



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:10 PM GMT

PDB ID : 4A1G  
Title : The crystal structure of the human Bub1 TPR domain in complex with the  
KI motif of Knl1  
Authors : Krenn, V.; Wehenkel, A.; Li, X.; Santaguida, S.; Musacchio, A.  
Deposited on : 2011-09-15  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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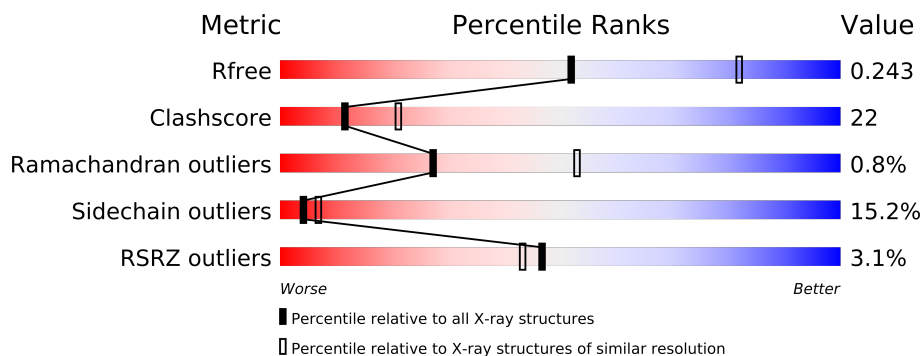
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance









The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	152	
1	B	152	
1	C	152	
1	D	152	
2	E	53	
2	F	53	
2	G	53	
2	H	53	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5497 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MITOTIC CHECKPOINT SERINE/THREONINE-PROTEIN KINASE BUB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1219	788	201	226	4			
1	B	149	Total	C	N	O	S	0	0	0
			1227	793	204	226	4			
1	C	149	Total	C	N	O	S	0	0	0
			1251	805	209	233	4			
1	D	148	Total	C	N	O	S	0	0	0
			1226	792	201	228	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP O43683
A	0	PRO	-	EXPRESSION TAG	UNP O43683
B	-1	GLY	-	EXPRESSION TAG	UNP O43683
B	0	PRO	-	EXPRESSION TAG	UNP O43683
C	-1	GLY	-	EXPRESSION TAG	UNP O43683
C	0	PRO	-	EXPRESSION TAG	UNP O43683
D	-1	GLY	-	EXPRESSION TAG	UNP O43683
D	0	PRO	-	EXPRESSION TAG	UNP O43683

- Molecule 2 is a protein called PROTEIN CASC5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	0	0	0
			90	58	14	18			
2	F	15	Total	C	N	O	0	0	0
			119	77	20	22			
2	G	15	Total	C	N	O	0	0	0
			119	77	20	22			
2	H	16	Total	C	N	O	0	0	0
			126	81	21	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	148	GLY	-	EXPRESSION TAG	UNP Q8NG31
E	149	PRO	-	EXPRESSION TAG	UNP Q8NG31
F	148	GLY	-	EXPRESSION TAG	UNP Q8NG31
F	149	PRO	-	EXPRESSION TAG	UNP Q8NG31
G	148	GLY	-	EXPRESSION TAG	UNP Q8NG31
G	149	PRO	-	EXPRESSION TAG	UNP Q8NG31
H	148	GLY	-	EXPRESSION TAG	UNP Q8NG31
H	149	PRO	-	EXPRESSION TAG	UNP Q8NG31

- Molecule 3 is water.

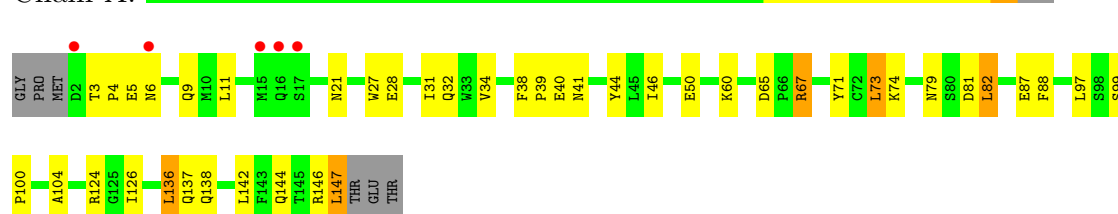
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	40	Total O 40 40	0	0
3	B	30	Total O 30 30	0	0
3	C	29	Total O 29 29	0	0
3	D	14	Total O 14 14	0	0
3	F	1	Total O 1 1	0	0
3	G	6	Total O 6 6	0	0

### 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 ( $RSRZ > 2$ ). 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.

