	0.68
1:A:212:ARG:HG3	2:A:343:HOH:O	1.93	0.67
1:A:152:HIS:CG	1:A:170:ARG:HH22	1.80	0.67
1:A:167:ILE:CG2	1:A:168:HIS:N	2.58	0.66
1:A:152:HIS:CE1	1:A:170:ARG:NH2	2.62	0.66
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.01	0.66
1:A:169:TYR:CE2	1:A:203:ILE:HG21	2.27	0.65
1:A:212:ARG:HG3	1:A:212:ARG:O	1.97	0.64
1:A:124:HIS:N	1:A:124:HIS:CD2	2.63	0.64
1:A:178:LEU:HG	1:A:179:THR:N	2.06	0.64
1:A:167:ILE:C	1:A:168:HIS:CD2	2.73	0.61
1:A:162:PHE:CE2	1:A:205:THR:OG1	2.55	0.60
1:A:152:HIS:CD2	1:A:170:ARG:NH2	2.62	0.60
1:A:170:ARG:HH11	1:A:170:ARG:HG3	1.65	0.60
1:A:174:ARG:NH1	1:A:174:ARG:HG2	2.07	0.59
1:A:213:LYS:NZ	2:A:343:HOH:O	2.28	0.59
1:A:170:ARG:NH1	1:A:170:ARG:HG3	2.17	0.59
1:A:180:ILE:CG1	1:A:184:VAL:H	2.14	0.59
1:A:130:GLN:HB2	2:A:326:HOH:O	2.04	0.58
1:A:167:ILE:C	1:A:168:HIS:HD2	2.06	0.57
1:A:181:ASP:N	1:A:181:ASP:OD1	2.37	0.57
1:A:180:ILE:O	1:A:180:ILE:CG1	2.52	0.57
1:A:152:HIS:O	1:A:155:ASP:HB2	2.03	0.57
1:A:211:LYS:NZ	2:A:311:HOH:O	2.34	0.57
1:A:178:LEU:HD11	1:A:180:ILE:O	2.04	0.56
1:A:169:TYR:CD2	1:A:203:ILE:HG21	2.38	0.56
1:A:117:LEU:O	1:A:120:MET:N	2.30	0.56
1:A:117:LEU:HD23	1:A:117:LEU:N	2.22	0.55
1:A:173:HIS:HD2	2:A:348:HOH:O	1.56	0.55
1:A:169:TYR:HD1	2:A:313:HOH:O	1.90	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HD12	1:A:167:ILE:N	2.21	0.55
1:A:174:ARG:O	1:A:175:ASP:OD2	2.24	0.55
1:A:151:ARG:NH2	2:A:319:HOH:O	2.40	0.55
1:A:200:LYS:HG2	1:A:201:GLY:N	2.22	0.54
1:A:200:LYS:HG2	1:A:201:GLY:H	1.73	0.54
1:A:180:ILE:HG13	1:A:184:VAL:H	1.71	0.53
1:A:189:LEU:O	1:A:191:ASP:N	2.42	0.53
1:A:117:LEU:CB	2:A:318:HOH:O	2.57	0.53
1:A:213:LYS:HE2	2:A:311:HOH:O	2.08	0.53
1:A:168:HIS:CD2	1:A:168:HIS:N	2.75	0.53
1:A:188:ASN:HB3	1:A:190:MET:CE	2.39	0.52
1:A:137:GLN:O	1:A:139:PRO:HD2	2.07	0.52
1:A:144:PHE:CD1	1:A:207:LEU:HD22	2.46	0.51
1:A:194:GLU:HG2	2:A:315:HOH:O	2.10	0.50
1:A:144:PHE:CG	1:A:207:LEU:HD22	2.48	0.49
1:A:174:ARG:N	1:A:176:GLY:O	2.43	0.49
1:A:178:LEU:HD11	1:A:181:ASP:N	2.28	0.49
1:A:212:ARG:O	1:A:213:LYS:CD	2.56	0.49
1:A:188:ASN:N	1:A:188:ASN:ND2	2.62	0.48
1:A:134:GLN:O	1:A:137:GLN:HB2	2.14	0.48
1:A:137:GLN:O	1:A:137:GLN:CD	2.51	0.48
1:A:117:LEU:CA	2:A:318:HOH:O	2.62	0.48
1:A:212:ARG:CG	2:A:343:HOH:O	2.58	0.47
1:A:178:LEU:HD22	1:A:185:PHE:CE2	2.49	0.47
1:A:129:GLY:O	1:A:132:ALA:N	2.45	0.47
1:A:167:ILE:HG21	1:A:169:TYR:CE1	2.48	0.46
1:A:169:TYR:CE2	1:A:203:ILE:HG23	2.33	0.46
1:A:146:VAL:C	1:A:146:VAL:CG1	2.83	0.46
1:A:200:LYS:O	1:A:201:GLY:C	2.54	0.46
1:A:180:ILE:HD11	1:A:184:VAL:H	1.80	0.46
1:A:174:ARG:C	1:A:176:GLY:H	2.19	0.45
1:A:137:GLN:O	1:A:137:GLN:CG	2.64	0.45
1:A:152:HIS:N	1:A:152:HIS:ND1	2.65	0.45
