



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 05:43 AM JST

PDB ID : 7WDC  
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC  
Authors : Furuike, Y.; Akiyama, S.  
Deposited on : 2021-12-21  
Resolution : 2.84 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : ?? (??), CSD ??CSD?? (????)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

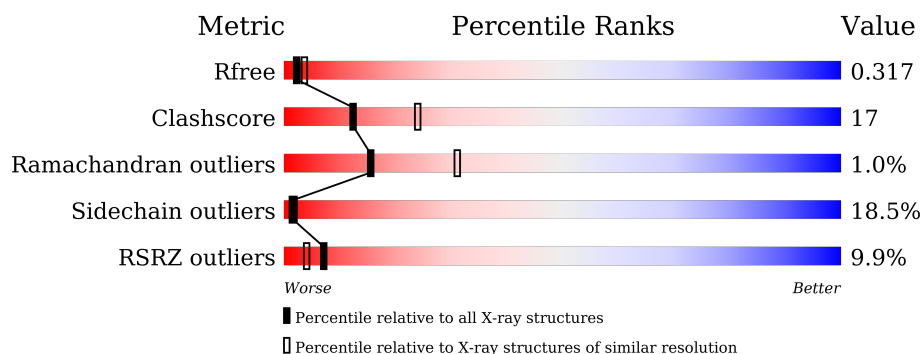
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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))
$R_{free}$	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	519	<div> <div>10%</div> <div>57%</div> <div>27%</div> <div>•</div> <div>12%</div> </div>
1	B	519	<div> <div>7%</div> <div>58%</div> <div>26%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6682 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.

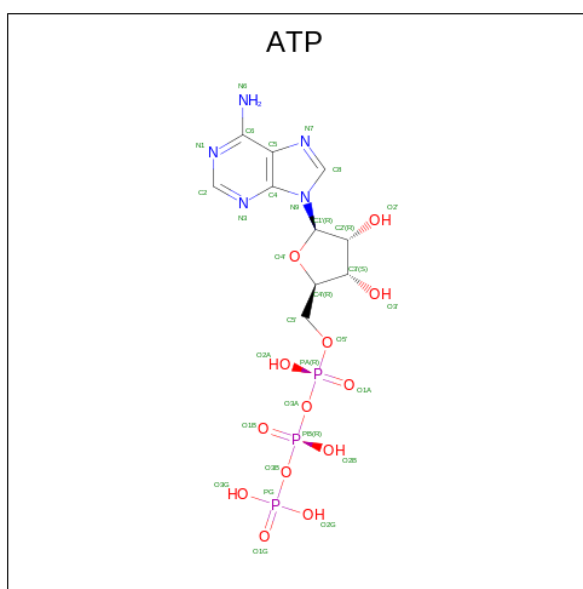
- Molecule 1 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3270	2057	573	627	13			
1	B	460	Total	C	N	O	S	0	0	0
			3267	2050	575	629	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	TRP	PHE	engineered mutation	UNP Q79PF4
B	419	TRP	PHE	engineered mutation	UNP Q79PF4