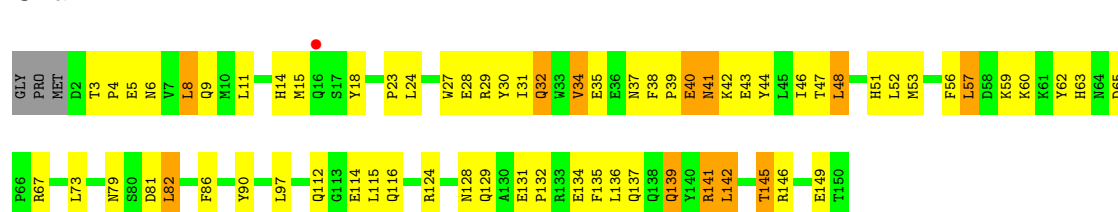
#### • Molecule 1: MITOTIC CHECKPOINT SERINE/THREONINE-PROTEINKINASE BUB1

Chain A:



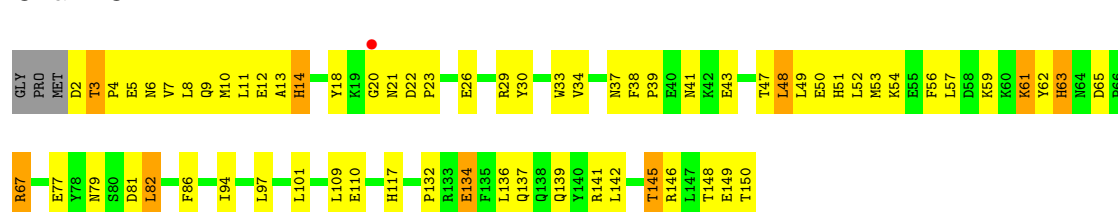
#### • Molecule 1: MITOTIC CHECKPOINT SERINE/THREONINE-PROTEINKINASE BUB1

Chain B:



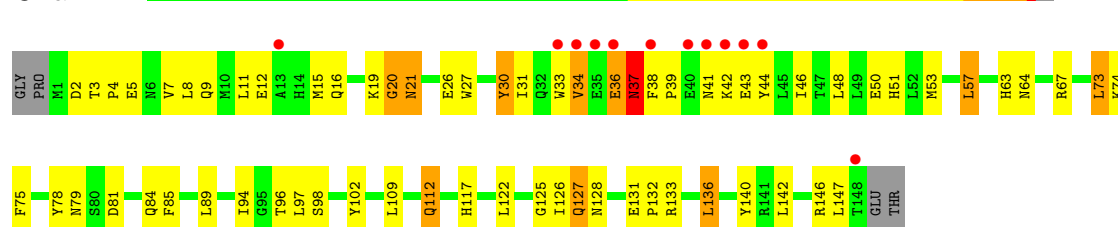
#### • Molecule 1: MITOTIC CHECKPOINT SERINE/THREONINE-PROTEINKINASE BUB1

Chain C:



#### • Molecule 1: MITOTIC CHECKPOINT SERINE/THREONINE-PROTEINKINASE BUB1

Chain D:



#### • Molecule 2: PROTEIN CASC5

Chain E: 

GLY	PRO	GLN	MET	ASP	LEU	THR	SER	SER	HIS	THR	VAL	MET	ILE	THR	LYS	GLY	LEU	LEU	ASP	ASN	PRO	ILE	SER	GLU	LYS	THR	K176	I177	D178	T179	F182	L183	A184	M185	L186	K187	LEU	HIS	THR	GLU	ASP	SER	ARG	MET	LYS	LYS	GLU	VAL	ASN
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- Molecule 2: PROTEIN CASC5

Chain F: 

GLY	PRO	GLN	MET	ASP	LEU	THR	SER	SER	HIS	THR	VAL	MET	ILE	THR	LYS	GLY	LEU	LEU	ASP	ASN	PRO	ILE	SER	GLU	LYS	SER	T175	K176	I177	D178	T179	F182	L183	L186	K187	L188	H189	THR	GLU	ASP	SER	ARG	MET	LYS	LYS	GLU	VAL	ASN
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- Molecule 2: PROTEIN CASC5

Chain G: 

GLY	PRO	GLN	MET	ASP	LEU	THR	SER	SER	HIS	THR	VAL	MET	ILE	THR	LYS	GLY	LEU	LEU	ASP	ASN	PRO	ILE	SER	GLU	LYS	SER	T175	K176	I177	D178	T179	F182	L183	L186	K187	L188	H189	THR	GLU	ASP	SER	ARG	MET	LYS	LYS	GLU	VAL	ASN
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- Molecule 2: PROTEIN CASC5

