



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:01 AM GMT

PDB ID : 2VN2  
Title : Crystal structure of the N-terminal domain of DnaD protein from *Geobacillus kaustophilus* HTA426  
Authors : Huang, C.-Y.; Chang, Y.-W.; Chen, W.-T.; Sun, Y.-J.; Hsiao, C.-D.  
Deposited on : 2008-01-30  
Resolution : 2.30 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

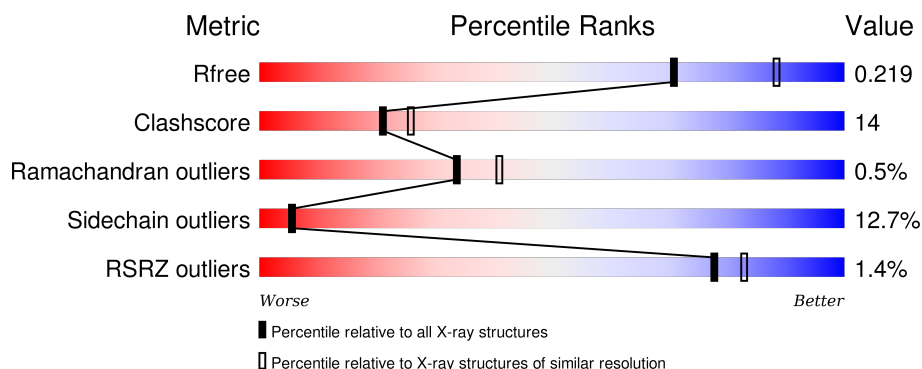
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	128	<div> <div>4%</div> <div>50%</div> <div>31%</div> <div>• •</div> <div>13%</div> </div>
1	B	128	<div> <div>%</div> <div>56%</div> <div>23%</div> <div>6%</div> <div>•</div> <div>13%</div> </div>
1	C	128	<div> <div>59%</div> <div>20%</div> <div>7%</div> <div>•</div> <div>14%</div> </div>
1	D	128	<div> <div>55%</div> <div>26%</div> <div>5%</div> <div>•</div> <div>14%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3650 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 CHROMOSOME REPLICATION INITIATION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	2
			877	567	146	157	7			
1	B	111	Total	C	N	O	S	0	0	2
			869	561	145	156	7			
1	C	110	Total	C	N	O	S	0	0	2
			861	556	144	155	6			
1	D	110	Total	C	N	O	S	0	0	2
			861	556	144	155	6			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

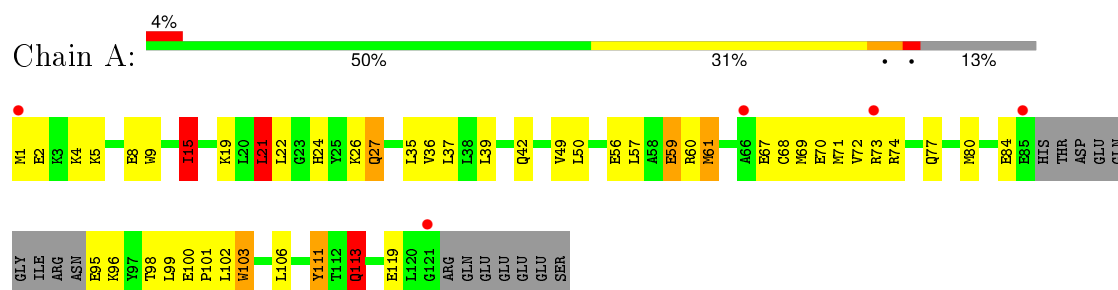
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	42	Total	O	0	0
			42	42		
3	C	45	Total	O	0	0
			45	45		
3	D	52	Total	O	0	0
			52	52		

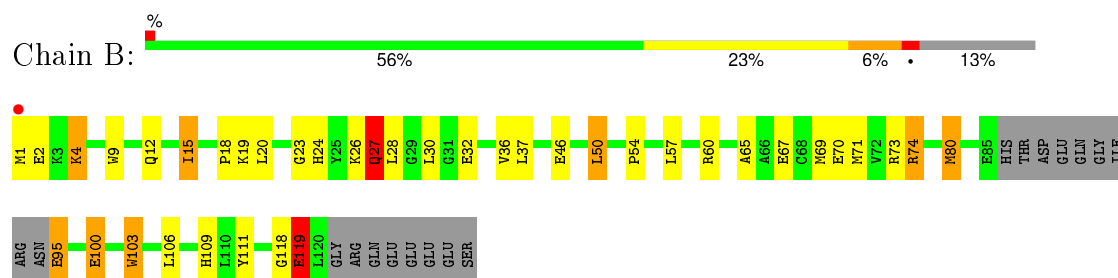
### 3 Residue-property plots

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.

