



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:35 PM GMT

PDB ID : 1BKN  
Title : CRYSTAL STRUCTURE OF AN N-TERMINAL 40KD FRAGMENT OF E.  
COLI DNA MISMATCH REPAIR PROTEIN MUTL  
Authors : Yang, W.; Ban, C.  
Deposited on : 1998-07-09  
Resolution : 2.90 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

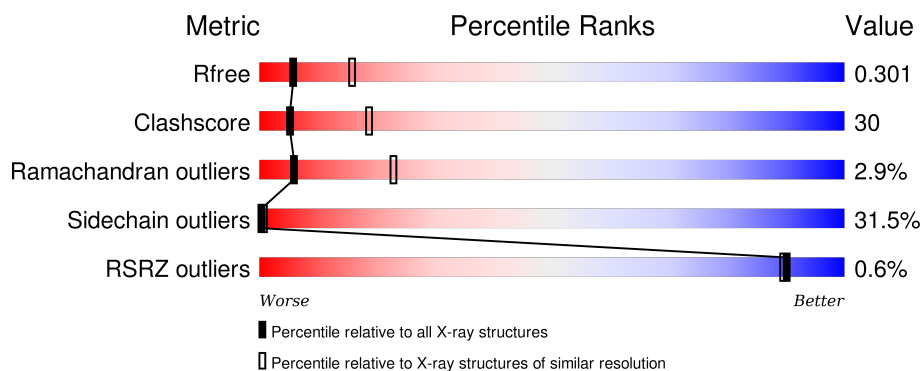
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	352	
1	B	352	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4292 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 MUTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2120	1329	385	400	6			
1	B	271	Total	C	N	O	S	0	0	0
			2117	1326	388	396	7			

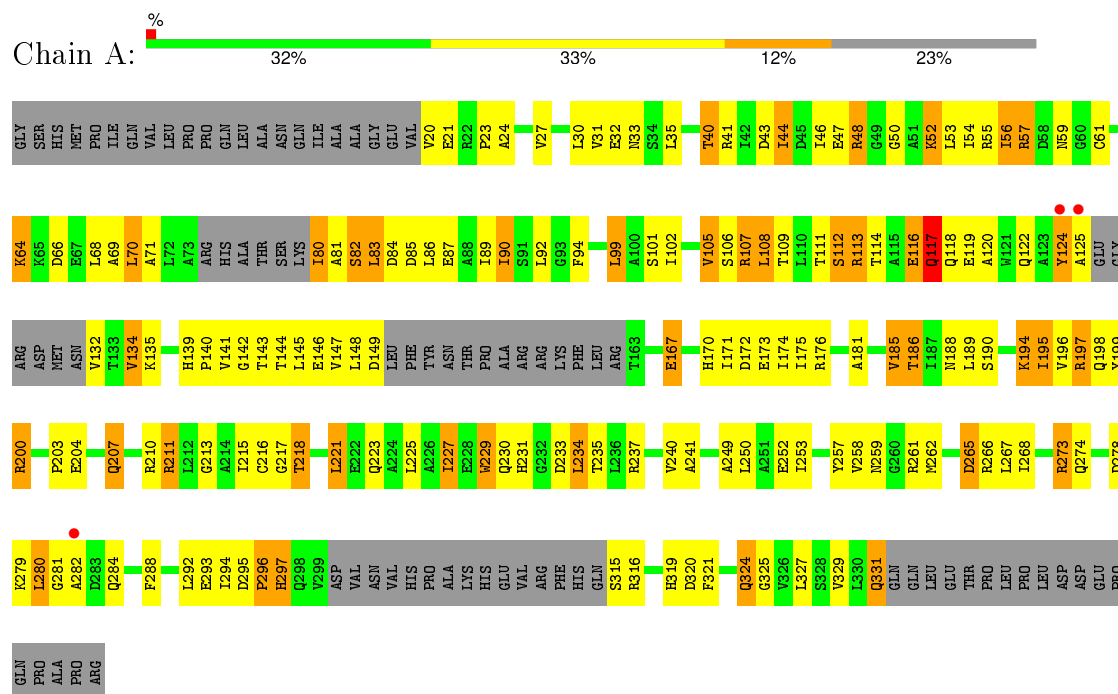
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	24	Total	O	0	0
			24	24		