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

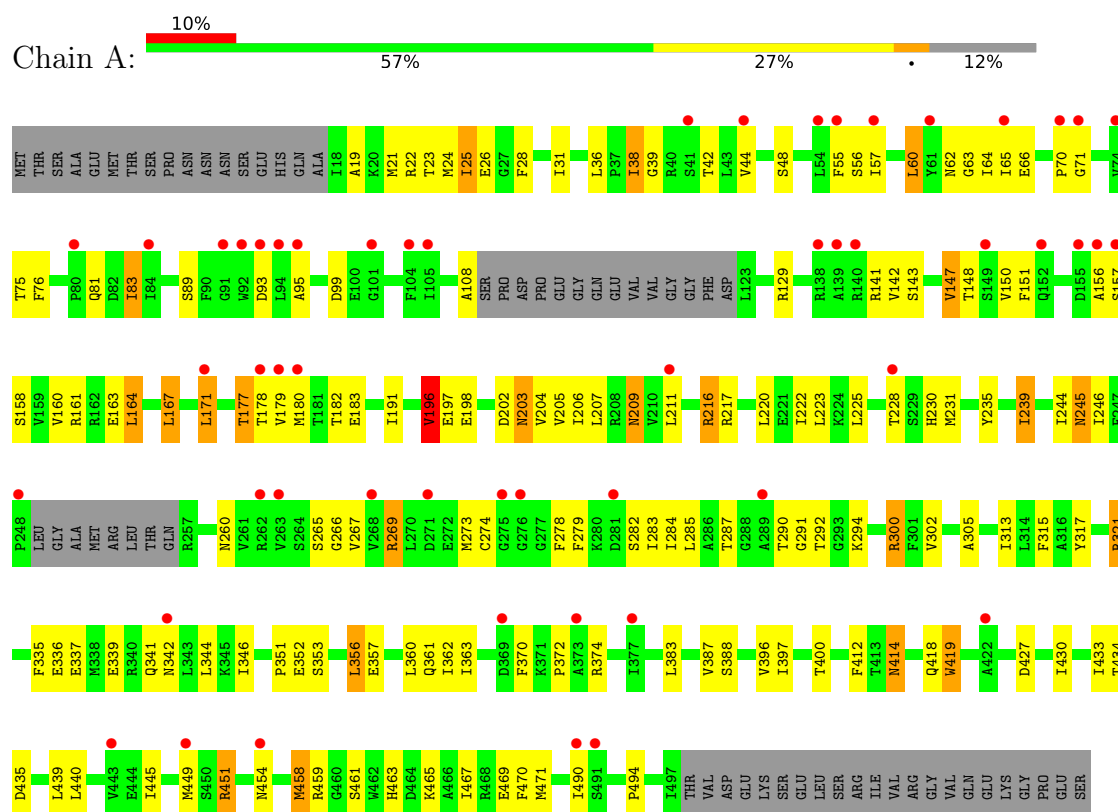
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	9	Total	O	0	0
			9	9		

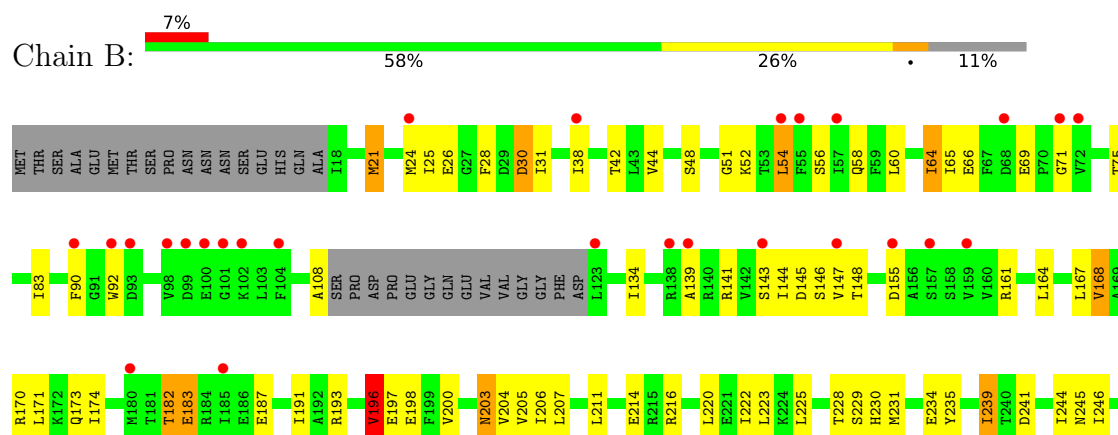
### 3 Residue-property plots

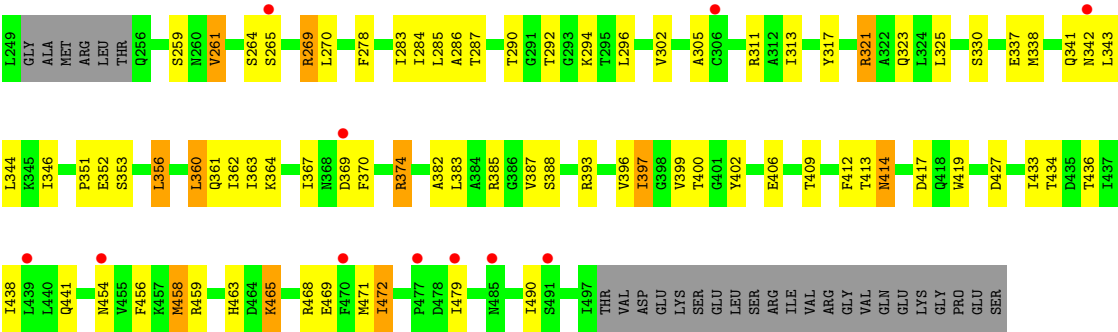
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Circadian clock protein kinase KaiC



