



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:59 am BST

PDB ID : 1BI7
Title : MECHANISM OF G1 CYCLIN DEPENDENT KINASE INHIBITION FROM
THE STRUCTURE OF THE CDK6-P16INK4A TUMOR SUPPRESSOR
COMPLEX
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Deposited on : 1998-06-22
Resolution : 3.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

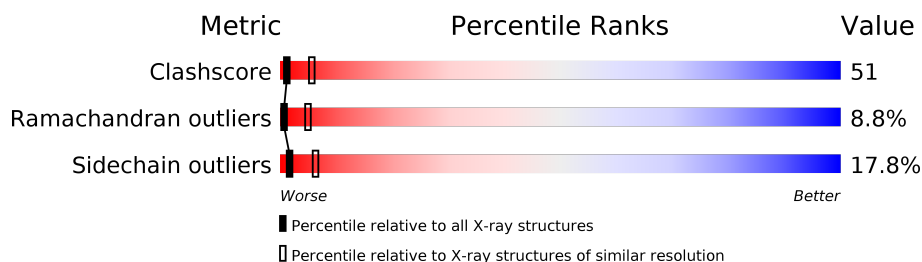
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	326	
2	B	156	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3087 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 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2143	1372	373	391	7			

- Molecule 2 is a protein called MULTIPLE TUMOR SUPPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			944	584	185	171	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	ASN	LEU	CONFLICT	UNP P42771

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.10 Å 123.10 Å 112.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.40	Depositor
% Data completeness (in resolution range)	94.7 (10.00-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.227 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3087	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

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	0.63	0/2190	0.89	4/2967 (0.1%)
2	B	0.58	0/962	0.89	1/1310 (0.1%)
All	All	0.62	0/3152	0.89	5/4277 (0.1%)

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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	202	LEU	CA-CB-CG	-7.69	97.61	115.30
1	A	114	GLU	N-CA-C	6.36	128.18	111.00
2	B	14	ASP	N-CA-C	-5.46	96.26	111.00
1	A	214	ARG	N-CA-C	5.29	125.28	111.00
1	A	37	GLY	N-CA-C	-5.10	100.36	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	TYR	Sidechain

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	2143	0	2148	218	0
2	B	944	0	938	116	0
All	All	3087	0	3086	316	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 51.