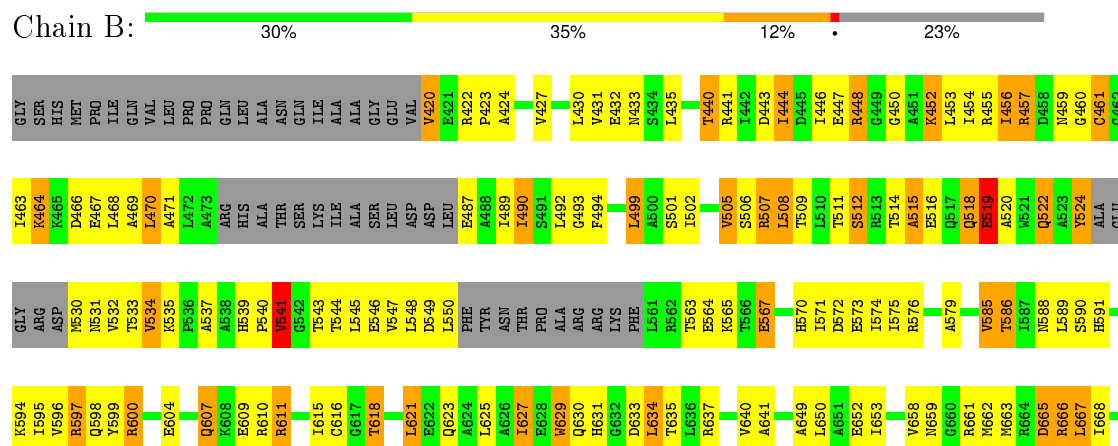
### 3 Residue-property plots

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: MUTL



#### • Molecule 1: MUTL



ASP	R673
ASP	R674
GLU	R678
PRO	K679
GLN	L680
PRO	G681
ALA	A682
PRO	D683
ARG	Q684
	F688
	L692
	E693
	I694
	D695
	P696
	H697
	Q698
	V699
ASP	VAL
ASN	VAL
VAL	HIS
PRO	PRO
ALA	ALA
LYS	LYS
HIS	HIS
GLU	GLU
VAL	VAL
ARG	ARG
PHI	PHI
	H713
	Q714
	S715
	R716
	H719
	D720
	F721
	Q724
	G725
	V726
	L727
	S728
	V729
	L730
	Q731
	GLN
	GLN
	LEU
	GLU
	THR
	PRO
	LEU
	PRO
	LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.20 Å 93.20 Å 221.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 28.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.90) 96.4 (28.19-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.72 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.248 , 0.300 0.254 , 0.301	Depositor DCC
$R_{free}$ test set	964 reflections (4.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.5	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 69.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 24322 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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	0.32	0/2149	0.52	0/2907
1	B	0.32	0/2147	0.52	0/2903
All	All	0.32	0/4296	0.52	0/5810

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	2120	0	2131	131	0
1	B	2117	0	2120	130	1
2	A	31	0	0	2	0
2	B	24	0	0	3	0
All	All	4292	0	4251	258	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 30.