#### • Molecule 1: Circadian clock protein kinase KaiC





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.26Å 95.26Å 182.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.13 – 2.84 46.09 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.13-2.84) 99.8 (46.09-2.84)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.283 , 0.325 0.286 , 0.317	Depositor DCC
$R_{free}$ test set	1035 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 66.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4832e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	0.69	0/3320	0.74	0/4511
1	B	0.69	0/3318	0.75	0/4509
All	All	0.69	0/6638	0.75	0/9020

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3270	0	2983	104	1
1	B	3267	0	2942	112	1
2	A	62	0	24	5	0
2	B	62	0	24	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	8	0	0	0	0
4	B	9	0	0	1	0
All	All	6682	0	5973	214	1

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 17.



All (214) 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:38:ILE:HA	1:A:177:THR:HG21	1.42	0.99
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.40	0.98
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.46	0.97
1:B:211:LEU:HD13	1:B:216:ARG:HD2	1.54	0.90
1:A:39:GLY:H	1:A:177:THR:HG22	1.35	0.90
1:B:305:ALA:HB2	1:B:374:ARG:HD3	1.57	0.85
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.59	0.82
1:B:31:ILE:HD12	1:B:246:ILE:HG21	1.61	0.82
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.60	0.81
1:B:170:ARG:O	1:B:174:ILE:HD12	1.80	0.81
1:A:38:ILE:HA	1:A:177:THR:CG2	2.13	0.79
1:A:24:MET:HG3	1:A:66:GLU:HG3	1.66	0.77
1:B:278:PHE:CD2	1:B:284:ILE:CD1	2.69	0.76
1:A:396:VAL:HG11	1:A:430:ILE:HG23	1.66	0.75
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.15	0.74
1:B:397:ILE:CD1	1:B:433:ILE:HD13	2.17	0.73
1:B:148:THR:HG21	1:B:183:GLU:HG3	1.71	0.73
1:B:225:LEU:HB3	1:B:228:THR:HG23	1.71	0.72
1:A:225:LEU:HB3	1:A:228:THR:HG23	1.71	0.72
1:B:225:LEU:HB3	1:B:228:THR:CG2	2.20	0.72
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.72	0.72
1:B:278:PHE:CG	1:B:284:ILE:CD1	2.72	0.71
1:A:167:LEU:HD12	1:A:171:LEU:HD22	1.71	0.71
1:A:57:ILE:HD11	1:A:83:ILE:HG23	1.72	0.71
1:A:211:LEU:HD13	1:A:216:ARG:HD2	1.72	0.70
1:A:39:GLY:N	1:A:177:THR:HG22	2.06	0.70
1:B:134:ILE:HA	1:B:139:ALA:HB2	1.74	0.69
1:A:435:ASP:HA	1:A:459:ARG:HD2	1.75	0.69
1:B:148:THR:OG1	1:B:182:THR:OG1	2.12	0.68
1:A:44:VAL:HG23	1:A:179:VAL:HG13	1.75	0.68
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.74	0.67
1:A:225:LEU:HB3	1:A:228:THR:CG2	2.25	0.67
1:B:360:LEU:O	1:B:364:LYS:HG3	1.95	0.67
1:A:419:TRP:HZ2	1:A:449:MET:HE1	1.59	0.66
1:B:278:PHE:CG	1:B:284:ILE:HD13	2.31	0.65