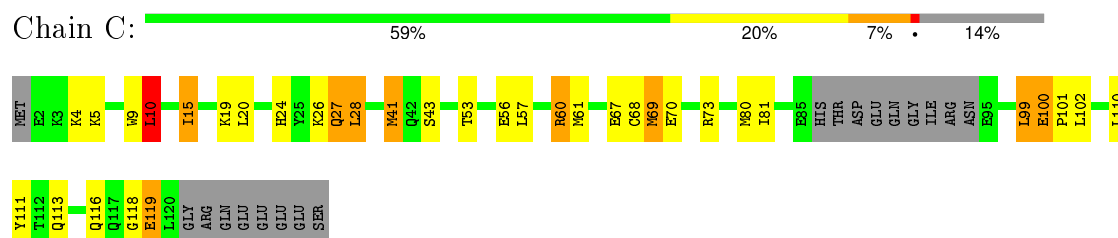
#### • Molecule 1: CHROMOSOME REPLICATION INITIATION PROTEIN



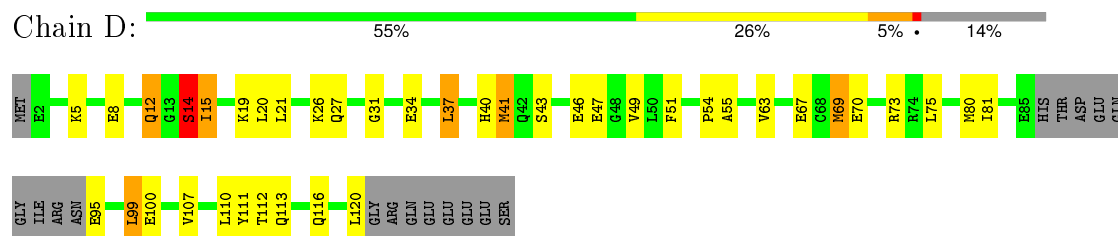
#### • Molecule 1: CHROMOSOME REPLICATION INITIATION PROTEIN



#### • Molecule 1: CHROMOSOME REPLICATION INITIATION PROTEIN



#### • Molecule 1: CHROMOSOME REPLICATION INITIATION PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.51Å 124.71Å 157.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.49 – 2.30 27.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (27.49-2.30) 97.4 (27.49-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.93 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.217 , 0.223 0.215 , 0.219	Depositor DCC
$R_{free}$ test set	2485 reflections (11.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	13 of 49039 reflections (0.027%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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 80.31 % 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 4.6013e-07. 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	1.67	13/893 (1.5%)	1.42	9/1202 (0.7%)
1	B	1.62	15/885 (1.7%)	1.24	3/1191 (0.3%)
1	C	1.62	12/877 (1.4%)	1.26	8/1181 (0.7%)
1	D	1.66	16/877 (1.8%)	1.30	4/1181 (0.3%)
All	All	1.64	56/3532 (1.6%)	1.31	24/4755 (0.5%)

