



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:35 PM GMT

PDB ID : 4YC6  
Title : CDK1/CKS1  
Authors : Brown, N.R.; Korolchuk, S.; Martin, M.P.; Stanley, W.; Moukhametzianov, R.; Noble, M.E.M.; Endicott, J.A.  
Deposited on : 2015-02-19  
Resolution : 2.60 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  
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

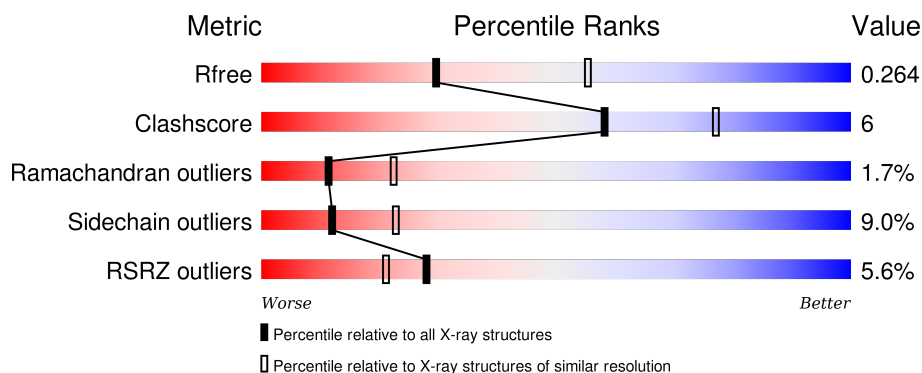
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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. 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	297	<div> <div>0%</div> <div>80% 12% . .</div> </div>
1	C	297	<div> <div>2%</div> <div>79% 13% . .</div> </div>
1	E	297	<div> <div>5%</div> <div>80% 12% . . .</div> </div>
1	G	297	<div> <div>14%</div> <div>74% 19% . .</div> </div>
2	B	85	<div> <div>2%</div> <div>61% 16% . . 18%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	85	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>64%</div><div>14%</div><div>• •</div><div>18%</div></div>
2	F	85	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>9%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>61%</div><div>16%</div><div>• •</div><div>18%</div></div>
2	H	85	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>64%</div><div>15%</div><div>• •</div><div>18%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12339 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 Cyclin-dependent kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	1	0
			2312	1490	389	425	8			
1	C	285	Total	C	N	O	S	0	1	0
			2312	1490	389	425	8			
1	E	285	Total	C	N	O	S	0	1	0
			2312	1490	389	425	8			
1	G	285	Total	C	N	O	S	0	1	0
			2312	1490	389	425	8			

- Molecule 2 is a protein called Cyclin-dependent kinases regulatory subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	70	Total	C	N	O	S	0	1	0
			613	396	104	110	3			
2	D	70	Total	C	N	O	S	0	1	0
			613	396	104	110	3			
2	F	70	Total	C	N	O	S	0	1	0
			613	396	104	110	3			
2	H	70	Total	C	N	O	S	0	1	0
			613	396	104	110	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	80	HIS	-	expression tag	UNP P61024
B	81	HIS	-	expression tag	UNP P61024
B	82	HIS	-	expression tag	UNP P61024
B	83	HIS	-	expression tag	UNP P61024
B	84	HIS	-	expression tag	UNP P61024
B	85	HIS	-	expression tag	UNP P61024
D	80	HIS	-	expression tag	UNP P61024
D	81	HIS	-	expression tag	UNP P61024

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Chain	Residue	Modelled	Actual	Comment	Reference
D	82	HIS	-	expression tag	UNP P61024
D	83	HIS	-	expression tag	UNP P61024
D	84	HIS	-	expression tag	UNP P61024
D	85	HIS	-	expression tag	UNP P61024
F	80	HIS	-	expression tag	UNP P61024
F	81	HIS	-	expression tag	UNP P61024
F	82	HIS	-	expression tag	UNP P61024
F	83	HIS	-	expression tag	UNP P61024
F	84	HIS	-	expression tag	UNP P61024
F	85	HIS	-	expression tag	UNP P61024
H	80	HIS	-	expression tag	UNP P61024
H	81	HIS	-	expression tag	UNP P61024
H	82	HIS	-	expression tag	UNP P61024
H	83	HIS	-	expression tag	UNP P61024
H	84	HIS	-	expression tag	UNP P61024
H	85	HIS	-	expression tag	UNP P61024