1:B:164:LEU:O	1:B:168:VAL:HG13	1.96	0.65
1:A:22:ARG:O	1:A:141:ARG:NH2	2.29	0.65
1:B:71:GLY:HA2	1:B:141:ARG:O	1.97	0.64
1:B:305:ALA:CB	1:B:374:ARG:HD3	2.28	0.64
1:B:317:TYR:HB3	1:B:351:PRO:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HG22	1:A:65:ILE:HD13	1.80	0.63
1:A:279:PHE:HB2	1:A:282:SER:HB3	1.81	0.62
1:A:191:ILE:HG21	1:A:198:GLU:HB3	1.81	0.62
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.29	0.62
1:A:31:ILE:HD12	1:A:246:ILE:HG21	1.82	0.62
1:B:148:THR:HG1	1:B:182:THR:HG1	1.49	0.61
1:A:147:VAL:HG21	1:A:180:MET:HE2	1.83	0.61
1:B:54:LEU:HD23	1:B:239:ILE:HG12	1.81	0.61
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.29	0.61
1:B:207:LEU:HD21	1:B:220:LEU:HD12	1.83	0.60
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.82	0.60
1:B:302:VAL:HG11	1:B:344:LEU:HD13	1.82	0.60
1:A:206:ILE:HD11	1:A:223:LEU:HD22	1.82	0.60
1:A:89:SER:OG	2:A:601:ATP:N6	2.34	0.60
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.84	0.60
1:B:397:ILE:HD11	1:B:433:ILE:HD13	1.84	0.60
1:A:211:LEU:CD1	1:A:216:ARG:HD2	2.32	0.59
1:B:302:VAL:CG1	1:B:344:LEU:HD13	2.32	0.59
1:B:296:LEU:CD2	1:B:472:ILE:HD13	2.33	0.59
1:A:55:PHE:CE1	1:A:179:VAL:HG11	2.38	0.59
1:B:31:ILE:CD1	1:B:246:ILE:HG21	2.31	0.58
1:B:311:ARG:HA	1:B:343:LEU:O	2.03	0.58
1:A:356:LEU:HD22	1:A:387:VAL:CG1	2.25	0.58
1:A:75:THR:O	1:A:108:ALA:HB3	2.04	0.58
1:B:383:LEU:O	1:B:387:VAL:HG21	2.04	0.57
1:B:211:LEU:CD1	1:B:216:ARG:HD2	2.31	0.57
1:A:23:THR:OG1	1:A:25:ILE:HG13	2.05	0.57
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.85	0.57
1:B:207:LEU:CD2	1:B:220:LEU:HD12	2.35	0.56
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.87	0.56
1:B:58:GLN:HG2	1:B:92:TRP:CH2	2.40	0.56
1:A:164:LEU:CD1	1:A:197:GLU:HA	2.36	0.56
2:A:602:ATP:O3G	1:B:459:ARG:NH2	2.38	0.56
1:B:31:ILE:CD1	1:B:246:ILE:CG2	2.84	0.56
1:A:225:LEU:HB2	1:A:230:HIS:HD2	1.71	0.56
1:B:239:ILE:HG21	2:B:601:ATP:C1'	2.36	0.56
1:A:269:ARG:O	1:A:273:MET:HG3	2.06	0.55
1:B:206:ILE:HD11	1:B:223:LEU:HD22	1.86	0.55
1:B:278:PHE:CD2	1:B:284:ILE:HD12	2.40	0.55
1:A:76:PHE:CE2	1:A:150:VAL:HG11	2.41	0.55
1:B:317:TYR:CD1	1:B:383:LEU:HD21	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:SER:HB2	1:B:261:VAL:HG12	1.89	0.54
1:A:44:VAL:CG2	1:A:179:VAL:HG13	2.37	0.54
1:A:239:ILE:HG21	2:A:601:ATP:C1'	2.38	0.54
1:B:402:TYR:O	1:B:406:GLU:HG2	2.08	0.54
1:A:265:SER:HB3	1:A:278:PHE:CE2	2.43	0.54
1:B:30:ASP:N	1:B:30:ASP:OD1	2.41	0.54
1:B:231:MET:HB3	1:B:235:TYR:OH	2.08	0.53
1:B:264:SER:O	1:B:374:ARG:NH1	2.35	0.53
1:B:24:MET:HG3	1:B:66:GLU:HG2	1.91	0.53
1:B:31:ILE:HD12	1:B:246:ILE:CG2	2.36	0.53
1:A:430:ILE:HD12	1:A:430:ILE:N	2.24	0.53