All (258) 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:B:634:LEU:HD22	1:B:694:ILE:HG22	1.32	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD22	1:A:294:ILE:HG22	1.34	1.05
1:A:186:THR:HG23	1:A:200:ARG:HA	1.46	0.98
1:A:227:ILE:HB	1:A:329:VAL:HG21	1.54	0.90
1:B:586:THR:HG23	1:B:600:ARG:HA	1.53	0.89
1:A:113:ARG:HB2	1:A:120:ALA:HA	1.54	0.89
1:A:80:ILE:HG12	1:A:83:LEU:HD11	1.56	0.85
1:A:86:LEU:HB3	1:A:89:ILE:HD11	1.57	0.85
1:B:597:ARG:HH11	1:B:597:ARG:HB3	1.42	0.83
1:A:27:VAL:HG21	1:A:171:ILE:HG12	1.62	0.81
1:B:427:VAL:HG21	1:B:571:ILE:HG12	1.61	0.81
1:B:627:ILE:HB	1:B:729:VAL:HG21	1.64	0.79
1:A:197:ARG:HH11	1:A:197:ARG:HB3	1.47	0.79
1:A:70:LEU:HD13	1:A:70:LEU:H	1.50	0.77
1:A:125:ALA:HB2	1:A:132:VAL:HG22	1.69	0.74
1:A:273:ARG:CZ	1:A:273:ARG:HB2	2.18	0.73
1:B:680:LEU:HD12	1:B:682:ALA:HB3	1.71	0.72
1:A:47:GLU:HB2	1:A:53:LEU:HB3	1.72	0.72
1:A:280:LEU:HD12	1:A:282:ALA:HB3	1.72	0.71
1:A:99:LEU:HA	1:A:102:ILE:HD12	1.71	0.71
1:B:673:ARG:CZ	1:B:673:ARG:HB2	2.19	0.70
1:A:90:ILE:HD13	1:A:90:ILE:H	1.54	0.70
1:B:470:LEU:HD13	1:B:470:LEU:H	1.55	0.70
1:B:447:GLU:HB2	1:B:453:LEU:HB3	1.74	0.69
1:B:522:GLN:O	1:B:534:VAL:HA	1.92	0.68
1:A:86:LEU:HB3	1:A:89:ILE:CD1	2.23	0.68
1:B:493:GLY:HA3	2:B:816:HOH:O	1.93	0.68
1:A:23:PRO:HG3	1:A:167:GLU:HG3	1.76	0.67
1:B:616:CYS:HB3	1:B:653:ILE:HD13	1.77	0.67
1:A:80:ILE:HG12	1:A:83:LEU:CD1	2.25	0.67
1:A:197:ARG:HD3	1:A:199:TYR:OH	1.95	0.67
1:B:665:ASP:HB2	1:B:668:ILE:HD12	1.78	0.66
1:B:597:ARG:HD3	1:B:599:TYR:OH	1.95	0.66
1:B:499:LEU:HA	1:B:502:ILE:HD12	1.78	0.66
1:B:490:ILE:H	1:B:490:ILE:HD13	1.60	0.66
1:B:424:ALA:HB1	1:B:574:ILE:HD12	1.77	0.66
1:A:196:VAL:HG12	1:A:197:ARG:HG2	1.78	0.65
1:A:216:CYS:HB3	1:A:253:ILE:HD13	1.78	0.65
1:B:731:GLN:HE21	1:B:731:GLN:HA	1.62	0.65
1:B:596:VAL:HG12	1:B:597:ARG:HG2	1.79	0.64
1:A:54:ILE:HB	1:A:147:VAL:HB	1.80	0.64
1:B:446:ILE:HD12	1:B:589:LEU:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:PRO:HG3	1:B:567:GLU:HG3	1.80	0.63
1:A:265:ASP:HB2	1:A:268:ILE:HD12	1.80	0.63
1:B:430:LEU:HD21	1:B:502:ILE:HD13	1.80	0.63
1:B:516:GLU:HB3	1:B:518:GLN:HG3	1.81	0.62
1:B:607:GLN:OE1	1:B:609:GLU:HB2	2.00	0.62
1:B:524:TYR:HB2	1:B:533:THR:OG1	1.98	0.62
1:A:32:GLU:HA	1:A:35:LEU:HD12	1.82	0.61