All (316) 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:171:SER:HB2	1:A:177:THR:HG23	1.25	1.13
1:A:169:ILE:HG12	1:A:181:VAL:HG23	1.24	1.11
1:A:166:LEU:HD12	2:B:22:ARG:HD2	1.40	1.03
1:A:211:GLU:HA	1:A:214:ARG:HB2	1.45	0.98
2:B:48:PRO:HA	2:B:51:VAL:HG12	1.51	0.92
1:A:13:TYR:CE2	1:A:97:VAL:HG21	2.06	0.90
1:A:192:LEU:HD13	1:A:228:LEU:HG	1.59	0.85
1:A:214:ARG:NH1	1:A:218:LEU:HA	1.93	0.83
1:A:272:LEU:HD13	1:A:298:PRO:HB2	1.62	0.81
2:B:64:LEU:HD12	2:B:96:VAL:HG12	1.64	0.79
1:A:214:ARG:HH11	1:A:218:LEU:HA	1.47	0.78
1:A:168:ARG:HG3	2:B:24:ARG:HD3	1.66	0.77
2:B:23:GLY:HA3	2:B:53:MET:CE	2.14	0.77
1:A:85:VAL:HB	1:A:93:LYS:HB2	1.67	0.76
1:A:237:LEU:HD23	1:A:238:PRO:HD2	1.65	0.76
2:B:71:ASN:HD21	2:B:102:ALA:HA	1.50	0.76
2:B:28:VAL:HG12	2:B:62:LEU:HD12	1.67	0.75
1:A:96:LEU:HB2	1:A:98:PHE:CE1	2.22	0.75
2:B:48:PRO:O	2:B:49:ILE:HG22	1.86	0.75
1:A:150:ASN:HB3	1:A:162:ALA:O	1.88	0.74
1:A:297:HIS:CE1	1:A:298:PRO:HG2	2.23	0.73
1:A:169:ILE:CG1	1:A:181:VAL:HG23	2.12	0.73
2:B:23:GLY:HA3	2:B:53:MET:HE3	1.70	0.72
2:B:49:ILE:HD11	2:B:97:LEU:HD11	1.71	0.72
1:A:101:VAL:HB	1:A:152:LEU:HD13	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:HB2	1:A:220:ARG:HH11	1.57	0.70
1:A:203:TRP:HZ2	1:A:231:ILE:HG12	1.57	0.70
2:B:80:ARG:O	2:B:83:HIS:HB2	1.92	0.70
1:A:155:SER:HB2	2:B:88:GLU:O	1.90	0.69
2:B:74:ASP:HB3	2:B:77:THR:OG1	1.91	0.69
2:B:64:LEU:HD11	2:B:97:LEU:HD12	1.73	0.69
1:A:19:ILE:HD11	1:A:27:VAL:HG22	1.75	0.69
2:B:53:MET:HG2	2:B:56:SER:HB2	1.73	0.69
1:A:187:ALA:HA	1:A:203:TRP:CD1	2.28	0.68
1:A:75:ASN:OD1	1:A:128:GLN:HB3	1.93	0.68
1:A:169:ILE:HG12	1:A:181:VAL:CG2	2.15	0.68
1:A:237:LEU:HD12	1:A:256:SER:N	2.09	0.67
1:A:289:ILE:HG12	1:A:290:SER:N	2.09	0.67
1:A:17:ALA:O	1:A:28:PHE:HB3	1.93	0.67
2:B:64:LEU:CD1	2:B:96:VAL:HG12	2.24	0.67
1:A:133:LEU:CD2	1:A:201:ASP:HB3	2.24	0.67
1:A:213:PHE:CZ	1:A:269:ILE:HG13	2.29	0.66
2:B:62:LEU:O	2:B:66:HIS:HB2	1.96	0.66
1:A:192:LEU:CD1	1:A:228:LEU:HG	2.25	0.66
1:A:218:LEU:HD13	1:A:219:PHE:CZ	2.31	0.66
1:A:214:ARG:NH2	1:A:216:LYS:HE3	2.11	0.66
2:B:71:ASN:ND2	2:B:102:ALA:HA	2.10	0.66
1:A:192:LEU:HB3	1:A:247:VAL:CG2	2.26	0.66
1:A:235:ILE:HG13	1:A:236:GLY:N	2.10	0.66
2:B:80:ARG:HE	2:B:106:VAL:HG21	1.61	0.65
1:A:19:ILE:HG12	1:A:27:VAL:O	1.96	0.64
1:A:192:LEU:HD12	1:A:249:LEU:HD23	1.77	0.64