1:B:265:SER:HB3	1:B:278:PHE:CE2	2.44	0.53
1:B:168:VAL:HA	1:B:171:LEU:HD12	1.90	0.53
1:B:204:VAL:HG11	1:B:223:LEU:HD23	1.91	0.52
1:B:285:LEU:HA	1:B:412:PHE:O	2.10	0.52
1:B:436:THR:HG23	1:B:458:MET:HG2	1.91	0.52
1:B:296:LEU:HD23	1:B:472:ILE:HD13	1.90	0.52
1:B:148:THR:CG2	1:B:183:GLU:HG3	2.39	0.51
1:A:225:LEU:HB2	1:A:230:HIS:CD2	2.46	0.51
1:B:397:ILE:HD11	1:B:433:ILE:CD1	2.41	0.51
1:A:274:CYS:HG	1:A:278:PHE:HE1	1.57	0.51
1:A:216:ARG:HH21	1:A:216:ARG:HG3	1.75	0.51
1:B:360:LEU:HD13	1:B:364:LYS:HD2	1.93	0.51
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.93	0.50
1:A:278:PHE:HB3	1:A:284:ILE:HD11	1.93	0.50
1:A:351:PRO:HB3	1:A:383:LEU:HD23	1.94	0.50
1:A:451:ARG:HD3	1:A:470:PHE:CE2	2.46	0.50
1:B:337:GLU:O	1:B:341:GLN:HG3	2.12	0.50
1:A:167:LEU:CD1	1:A:171:LEU:HD22	2.40	0.50
1:B:278:PHE:HB3	1:B:284:ILE:HD11	1.92	0.50
1:A:305:ALA:HB2	1:A:374:ARG:CD	2.40	0.49
1:B:338:MET:HB3	1:B:344:LEU:HB3	1.93	0.49
1:B:170:ARG:O	1:B:173:GLN:HB2	2.11	0.49
1:A:317:TYR:HB3	1:A:351:PRO:HG3	1.94	0.49
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.37	0.49
1:B:269:ARG:HB3	1:B:479:ILE:HD12	1.95	0.49
1:A:147:VAL:HG21	1:A:180:MET:CE	2.43	0.49
1:A:315:PHE:CZ	1:A:363:ILE:HA	2.47	0.49
2:A:601:ATP:C2	1:B:229:SER:HB3	2.48	0.48
1:B:64:ILE:HG23	1:B:69:GLU:O	2.13	0.48
1:B:313:ILE:HD11	1:B:370:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:MET:SD	1:B:141:ARG:NE	2.85	0.48
1:A:454:ASN:HB2	1:A:467:ILE:HA	1.96	0.48
1:B:161:ARG:HB2	1:B:196:VAL:CG1	2.44	0.48
1:B:363:ILE:O	1:B:367:ILE:HG13	2.13	0.48
1:B:287:THR:HG22	1:B:414:ASN:HD22	1.79	0.47
1:A:24:MET:HB2	1:A:62:ASN:HB3	1.97	0.47
1:B:58:GLN:CG	1:B:92:TRP:CH2	2.98	0.47
1:B:351:PRO:HG2	1:B:382:ALA:HB1	1.96	0.47
1:A:397:ILE:HD11	1:A:433:ILE:CD1	2.45	0.47
1:A:335:PHE:O	1:A:339:GLU:HG3	2.13	0.47
1:A:458:MET:HB2	1:A:463:HIS:CD2	2.50	0.47
1:A:211:LEU:HD13	1:A:216:ARG:CD	2.43	0.47
1:B:278:PHE:CG	1:B:284:ILE:HD11	2.50	0.47
1:A:31:ILE:CD1	1:A:246:ILE:CG2	2.93	0.46
1:B:54:LEU:C	1:B:54:LEU:HD12	2.36	0.46
1:A:445:ILE:CD1	1:A:494:PRO:HG3	2.46	0.46
1:B:458:MET:HB2	1:B:463:HIS:CD2	2.50	0.46
1:A:44:VAL:HA	1:A:205:VAL:O	2.15	0.46
1:A:313:ILE:HG13	1:A:372:PRO:HB3	1.97	0.46
1:A:445:ILE:HD11	1:A:494:PRO:HG3	1.97	0.46
1:B:58:GLN:CG	1:B:92:TRP:HH2	2.29	0.46
1:B:191:ILE:HG21	1:B:198:GLU:HB3	1.97	0.46
1:A:164:LEU:HD12	1:A:197:GLU:HG3	1.98	0.46
1:B:351:PRO:HB3	1:B:383:LEU:HD23	1.97	0.46
1:A:266:GLY:O	1:A:300:ARG:NH2	2.48	0.45
1:A:290:THR:HG22	1:B:456:PHE:HE2	1.80	0.45
1:B:51:GLY:HA2	2:B:601:ATP:O2A	2.17	0.45
1:B:323:GLN:NE2	4:B:703:HOH:O	2.48	0.45
1:A:209:ASN:O	1:A:216:ARG:NH2	2.50	0.45
1:B:28:PHE:HB2	1:B:246:ILE:HD12	1.98	0.45
1:B:269:ARG:HG3	1:B:269:ARG:HH11	1.80	0.45