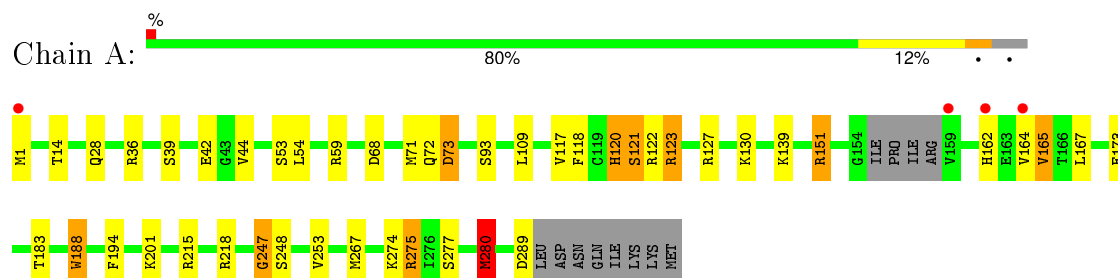
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	147	Total O 147 147	0	0
3	B	42	Total O 42 42	0	0
3	C	118	Total O 118 118	0	0
3	D	48	Total O 48 48	0	0
3	E	128	Total O 128 128	0	0
3	F	16	Total O 16 16	0	0
3	G	115	Total O 115 115	0	0
3	H	25	Total O 25 25	0	0

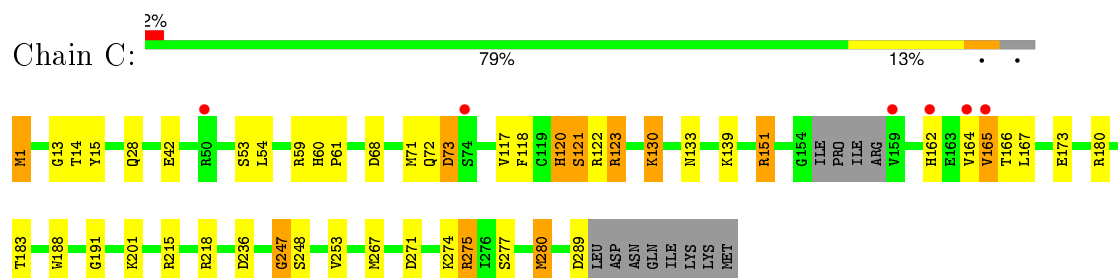
### 3 Residue-property plots

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.

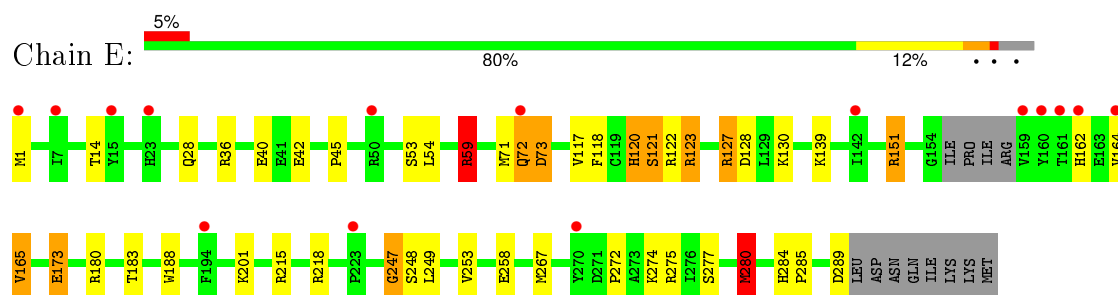
#### • Molecule 1: Cyclin-dependent kinase 1



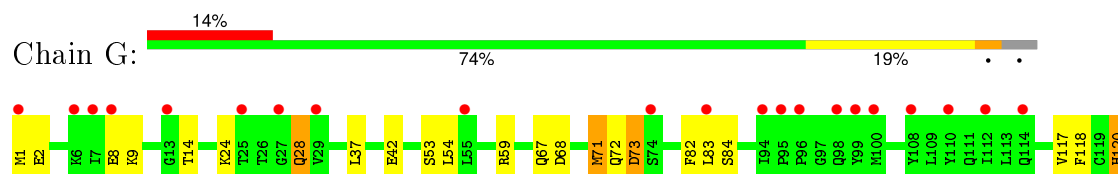
#### • Molecule 1: Cyclin-dependent kinase 1