Chain H: 

GLY	PRO	GLN	MET	ASP	LEU	THR	SER	SER	HIS	THR	VAL	MET	ILE	THR	LYS	GLY	LEU	LEU	ASP	ASN	PRO	ILE	SER	GLU	LYS	SER	T175	K176	I177	D178	T179	T180	S181	F182	L186	K187	L188	H189	T190	GLU	ASP	SER	ARG	MET	LYS	LYS	GLU	VAL	ASN
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.28Å 130.97Å 74.96Å 90.00° 110.17° 90.00°	Depositor
Resolution (Å)	61.98 – 2.60 61.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (61.98-2.60) 98.5 (61.98-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.186 , 0.244 0.186 , 0.243	Depositor DCC
$R_{free}$ test set	1652 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 32541 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.46	0/1255	0.58	0/1700
1	B	0.46	0/1263	0.60	0/1714
1	C	0.48	0/1287	0.59	0/1743
1	D	0.47	0/1262	0.56	0/1711
2	E	0.41	0/90	0.57	0/121
2	F	0.51	0/120	0.66	0/161
2	G	0.44	0/120	0.69	0/161
2	H	0.35	0/127	0.60	0/171
All	All	0.46	0/5524	0.59	0/7482

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1219	0	1137	33	0
1	B	1227	0	1137	62	0
1	C	1251	0	1173	62	0
1	D	1226	0	1139	68	0
2	E	90	0	90	10	0
2	F	119	0	126	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	119	0	126	8	0
2	H	126	0	133	16	0
3	A	40	0	0	3	0
3	B	30	0	0	1	0
3	C	29	0	0	1	0
3	D	14	0	0	1	0
3	F	1	0	0	0	0
3	G	6	0	0	1	0
All	All	5497	0	5061	230	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (230) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:ARG:NE	1:B:149:GLU:OE2	1.85	1.09
1:D:112:GLN:HA	1:D:112:GLN:HE21	1.23	1.03
1:C:65:ASP:OD1	1:C:67:ARG:HG2	1.61	1.00
1:B:81:ASP:H	2:F:179:THR:HG21	1.34	0.91
1:B:79:ASN:OD1	2:F:179:THR:HB	1.71	0.90
1:B:81:ASP:H	2:F:179:THR:CG2	1.86	0.87
3:A:2037:HOH:O	1:B:139:GLN:HG3	1.78	0.82
1:B:53:MET:O	1:B:57:LEU:HB2	1.81	0.81
1:D:37:ASN:HB3	1:D:38:PHE:CD1	2.18	0.79
1:C:18:TYR:HE2	1:C:20:GLY:O	1.66	0.78
1:B:31:ILE:O	1:B:35:GLU:HB2	1.86	0.75
1:B:31:ILE:HG12	1:B:48:LEU:HD13	1.68	0.75
1:D:112:GLN:CA	1:D:112:GLN:HE21	2.00	0.75
1:D:81:ASP:H	2:H:179:THR:CG2	2.01	0.74
1:C:82:LEU:HD12	1:C:86:PHE:CE2	2.23	0.73
1:C:81:ASP:H	2:G:179:THR:CG2	2.01	0.73
1:A:5:GLU:O	1:A:9:GLN:HG3	1.87	0.73
1:A:146:ARG:CZ	1:B:149:GLU:OE2	2.37	0.73
1:D:81:ASP:H	2:H:179:THR:HG21	1.53	0.73
1:C:79:ASN:OD1	2:G:179:THR:HB	1.89	0.72
1:C:81:ASP:H	2:G:179:THR:HG21	1.55	0.72
1:D:112:GLN:HA	1:D:112:GLN:NE2	2.03	0.71
1:B:67:ARG:HG3	1:B:67:ARG:HH11	1.55	0.71
1:D:41:ASN:ND2	1:D:43:GLU:HB3	2.06	0.71
2:H:186:LEU:HD12	2:H:186:LEU:H	1.56	0.71
1:D:74:LYS:HE3	3:D:2007:HOH:O	1.91	0.70
1:C:57:LEU:CD1	2:G:186:LEU:HD21	2.21	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:4:PRO:HD3	1:D:44:TYR:CE1	2.27	0.69
1:C:41:ASN:HD21	1:C:43:GLU:HB2	1.56	0.69
1:D:109:LEU:HD13	1:D:117:HIS:HB3	1.75	0.69
1:D:33:TRP:O	1:D:37:ASN:HB2	1.94	0.68
1:B:52:LEU:HD12	1:B:56:PHE:HD2	1.57	0.68
1:C:149:GLU:OE2	1:D:146:ARG:NE	2.25	0.68
1:C:3:THR:HG22	1:C:6:ASN:CG	2.14	0.67
1:A:28:GLU:HG2	1:A:32:GLN:HE21	1.60	0.67