1:A:63:GLY:HA3	1:A:141:ARG:HD2	1.99	0.45
1:A:231:MET:HB3	1:A:235:TYR:OH	2.16	0.45
1:B:54:LEU:CD2	1:B:239:ILE:HG12	2.46	0.45
1:B:278:PHE:CD1	1:B:284:ILE:HD13	2.51	0.45
1:A:287:THR:OG1	1:A:414:ASN:ND2	2.50	0.45
1:A:285:LEU:HA	1:A:412:PHE:O	2.18	0.44
1:A:440:LEU:HD22	1:A:470:PHE:CZ	2.53	0.44
1:B:203:ASN:HB3	1:B:225:LEU:CD2	2.41	0.44
1:A:19:ALA:O	1:A:38:ILE:HG13	2.17	0.44
1:A:56:SER:HB2	1:A:143:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLU:OE2	1:B:197:GLU:N	2.44	0.44
1:B:284:ILE:HG23	1:B:436:THR:HB	2.00	0.44
1:A:419:TRP:CZ2	1:A:449:MET:HE1	2.46	0.44
1:B:168:VAL:HG11	1:B:200:VAL:HG12	1.99	0.43
1:A:321:ARG:HG3	1:A:346:ILE:HG21	2.00	0.43
2:A:601:ATP:C2	1:B:229:SER:CB	3.01	0.43
1:A:204:VAL:HB	1:A:223:LEU:HB3	1.99	0.43
1:A:397:ILE:CD1	1:A:433:ILE:CD1	2.97	0.43
1:B:352:GLU:OE1	1:B:385:ARG:NH1	2.35	0.43
1:A:19:ALA:C	1:A:38:ILE:HG13	2.39	0.43
1:A:287:THR:HA	1:A:414:ASN:O	2.19	0.43
1:A:28:PHE:CZ	1:A:36:LEU:HD21	2.54	0.43
1:B:321:ARG:HG3	1:B:346:ILE:HG21	2.01	0.43
1:B:54:LEU:HD12	1:B:54:LEU:O	2.19	0.43
1:B:245:ASN:ND2	1:B:361:GLN:OE1	2.52	0.43
1:B:278:PHE:CB	1:B:284:ILE:HD11	2.49	0.43
1:A:449:MET:N	1:B:465:LYS:O	2.46	0.43
1:A:95:ALA:O	1:A:99:ASP:N	2.51	0.42
1:A:245:ASN:OD1	1:A:361:GLN:NE2	2.52	0.42
1:A:313:ILE:HD11	1:A:370:PHE:HB3	2.01	0.42
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.88	0.42
1:A:156:ALA:O	1:A:158:SER:N	2.52	0.42
1:B:58:GLN:HG3	1:B:92:TRP:HH2	1.83	0.42
1:A:160:VAL:O	1:A:164:LEU:HB2	2.20	0.42
1:B:90:PHE:HA	1:B:241:ASP:O	2.20	0.42
1:A:21:MET:SD	1:A:141:ARG:NE	2.92	0.42
1:B:60:LEU:HD22	1:B:71:GLY:HA3	2.01	0.42
1:B:170:ARG:C	1:B:174:ILE:HD12	2.38	0.42
1:B:225:LEU:CB	1:B:228:THR:HG23	2.47	0.42
1:A:337:GLU:O	1:A:341:GLN:HG3	2.20	0.42
1:B:44:VAL:HA	1:B:205:VAL:O	2.20	0.42
1:A:458:MET:HE2	1:A:461:SER:HB3	2.02	0.42
1:B:321:ARG:CZ	1:B:325:LEU:HD11	2.50	0.42
1:A:64:ILE:HD11	1:A:71:GLY:N	2.35	0.41
1:A:142:VAL:O	1:A:178:THR:HA	2.20	0.41
1:A:42:THR:O	1:A:179:VAL:HA	2.19	0.41
1:B:265:SER:CB	1:B:278:PHE:CE2	3.03	0.41
1:B:52:LYS:HB2	1:B:52:LYS:HE2	1.83	0.41
1:A:150:VAL:O	1:A:150:VAL:HG22	2.19	0.41
1:A:245:ASN:HD22	1:A:245:ASN:HA	1.62	0.41
1:A:383:LEU:O	1:A:387:VAL:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD21	1:A:220:LEU:HD12	2.03	0.41
1:B:75:THR:O	1:B:108:ALA:HB3	2.20	0.41
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.93	0.40
1:A:291:GLY:O	1:A:451:ARG:NH1	2.54	0.40
1:B:167:LEU:CD1	1:B:171:LEU:HD11	2.51	0.40
1:B:286:ALA:HA	1:B:438:ILE:O	2.20	0.40
1:B:145:ASP:HA	1:B:146:SER:HA	1.64	0.40
1:A:148:THR:HB	1:A:183:GLU:HG3	2.02	0.40
1:A:302:VAL:CG1	1:A:344:LEU:HD13	2.51	0.40
1:B:42:THR:HG1	1:B:203:ASN:HD22	1.63	0.40