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	C	0	1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TYR	CE2-CZ	9.62	1.51	1.38
1	B	111	TYR	CD2-CE2	9.06	1.52	1.39
1	A	59	GLU	CG-CD	8.53	1.64	1.51
1	A	72	VAL	CB-CG2	8.40	1.70	1.52
1	D	14	SER	CB-OG	-7.96	1.31	1.42
1	B	100	GLU	CG-CD	7.15	1.62	1.51
1	D	67	GLU	CD-OE1	7.04	1.33	1.25
1	D	100	GLU	CG-CD	7.02	1.62	1.51
1	B	74	ARG	CG-CD	6.90	1.69	1.51
1	B	27	GLN	CG-CD	6.80	1.66	1.51
1	A	103	TRP	CE3-CZ3	6.72	1.49	1.38
1	D	111	TYR	CE2-CZ	6.71	1.47	1.38
1	C	111	TYR	CG-CD1	6.70	1.47	1.39
1	C	67	GLU	CB-CG	-6.70	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	TYR	CE2-CZ	6.69	1.47	1.38
1	A	36	VAL	CB-CG1	6.66	1.66	1.52
1	C	43	SER	CB-OG	-6.64	1.33	1.42
1	C	111	TYR	CD1-CE1	6.55	1.49	1.39
1	C	67	GLU	CD-OE1	6.52	1.32	1.25
1	B	111	TYR	CD1-CE1	6.52	1.49	1.39
1	A	27	GLN	CG-CD	6.39	1.65	1.51
1	D	69	MET	CG-SD	6.27	1.97	1.81
1	C	111	TYR	CD2-CE2	6.23	1.48	1.39
1	A	74	ARG	CG-CD	6.20	1.67	1.51
1	D	63	VAL	CB-CG1	6.08	1.65	1.52
1	B	46	GLU	CD-OE2	6.07	1.32	1.25
1	D	67	GLU	CD-OE2	5.96	1.32	1.25
1	C	69	MET	CG-SD	5.94	1.96	1.81
1	C	100	GLU	CG-CD	5.94	1.60	1.51
1	A	113	GLN	CG-CD	5.92	1.64	1.51
1	A	8	GLU	CD-OE2	5.92	1.32	1.25
1	D	70	GLU	CG-CD	5.89	1.60	1.51
1	D	55	ALA	CA-CB	5.88	1.64	1.52
1	D	43	SER	CB-OG	-5.87	1.34	1.42
1	D	70	GLU	CD-OE1	5.86	1.32	1.25
1	B	119	GLU	CG-CD	5.81	1.60	1.51
1	D	34	GLU	CB-CG	5.79	1.63	1.52
1	B	23	GLY	CA-C	5.78	1.61	1.51
1	C	67	GLU	CD-OE2	5.76	1.31	1.25
1	A	56	GLU	CB-CG	5.69	1.62	1.52
1	A	49	VAL	CB-CG2	5.62	1.64	1.52
1	C	111	TYR	CE1-CZ	-5.55	1.31	1.38
1	B	70	GLU	CG-CD	5.46	1.60	1.51
1	B	111	TYR	CG-CD1	5.44	1.46	1.39
1	A	111	TYR	CE2-CZ	5.43	1.45	1.38
1	B	103	TRP	CE3-CZ3	5.38	1.47	1.38
1	D	49	VAL	CB-CG2	5.37	1.64	1.52
1	A	50	LEU	C-O	5.33	1.33	1.23
1	A	26	LYS	CE-NZ	5.30	1.62	1.49
1	D	46	GLU	CD-OE2	5.22	1.31	1.25
1	B	70	GLU	CD-OE1	5.19	1.31	1.25
1	D	8	GLU	CD-OE2	5.15	1.31	1.25
1	B	65	ALA	CA-CB	5.11	1.63	1.52
1	B	95	GLU	CA-C	5.10	1.66	1.52
1	D	107	VAL	CB-CG2	5.03	1.63	1.52
1	C	10	LEU	C-O	-5.00	1.13	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	MET	CG-SD-CE	-15.55	75.31	100.20
1	A	60	ARG	NE-CZ-NH1	13.02	126.81	120.30
1	D	80	MET	CG-SD-CE	-11.55	81.72	100.20
1	A	60	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	C	80	MET	CG-SD-CE	-8.42	86.73	100.20
1	C	10	LEU	CA-CB-CG	7.33	132.15	115.30
1	C	67	GLU	OE1-CD-OE2	6.68	131.32	123.30
1	A	80	MET	CG-SD-CE	-6.50	89.80	100.20
1	B	80	MET	CG-SD-CE	-6.36	90.03	100.20
1	A	15	ILE	CG1-CB-CG2	-6.06	98.06	111.40
1	A	21	LEU	CB-CG-CD2	5.96	121.13	111.00
1	C	69	MET	CG-SD-CE	5.93	109.68	100.20
1	C	28	LEU	CA-CB-CG	5.85	128.75	115.30
1	D	21	LEU	CB-CG-CD2	5.74	120.76	111.00
1	C	41	MET	CA-CB-CG	5.65	122.90	113.30
1	B	95	GLU	N-CA-C	5.39	125.56	111.00
1	D	5	LYS	CD-CE-NZ	-5.37	99.36	111.70
1	B	27	GLN	CA-CB-CG	5.25	124.95	113.40
1	C	69	MET	CA-CB-CG	5.24	122.21	113.30
1	D	41	MET	CA-CB-CG	5.16	122.07	113.30
1	A	113	GLN	CA-CB-CG	5.11	124.63	113.40
1	A	69	MET	CG-SD-CE	5.10	108.36	100.20
1	A	60	ARG	CD-NE-CZ	5.04	130.66	123.60
1	C	119	GLU	CA-C-N	5.02	128.24	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	118	GLY	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	877	0	901	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	869	0	890	36	0
1	C	861	0	878	25	0
1	D	861	0	878	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	39	0	0	5	0
3	B	42	0	0	8	0
3	C	45	0	0	5	0
3	D	52	0	0	5	0
All	All	3650	0	3547	100	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 14.