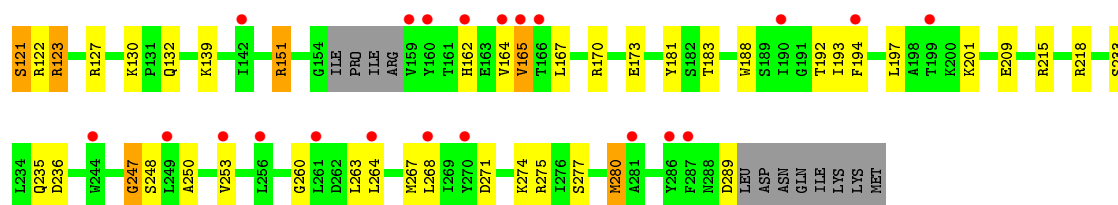


#### • Molecule 1: Cyclin-dependent kinase 1

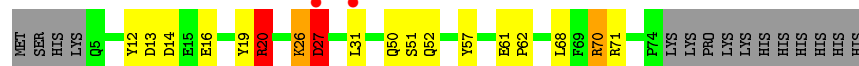


#### • Molecule 1: Cyclin-dependent kinase 1

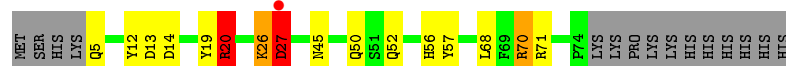




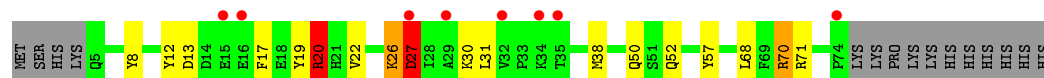
- Molecule 2: Cyclin-dependent kinases regulatory subunit 1



- Molecule 2: Cyclin-dependent kinases regulatory subunit 1



- Molecule 2: Cyclin-dependent kinases regulatory subunit 1



- Molecule 2: Cyclin-dependent kinases regulatory subunit 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.82Å 147.53Å 87.30Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	75.09 – 2.60 66.77 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (75.09-2.60) 97.0 (66.77-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.225 , 0.267 0.228 , 0.264	Depositor DCC
$R_{free}$ test set	1787 reflections (3.68%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.6	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 50430 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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	0.85	1/2364 (0.0%)	0.98	6/3194 (0.2%)
1	C	0.82	0/2364	0.96	6/3194 (0.2%)
1	E	0.79	1/2364 (0.0%)	0.96	5/3194 (0.2%)
1	G	0.76	0/2362	0.95	4/3188 (0.1%)
2	B	0.80	0/634	1.02	2/860 (0.2%)
2	D	0.93	0/634	1.08	4/860 (0.5%)
2	F	0.65	0/634	0.98	2/860 (0.2%)
2	H	0.72	0/634	1.02	4/860 (0.5%)
All	All	0.80	2/11990 (0.0%)	0.98	33/16210 (0.2%)

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	2
1	C	0	2
1	E	0	2
1	G	0	2
2	B	0	2
2	D	0	2
2	F	0	2
2	H	0	2
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	188	TRP	CB-CG	-5.37	1.40	1.50
1	A	188	TRP	CB-CG	-5.36	1.40	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	20	ARG	NE-CZ-NH2	-9.55	115.52	120.30
2	H	20	ARG	NE-CZ-NH2	-9.29	115.66	120.30
2	F	20	ARG	NE-CZ-NH2	-7.96	116.32	120.30
2	B	20	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	G	218	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	E	123	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	C	218	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	C	123	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	123	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	E	218	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	E	151	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	D	71	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	218	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	D	71	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	H	71	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	B	71	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	E	280	MET	CG-SD-CE	5.72	109.35	100.20
1	A	151	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	275	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	C	151	ARG	NE-CZ-NH1	5.37	122.98	120.30
2	F	71	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	G	123	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	280	MET	CG-SD-CE	5.24	108.59	100.20
1	G	68	ASP	CB-CG-OD1	5.24	123.02	118.30
2	H	20	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	271	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	275	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	G	271	ASP	CB-CG-OD2	-5.09	113.72	118.30
2	H	71	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	68	ASP	CB-CG-OD1	5.08	122.87	118.30
2	D	14	ASP	CB-CA-C	-5.06	100.28	110.40
1	C	68	ASP	CB-CG-OD1	5.03	122.83	118.30
1	E	59	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	HIS	Peptide
1	A	247	GLY	Peptide
2	B	26	LYS	Peptide
2	B	27[B]	ASP	Peptide
1	C	120	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	C	247	GLY	Peptide
2	D	26	LYS	Peptide
2	D	27[B]	ASP	Peptide
1	E	120	HIS	Peptide
1	E	247	GLY	Peptide
2	F	26	LYS	Peptide
2	F	27[B]	ASP	Peptide
1	G	120	HIS	Peptide
1	G	247	GLY	Peptide
2	H	26	LYS	Peptide
2	H	27[B]	ASP	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	2312	0	2334	24	0
1	C	2312	0	2334	22	0
1	E	2312	0	2334	24	0
1	G	2312	0	2332	51	0
2	B	613	0	584	8	0
2	D	613	0	584	6	0
2	F	613	0	584	12	0
2	H	613	0	584	6	0
3	A	147	0	0	1	0
3	B	42	0	0	0	0
3	C	118	0	0	6	0
3	D	48	0	0	3	0
3	E	128	0	0	7	0
3	F	16	0	0	6	0
3	G	115	0	0	23	0
3	H	25	0	0	1	0
All	All	12339	0	11670	138	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 6.