All (1) 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:217:ARG:NH2	1:B:214:GLU:OE1[2_455]	2.14	0.06

## 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	452/519 (87%)	411 (91%)	36 (8%)	5 (1%)	14	30
1	B	454/519 (88%)	416 (92%)	34 (8%)	4 (1%)	17	34
All	All	906/1038 (87%)	827 (91%)	70 (8%)	9 (1%)	15	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	SER
1	B	65	ILE
1	B	26	GLU

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Mol	Chain	Res	Type
1	A	26	GLU
1	A	353	SER
1	B	353	SER
1	A	70	PRO
1	B	196	VAL
1	A	196	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	302/444 (68%)	250 (83%)	52 (17%)	2	2
1	B	298/444 (67%)	239 (80%)	59 (20%)	1	1
All	All	600/888 (68%)	489 (82%)	111 (18%)	1	2

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	38	ILE
1	A	48	SER
1	A	60	LEU
1	A	81	GLN
1	A	83	ILE
1	A	93	ASP
1	A	129	ARG
1	A	147	VAL
1	A	151	PHE
1	A	163	GLU
1	A	164	LEU
1	A	167	LEU
1	A	171	LEU
1	A	177	THR
1	A	182	THR
1	A	196	VAL

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Mol	Chain	Res	Type
1	A	202	ASP
1	A	203	ASN
1	A	209	ASN
1	A	216	ARG
1	A	222	ILE
1	A	239	ILE
1	A	244	ILE
1	A	245	ASN
1	A	260	ASN
1	A	267	VAL
1	A	269	ARG
1	A	292	THR
1	A	294	LYS
1	A	300	ARG
1	A	321	ARG
1	A	336	GLU
1	A	342	ASN
1	A	352	GLU
1	A	356	LEU
1	A	357	GLU
1	A	360	LEU
1	A	362	ILE
1	A	388	SER
1	A	414	ASN
1	A	418	GLN
1	A	419	TRP
1	A	427	ASP
1	A	434	THR
1	A	439	LEU
1	A	451	ARG
1	A	458	MET
1	A	465	LYS
1	A	469	GLU
1	A	471	MET
1	A	490	ILE
1	B	21	MET
1	B	25	ILE
1	B	30	ASP
1	B	38	ILE
1	B	48	SER
1	B	54	LEU
1	B	56	SER

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Mol	Chain	Res	Type
1	B	64	ILE
1	B	83	ILE
1	B	143	SER
1	B	144	ILE
1	B	147	VAL
1	B	155	ASP
1	B	168	VAL
1	B	182	THR
1	B	183	GLU
1	B	187	GLU
1	B	193	ARG
1	B	196	VAL
1	B	203	ASN
1	B	222	ILE
1	B	234	GLU
1	B	239	ILE
1	B	244	ILE
1	B	261	VAL
1	B	269	ARG
1	B	270	LEU
1	B	290	THR
1	B	292	THR
1	B	294	LYS
1	B	321	ARG
1	B	330	SER
1	B	342	ASN
1	B	356	LEU
1	B	360	LEU
1	B	362	ILE
1	B	369	ASP
1	B	374	ARG
1	B	388	SER
1	B	393	ARG
1	B	396	VAL
1	B	397	ILE
1	B	399	VAL
1	B	409	THR
1	B	413	THR
1	B	414	ASN
1	B	417	ASP
1	B	419	TRP
1	B	427	ASP