2:B:69:GLU:H	2:B:69:GLU:CD	2.01	0.64
1:A:45:VAL:HG22	1:A:94:LEU:HB2	1.79	0.64
2:B:94:LEU:HD21	2:B:130:LEU:HD21	1.78	0.64
2:B:39:ASN:HB3	2:B:69:GLU:OE1	1.98	0.64
1:A:168:ARG:HH12	1:A:170:TYR:HB2	1.61	0.64
1:A:142:VAL:HG22	1:A:198:THR:HA	1.79	0.64
1:A:168:ARG:HG3	2:B:24:ARG:CD	2.28	0.63
1:A:154:THR:HG23	1:A:158:GLN:O	1.98	0.63
1:A:129:LEU:HD23	1:A:161:LEU:HD21	1.79	0.63
1:A:231:ILE:O	1:A:235:ILE:HG12	1.99	0.63
2:B:95:VAL:HG22	2:B:129:TYR:CE2	2.34	0.63
1:A:243:TRP:HH2	1:A:254:PHE:CD2	2.17	0.63
2:B:84:ASP:HA	2:B:87:ARG:HG2	1.82	0.62
2:B:87:ARG:O	2:B:123:HIS:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:O	1:A:91:GLU:HB3	2.00	0.61
1:A:284:ASN:HB3	1:A:287:LYS:HB2	1.82	0.61
2:B:16:LEU:CD1	2:B:48:PRO:HG3	2.30	0.61
1:A:103:GLN:O	1:A:103:GLN:HG3	2.01	0.61
1:A:255:HIS:O	1:A:257:LYS:N	2.33	0.60
1:A:237:LEU:CD2	1:A:238:PRO:HD2	2.32	0.60
1:A:123:LYS:HG3	1:A:299:TYR:CE2	2.37	0.60
1:A:261:PRO:HD2	1:A:264:LYS:HD2	1.82	0.60
1:A:17:ALA:HB2	2:B:51:VAL:HG21	1.82	0.60
2:B:46:ARG:HD3	2:B:75:PRO:HD2	1.84	0.60
2:B:47:ARG:O	2:B:50:GLN:HB3	2.02	0.60
1:A:166:LEU:HD12	2:B:22:ARG:CD	2.24	0.59
1:A:28:PHE:HE2	2:B:44:TYR:HH	1.48	0.59
1:A:172:PHE:HB2	1:A:178:SER:H	1.66	0.59
1:A:237:LEU:HD13	1:A:251:ARG:CZ	2.32	0.59
1:A:11:GLN:HG2	1:A:95:THR:HG21	1.84	0.59
2:B:80:ARG:HH21	2:B:106:VAL:HG21	1.67	0.58
1:A:45:VAL:CG2	1:A:94:LEU:HB2	2.33	0.58
2:B:23:GLY:HA3	2:B:53:MET:HE2	1.85	0.58
2:B:12:SER:HA	2:B:15:TRP:CD1	2.38	0.58
1:A:219:PHE:HE1	1:A:234:VAL:HB	1.67	0.58
1:A:96:LEU:HB2	1:A:98:PHE:HE1	1.67	0.58
1:A:112:VAL:HG13	1:A:113:PRO:HD2	1.86	0.57
1:A:129:LEU:CD2	1:A:161:LEU:HD21	2.34	0.57
2:B:124:ARG:O	2:B:127:ALA:HB3	2.05	0.57
2:B:50:GLN:NE2	2:B:72:CYS:HB2	2.19	0.57
1:A:143:HIS:HB3	1:A:201:ASP:OD1	2.05	0.56
1:A:232:LEU:O	1:A:236:GLY:N	2.38	0.56
1:A:192:LEU:HB3	1:A:247:VAL:HG21	1.87	0.56
1:A:218:LEU:HD13	1:A:219:PHE:CE2	2.40	0.56
1:A:228:LEU:O	1:A:232:LEU:HG	2.06	0.56
1:A:235:ILE:HG13	1:A:236:GLY:H	1.69	0.56
1:A:13:TYR:CE1	1:A:97:VAL:HG11	2.40	0.56
1:A:137:HIS:CG	1:A:198:THR:HG23	2.40	0.56
1:A:28:PHE:CD1	1:A:28:PHE:N	2.71	0.56
1:A:148:PRO:HD3	1:A:185:TYR:CE2	2.41	0.56
2:B:27:GLU:O	2:B:31:LEU:HB2	2.05	0.56
2:B:64:LEU:HA	2:B:68:ALA:HB3	1.88	0.56
2:B:12:SER:O	2:B:15:TRP:HD1	1.88	0.56
1:A:220:ARG:NH1	1:A:220:ARG:HB2	2.20	0.55