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:G:193:ILE:O	3:G:396:HOH:O	1.68	1.08
1:G:188:TRP:O	3:G:390:HOH:O	1.75	1.04
1:G:8:GLU:C	1:G:9:LYS:N	2.13	1.02
2:F:17:PHE:O	3:F:112:HOH:O	1.92	0.86
1:C:1:MET:N	3:C:380:HOH:O	2.00	0.85
1:G:260:GLY:HA2	3:G:408:HOH:O	1.77	0.84
1:E:277:SER:OG	1:E:280:MET:SD	2.35	0.83
2:F:19:TYR:CE2	3:F:112:HOH:O	2.35	0.79
1:G:83:LEU:C	1:G:84:SER:N	2.40	0.76
1:A:73:ASP:HB2	1:G:235:GLN:HB3	1.67	0.75
1:G:197:LEU:CB	3:G:396:HOH:O	2.35	0.75
1:G:197:LEU:HB2	3:G:396:HOH:O	1.85	0.75
1:G:24:LYS:O	3:G:301:HOH:O	2.08	0.71
1:A:247:GLY:HA2	1:A:248:SER:HB3	1.73	0.71
1:G:194:PHE:O	3:G:396:HOH:O	2.08	0.70
1:E:247:GLY:HA2	1:E:248:SER:HB3	1.73	0.70
1:A:73:ASP:OD2	1:G:233:SER:O	2.10	0.70
1:G:132[B]:GLN:OE1	1:G:132[B]:GLN:N	2.22	0.69
1:C:247:GLY:HA2	1:C:248:SER:HB3	1.74	0.69
1:G:247:GLY:HA2	1:G:248:SER:HB3	1.74	0.68
1:G:268:LEU:HD21	3:G:390:HOH:O	1.93	0.68
1:G:192:THR:HG23	3:G:390:HOH:O	1.95	0.66
1:G:192:THR:N	3:G:390:HOH:O	2.28	0.66
1:G:263:LEU:HG	3:G:356:HOH:O	1.96	0.66
2:F:19:TYR:HE2	3:F:112:HOH:O	1.77	0.62
1:G:24:LYS:NZ	3:G:391:HOH:O	2.35	0.60
1:C:120:HIS:CE1	1:C:183:THR:HB	2.37	0.59
1:A:164:VAL:C	1:A:165:VAL:N	2.56	0.59
1:G:277:SER:OG	1:G:280:MET:HG2	2.02	0.59
1:G:28:GLN:OE1	1:G:67:GLN:NE2	2.36	0.58
1:G:194:PHE:C	3:G:396:HOH:O	2.42	0.58
1:A:117:VAL:O	1:A:121:SER:CB	2.52	0.58
1:E:164:VAL:C	1:E:165:VAL:N	2.57	0.58
1:G:117:VAL:O	1:G:121:SER:CB	2.51	0.58
1:E:117:VAL:O	1:E:121:SER:CB	2.52	0.58
1:C:117:VAL:O	1:C:121:SER:CB	2.53	0.57
1:E:128:ASP:HB2	3:E:369:HOH:O	2.05	0.57
1:G:37:LEU:HB2	3:G:332:HOH:O	2.03	0.56
1:A:117:VAL:O	1:A:121:SER:HB2	2.06	0.56
1:A:277:SER:OG	1:A:280:MET:HG2	2.06	0.56
1:G:120:HIS:CE1	1:G:183:THR:HB	2.40	0.55
1:E:117:VAL:O	1:E:121:SER:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:VAL:O	1:G:121:SER:HB2	2.07	0.55
1:E:120:HIS:CE1	1:E:183:THR:HB	2.42	0.55
1:A:73:ASP:HB2	1:G:235:GLN:CB	2.34	0.54
1:C:191:GLY:HA3	3:C:375:HOH:O	2.07	0.54
1:A:73:ASP:CB	1:G:235:GLN:HB3	2.36	0.54
2:D:20:ARG:HE	2:D:50:GLN:HE21	1.56	0.54
1:A:120:HIS:CE1	1:A:183:THR:HB	2.44	0.53
1:G:2:GLU:HG2	3:G:318:HOH:O	2.08	0.53
1:E:127:ARG:HD3	3:E:339:HOH:O	2.08	0.53
1:E:277:SER:OG	1:E:280:MET:HG2	2.09	0.52
1:G:197:LEU:N	3:G:396:HOH:O	2.09	0.52
1:C:277:SER:OG	1:C:280:MET:HG2	2.09	0.52
1:C:117:VAL:O	1:C:121:SER:HB2	2.09	0.52
1:G:117:VAL:O	1:G:121:SER:HB3	2.11	0.51
1:C:188:TRP:HA	3:C:375:HOH:O	2.10	0.51
1:A:73:ASP:O	1:G:235:GLN:HB3	2.11	0.51
1:A:36:ARG:NH2	1:G:236:ASP:OD1	2.42	0.51
2:B:20:ARG:HE	2:B:50:GLN:HE21	1.57	0.51
1:C:117:VAL:O	1:C:121:SER:HB3	2.11	0.50
1:G:83:LEU:C	1:G:84:SER:CA	2.80	0.50
2:F:20:ARG:HE	2:F:50:GLN:HE21	1.59	0.50
1:C:164:VAL:C	1:C:165:VAL:N	2.65	0.50
1:C:267:MET:HB3	3:C:375:HOH:O	2.11	0.50
1:E:277:SER:OG	1:E:280:MET:CG	2.60	0.49
1:C:73:ASP:OD1	1:C:73:ASP:N	2.46	0.49
1:A:36:ARG:NH2	1:G:236:ASP:OD2	2.44	0.49
1:E:73:ASP:OD1	1:E:73:ASP:N	2.45	0.49
2:H:12:TYR:CD1	2:H:19:TYR:HB2	2.48	0.49
1:A:118:PHE:O	1:A:121:SER:HB3	2.13	0.49
2:D:56:HIS:HE1	3:D:113:HOH:O	1.96	0.49
2:B:31:LEU:HD12	2:F:31:LEU:HD12	1.94	0.49
1:A:73:ASP:N	1:A:73:ASP:OD1	2.46	0.48