1:A:296:PRO:HD3	2:A:838:HOH:O	1.99	0.61
1:B:630:GLN:O	1:B:631:HIS:HD2	1.83	0.61
1:A:230:GLN:O	1:A:231:HIS:HD2	1.83	0.61
1:A:234:LEU:HB3	1:A:321:PHE:CE2	2.36	0.60
1:B:446:ILE:CD1	1:B:571:ILE:HG21	2.30	0.60
1:A:23:PRO:CG	1:A:167:GLU:HG3	2.31	0.60
1:A:86:LEU:HB3	1:A:89:ILE:CG1	2.31	0.60
1:B:524:TYR:O	1:B:532:VAL:HA	2.02	0.60
1:A:297:HIS:HB3	2:A:819:HOH:O	2.01	0.60
1:A:89:ILE:HD12	1:A:90:ILE:N	2.17	0.60
1:B:432:GLU:HA	1:B:435:LEU:HD12	1.83	0.60
1:B:539:HIS:ND1	1:B:540:PRO:HD2	2.17	0.59
1:A:108:LEU:HD13	1:A:109:THR:N	2.18	0.59
1:A:80:ILE:O	1:A:83:LEU:HG	2.02	0.58
1:A:46:ILE:HG23	1:A:50:GLY:HA2	1.84	0.58
1:B:506:SER:OG	1:B:547:VAL:HG13	2.03	0.58
1:A:223:GLN:O	1:A:241:ALA:HA	2.03	0.58
1:B:623:GLN:O	1:B:641:ALA:HA	2.02	0.58
1:A:83:LEU:HA	1:A:86:LEU:HD12	1.86	0.58
1:B:508:LEU:HD13	1:B:509:THR:N	2.18	0.58
1:A:176:ARG:HG3	1:A:215:ILE:CG2	2.34	0.57
1:A:106:SER:CB	1:A:149:ASP:HA	2.34	0.57
1:B:516:GLU:HB3	1:B:518:GLN:CG	2.34	0.57
1:A:52:LYS:O	1:A:148:LEU:HA	2.04	0.57
1:B:713:HIS:HA	1:B:716:ARG:HB3	1.86	0.57
1:A:24:ALA:HB1	1:A:174:ILE:HD12	1.86	0.57
1:B:430:LEU:HB2	1:B:456:ILE:HD13	1.87	0.57
1:B:611:ARG:O	1:B:615:ILE:HG13	2.05	0.57
1:B:446:ILE:HD13	1:B:571:ILE:HD13	1.86	0.57
1:A:211:ARG:O	1:A:215:ILE:HG13	2.04	0.57
1:B:564:GLU:HG3	1:B:565:LYS:N	2.20	0.56
1:A:46:ILE:HD12	1:A:189:LEU:HD11	1.87	0.56
1:B:683:ASP:HB3	2:B:826:HOH:O	2.05	0.56
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HB2	1:A:56:ILE:HD13	1.88	0.55
1:B:634:LEU:HD23	1:B:634:LEU:N	2.22	0.55
1:A:320:ASP:O	1:A:324:GLN:HB2	2.06	0.55
1:B:634:LEU:CD2	1:B:694:ILE:HG22	2.22	0.55
1:B:727:LEU:HD12	1:B:727:LEU:O	2.07	0.55
1:B:585:VAL:O	1:B:611:ARG:NH2	2.40	0.55
1:B:720:ASP:O	1:B:724:GLN:HB2	2.08	0.54
1:A:24:ALA:HA	1:A:171:ILE:HG13	1.89	0.54
1:B:446:ILE:HG23	1:B:450:GLY:HA2	1.88	0.54
1:B:457:ARG:HA	1:B:543:THR:O	2.07	0.54
1:A:125:ALA:CB	1:A:132:VAL:HG22	2.37	0.54
1:B:499:LEU:HD11	1:B:545:LEU:CD2	2.38	0.54
1:A:64:LYS:HE3	1:A:114:THR:HG21	1.88	0.54
1:A:234:LEU:HD23	1:A:234:LEU:N	2.23	0.54
1:A:106:SER:HB2	1:A:149:ASP:HA	1.90	0.54
1:B:607:GLN:HA	1:B:607:GLN:NE2	2.22	0.54
1:B:489:ILE:HD12	1:B:490:ILE:N	2.24	0.53
1:B:423:PRO:CG	1:B:567:GLU:HG3	2.38	0.53
1:A:185:VAL:O	1:A:211:ARG:NH2	2.42	0.53