2:B:47:ARG:N	2:B:50:GLN:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LEU:HD12	2:B:62:LEU:CD1	2.36	0.55
2:B:60:ALA:HB2	2:B:93:THR:HG22	1.89	0.55
1:A:168:ARG:HA	2:B:22:ARG:HH22	1.73	0.54
1:A:299:TYR:CE2	1:A:300:PHE:CE1	2.95	0.54
1:A:35:ASN:O	1:A:37:GLY:N	2.40	0.54
1:A:123:LYS:HG3	1:A:299:TYR:CZ	2.42	0.54
1:A:179:VAL:HG22	1:A:180:VAL:N	2.23	0.54
1:A:73:HIS:CD2	1:A:75:ASN:H	2.25	0.54
1:A:202:LEU:O	1:A:205:VAL:HG22	2.07	0.54
1:A:266:VAL:HG11	1:A:269:ILE:HD12	1.89	0.54
1:A:31:ARG:HA	1:A:38:ARG:O	2.07	0.54
1:A:192:LEU:HB3	1:A:247:VAL:HG22	1.88	0.54
1:A:220:ARG:H	1:A:220:ARG:CZ	2.20	0.54
2:B:69:GLU:N	2:B:69:GLU:CD	2.61	0.54
2:B:24:ARG:HA	2:B:24:ARG:NE	2.22	0.53
1:A:193:GLN:O	1:A:247:VAL:HG23	2.08	0.53
1:A:202:LEU:HA	1:A:205:VAL:HG13	1.90	0.53
1:A:241:GLU:HG3	1:A:242:ASP:H	1.72	0.53
2:B:12:SER:HA	2:B:15:TRP:HD1	1.72	0.53
1:A:32:ASP:OD2	1:A:34:LYS:HG2	2.09	0.53
1:A:183:LEU:H	1:A:183:LEU:CD2	2.20	0.53
1:A:243:TRP:CH2	1:A:254:PHE:CD2	2.97	0.53
1:A:170:TYR:O	1:A:179:VAL:HA	2.09	0.53
1:A:88:THR:OG1	1:A:91:GLU:HG3	2.09	0.53
1:A:183:LEU:HD23	1:A:183:LEU:H	1.73	0.52
1:A:214:ARG:HH21	1:A:216:LYS:HB3	1.73	0.52
2:B:42:ASN:C	2:B:44:TYR:H	2.11	0.52
1:A:137:HIS:CD2	1:A:198:THR:HG23	2.44	0.52
1:A:42:LEU:HD22	1:A:97:VAL:HG22	1.91	0.52
2:B:16:LEU:HD13	2:B:48:PRO:HG3	1.92	0.52
1:A:249:LEU:H	1:A:249:LEU:HD22	1.75	0.52
1:A:187:ALA:HB1	1:A:189:GLU:OE2	2.09	0.52
2:B:49:ILE:HD11	2:B:97:LEU:CD1	2.39	0.52
1:A:16:VAL:HG12	1:A:29:LYS:C	2.30	0.52
1:A:169:ILE:HA	1:A:181:VAL:HA	1.92	0.52
1:A:177:THR:HG22	1:A:177:THR:O	2.09	0.52
1:A:214:ARG:HH22	1:A:216:LYS:HE3	1.74	0.51
1:A:106:THR:HG21	2:B:24:ARG:HH22	1.76	0.51
2:B:64:LEU:HD13	2:B:100:ALA:HB2	1.91	0.51
1:A:234:VAL:HG13	1:A:265:PHE:CE1	2.45	0.51
2:B:38:PRO:HG2	2:B:39:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:PRO:HG2	2:B:12:SER:H	1.76	0.51
1:A:103:GLN:HA	2:B:53:MET:SD	2.50	0.51
1:A:87:ARG:HA	1:A:87:ARG:HE	1.75	0.51
1:A:123:LYS:O	1:A:127:PHE:HB2	2.11	0.51
1:A:210:ALA:O	1:A:214:ARG:HG3	2.10	0.51
1:A:214:ARG:HB3	1:A:216:LYS:O	2.11	0.51
1:A:32:ASP:OD1	1:A:35:ASN:HB2	2.11	0.51
1:A:214:ARG:NH2	1:A:216:LYS:HB3	2.26	0.51
1:A:297:HIS:CG	1:A:298:PRO:HD2	2.46	0.51
1:A:133:LEU:HD11	1:A:146:LEU:HD21	1.93	0.50
1:A:85:VAL:HB	1:A:93:LYS:CB	2.39	0.50