1:E:117:VAL:O	1:E:121:SER:HB3	2.13	0.48
2:F:12:TYR:CD1	2:F:19:TYR:HB2	2.48	0.48
1:A:117:VAL:O	1:A:121:SER:HB3	2.13	0.48
2:B:12:TYR:CD1	2:B:19:TYR:HB2	2.49	0.48
1:E:45:PRO:HD2	3:E:386:HOH:O	2.12	0.47
1:C:236:ASP:OD1	1:E:36:ARG:NH2	2.47	0.47
1:G:264:LEU:HA	3:G:356:HOH:O	2.14	0.47
1:E:118:PHE:O	1:E:121:SER:HB3	2.14	0.47
2:D:12:TYR:CD1	2:D:19:TYR:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:ARG:O	3:G:349:HOH:O	2.20	0.47
1:G:73:ASP:N	1:G:73:ASP:OD1	2.48	0.47
1:G:118:PHE:O	1:G:121:SER:HB3	2.15	0.46
1:G:247:GLY:CA	1:G:248:SER:HB3	2.45	0.46
1:C:280:MET:CE	3:C:390:HOH:O	2.64	0.46
1:E:59:ARG:NH1	3:E:385:HOH:O	2.49	0.46
2:B:57:TYR:CD1	2:B:70:ARG:HB3	2.52	0.45
2:H:36:HIS:ND1	3:H:121:HOH:O	2.36	0.45
1:C:118:PHE:O	1:C:121:SER:HB3	2.17	0.45
1:A:164:VAL:HG12	3:A:368:HOH:O	2.17	0.45
1:G:164:VAL:C	1:G:165:VAL:N	2.70	0.45
1:G:197:LEU:CG	3:G:396:HOH:O	2.64	0.44
1:A:247:GLY:CA	1:A:248:SER:HB3	2.46	0.44
2:D:5:GLN:N	3:D:111:HOH:O	2.50	0.44
1:G:268:LEU:CD2	3:G:390:HOH:O	2.58	0.44
2:H:20:ARG:HE	2:H:50:GLN:HE21	1.65	0.44
1:C:166:THR:HG21	3:C:348:HOH:O	2.18	0.44
2:B:51:SER:H	2:B:51:SER:HG	1.57	0.44
1:A:93:SER:HB2	3:D:148:HOH:O	2.18	0.43
2:F:57:TYR:CD1	2:F:70:ARG:HB3	2.53	0.43
1:C:188:TRP:CD1	1:C:188:TRP:C	2.92	0.43
1:G:71:MET:HE1	3:G:332:HOH:O	2.18	0.43
1:G:188:TRP:CD1	1:G:188:TRP:C	2.92	0.43
2:H:61:GLU:N	2:H:62:PRO:CD	2.81	0.43
1:G:209:GLU:HB2	2:H:63:GLU:CD	2.39	0.42
1:E:173:GLU:CG	1:E:272:PRO:HG3	2.49	0.42
1:A:44:VAL:HG21	1:G:151:ARG:CD	2.50	0.42
1:G:132[B]:GLN:CD	1:G:132[B]:GLN:H	2.18	0.42
1:A:188:TRP:CD1	1:A:188:TRP:C	2.93	0.42
1:E:180:ARG:NH1	3:E:378:HOH:O	2.53	0.42
1:G:194:PHE:CA	3:G:396:HOH:O	2.69	0.41
2:F:8:TYR:HD1	2:F:22:VAL:HG22	1.85	0.41
1:C:267:MET:O	1:C:275:ARG:HD3	2.21	0.41
1:E:164:VAL:O	1:E:165:VAL:N	2.54	0.41
2:B:31:LEU:HD12	2:F:31:LEU:CD1	2.50	0.41
1:E:267:MET:O	1:E:275:ARG:HD3	2.21	0.41
1:E:284:HIS:CG	1:E:285:PRO:HD2	2.56	0.41
2:F:19:TYR:CD2	3:F:112:HOH:O	2.69	0.41
1:C:180:ARG:HA	1:E:40:GLU:O	2.21	0.41
2:B:14:ASP:HB3	2:B:16:GLU:H	1.86	0.41
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:TYR:CD1	2:D:70:ARG:HB3	2.55	0.41
2:D:45:ASN:O	2:H:31:LEU:HD22	2.21	0.41
1:E:249:LEU:N	3:E:301:HOH:O	2.48	0.41
1:G:250:ALA:N	3:G:355:HOH:O	2.55	0.40
2:F:30:LYS:NZ	3:F:101:HOH:O	2.54	0.40
1:A:267:MET:O	1:A:275:ARG:HD3	2.21	0.40
1:A:39:SER:OG	1:G:181:TYR:HD1	2.04	0.40
1:C:13:GLY:O	1:C:15:TYR:N	2.46	0.40
2:F:38:MET:HE3	3:F:114:HOH:O	2.21	0.40
1:C:130:LYS:HG2	1:C:133:ASN:ND2	2.36	0.40
2:B:61:GLU:N	2:B:62:PRO:CD	2.85	0.40
1:E:72:GLN:HA	3:E:317:HOH:O	2.21	0.40
1:A:109:LEU:HD22	1:A:194:PHE:CD1	2.56	0.40
1:G:267:MET:O	1:G:275:ARG:HD3	2.21	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	280/297 (94%)	246 (88%)	30 (11%)	4 (1%)	14	28
1	C	280/297 (94%)	246 (88%)	31 (11%)	3 (1%)	17	36
1	E	280/297 (94%)	244 (87%)	32 (11%)	4 (1%)	14	28
1	G	276/297 (93%)	239 (87%)	32 (12%)	5 (2%)	11	21
2	B	69/85 (81%)	64 (93%)	2 (3%)	3 (4%)	3	4
2	D	69/85 (81%)	65 (94%)	1 (1%)	3 (4%)	3	4
2	F	69/85 (81%)	64 (93%)	2 (3%)	3 (4%)	3	4
2	H	69/85 (81%)	64 (93%)	2 (3%)	3 (4%)	3	4
All	All	1392/1528 (91%)	1232 (88%)	132 (10%)	28 (2%)	11	18