All (100) 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:42:GLN:HG3	3:A:2021:HOH:O	1.23	1.31
1:D:69:MET:HG3	3:D:2039:HOH:O	1.38	1.23
1:A:73:ARG:HD2	3:A:2030:HOH:O	1.61	0.97
1:C:69:MET:HG3	3:C:2034:HOH:O	1.66	0.95
1:B:50:LEU:H	1:B:50:LEU:HD12	1.34	0.93
1:C:70:GLU:OE1	3:C:2035:HOH:O	1.94	0.85
1:B:27:GLN:OE1	1:B:109:HIS:NE2	2.07	0.85
1:A:73:ARG:CD	3:A:2030:HOH:O	2.26	0.79
1:B:54:PRO:HG2	1:B:69:MET:CE	2.18	0.73
1:D:12:GLN:HE21	1:D:12:GLN:HA	1.51	0.73
1:B:103:TRP:CZ3	1:B:106:LEU:HD23	2.26	0.71
1:B:54:PRO:HG2	1:B:69:MET:HE2	1.72	0.71
1:B:24:HIS:HD2	1:B:27:GLN:OE1	1.75	0.69
1:B:27:GLN:HG2	1:B:109:HIS:CE1	2.29	0.67
1:B:1:MET:HB3	3:B:2002:HOH:O	1.96	0.66
1:A:111:TYR:HD1	1:C:9:TRP:HH2	1.43	0.66
1:C:20:LEU:HD13	1:C:110:LEU:HD11	1.77	0.66
1:B:30:LEU:HD21	1:B:80:MET:HG3	1.78	0.65
1:A:57:LEU:O	1:A:61:MET:HE2	1.97	0.65
1:A:100:GLU:HB2	1:A:101:PRO:HD3	1.78	0.64
1:B:27:GLN:HG2	1:B:109:HIS:HE1	1.63	0.63
1:A:27:GLN:NE2	1:A:113:GLN:HE22	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:H	1:B:50:LEU:CD1	2.02	0.63
1:C:20:LEU:HD13	1:C:110:LEU:CD1	2.29	0.62
1:D:120:LEU:N	3:D:2051:HOH:O	2.32	0.62
1:B:118:GLY:O	1:B:119:GLU:HB2	1.98	0.62
1:B:60:ARG:NH1	3:B:2024:HOH:O	2.31	0.62
1:A:57:LEU:O	1:A:61:MET:CE	2.47	0.61
1:A:27:GLN:HE22	1:A:113:GLN:HE22	1.45	0.61
1:C:53:THR:OG1	1:C:56:GLU:HG3	2.02	0.59
1:A:9:TRP:HB3	1:C:20:LEU:HD11	1.84	0.59
1:C:10:LEU:O	1:C:10:LEU:HD12	2.02	0.59
1:B:103:TRP:CE3	1:B:106:LEU:HD23	2.38	0.58
1:A:84:GLU:HB2	1:A:96:LYS:HZ2	1.67	0.58
1:C:81:ILE:HG22	1:C:99:LEU:HD12	1.85	0.58
1:A:24:HIS:CE1	1:A:113:GLN:OE1	2.57	0.57
1:D:40:HIS:HD2	3:D:2027:HOH:O	1.88	0.56
1:B:69:MET:HG2	3:B:2013:HOH:O	2.05	0.56
1:A:67:GLU:O	1:A:71:MET:HG3	2.07	0.55
1:A:24:HIS:HE1	1:A:113:GLN:OE1	1.89	0.55
1:A:111:TYR:CD1	1:C:9:TRP:HH2	2.23	0.55
1:A:27:GLN:HE22	1:A:113:GLN:NE2	2.05	0.54
1:D:81:ILE:HG22	1:D:99:LEU:HD12	1.89	0.54
1:D:31:GLY:HA3	3:D:2023:HOH:O	2.07	0.54
1:A:103:TRP:CZ3	1:A:106:LEU:HD23	2.43	0.54
1:B:19:LYS:HE2	1:D:15:ILE:CD1	2.38	0.53
1:C:100:GLU:HB3	1:C:101:PRO:HD3	1.89	0.53
1:A:15:ILE:HD12	1:C:19:LYS:HE2	1.91	0.53
1:B:67:GLU:O	1:B:71:MET:HG3	2.09	0.53
1:A:73:ARG:CG	3:A:2030:HOH:O	2.57	0.52
1:A:73:ARG:HG2	3:A:2030:HOH:O	2.10	0.51
1:B:4:LYS:C	1:B:4:LYS:HD2	2.30	0.51
1:B:37:LEU:HD11	1:B:57:LEU:HD13	1.93	0.51
1:A:15:ILE:CD1	1:C:19:LYS:HE2	2.41	0.50
1:A:67:GLU:O	1:A:70:GLU:HB3	2.12	0.50
1:C:24:HIS:CE1	1:C:113:GLN:OE1	2.65	0.50