2:B:74:ASP:O	2:B:75:PRO:C	2.49	0.50
1:A:107:THR:O	1:A:111:LYS:HB2	2.11	0.50
1:A:166:LEU:HD12	2:B:22:ARG:HH11	1.76	0.50
1:A:17:ALA:CB	2:B:51:VAL:HG21	2.41	0.50
1:A:28:PHE:HE2	2:B:44:TYR:OH	1.93	0.50
1:A:146:LEU:HD11	1:A:161:LEU:HD22	1.93	0.50
2:B:74:ASP:HB3	2:B:77:THR:HG1	1.77	0.50
1:A:202:LEU:HD23	1:A:202:LEU:O	2.11	0.49
1:A:232:LEU:HD21	1:A:283:PHE:HE2	1.78	0.49
1:A:164:PHE:C	1:A:166:LEU:H	2.15	0.49
1:A:237:LEU:HD12	1:A:256:SER:HA	1.95	0.49
2:B:70:PRO:HB2	2:B:102:ALA:HB2	1.94	0.49
1:A:198:THR:HB	1:A:199:PRO:HD3	1.95	0.49
1:A:167:ALA:O	1:A:169:ILE:HG13	2.13	0.49
1:A:246:ASP:CG	1:A:247:VAL:N	2.66	0.49
1:A:279:LYS:O	1:A:289:ILE:HG22	2.12	0.49
1:A:171:SER:CB	1:A:177:THR:HG23	2.18	0.49
1:A:164:PHE:HB2	1:A:166:LEU:HD22	1.95	0.49
1:A:133:LEU:HD21	1:A:201:ASP:HB3	1.94	0.48
1:A:210:ALA:HB2	1:A:277:LEU:HD11	1.94	0.48
1:A:102:ASP:O	2:B:54:MET:O	2.31	0.48
2:B:52:MET:O	2:B:54:MET:HE2	2.13	0.48
1:A:133:LEU:HD13	1:A:205:VAL:CG1	2.44	0.48
1:A:272:LEU:CD1	1:A:298:PRO:HB2	2.39	0.48
2:B:38:PRO:HG2	2:B:39:ASN:HD22	1.78	0.48
2:B:130:LEU:C	2:B:132:ALA:H	2.16	0.48
2:B:81:PRO:O	2:B:83:HIS:N	2.46	0.48
1:A:170:TYR:HB3	1:A:180:VAL:HG13	1.95	0.48
1:A:278:LEU:O	1:A:282:THR:HG23	2.12	0.48
2:B:32:LEU:C	2:B:34:ALA:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:TYR:HA	1:A:200:VAL:HG21	1.95	0.48
1:A:237:LEU:CB	1:A:256:SER:HA	2.43	0.48
1:A:171:SER:HA	1:A:178:SER:O	2.14	0.48
1:A:220:ARG:H	1:A:220:ARG:NH1	2.12	0.48
1:A:20:GLY:HA2	1:A:166:LEU:HA	1.96	0.47
1:A:31:ARG:HB3	1:A:37:GLY:O	2.14	0.47
2:B:91:LEU:HD12	2:B:95:VAL:HG23	1.96	0.47
2:B:29:ARG:O	2:B:32:LEU:HB2	2.14	0.47
1:A:98:PHE:CD1	1:A:98:PHE:N	2.82	0.47
1:A:241:GLU:HG3	1:A:242:ASP:N	2.28	0.47
2:B:113:LEU:HB2	2:B:116:ASP:OD2	2.15	0.47
1:A:299:TYR:HE2	1:A:300:PHE:CE1	2.31	0.47
1:A:123:LYS:HD3	1:A:299:TYR:O	2.15	0.47
2:B:56:SER:O	2:B:59:VAL:N	2.48	0.47
1:A:168:ARG:HB2	2:B:22:ARG:HH12	1.79	0.47
1:A:129:LEU:HD22	1:A:133:LEU:HD12	1.97	0.46
1:A:269:ILE:HG23	1:A:269:ILE:O	2.15	0.46
2:B:49:ILE:O	2:B:49:ILE:HG23	2.15	0.46
1:A:13:TYR:OH	1:A:81:ASP:HB3	2.16	0.46
2:B:46:ARG:HD2	2:B:74:ASP:OD2	2.15	0.46
1:A:40:VAL:HG21	1:A:97:VAL:HG12	1.97	0.46
1:A:172:PHE:HD1	1:A:178:SER:O	1.98	0.46
1:A:78:ARG:N	1:A:99:GLU:HG2	2.30	0.46
1:A:13:TYR:CZ	1:A:97:VAL:HG11	2.49	0.46