1:A:146:ARG:NH2	1:B:149:GLU:OE2	2.27	0.66
1:C:18:TYR:CE2	1:C:20:GLY:O	2.47	0.66
1:A:144:GLN:HA	1:A:147:LEU:HD22	1.77	0.66
1:C:57:LEU:HD22	1:C:94:ILE:CD1	2.26	0.65
1:D:34:VAL:HG11	1:D:48:LEU:HD11	1.78	0.65
1:C:141:ARG:O	1:C:145:THR:HG22	1.96	0.64
1:B:24:LEU:HD22	1:B:62:TYR:CD1	2.33	0.64
1:A:146:ARG:HE	1:B:149:GLU:CD	1.97	0.64
1:B:52:LEU:HD12	1:B:56:PHE:CD2	2.33	0.63
1:C:50:GLU:O	1:C:54:LYS:HG3	1.98	0.63
1:B:27:TRP:O	1:B:31:ILE:HG13	1.98	0.63
1:D:38:PHE:CD2	1:D:44:TYR:HE2	2.16	0.62
1:C:41:ASN:ND2	1:C:43:GLU:HB2	2.15	0.62
2:F:188:LEU:HD12	2:F:189:HIS:ND1	2.14	0.62
2:F:182:PHE:CE2	2:F:186:LEU:HD22	2.36	0.61
1:B:141:ARG:O	1:B:145:THR:HG22	2.00	0.61
1:B:57:LEU:HD13	2:F:186:LEU:HD21	1.80	0.61
1:D:36:GLU:CD	1:D:36:GLU:O	2.39	0.61
1:A:38:PHE:N	1:A:39:PRO:HD3	2.16	0.61
1:D:37:ASN:HB3	1:D:38:PHE:HD1	1.67	0.60
1:C:57:LEU:HD12	2:G:186:LEU:HD21	1.84	0.60
1:B:81:ASP:N	2:F:179:THR:CG2	2.63	0.60
1:B:81:ASP:N	2:F:179:THR:HG21	2.12	0.60
1:C:57:LEU:HD22	1:C:94:ILE:HD13	1.83	0.59
1:D:36:GLU:O	1:D:37:ASN:HB2	2.02	0.59
1:D:127:GLN:HG3	1:D:128:ASN:N	2.18	0.59
1:C:53:MET:O	1:C:57:LEU:HG	2.03	0.59
1:C:132:PRO:HG2	1:D:73:LEU:HB3	1.82	0.59
1:A:81:ASP:H	2:E:179:THR:CG2	2.15	0.59
1:C:14:HIS:ND1	1:C:14:HIS:C	2.55	0.59
1:B:82:LEU:HD23	1:B:86:PHE:CE2	2.38	0.58
1:D:27:TRP:O	1:D:31:ILE:HG13	2.03	0.58
1:C:61:LYS:HD2	1:C:62:TYR:CZ	2.40	0.57
1:D:57:LEU:HD23	2:H:186:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:177:ILE:O	2:F:177:ILE:HG13	2.03	0.57
1:D:78:TYR:O	2:H:176:LYS:HB3	2.03	0.57
1:A:81:ASP:H	2:E:179:THR:HG21	1.70	0.56
1:C:3:THR:HG22	1:C:6:ASN:H	1.71	0.56
1:D:57:LEU:HD12	1:D:94:ILE:HD13	1.88	0.56
1:B:3:THR:HB	1:B:6:ASN:ND2	2.21	0.56
1:A:28:GLU:CG	1:A:32:GLN:HE21	2.18	0.56
2:E:177:ILE:HG12	2:E:178:ASP:N	2.21	0.55
1:D:38:PHE:N	1:D:39:PRO:HD3	2.21	0.55
1:D:75:PHE:CZ	2:H:177:ILE:HD11	2.42	0.55
1:D:42:LYS:O	1:D:46:ILE:HG13	2.06	0.54
1:B:14:HIS:NE2	1:C:33:TRP:HH2	2.05	0.54
1:C:18:TYR:CE1	1:C:26:GLU:HG2	2.43	0.54
2:F:182:PHE:CZ	2:F:186:LEU:HD22	2.42	0.54
1:C:38:PHE:N	1:C:39:PRO:HD3	2.22	0.54
1:D:53:MET:O	1:D:57:LEU:HB2	2.08	0.53
1:B:3:THR:HG22	1:B:5:GLU:H	1.73	0.53
1:C:82:LEU:CD1	1:C:86:PHE:CE2	2.92	0.53
1:C:3:THR:HG23	1:C:5:GLU:H	1.72	0.53
1:B:5:GLU:O	1:B:9:GLN:HG3	2.09	0.53
1:B:42:LYS:O	1:B:46:ILE:HG13	2.09	0.53
1:B:14:HIS:O	1:B:18:TYR:N	2.42	0.52
1:A:28:GLU:HG3	1:A:71:TYR:OH	2.10	0.52
1:B:41:ASN:HD21	1:B:44:TYR:HD1	1.55	0.52
1:D:38:PHE:HB2	1:D:44:TYR:HD2	1.74	0.52
1:C:3:THR:OG1	1:C:4:PRO:HD2	2.10	0.52
1:A:38:PHE:N	1:A:39:PRO:CD	2.73	0.52
2:E:182:PHE:CD2	2:E:183:LEU:HD13	2.45	0.52
1:D:19:LYS:O	1:D:20:GLY:O	2.29	0.51
1:C:57:LEU:O	1:C:63:HIS:HE1	1.92	0.51
1:D:112:GLN:CA	1:D:112:GLN:NE2	2.66	0.51
1:B:57:LEU:O	1:B:63:HIS:HE1	1.94	0.51
1:D:37:ASN:C	1:D:39:PRO:HD3	2.31	0.50
1:D:8:LEU:HD13	1:D:48:LEU:HD23	1.92	0.50
3:A:2023:HOH:O	1:B:146:ARG:HD3	2.11	0.50
1:C:5:GLU:O	1:C:9:GLN:HB2	2.12	0.50
2:H:189:HIS:CD2	2:H:189:HIS:N	2.80	0.50