1:B:649:ALA:O	1:B:652:GLU:HB2	2.09	0.53
1:B:440:THR:HG23	1:B:441:ARG:HG3	1.90	0.53
1:A:249:ALA:O	1:A:252:GLU:HB2	2.09	0.53
1:A:55:ARG:HA	1:A:145:LEU:O	2.09	0.53
1:A:316:ARG:O	1:A:319:HIS:HB3	2.09	0.52
1:A:140:PRO:O	1:A:142:GLY:N	2.42	0.52
1:A:194:LYS:NZ	1:B:600:ARG:HE	2.08	0.52
1:B:487:GLU:O	1:B:490:ILE:HD13	2.10	0.52
1:A:327:LEU:O	1:A:327:LEU:HD12	2.09	0.52
1:A:70:LEU:HD22	1:A:71:ALA:N	2.25	0.52
1:B:489:ILE:HD12	1:B:490:ILE:HG23	1.92	0.51
1:B:731:GLN:CA	1:B:731:GLN:HE21	2.21	0.51
1:A:234:LEU:CD2	1:A:294:ILE:HG22	2.24	0.51
1:B:634:LEU:HB3	1:B:721:PHE:CE2	2.46	0.51
1:B:629:TRP:CE2	1:B:725:GLY:HA2	2.46	0.51
1:B:433:ASN:HD22	1:B:433:ASN:N	2.09	0.51
1:A:86:LEU:HD13	1:A:89:ILE:HD11	1.93	0.51
1:A:327:LEU:O	1:A:331:GLN:HG3	2.11	0.51
1:A:113:ARG:HB2	1:A:120:ALA:CA	2.35	0.51
1:B:470:LEU:HD22	1:B:471:ALA:N	2.26	0.51
1:A:108:LEU:HD13	1:A:109:THR:H	1.76	0.50
1:A:89:ILE:HD12	1:A:90:ILE:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:ARG:O	1:B:719:HIS:HB3	2.10	0.50
1:A:173:GLU:O	1:A:176:ARG:HB3	2.12	0.50
1:A:86:LEU:O	1:A:89:ILE:HG13	2.12	0.50
1:B:679:LYS:HD3	1:B:680:LEU:HD23	1.94	0.50
1:A:44:ILE:O	1:A:44:ILE:HG13	2.12	0.50
1:B:534:VAL:O	1:B:534:VAL:CG1	2.59	0.50
1:A:116:GLU:O	1:A:117:GLN:C	2.50	0.50
1:A:33:ASN:N	1:A:33:ASN:HD22	2.09	0.50
1:A:279:LYS:HD3	1:A:280:LEU:HD23	1.94	0.49
1:A:118:GLN:HG2	1:A:119:GLU:O	2.13	0.49
1:A:172:ASP:OD1	1:A:197:ARG:HD2	2.12	0.49
1:A:50:GLY:O	1:A:54:ILE:HG13	2.13	0.49
1:B:573:GLU:O	1:B:576:ARG:HB3	2.13	0.49
1:B:422:ARG:HB3	1:B:423:PRO:HD2	1.95	0.49
1:A:295:ASP:OD1	1:A:296:PRO:HD2	2.13	0.48
1:B:515:ALA:HA	1:B:541:VAL:CG1	2.42	0.48
1:A:40:THR:HG23	1:A:41:ARG:HG3	1.94	0.48
1:A:229:TRP:CE2	1:A:325:GLY:HA2	2.48	0.48
1:A:70:LEU:H	1:A:70:LEU:CD1	2.24	0.48
1:B:665:ASP:CB	1:B:668:ILE:HD12	2.43	0.48
1:B:446:ILE:O	1:B:591:HIS:HD2	1.96	0.48
1:B:514:THR:O	1:B:516:GLU:N	2.44	0.48
1:B:512:SER:HB2	1:B:543:THR:HG23	1.96	0.48
1:B:487:GLU:O	1:B:490:ILE:CD1	2.61	0.48
1:B:550:LEU:HD12	1:B:550:LEU:O	2.14	0.48
1:A:40:THR:HG22	1:A:59:ASN:ND2	2.29	0.48
1:A:23:PRO:HD2	1:A:167:GLU:OE2	2.13	0.47
1:B:576:ARG:HG3	1:B:615:ILE:CG2	2.43	0.47
1:A:194:LYS:HZ3	1:B:600:ARG:HE	1.61	0.47
1:A:106:SER:OG	1:A:147:VAL:HG13	2.14	0.47
1:B:544:THR:C	1:B:545:LEU:HD12	2.34	0.47