2:B:87:ARG:O	2:B:123:HIS:CE1	2.67	0.46
1:A:191:LEU:HD11	1:A:227:GLN:HG3	1.98	0.46
1:A:131:ARG:N	1:A:295:LEU:HD11	2.31	0.46
2:B:46:ARG:CD	2:B:75:PRO:HD2	2.46	0.46
1:A:124:ASP:O	1:A:128:GLN:HG3	2.16	0.46
1:A:144:ARG:HD3	1:A:190:VAL:HG11	1.98	0.45
1:A:202:LEU:HD23	1:A:280:CYS:HB3	1.97	0.45
1:A:85:VAL:N	1:A:93:LYS:O	2.49	0.45
1:A:218:LEU:HD22	1:A:219:PHE:CE1	2.51	0.45
1:A:133:LEU:HD13	1:A:205:VAL:HG12	1.97	0.45
1:A:172:PHE:CD1	1:A:178:SER:HB2	2.51	0.45
1:A:262:ILE:HG12	1:A:278:LEU:HD21	1.99	0.45
1:A:73:HIS:CE1	1:A:131:ARG:HG2	2.51	0.45
2:B:25:VAL:HA	2:B:59:VAL:HG22	1.98	0.45
1:A:276:LEU:HG	1:A:276:LEU:O	2.16	0.45
1:A:42:LEU:CD2	1:A:97:VAL:HG22	2.47	0.45
2:B:109:ALA:HB3	2:B:110:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:OG	1:A:196:TYR:N	2.49	0.45
1:A:47:VAL:HB	1:A:48:GLN:OE1	2.16	0.45
2:B:104:LEU:N	2:B:104:LEU:HD12	2.32	0.45
2:B:47:ARG:HB2	2:B:48:PRO:HD2	1.97	0.45
2:B:81:PRO:O	2:B:82:VAL:C	2.55	0.45
1:A:228:LEU:HD12	1:A:254:PHE:CE2	2.51	0.45
1:A:13:TYR:CE1	1:A:32:ASP:OD2	2.70	0.44
1:A:73:HIS:CG	1:A:74:PRO:HD2	2.52	0.44
2:B:64:LEU:HD12	2:B:96:VAL:CG1	2.43	0.44
2:B:88:GLU:HB3	2:B:90:PHE:CE2	2.52	0.44
2:B:60:ALA:CB	2:B:93:THR:HG22	2.46	0.44
2:B:83:HIS:O	2:B:86:ALA:HB3	2.17	0.44
1:A:170:TYR:CG	1:A:171:SER:N	2.85	0.44
2:B:104:LEU:HD12	2:B:104:LEU:H	1.82	0.44
1:A:37:GLY:HA3	2:B:77:THR:HG22	1.99	0.44
1:A:180:VAL:HG22	1:A:182:THR:H	1.83	0.44
2:B:45:GLY:O	2:B:46:ARG:NE	2.51	0.44
1:A:143:HIS:CE1	1:A:146:LEU:HD12	2.53	0.44
1:A:15:CYS:SG	1:A:28:PHE:CG	3.11	0.44
1:A:173:GLN:O	1:A:175:ALA:N	2.51	0.43
2:B:12:SER:O	2:B:15:TRP:CD1	2.69	0.43
2:B:24:ARG:O	2:B:25:VAL:C	2.56	0.43
2:B:52:MET:HG2	2:B:54:MET:HE2	2.01	0.43
2:B:80:ARG:NE	2:B:106:VAL:HG21	2.31	0.43
1:A:123:LYS:HE3	1:A:123:LYS:HB2	1.88	0.43
1:A:12:GLN:NE2	1:A:34:LYS:HB3	2.33	0.43
1:A:203:TRP:CZ2	1:A:231:ILE:HG12	2.45	0.43
1:A:166:LEU:HD23	1:A:167:ALA:H	1.84	0.43
1:A:180:VAL:CG2	1:A:183:LEU:HD22	2.49	0.43
1:A:184:TRP:N	1:A:184:TRP:CD1	2.87	0.43
1:A:209:PHE:CE1	1:A:213:PHE:CE2	3.06	0.43
1:A:289:ILE:CD1	1:A:294:ALA:HA	2.48	0.43
1:A:24:TYR:CE1	1:A:43:LYS:HE3	2.54	0.43
2:B:107:ARG:NH2	2:B:113:LEU:HD22	2.34	0.43
2:B:80:ARG:HB3	2:B:81:PRO:HD2	2.00	0.43
2:B:49:ILE:CD1	2:B:97:LEU:HD11	2.44	0.43
1:A:107:THR:HA	1:A:110:ASP:HB3	2.01	0.42
1:A:12:GLN:HE22	1:A:34:LYS:HD3	1.84	0.42