1:D:37:ASN:HB3	1:D:38:PHE:CE1	2.47	0.50
2:G:187:LYS:NZ	3:G:2003:HOH:O	2.45	0.50
1:D:84:GLN:HE22	2:H:180:THR:HB	1.76	0.50
1:B:11:LEU:O	1:B:15:MET:HB2	2.12	0.49
1:B:38:PHE:N	1:B:39:PRO:HD3	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:38:PHE:CB	1:D:44:TYR:CD2	2.96	0.49
2:H:189:HIS:CD2	2:H:189:HIS:H	2.29	0.49
1:C:67:ARG:HD3	1:D:67:ARG:HE	1.77	0.49
1:D:3:THR:O	1:D:7:VAL:HG12	2.11	0.49
1:C:34:VAL:HG21	1:C:48:LEU:HD11	1.94	0.49
1:D:38:PHE:CB	1:D:44:TYR:HD2	2.26	0.49
1:C:11:LEU:HD22	1:C:30:TYR:CG	2.47	0.49
1:D:38:PHE:CD2	1:D:44:TYR:CE2	3.01	0.48
1:C:57:LEU:HD22	1:C:94:ILE:HD11	1.93	0.48
2:H:187:LYS:HD3	2:H:188:LEU:N	2.28	0.48
1:A:65:ASP:OD1	1:A:67:ARG:HG2	2.13	0.48
1:C:77:GLU:HG2	1:C:77:GLU:O	2.12	0.48
1:B:52:LEU:CD1	1:B:56:PHE:CD2	2.95	0.48
1:D:2:ASP:OD2	1:D:5:GLU:HB2	2.13	0.48
1:D:38:PHE:N	1:D:38:PHE:CD1	2.81	0.48
1:D:2:ASP:OD2	1:D:4:PRO:HG2	2.14	0.48
1:C:3:THR:CG2	1:C:6:ASN:H	2.27	0.47
2:E:179:THR:O	2:E:183:LEU:HD22	2.14	0.47
1:C:109:LEU:HD13	1:C:117:HIS:HB3	1.95	0.47
1:A:28:GLU:O	1:A:32:GLN:HG3	2.15	0.47
1:D:122:LEU:HD13	1:D:140:TYR:HA	1.95	0.47
1:D:3:THR:N	1:D:4:PRO:HD2	2.30	0.47
1:A:28:GLU:HG2	1:A:32:GLN:NE2	2.27	0.47
2:E:182:PHE:HD2	2:E:183:LEU:HD13	1.79	0.47
1:A:60:LYS:HD2	1:D:96:THR:HG21	1.97	0.47
1:B:28:GLU:O	1:B:32:GLN:HB2	2.15	0.47
1:B:47:THR:O	1:B:51:HIS:HD2	1.97	0.47
1:D:5:GLU:O	1:D:9:GLN:HG3	2.14	0.46
1:B:3:THR:HG23	1:B:4:PRO:HD2	1.98	0.46
1:D:34:VAL:HG23	1:D:34:VAL:O	2.15	0.46
1:B:65:ASP:OD1	1:B:67:ARG:HB2	2.15	0.46
1:C:23:PRO:HD2	1:C:62:TYR:OH	2.15	0.46
1:A:3:THR:O	1:A:6:ASN:HB2	2.16	0.46
1:B:128:ASN:O	1:B:129:GLN:HB2	2.16	0.46
1:A:46:ILE:O	1:A:50:GLU:HG3	2.16	0.46
1:A:126:ILE:HG12	1:A:136:LEU:HD13	1.98	0.46
1:D:79:ASN:HB3	2:H:179:THR:CG2	2.46	0.46
1:D:85:PHE:O	1:D:89:LEU:HG	2.16	0.46
1:D:4:PRO:HD3	1:D:44:TYR:CD1	2.51	0.45
1:D:15:MET:HE3	1:D:26:GLU:HB2	1.99	0.45
1:C:47:THR:O	1:C:51:HIS:HD2	1.98	0.45
1:C:57:LEU:HD23	1:C:57:LEU:HA	1.60	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:142:LEU:HA	1:B:145:THR:HG23	1.98	0.45
1:C:110:GLU:OE2	1:C:146:ARG:HD2	2.16	0.45
3:A:2006:HOH:O	1:B:145:THR:HG21	2.16	0.45
1:B:60:LYS:HA	1:B:63:HIS:CD2	2.52	0.45
1:C:14:HIS:O	1:C:14:HIS:ND1	2.49	0.45
1:C:8:LEU:HD22	1:C:47:THR:HG22	1.98	0.45
1:C:52:LEU:HD12	1:C:56:PHE:CD2	2.52	0.45
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.81	0.45
1:D:53:MET:HE3	1:D:57:LEU:HD13	1.99	0.45
1:C:49:LEU:O	1:C:53:MET:HG2	2.17	0.45
1:C:57:LEU:HD12	2:G:186:LEU:HD11	1.99	0.45
1:A:88:PHE:CD2	2:E:183:LEU:HG	2.52	0.45
2:H:176:LYS:HA	2:H:176:LYS:HD2	1.46	0.45
1:C:67:ARG:CD	1:D:67:ARG:HE	2.30	0.45
1:D:57:LEU:HD12	1:D:94:ILE:CD1	2.46	0.45
1:B:23:PRO:HD2	1:B:62:TYR:OH	2.17	0.44
1:D:20:GLY:O	1:D:21:ASN:CB	2.65	0.44
1:C:8:LEU:O	1:C:12:GLU:HB2	2.17	0.44
1:C:11:LEU:HD13	1:C:30:TYR:HB3	1.99	0.44
1:B:30:TYR:O	1:B:34:VAL:HG12	2.16	0.44
2:E:176:LYS:HG2	2:E:176:LYS:HZ2	1.70	0.44
1:D:8:LEU:HD21	1:D:51:HIS:CE1	2.52	0.44