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	C	121	SER
1	E	121	SER
1	G	14	THR
1	G	82	PHE
1	G	121	SER
1	A	14	THR
2	B	26	LYS
1	C	14	THR
2	D	26	LYS
1	E	14	THR
2	F	26	LYS
2	H	26	LYS
1	A	127	ARG
2	F	27[A]	ASP
2	F	27[B]	ASP
2	H	27[A]	ASP
2	H	27[B]	ASP
2	B	27[A]	ASP
2	B	27[B]	ASP
2	D	27[A]	ASP
2	D	27[B]	ASP
1	C	42	GLU
1	E	42	GLU
1	E	127	ARG
1	G	42	GLU
1	A	42	GLU
1	G	127	ARG

### 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	256/267 (96%)	233 (91%)	23 (9%)	12	23
1	C	256/267 (96%)	233 (91%)	23 (9%)	12	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	256/267 (96%)	233 (91%)	23 (9%)	12	23
1	G	256/267 (96%)	233 (91%)	23 (9%)	12	23
2	B	68/82 (83%)	61 (90%)	7 (10%)	9	16
2	D	68/82 (83%)	61 (90%)	7 (10%)	9	16
2	F	68/82 (83%)	61 (90%)	7 (10%)	9	16
2	H	68/82 (83%)	61 (90%)	7 (10%)	9	16
All	All	1296/1396 (93%)	1176 (91%)	120 (9%)	12	21