1:B:650:LEU:C	1:B:652:GLU:H	2.18	0.47
1:B:572:ASP:OD1	1:B:597:ARG:HD2	2.14	0.47
1:B:508:LEU:HD13	1:B:509:THR:H	1.78	0.47
1:B:450:GLY:O	1:B:454:ILE:HG13	2.15	0.47
1:B:727:LEU:O	1:B:731:GLN:HG2	2.15	0.47
1:B:440:THR:HG22	1:B:459:ASN:ND2	2.29	0.47
1:B:588:ASN:OD1	1:B:598:GLN:HG3	2.15	0.47
1:B:507:ARG:HB2	1:B:548:LEU:HD13	1.95	0.47
1:A:46:ILE:CD1	1:A:171:ILE:HG21	2.44	0.47
1:A:107:ARG:HB2	1:A:148:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:LEU:N	1:B:634:LEU:CD2	2.77	0.46
1:B:444:ILE:O	1:B:444:ILE:HG13	2.12	0.46
1:B:463:ILE:CG2	1:B:467:GLU:HB2	2.45	0.46
1:A:44:ILE:HB	1:A:56:ILE:HG13	1.98	0.46
1:A:250:LEU:C	1:A:252:GLU:H	2.18	0.46
1:B:505:VAL:O	1:B:505:VAL:HG12	2.16	0.46
1:A:234:LEU:CD2	1:A:234:LEU:N	2.78	0.46
1:B:433:ASN:ND2	1:B:433:ASN:N	2.64	0.46
1:A:188:ASN:OD1	1:A:198:GLN:HG3	2.16	0.46
1:B:680:LEU:C	1:B:682:ALA:H	2.19	0.46
1:A:181:ALA:HB2	1:A:257:TYR:CE2	2.51	0.46
1:A:265:ASP:CB	1:A:268:ILE:HD12	2.46	0.46
1:A:229:TRP:HD1	1:A:321:PHE:CE1	2.34	0.46
1:A:108:LEU:HD22	1:A:147:VAL:HG22	1.97	0.46
1:A:31:VAL:O	1:A:35:LEU:HD12	2.16	0.45
1:A:86:LEU:CB	1:A:89:ILE:HD11	2.39	0.45
1:A:134:VAL:CG1	1:A:134:VAL:O	2.64	0.45
1:B:695:ASP:OD1	1:B:696:PRO:HD2	2.17	0.45
1:B:679:LYS:HG3	1:B:730:LEU:HB3	1.97	0.45
1:A:33:ASN:ND2	1:A:33:ASN:N	2.64	0.45
1:B:519:GLU:HG3	1:B:519:GLU:H	1.39	0.45
1:A:44:ILE:HD11	1:A:46:ILE:HG13	1.99	0.44
1:A:280:LEU:C	1:A:282:ALA:H	2.20	0.44
1:B:431:VAL:O	1:B:435:LEU:HD12	2.17	0.44
1:B:440:THR:HG22	1:B:459:ASN:HD21	1.82	0.44
1:A:124:TYR:O	1:A:132:VAL:N	2.50	0.44
1:B:534:VAL:HG12	1:B:534:VAL:O	2.18	0.44
1:A:324:GLN:NE2	1:A:324:GLN:HA	2.33	0.44
1:A:288:PHE:CD1	1:A:288:PHE:C	2.90	0.44
1:A:186:THR:HA	1:A:199:TYR:O	2.17	0.44
1:A:124:TYR:O	1:A:125:ALA:HB3	2.17	0.44
1:B:692:LEU:HD12	1:B:693:GLU:H	1.82	0.44
1:B:597:ARG:NH1	1:B:597:ARG:HB3	2.21	0.43
1:B:470:LEU:H	1:B:470:LEU:CD1	2.28	0.43
1:A:112:SER:HB2	1:A:143:THR:HG23	1.98	0.43
1:A:24:ALA:HA	1:A:171:ILE:CG1	2.48	0.43
1:B:454:ILE:HB	1:B:547:VAL:HB	2.00	0.43
1:B:508:LEU:HD22	1:B:547:VAL:HG22	2.00	0.43
1:A:225:LEU:HB2	1:A:240:VAL:O	2.19	0.43
1:B:625:LEU:HB2	1:B:640:VAL:O	2.18	0.43
1:A:194:LYS:HD3	2:B:815:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ILE:O	1:B:591:HIS:HA	2.19	0.43