1:A:38:PHE:CD1	1:A:44:TYR:CE2	3.06	0.44
2:H:178:ASP:OD2	2:H:181:SER:HB3	2.18	0.44
2:F:188:LEU:HD12	2:F:189:HIS:CE1	2.53	0.43
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.74	0.43
1:B:41:ASN:OD1	1:B:43:GLU:HB2	2.18	0.43
1:B:11:LEU:HD21	1:B:27:TRP:CD2	2.54	0.43
1:B:37:ASN:HB2	1:B:38:PHE:CD1	2.53	0.43
1:D:79:ASN:HB3	2:H:179:THR:HG21	2.01	0.43
1:B:67:ARG:CG	1:B:67:ARG:HH11	2.26	0.43
1:B:90:TYR:CZ	1:B:124:ARG:HD2	2.54	0.43
1:D:102:TYR:CZ	1:D:125:GLY:HA2	2.53	0.43
1:D:11:LEU:HD12	1:D:30:TYR:HB3	2.01	0.43
1:A:27:TRP:O	1:A:31:ILE:HG13	2.18	0.43
1:B:112:GLN:HB2	1:B:114:GLU:HG2	2.00	0.43
1:A:4:PRO:HA	1:A:44:TYR:CD1	2.54	0.43
1:C:10:MET:O	1:C:13:ALA:HB3	2.19	0.43
1:C:7:VAL:HA	1:C:10:MET:HE3	1.99	0.43
1:C:30:TYR:O	1:C:34:VAL:HG23	2.18	0.42
1:B:142:LEU:HA	1:B:145:THR:CG2	2.49	0.42
1:B:145:THR:O	1:B:149:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:23:PRO:O	1:C:26:GLU:HB2	2.19	0.42
1:B:8:LEU:O	1:B:11:LEU:HB3	2.20	0.42
1:C:49:LEU:HA	1:C:49:LEU:HD23	1.95	0.42
1:D:64:ASN:OD1	1:D:97:LEU:HB2	2.19	0.42
1:B:8:LEU:O	1:B:11:LEU:N	2.52	0.42
1:B:39:PRO:O	1:B:40:GLU:C	2.57	0.42
2:F:183:LEU:HA	2:F:183:LEU:HD12	1.90	0.42
1:D:36:GLU:O	1:D:37:ASN:CB	2.68	0.42
1:D:126:ILE:HG13	1:D:136:LEU:HD13	2.01	0.42
1:D:126:ILE:O	1:D:133:ARG:NH2	2.53	0.42
2:G:177:ILE:HD13	2:G:182:PHE:HB2	2.00	0.42
1:A:73:LEU:HB3	1:B:132:PRO:HG2	2.01	0.42
1:B:11:LEU:O	1:B:15:MET:N	2.48	0.41
1:C:11:LEU:CD1	1:C:30:TYR:HB3	2.50	0.41
1:C:134:GLU:HG3	3:C:2024:HOH:O	2.19	0.41
1:A:99:SER:N	1:A:100:PRO:CD	2.83	0.41
1:A:79:ASN:HB3	2:E:179:THR:HG21	2.01	0.41
1:A:104:ALA:HA	1:B:135:PHE:CE1	2.56	0.41
1:C:59:LYS:HB3	1:C:59:LYS:HE3	1.75	0.41
1:D:131:GLU:HB3	1:D:132:PRO:HA	2.02	0.41
1:C:56:PHE:HA	1:C:59:LYS:HG3	2.02	0.41
1:A:124:ARG:HD3	1:A:124:ARG:HA	1.68	0.41
1:D:50:GLU:HG3	2:H:182:PHE:HE1	1.86	0.41
1:D:38:PHE:HD2	1:D:44:TYR:HE2	1.67	0.40
1:D:79:ASN:OD1	2:H:179:THR:HB	2.21	0.40
1:B:67:ARG:NH1	1:B:67:ARG:HG3	2.29	0.40
1:A:3:THR:N	1:A:4:PRO:HD2	2.35	0.40
1:B:81:ASP:HB2	3:B:2008:HOH:O	2.20	0.40
1:C:149:GLU:CD	1:D:146:ARG:HE	2.19	0.40
1:A:81:ASP:H	2:E:179:THR:HG23	1.85	0.40
1:C:22:ASP:OD2	1:C:67:ARG:NH2	2.49	0.40
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.87	0.40
1:C:33:TRP:CE2	1:C:37:ASN:ND2	2.90	0.40
1:A:38:PHE:H	1:A:39:PRO:HD3	1.84	0.40
1:B:14:HIS:HE1	1:C:38:PHE:CZ	2.40	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	144/152 (95%)	140 (97%)	3 (2%)	1 (1%)	30	58
1	B	147/152 (97%)	141 (96%)	5 (3%)	1 (1%)	30	58
1	C	147/152 (97%)	138 (94%)	9 (6%)	0	100	100
1	D	146/152 (96%)	138 (94%)	5 (3%)	3 (2%)	11	19
2	E	10/53 (19%)	9 (90%)	1 (10%)	0	100	100
2	F	13/53 (24%)	12 (92%)	1 (8%)	0	100	100
2	G	13/53 (24%)	11 (85%)	2 (15%)	0	100	100
2	H	14/53 (26%)	11 (79%)	3 (21%)	0	100	100
All	All	634/820 (77%)	600 (95%)	29 (5%)	5 (1%)	27	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	20	GLY
1	D	37	ASN
1	D	21	ASN
1	A	40	GLU
1	B	40	GLU