1:B:1:MET:CB	3:B:2002:HOH:O	2.57	0.50
1:B:9:TRP:HB3	1:D:20:LEU:HD11	1.94	0.50
1:A:99:LEU:O	1:A:102:LEU:HB3	2.12	0.49
1:A:57:LEU:HB2	1:A:68:CYS:SG	2.52	0.49
1:B:67:GLU:OE2	3:B:2031:HOH:O	2.19	0.48
1:B:54:PRO:HG2	1:B:69:MET:HE1	1.95	0.48
1:A:21:LEU:HD13	1:A:35:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ARG:NH2	3:C:2028:HOH:O	2.47	0.47
1:C:116:GLN:O	3:C:2045:HOH:O	2.21	0.47
1:B:15:ILE:HD12	1:D:19:LYS:CG	2.45	0.46
1:A:37:LEU:C	1:A:37:LEU:HD23	2.36	0.46
1:B:27:GLN:CG	1:B:109:HIS:CE1	2.98	0.46
1:B:20:LEU:HD21	1:D:12:GLN:HG3	1.97	0.46
1:B:74:ARG:HD2	3:B:2033:HOH:O	2.16	0.45
1:B:19:LYS:HE2	1:D:15:ILE:HD11	1.99	0.45
1:D:37:LEU:HD22	1:D:41:MET:HE1	1.98	0.44
1:D:26:LYS:HE2	1:D:26:LYS:HB3	1.81	0.44
1:A:99:LEU:HD23	1:A:102:LEU:HD23	1.98	0.44
1:A:9:TRP:HB3	1:C:20:LEU:CD1	2.48	0.44
1:C:61:MET:HE2	1:C:68:CYS:SG	2.57	0.44
1:C:60:ARG:CZ	3:C:2028:HOH:O	2.66	0.44
1:D:37:LEU:HD13	1:D:75:LEU:HD12	2.00	0.43
1:A:84:GLU:HB2	1:A:96:LYS:NZ	2.33	0.43
1:B:74:ARG:CD	3:B:2033:HOH:O	2.66	0.43
1:B:18:PRO:HA	1:D:14:SER:HB3	2.00	0.43
1:B:24:HIS:CD2	1:B:27:GLN:OE1	2.63	0.43
1:D:37:LEU:HD13	1:D:75:LEU:CD1	2.49	0.43
1:B:19:LYS:HE2	1:D:15:ILE:HD12	1.99	0.43
1:B:2:GLU:HB3	3:B:2001:HOH:O	2.18	0.43
1:C:27:GLN:HE21	1:C:27:GLN:HB2	1.69	0.43
1:A:98:THR:OG1	1:A:100:GLU:HG2	2.19	0.42
1:D:75:LEU:HB3	1:D:81:ILE:HG12	2.01	0.42
1:D:37:LEU:HD22	1:D:41:MET:CE	2.50	0.42
1:C:20:LEU:O	1:C:24:HIS:HD2	2.02	0.42
1:A:22:LEU:CD2	1:C:15:ILE:HD13	2.50	0.42
1:B:24:HIS:HD2	1:B:109:HIS:HE2	1.68	0.41
1:B:54:PRO:CG	1:B:69:MET:HE1	2.49	0.41
1:C:57:LEU:O	1:C:61:MET:HG3	2.20	0.41
1:C:99:LEU:O	1:C:102:LEU:N	2.53	0.41
1:D:112:THR:O	1:D:116:GLN:HG3	2.21	0.41
1:A:73:ARG:HD3	3:D:2052:HOH:O	2.21	0.41
1:A:19:LYS:CG	1:C:15:ILE:HD12	2.51	0.40
1:B:32:GLU:O	1:B:36:VAL:HG23	2.22	0.40
1:D:27:GLN:HG3	1:D:27:GLN:H	1.69	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	108/128 (84%)	107 (99%)	1 (1%)	0	100	100
1	B	107/128 (84%)	103 (96%)	3 (3%)	1 (1%)	21	24
1	C	106/128 (83%)	102 (96%)	3 (3%)	1 (1%)	21	24
1	D	106/128 (83%)	103 (97%)	3 (3%)	0	100	100
All	All	427/512 (83%)	415 (97%)	10 (2%)	2 (0%)	34	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119	GLU
1	C	119	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	92/108 (85%)	80 (87%)	12 (13%)	5	5
1	B	91/108 (84%)	80 (88%)	11 (12%)	6	6
1	C	90/108 (83%)	79 (88%)	11 (12%)	6	6
1	D	90/108 (83%)	78 (87%)	12 (13%)	5	5
All	All	363/432 (84%)	317 (87%)	46 (13%)	5	5