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Mol	Chain	Res	Type
1	B	434	THR
1	B	441	GLN
1	B	454	ASN
1	B	458	MET
1	B	465	LYS
1	B	468	ARG
1	B	469	GLU
1	B	471	MET
1	B	472	ILE
1	B	490	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	230	HIS
1	A	245	ASN
1	A	304	ASN
1	A	323	GLN
1	A	361	GLN
1	A	414	ASN
1	A	418	GLN
1	B	203	ASN
1	B	414	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	458/519 (88%)	0.63	53 (11%) <b>4</b> <b>2</b>	54, 79, 114, 141	0
1	B	460/519 (88%)	0.53	38 (8%) <b>11</b> <b>6</b>	52, 79, 122, 139	0
All	All	918/1038 (88%)	0.58	91 (9%) <b>7</b> <b>4</b>	52, 79, 119, 141	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	LEU	7.9
1	A	92	TRP	7.7
1	A	152	GLN	5.7
1	A	95	ALA	5.3
1	B	139	ALA	4.7
1	A	156	ALA	4.7
1	A	262	ARG	4.6
1	B	92	TRP	4.5
1	A	139	ALA	4.5
1	A	104	PHE	4.3
1	B	72	VAL	4.3
1	A	91	GLY	4.0
1	A	180	MET	4.0
1	A	157	SER	4.0
1	B	155	ASP	4.0
1	B	99	ASP	3.9
1	B	71	GLY	3.9
1	B	138	ARG	3.7
1	A	179	VAL	3.6
1	A	84	ILE	3.6
1	B	93	ASP	3.6
1	A	101	GLY	3.6
1	A	276	GLY	3.6
1	B	157	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	479	ILE	3.4
1	B	101	GLY	3.4
1	A	138	ARG	3.2
1	B	68	ASP	3.1
1	B	491	SER	3.1
1	A	155	ASP	3.1
1	B	57	ILE	3.1
1	B	90	PHE	3.0
1	A	65	ILE	3.0
1	A	41	SER	2.9
1	B	159	VAL	2.9
1	A	80	PRO	2.9
1	A	71	GLY	2.8
1	A	369	ASP	2.8
1	A	263	VAL	2.8
1	A	268	VAL	2.8
1	B	38	ILE	2.8
1	A	74	VAL	2.8
1	B	180	MET	2.7
1	A	93	ASP	2.7
1	A	342	ASN	2.7
1	B	54	LEU	2.7
1	A	422	ALA	2.6
1	B	439	LEU	2.6
1	A	57	ILE	2.5
1	B	185	ILE	2.5
1	A	54	LEU	2.5
1	A	490	ILE	2.5
1	B	306	CYS	2.5
1	B	98	VAL	2.4
1	B	147	VAL	2.4
1	B	454	ASN	2.4
1	B	102	LYS	2.4
1	A	377	ILE	2.4
1	A	44	VAL	2.3
1	B	369	ASP	2.3
1	B	143	SER	2.3
1	B	265	SER	2.3
1	A	373	ALA	2.3
1	A	55	PHE	2.3
1	A	454	ASN	2.3
1	A	281	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	140	ARG	2.3
1	A	289	ALA	2.2
1	A	105	ILE	2.2
1	A	248	PRO	2.2
1	B	123	LEU	2.2
1	B	55	PHE	2.1
1	A	149	SER	2.1
1	B	485	ASN	2.1
1	A	211	LEU	2.1
1	B	477	PRO	2.1
1	A	491	SER	2.1
1	B	342	ASN	2.1
1	B	24	MET	2.1
1	A	449	MET	2.1
1	B	100	GLU	2.1
1	A	171	LEU	2.1
1	A	271	ASP	2.1
1	B	104	PHE	2.1
1	B	470	PHE	2.0
1	A	228	THR	2.0
1	A	443	VAL	2.0
1	A	275	GLY	2.0
1	A	61	TYR	2.0
1	A	70	PRO	2.0
1	A	178	THR	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	603	1/1	0.90	0.13	62,62,62,62	0
2	ATP	A	601	31/31	0.92	0.18	76,81,97,99	0
2	ATP	B	601	31/31	0.93	0.20	77,82,101,102	0
2	ATP	B	602	31/31	0.95	0.15	52,54,72,73	0
2	ATP	A	602	31/31	0.95	0.14	49,52,70,72	0
3	MG	A	604	1/1	0.96	0.11	48,48,48,48	0
3	MG	B	603	1/1	0.97	0.06	64,64,64,64	0
3	MG	B	604	1/1	0.98	0.10	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.