### 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	127/136 (93%)	112 (88%)	15 (12%)	8	14
1	B	126/136 (93%)	106 (84%)	20 (16%)	4	6
1	C	132/136 (97%)	112 (85%)	20 (15%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	127/136 (93%)	112 (88%)	15 (12%)	8	14
2	E	10/50 (20%)	6 (60%)	4 (40%)	0	0
2	F	14/50 (28%)	10 (71%)	4 (29%)	0	1
2	G	14/50 (28%)	10 (71%)	4 (29%)	0	1
2	H	15/50 (30%)	11 (73%)	4 (27%)	1	1
All	All	565/744 (76%)	479 (85%)	86 (15%)	4	7

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	21	ASN
1	A	34	VAL
1	A	41	ASN
1	A	67	ARG
1	A	73	LEU
1	A	74	LYS
1	A	82	LEU
1	A	87	GLU
1	A	97	LEU
1	A	136	LEU
1	A	137	GLN
1	A	138	GLN
1	A	142	LEU
1	A	147	LEU
1	B	8	LEU
1	B	29	ARG
1	B	32	GLN
1	B	34	VAL
1	B	41	ASN
1	B	48	LEU
1	B	57	LEU
1	B	59	LYS
1	B	73	LEU
1	B	82	LEU
1	B	97	LEU
1	B	116	GLN
1	B	131	GLU
1	B	134	GLU
1	B	136	LEU