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	28	GLN
1	A	53	SER
1	A	54	LEU
1	A	59	ARG
1	A	71	MET
1	A	72	GLN
1	A	73	ASP
1	A	122	ARG
1	A	123	ARG
1	A	130	LYS
1	A	139	LYS
1	A	151	ARG
1	A	162	HIS
1	A	165	VAL
1	A	167	LEU
1	A	173	GLU
1	A	201	LYS
1	A	215	ARG
1	A	253	VAL
1	A	274	LYS
1	A	280	MET
1	A	289	ASP
2	B	13	ASP
2	B	20	ARG
2	B	27[A]	ASP
2	B	27[B]	ASP
2	B	52	GLN
2	B	68	LEU

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Mol	Chain	Res	Type
2	B	70	ARG
1	C	1	MET
1	C	28	GLN
1	C	53	SER
1	C	54	LEU
1	C	59	ARG
1	C	71	MET
1	C	72	GLN
1	C	73	ASP
1	C	122	ARG
1	C	123	ARG
1	C	130	LYS
1	C	139	LYS
1	C	151	ARG
1	C	162	HIS
1	C	165	VAL
1	C	167	LEU
1	C	173	GLU
1	C	201	LYS
1	C	215	ARG
1	C	253	VAL
1	C	274	LYS
1	C	280	MET
1	C	289	ASP
2	D	13	ASP
2	D	20	ARG
2	D	27[A]	ASP
2	D	27[B]	ASP
2	D	52	GLN
2	D	68	LEU
2	D	70	ARG
1	E	1	MET
1	E	28	GLN
1	E	53	SER
1	E	54	LEU
1	E	59	ARG
1	E	71	MET
1	E	72	GLN
1	E	73	ASP
1	E	122	ARG
1	E	123	ARG
1	E	130	LYS

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Mol	Chain	Res	Type
1	E	139	LYS
1	E	151	ARG
1	E	162	HIS
1	E	165	VAL
1	E	173	GLU
1	E	201	LYS
1	E	215	ARG
1	E	253	VAL
1	E	258	GLU
1	E	274	LYS
1	E	280	MET
1	E	289	ASP
2	F	13	ASP
2	F	20	ARG
2	F	27[A]	ASP
2	F	27[B]	ASP
2	F	52	GLN
2	F	68	LEU
2	F	70	ARG
1	G	1	MET
1	G	28	GLN
1	G	53	SER
1	G	54	LEU
1	G	59	ARG
1	G	71	MET
1	G	72	GLN
1	G	73	ASP
1	G	122	ARG
1	G	123	ARG
1	G	130	LYS
1	G	139	LYS
1	G	151	ARG
1	G	162	HIS
1	G	165	VAL
1	G	167	LEU
1	G	173	GLU
1	G	201	LYS
1	G	215	ARG
1	G	253	VAL
1	G	274	LYS
1	G	280	MET
1	G	289	ASP