1:B:520:ALA:HB3	1:B:537:ALA:O	2.19	0.43
1:A:57:ARG:HA	1:A:143:THR:O	2.19	0.43
1:B:699:VAL:HG21	1:B:715:SER:OG	2.19	0.43
1:B:460:GLY:O	1:B:461:CYS:C	2.56	0.43
1:A:325:GLY:O	1:A:329:VAL:HG23	2.18	0.43
1:A:48:ARG:HB2	1:A:52:LYS:HB2	2.00	0.43
1:B:618:THR:HA	1:B:621:LEU:HB3	2.01	0.43
1:A:292:LEU:HD12	1:A:293:GLU:H	1.82	0.43
1:B:444:ILE:HD11	1:B:446:ILE:HG13	2.01	0.43
1:B:499:LEU:HD13	1:B:499:LEU:HA	1.86	0.43
1:A:134:VAL:HG12	1:A:134:VAL:O	2.19	0.43
1:A:124:TYR:OH	1:B:519:GLU:HG2	2.19	0.43
1:B:579:ALA:O	1:B:611:ARG:NH1	2.51	0.43
1:A:82:SER:O	1:A:86:LEU:HG	2.18	0.42
1:B:724:GLN:HA	1:B:724:GLN:NE2	2.34	0.42
1:A:174:ILE:HG22	1:A:175:ILE:N	2.33	0.42
1:B:539:HIS:CG	1:B:540:PRO:HD2	2.54	0.42
1:B:574:ILE:HG22	1:B:575:ILE:N	2.35	0.42
1:B:464:LYS:HE3	1:B:514:THR:HG21	2.01	0.42
1:A:213:GLY:O	1:A:217:GLY:N	2.53	0.42
1:B:448:ARG:HB2	1:B:452:LYS:HB2	2.02	0.42
1:B:543:THR:HG22	1:B:544:THR:N	2.35	0.42
1:A:218:THR:HA	1:A:221:LEU:HB3	2.01	0.42
1:B:666:ARG:HG2	1:B:667:LEU:N	2.35	0.42
1:A:144:THR:C	1:A:145:LEU:HD12	2.40	0.41
1:A:40:THR:HG22	1:A:59:ASN:HD21	1.84	0.41
1:A:295:ASP:O	1:A:296:PRO:C	2.59	0.41
1:B:688:PHE:C	1:B:688:PHE:CD1	2.93	0.41
1:A:20:VAL:HG23	1:A:20:VAL:O	2.20	0.41
1:B:456:ILE:O	1:B:544:THR:HA	2.21	0.41
1:A:105:VAL:HG12	1:A:105:VAL:O	2.20	0.41
1:B:680:LEU:O	1:B:682:ALA:N	2.53	0.41
1:B:455:ARG:HA	1:B:545:LEU:O	2.21	0.41
1:B:629:TRP:HD1	1:B:721:PHE:CE1	2.39	0.41
1:B:586:THR:HA	1:B:599:TYR:O	2.19	0.41
1:A:56:ILE:O	1:A:144:THR:HA	2.21	0.41
1:A:280:LEU:O	1:A:282:ALA:N	2.54	0.41
1:B:658:VAL:HG23	1:B:663:MET:HB2	2.02	0.41
1:A:106:SER:HB3	1:A:149:ASP:HA	2.03	0.41
1:B:658:VAL:O	1:B:659:ASN:HB2	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ASN:ND2	1:B:433:ASN:H	2.20	0.40
1:A:171:ILE:O	1:A:175:ILE:HG12	2.21	0.40
1:B:446:ILE:HD11	1:B:571:ILE:HG21	2.02	0.40
1:A:250:LEU:C	1:A:252:GLU:N	2.74	0.40
1:A:139:HIS:ND1	1:A:140:PRO:HD2	2.36	0.40
1:A:81:ALA:O	1:A:84:ASP:HB2	2.22	0.40
1:B:456:ILE:O	1:B:456:ILE:HG22	2.20	0.40
1:B:650:LEU:C	1:B:652:GLU:N	2.74	0.40
1:A:195:ILE:HG22	1:A:195:ILE:O	2.21	0.40
1:A:258:VAL:O	1:A:259:ASN:HB2	2.21	0.40
1:A:279:LYS:HD3	1:A:280:LEU:CD2	2.52	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:B:420:VAL:CG2	1:B:420:VAL:CG2[6_855]	2.08	0.12