1:A:117:LEU:HD22	1:A:117:LEU:HA	1.59	0.45
1:A:173:HIS:HA	1:A:176:GLY:O	2.17	0.45
1:A:174:ARG:C	1:A:175:ASP:OD2	2.54	0.45
1:A:206:LYS:N	2:A:310:HOH:O	2.46	0.45
1:A:180:ILE:CD1	1:A:184:VAL:H	2.30	0.45
1:A:213:LYS:HD3	2:A:316:HOH:O	2.18	0.44
1:A:169:TYR:CD2	1:A:203:ILE:HG23	2.48	0.44
1:A:178:LEU:HD11	1:A:181:ASP:CA	2.48	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:C	1:A:128:SER:O	2.56	0.43
1:A:208:VAL:HG12	1:A:209:ARG:N	2.34	0.42
1:A:170:ARG:HH11	1:A:170:ARG:CG	2.32	0.42
1:A:205:THR:CG2	2:A:310:HOH:O	1.82	0.42
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.94	0.42
1:A:145:LEU:C	1:A:145:LEU:HD12	2.40	0.42
1:A:125:GLY:O	1:A:147:ARG:HB2	2.20	0.42
1:A:180:ILE:HD13	2:A:304:HOH:O	2.20	0.41
1:A:122:TRP:HB3	1:A:210:PRO:HB3	2.02	0.41
1:A:124:HIS:N	1:A:124:HIS:HD2	2.12	0.41
1:A:123:PHE:C	1:A:124:HIS:HD2	2.24	0.41
1:A:120:MET:HA	1:A:121:PRO:HD3	1.68	0.41
1:A:178:LEU:CD2	1:A:181:ASP:HA	2.50	0.41
1:A:171:VAL:HG21	1:A:192:MET:HE1	2.02	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:CZ	1:A:182:GLU:CG[4_546]	0.80	1.40
1:A:164:ARG:NH2	1:A:182:GLU:CG[4_546]	1.00	1.20
1:A:164:ARG:NH1	1:A:182:GLU:CD[4_546]	1.04	1.16
1:A:164:ARG:NH1	1:A:182:GLU:OE1[4_546]	1.18	1.02
1:A:164:ARG:NH1	1:A:182:GLU:CG[4_546]	1.36	0.84
1:A:164:ARG:CZ	1:A:182:GLU:CD[4_546]	1.54	0.66
1:A:211:LYS:NZ	2:A:340:HOH:O[1_554]	1.58	0.62
1:A:164:ARG:NH2	1:A:182:GLU:CB[4_546]	1.64	0.56
2:A:311:HOH:O	2:A:340:HOH:O[1_554]	1.72	0.48
1:A:182:GLU:O	1:A:187:CYS:SG[2_656]	2.06	0.14
2:A:326:HOH:O	2:A:326:HOH:O[2_555]	2.07	0.13
1:A:164:ARG:NE	1:A:182:GLU:CG[4_546]	2.10	0.10

## 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	95/97 (98%)	69 (73%)	16 (17%)	10 (10%)	1	0

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	ASP
1	A	191	ASP
1	A	140	GLU
1	A	182	GLU
1	A	201	GLY
1	A	202	ALA
1	A	139	PRO
1	A	190	MET
1	A	183	ALA
1	A	193	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	86/86 (100%)	65 (76%)	21 (24%)	1	1

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	118	SER
1	A	119	LEU
1	A	126	LYS
1	A	131	GLU
1	A	137	GLN
1	A	143	LEU
1	A	149	SER
1	A	151	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	152	HIS
1	A	155	ASP
1	A	174	ARG
1	A	175	ASP
1	A	177	HIS
1	A	178	LEU
1	A	181	ASP
1	A	188	ASN
1	A	191	ASP
1	A	203	ILE
1	A	211	LYS
1	A	213	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	130	GLN
1	A	168	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 [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	96/97 (98%)	-0.32	0 <a href="#">100</a> <a href="#">100</a>	15, 32, 45, 59	5 (5%)

There are no RSRZ outliers to report.

### 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.