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Mol	Chain	Res	Type
2	H	13	ASP
2	H	20	ARG
2	H	27[A]	ASP
2	H	27[B]	ASP
2	H	52	GLN
2	H	68	LEU
2	H	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	111	GLN
1	A	133	ASN
1	A	239	ASN
2	B	36	HIS
2	B	50	GLN
1	C	28	GLN
1	C	111	GLN
1	C	133	ASN
1	C	239	ASN
2	D	36	HIS
2	D	50	GLN
1	E	28	GLN
1	E	111	GLN
1	E	133	ASN
1	E	239	ASN
2	F	36	HIS
2	F	50	GLN
1	G	111	GLN
1	G	133	ASN
1	G	239	ASN
2	H	36	HIS
2	H	50	GLN

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	3
1	A	1
1	C	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	164:VAL	C	165:VAL	N	2.70
1	C	164:VAL	C	165:VAL	N	2.65
1	E	164:VAL	C	165:VAL	N	2.57
1	A	164:VAL	C	165:VAL	N	2.56
1	G	83:LEU	C	84:SER	N	2.40
1	G	8:GLU	C	9:LYS	N	2.13

## 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	285/297 (95%)	-0.03	4 (1%) 78 74	44, 77, 121, 179	0
1	C	285/297 (95%)	0.05	6 (2%) 67 61	46, 80, 136, 187	0
1	E	285/297 (95%)	0.34	15 (5%) 30 23	60, 96, 137, 212	0
1	G	285/297 (95%)	0.79	42 (14%) 3 2	76, 120, 167, 188	0
2	B	70/85 (82%)	0.01	2 (2%) 55 48	52, 77, 126, 159	0
2	D	70/85 (82%)	-0.25	1 (1%) 78 74	44, 65, 101, 122	0
2	F	70/85 (82%)	0.60	8 (11%) 7 4	90, 127, 170, 187	0
2	H	70/85 (82%)	0.01	2 (2%) 55 48	66, 91, 131, 144	0
All	All	1420/1528 (92%)	0.25	80 (5%) 28 21	44, 94, 152, 212	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	164	VAL	12.1
1	E	162	HIS	9.0
1	E	159	VAL	8.7
2	B	27[A]	ASP	8.5
1	C	162	HIS	8.1
1	E	164	VAL	7.9
1	G	162	HIS	7.4
1	G	13	GLY	7.0
1	E	1	MET	6.4
1	G	159	VAL	6.1
1	G	287	PHE	4.8
1	G	25	THR	4.7
1	G	112	ILE	4.7
1	A	1	MET	4.6
1	E	160	TYR	4.4
2	F	34	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	74	SER	4.3
2	H	27[A]	ASP	4.3
1	G	1	MET	4.3
1	G	100	MET	4.2
1	G	261	LEU	4.0
1	G	160	TYR	4.0
1	G	8	GLU	4.0
1	C	159	VAL	4.0
2	F	16	GLU	3.7
2	F	27[A]	ASP	3.7
1	G	264	LEU	3.7
1	G	270	TYR	3.6
1	G	194	PHE	3.5
1	G	6	LYS	3.5
1	G	99	TYR	3.4
1	C	164	VAL	3.4
1	G	110	TYR	3.3
2	F	32	VAL	3.2
1	A	162	HIS	3.2
1	G	249	LEU	3.2
1	E	23	HIS	3.2
1	G	166	THR	3.2
1	G	256	LEU	3.1
1	G	94	ILE	3.1
1	G	142	ILE	3.1
1	E	15	TYR	3.1
1	G	286	TYR	3.1
1	G	244	TRP	3.1
1	C	50	ARG	3.0
1	G	199	THR	3.0
1	E	270	TYR	3.0
1	G	7	ILE	2.9
1	G	95	PRO	2.8
1	G	253	VAL	2.8
1	G	27	GLY	2.8
1	A	164	VAL	2.7
2	F	74	PRO	2.7
1	A	159	VAL	2.6
1	G	108	TYR	2.6
2	F	35	THR	2.6
2	B	31	LEU	2.6
1	G	281	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	194	PHE	2.5
1	G	29	VAL	2.4
1	E	142	ILE	2.4
1	E	161	THR	2.4
2	F	15	GLU	2.3
1	G	190	ILE	2.3
2	H	30	LYS	2.3
1	G	96	PRO	2.3
2	D	27[A]	ASP	2.3
1	E	7	ILE	2.3
1	C	165	VAL	2.3
1	C	74	SER	2.3
1	G	165	VAL	2.2
1	E	50	ARG	2.2
1	E	223	PRO	2.2
1	G	268	LEU	2.2
1	G	98	GLN	2.2
1	E	72	GLN	2.1
2	F	29	ALA	2.1
1	G	114	GLN	2.1
1	G	83	LEU	2.0
1	G	55	LEU	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.