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	4	LYS
1	A	5	LYS
1	A	15	ILE
1	A	21	LEU
1	A	39	LEU
1	A	59	GLU
1	A	77	GLN
1	A	95	GLU
1	A	113	GLN
1	A	119	GLU
1	B	4	LYS
1	B	12	GLN
1	B	15	ILE
1	B	26	LYS
1	B	27	GLN
1	B	28	LEU
1	B	50	LEU
1	B	73	ARG
1	B	95	GLU
1	B	100	GLU
1	B	119	GLU
1	C	4	LYS
1	C	5	LYS
1	C	10	LEU
1	C	15	ILE
1	C	26	LYS
1	C	27	GLN
1	C	28	LEU
1	C	41	MET
1	C	60	ARG
1	C	73	ARG
1	C	99	LEU
1	D	12	GLN
1	D	14	SER
1	D	15	ILE
1	D	37	LEU
1	D	47	GLU
1	D	51	PHE
1	D	54	PRO
1	D	73	ARG
1	D	95	GLU

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Mol	Chain	Res	Type
1	D	99	LEU
1	D	110	LEU
1	D	113	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	27	GLN
1	B	24	HIS
1	C	24	HIS
1	D	12	GLN
1	D	24	HIS
1	D	40	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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	112/128 (87%)	0.07	5 (4%) 37 46	18, 33, 56, 66	0
1	B	111/128 (86%)	0.09	1 (0%) 85 89	18, 33, 55, 73	0
1	C	110/128 (85%)	-0.17	0 100 100	19, 30, 51, 59	0
1	D	110/128 (85%)	-0.18	0 100 100	20, 30, 49, 60	0
All	All	443/512 (86%)	-0.05	6 (1%) 78 83	18, 31, 52, 73	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	10.0
1	A	1	MET	4.0
1	A	121	GLY	3.3
1	A	73	ARG	2.8
1	A	85	GLU	2.4
1	A	66	ALA	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](#)

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	C	1120	1/1	0.97	0.12	-	18,18,18,18	0
2	MG	D	1120	1/1	0.97	0.07	-	23,23,23,23	0
2	MG	A	1120	1/1	0.93	0.10	-	35,35,35,35	0
2	MG	B	1120	1/1	0.90	0.10	-	21,21,21,21	0

## 6.5 Other polymers

There are no such residues in this entry.