## 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	262/352 (74%)	218 (83%)	37 (14%)	7 (3%)	6	25
1	B	261/352 (74%)	214 (82%)	39 (15%)	8 (3%)	5	21
All	All	523/704 (74%)	432 (83%)	76 (14%)	15 (3%)	6	23

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	141	VAL

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Mol	Chain	Res	Type
1	B	515	ALA
1	B	519	GLU
1	B	541	VAL
1	A	69	ALA
1	A	296	PRO
1	B	469	ALA
1	B	696	PRO
1	B	461	CYS
1	B	681	GLY
1	A	105	VAL
1	A	281	GLY
1	B	505	VAL
1	A	203	PRO

### 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	223/293 (76%)	153 (69%)	70 (31%)	0	1
1	B	222/293 (76%)	152 (68%)	70 (32%)	0	1
All	All	445/586 (76%)	305 (68%)	140 (32%)	0	1

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	40	THR
1	A	43	ASP
1	A	44	ILE
1	A	48	ARG
1	A	52	LYS
1	A	56	ILE
1	A	57	ARG
1	A	61	CYS
1	A	64	LYS

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Mol	Chain	Res	Type
1	A	66	ASP
1	A	68	LEU
1	A	70	LEU
1	A	80	ILE
1	A	82	SER
1	A	83	LEU
1	A	85	ASP
1	A	87	GLU
1	A	90	ILE
1	A	92	LEU
1	A	94	PHE
1	A	99	LEU
1	A	101	SER
1	A	107	ARG
1	A	108	LEU
1	A	111	THR
1	A	112	SER
1	A	113	ARG
1	A	116	GLU
1	A	117	GLN
1	A	122	GLN
1	A	124	TYR
1	A	134	VAL
1	A	135	LYS
1	A	146	GLU
1	A	167	GLU
1	A	170	HIS
1	A	185	VAL
1	A	186	THR
1	A	190	SER
1	A	194	LYS
1	A	195	ILE
1	A	197	ARG
1	A	200	ARG
1	A	204	GLU
1	A	207	GLN
1	A	210	ARG
1	A	211	ARG
1	A	218	THR
1	A	221	LEU
1	A	227	ILE
1	A	229	TRP

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Mol	Chain	Res	Type
1	A	233	ASP
1	A	234	LEU
1	A	235	THR
1	A	237	ARG
1	A	261	ARG
1	A	262	MET
1	A	265	ASP
1	A	266	ARG
1	A	267	LEU
1	A	273	ARG
1	A	274	GLN
1	A	278	ASP
1	A	280	LEU
1	A	284	GLN
1	A	297	HIS
1	A	315	SER
1	A	324	GLN
1	A	331	GLN
1	B	420	VAL
1	B	440	THR
1	B	443	ASP
1	B	444	ILE
1	B	448	ARG
1	B	452	LYS
1	B	456	ILE
1	B	457	ARG
1	B	464	LYS
1	B	466	ASP
1	B	468	LEU
1	B	470	LEU
1	B	490	ILE
1	B	492	LEU
1	B	494	PHE
1	B	499	LEU
1	B	501	SER
1	B	507	ARG
1	B	508	LEU
1	B	511	THR
1	B	512	SER
1	B	518	GLN
1	B	519	GLU
1	B	522	GLN

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Mol	Chain	Res	Type
1	B	524	TYR
1	B	530	MET
1	B	531	ASN
1	B	534	VAL
1	B	535	LYS
1	B	541	VAL
1	B	546	GLU
1	B	549	ASP
1	B	563	THR
1	B	567	GLU
1	B	570	HIS
1	B	585	VAL
1	B	586	THR
1	B	590	SER
1	B	594	LYS
1	B	595	ILE
1	B	597	ARG
1	B	600	ARG
1	B	604	GLU
1	B	607	GLN
1	B	610	ARG
1	B	611	ARG
1	B	618	THR
1	B	621	LEU
1	B	627	ILE
1	B	629	TRP
1	B	633	ASP
1	B	634	LEU
1	B	635	THR
1	B	637	ARG
1	B	661	ARG
1	B	662	MET
1	B	665	ASP
1	B	666	ARG
1	B	667	LEU
1	B	673	ARG
1	B	674	GLN
1	B	678	ASP
1	B	680	LEU
1	B	684	GLN
1	B	697	HIS
1	B	714	GLN

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Mol	Chain	Res	Type
1	B	715	SER
1	B	724	GLN
1	B	728	SER
1	B	731	GLN

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

Mol	Chain	Res	Type
1	A	33	ASN
1	A	231	HIS
1	A	245	HIS
1	A	269	ASN
1	B	433	ASN
1	B	591	HIS
1	B	631	HIS
1	B	645	HIS
1	B	669	ASN
1	B	731	GLN

### 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 [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	272/352 (77%)	0.00	3 (1%) 82 80	26, 76, 100, 100	0
1	B	271/352 (76%)	0.02	0 100 100	25, 78, 100, 100	0
All	All	543/704 (77%)	0.01	3 (0%) 90 89	25, 77, 100, 100	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	ALA	6.6
1	A	282	ALA	2.5
1	A	124	TYR	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.