2:B:80:ARG:NH2	2:B:106:VAL:HG21	2.33	0.42
1:A:298:PRO:O	1:A:301:GLN:HB2	2.19	0.42
1:A:15:CYS:HB3	2:B:44:TYR:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HD11	1:A:294:ALA:HA	2.01	0.42
2:B:37:ASN:OD1	2:B:38:PRO:HD2	2.19	0.42
1:A:187:ALA:HB3	1:A:190:VAL:HG22	2.01	0.42
1:A:170:TYR:N	1:A:180:VAL:O	2.53	0.42
1:A:218:LEU:O	1:A:220:ARG:NH2	2.52	0.42
1:A:239:GLY:O	1:A:241:GLU:N	2.53	0.42
1:A:262:ILE:CG1	1:A:278:LEU:HD21	2.49	0.42
2:B:24:ARG:HB3	2:B:27:GLU:HB2	2.02	0.42
2:B:12:SER:CA	2:B:15:TRP:HD1	2.32	0.42
1:A:237:LEU:HD12	1:A:256:SER:CA	2.50	0.42
1:A:130:LEU:HD22	1:A:294:ALA:HB3	2.02	0.42
1:A:27:VAL:O	1:A:27:VAL:HG13	2.20	0.42
1:A:289:ILE:HG12	1:A:290:SER:H	1.79	0.42
2:B:103:ARG:O	2:B:106:VAL:HG23	2.19	0.42
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.90	0.41
2:B:15:TRP:CB	2:B:31:LEU:HD21	2.49	0.41
2:B:64:LEU:HD11	2:B:97:LEU:HA	2.01	0.41
1:A:280:CYS:HA	1:A:289:ILE:HG22	2.02	0.41
2:B:18:THR:O	2:B:22:ARG:N	2.46	0.41
1:A:261:PRO:HD2	1:A:264:LYS:CD	2.50	0.41
2:B:91:LEU:CD1	2:B:95:VAL:HG23	2.51	0.41
1:A:218:LEU:HD23	1:A:218:LEU:O	2.20	0.41
2:B:71:ASN:C	2:B:72:CYS:SG	2.99	0.41
2:B:32:LEU:HD21	2:B:38:PRO:HB3	2.03	0.41
2:B:74:ASP:HB2	2:B:79:THR:O	2.21	0.41
1:A:194:SER:O	1:A:195:SER:HB2	2.21	0.41
1:A:19:ILE:HG12	1:A:28:PHE:HA	2.03	0.41
1:A:82:VAL:HG22	1:A:96:LEU:HD22	2.03	0.41
2:B:97:LEU:O	2:B:100:ALA:HB3	2.21	0.41
2:B:47:ARG:O	2:B:50:GLN:CB	2.68	0.41
2:B:32:LEU:HD11	2:B:63:LEU:HD23	2.03	0.41
2:B:61:GLU:CA	2:B:96:VAL:HG11	2.51	0.41
1:A:133:LEU:HD11	1:A:146:LEU:CD2	2.51	0.41
1:A:143:HIS:ND1	1:A:146:LEU:HD12	2.36	0.40
1:A:203:TRP:HZ2	1:A:231:ILE:CG1	2.30	0.40
1:A:266:VAL:HG21	1:A:277:LEU:HD21	2.04	0.40
1:A:122:ILE:O	1:A:123:LYS:C	2.60	0.40
1:A:179:VAL:CG2	1:A:180:VAL:N	2.84	0.40
1:A:22:GLY:N	1:A:25:GLY:O	2.53	0.40
1:A:27:VAL:HA	1:A:42:LEU:O	2.22	0.40
2:B:109:ALA:HB3	2:B:110:TRP:CE3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:TRP:CE3	2:B:110:TRP:N	2.90	0.40
2:B:20:ALA:C	2:B:52:MET:HA	2.42	0.40
1:A:22:GLY:HA3	1:A:24:TYR:CE1	2.56	0.40
1:A:37:GLY:HA3	2:B:77:THR:CG2	2.52	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	265/326 (81%)	197 (74%)	44 (17%)	24 (9%)	1	4
2	B	123/156 (79%)	79 (64%)	34 (28%)	10 (8%)	1	5
All	All	388/482 (80%)	276 (71%)	78 (20%)	34 (9%)	1	5