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Mol	Chain	Res	Type
1	B	137	GLN
1	B	139	GLN
1	B	141	ARG
1	B	142	LEU
1	B	145	THR
1	C	2	ASP
1	C	3	THR
1	C	14	HIS
1	C	21	ASN
1	C	29	ARG
1	C	48	LEU
1	C	61	LYS
1	C	63	HIS
1	C	67	ARG
1	C	82	LEU
1	C	97	LEU
1	C	101	LEU
1	C	134	GLU
1	C	136	LEU
1	C	137	GLN
1	C	139	GLN
1	C	142	LEU
1	C	145	THR
1	C	148	THR
1	C	150	THR
1	D	12	GLU
1	D	16	GLN
1	D	30	TYR
1	D	34	VAL
1	D	36	GLU
1	D	37	ASN
1	D	57	LEU
1	D	63	HIS
1	D	73	LEU
1	D	98	SER
1	D	112	GLN
1	D	127	GLN
1	D	136	LEU
1	D	142	LEU
1	D	147	LEU
2	E	177	ILE
2	E	179	THR

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Mol	Chain	Res	Type
2	E	183	LEU
2	E	185	ASN
2	F	179	THR
2	F	183	LEU
2	F	188	LEU
2	F	189	HIS
2	G	177	ILE
2	G	179	THR
2	G	183	LEU
2	G	188	LEU
2	H	176	LYS
2	H	177	ILE
2	H	179	THR
2	H	186	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	21	ASN
1	A	32	GLN
1	A	51	HIS
1	A	137	GLN
1	A	138	GLN
1	A	139	GLN
1	B	6	ASN
1	B	14	HIS
1	B	21	ASN
1	B	51	HIS
1	B	63	HIS
1	B	84	GLN
1	C	21	ASN
1	C	51	HIS
1	C	63	HIS
1	C	84	GLN
1	D	14	HIS
1	D	51	HIS
1	D	92	HIS
1	D	112	GLN
1	D	127	GLN
1	D	137	GLN
2	E	185	ASN

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Mol	Chain	Res	Type
2	G	189	HIS
2	H	189	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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 ⓘ

### 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	146/152 (96%)	-0.03	5 (3%) 43 39	33, 51, 78, 90	0
1	B	149/152 (98%)	-0.27	1 (0%) 84 86	31, 47, 103, 116	0
1	C	149/152 (98%)	-0.28	1 (0%) 84 86	29, 48, 96, 101	0
1	D	148/152 (97%)	0.15	12 (8%) 12 9	32, 52, 98, 120	0
2	E	12/53 (22%)	-0.45	0 100 100	58, 65, 80, 90	0
2	F	15/53 (28%)	-0.38	0 100 100	36, 44, 84, 92	0
2	G	15/53 (28%)	-0.30	0 100 100	39, 49, 76, 90	0
2	H	16/53 (30%)	0.15	1 (6%) 19 16	60, 73, 119, 120	0
All	All	650/820 (79%)	-0.12	20 (3%) 47 43	29, 52, 98, 120	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	148	THR	4.7
1	D	33	TRP	4.5
1	D	42	LYS	3.7
1	D	43	GLU	3.7
2	H	175	THR	3.6
1	C	20	GLY	3.5
1	D	40	GLU	3.4
1	D	35	GLU	3.3
1	D	38	PHE	3.0
1	A	16	GLN	2.9
1	B	16	GLN	2.8
1	A	2	ASP	2.6
1	D	44	TYR	2.5
1	D	13	ALA	2.5
1	D	36	GLU	2.4
1	D	41	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	17	SER	2.3
1	D	34	VAL	2.2
1	A	15	MET	2.1
1	A	6	ASN	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.