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLU
1	A	173	GLN
1	A	177	THR
1	A	248	ALA
1	A	256	SER
1	A	259	ALA
2	B	11	PRO
2	B	75	PRO
1	A	36	GLY
1	A	114	GLU
1	A	174	MET
1	A	182	THR
1	A	255	HIS
1	A	299	TYR

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Mol	Chain	Res	Type
2	B	45	GLY
2	B	46	ARG
1	A	47	VAL
1	A	73	HIS
1	A	103	GLN
1	A	240	GLU
1	A	247	VAL
1	A	257	LYS
2	B	104	LEU
1	A	90	ARG
1	A	149	GLN
1	A	241	GLU
1	A	258	SER
2	B	39	ASN
2	B	76	ALA
1	A	140	ARG
2	B	33	GLU
2	B	25	VAL
1	A	165	GLY
2	B	49	ILE

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	235/289 (81%)	196 (83%)	39 (17%)	2	8
2	B	91/113 (80%)	72 (79%)	19 (21%)	1	3
All	All	326/402 (81%)	268 (82%)	58 (18%)	2	6

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	12	GLN
1	A	15	CYS

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Mol	Chain	Res	Type
1	A	28	PHE
1	A	32	ASP
1	A	38	ARG
1	A	48	GLN
1	A	88	THR
1	A	91	GLU
1	A	103	GLN
1	A	129	LEU
1	A	133	LEU
1	A	138	SER
1	A	140	ARG
1	A	146	LEU
1	A	158	GLN
1	A	166	LEU
1	A	168	ARG
1	A	183	LEU
1	A	192	LEU
1	A	202	LEU
1	A	205	VAL
1	A	216	LYS
1	A	218	LEU
1	A	220	ARG
1	A	237	LEU
1	A	246	ASP
1	A	249	LEU
1	A	255	HIS
1	A	257	LYS
1	A	262	ILE
1	A	265	PHE
1	A	267	THR
1	A	268	ASP
1	A	271	GLU
1	A	274	LYS
1	A	276	LEU
1	A	282	THR
1	A	296	SER
2	B	16	LEU
2	B	24	ARG
2	B	25	VAL
2	B	31	LEU
2	B	39	ASN
2	B	46	ARG

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Mol	Chain	Res	Type
2	B	49	ILE
2	B	69	GLU
2	B	72	CYS
2	B	74	ASP
2	B	75	PRO
2	B	77	THR
2	B	93	THR
2	B	97	LEU
2	B	104	LEU
2	B	105	ASP
2	B	113	LEU
2	B	124	ARG
2	B	125	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	137	HIS
1	A	150	ASN
1	A	255	HIS
2	B	39	ASN
2	B	71	ASN
2	B	98	HIS
2	B	123	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.