



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 07:01 AM EST

PDB ID : 1T94  
Title : Crystal structure of the catalytic core of human DNA polymerase kappa  
Authors : Uljon, S.N.; Johnson, R.E.; Edwards, T.A.; Prakash, S.; Prakash, L.; Aggarwal, A.K.  
Deposited on : 2004-05-14  
Resolution : 2.40 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](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.

---

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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

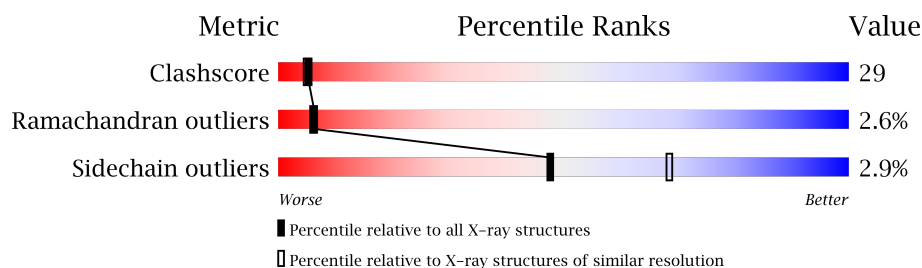
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	459	
1	B	459	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6532 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 polymerase (DNA directed) kappa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3185	2012	557	597	19			
1	B	382	Total	C	N	O	S	0	0	0
			2987	1889	525	555	18			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	187	Total	O	0	0
			187	187		
2	B	173	Total	O	0	0
			173	173		



I478	I480	I481	I482	I483	I484	I485	I486	I487	I488	I489	I490	I491	I492	I493	I494	I495	I496	I497	I498	I499	I500	I501	I502	I503	I504	I505	I506	I507	I508	I509	I510	I511	I512	I513	I514	I515	I516	I517	ASN	GLU	GLU	ASP	ARG	LYS	HIS	GLN	GLN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.21 Å   109.46 Å   111.20 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.03 – 2.40	Depositor
% Data completeness (in resolution range)	91.2 (20.03-2.40)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.246 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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	0.48	2/3232 (0.1%)	0.82	12/4358 (0.3%)
1	B	0.39	0/3036	0.70	2/4097 (0.0%)
All	All	0.44	2/6268 (0.0%)	0.76	14/8455 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	GLU	CD-OE2	7.28	1.33	1.25
1	A	455	THR	N-CA	6.36	1.59	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	516	PHE	C-N-CD	-10.41	97.70	120.60
1	A	475	SER	N-CA-C	8.00	132.59	111.00
1	A	451	LEU	N-CA-C	7.27	130.64	111.00
1	A	452	LYS	N-CA-C	6.66	128.99	111.00
1	B	449	GLU	N-CA-C	-6.58	93.23	111.00
1	A	230	GLU	C-N-CA	6.48	137.89	121.70
1	A	478	VAL	N-CA-C	5.69	126.36	111.00
1	A	499	ASP	N-CA-C	-5.53	96.08	111.00
1	A	416	MET	N-CA-C	-5.49	96.18	111.00
1	A	483	GLU	CA-C-N	-5.43	105.26	117.20
1	A	452	LYS	CA-C-N	5.42	127.03	116.20
1	A	498	ALA	N-CA-C	-5.35	96.55	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	VAL	C-N-CA	5.21	134.73	121.70
1	A	451	LEU	C-N-CA	-5.09	108.97	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	474	VAL	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	3185	0	3153	159	0
1	B	2987	0	2961	198	0
2	A	187	0	0	19	0
2	B	173	0	0	20	0
All	All	6532	0	6114	357	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 29.

All (357) 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:416:MET:HB2	1:B:513:ILE:HG22	1.28	1.14
1:B:305:THR:HG22	1:B:306:THR:H	1.11	1.13
1:A:451:LEU:O	1:A:452:LYS:CB	1.96	1.09
1:A:470:ARG:NH2	1:A:494:THR:HB	1.75	1.00
1:A:461:LYS:HB2	1:A:508:LEU:HB3	1.45	0.98
1:A:470:ARG:HH22	1:A:494:THR:HB	1.23	0.97
1:B:416:MET:HB2	1:B:513:ILE:CG2	1.94	0.97
1:A:474:VAL:O	1:A:475:SER:CB	2.09	0.97
1:A:170:ASN:ND2	1:A:173:LYS:HB2	1.79	0.96
1:B:409:ARG:CD	1:B:413:ARG:HH12	1.80	0.93

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LYS:HB3	1:A:329:PRO:CD	1.99	0.93
1:A:328:LYS:HB3	1:A:329:PRO:HD3	1.49	0.92
1:B:106:ILE:HD11	1:B:185:LEU:HD11	1.54	0.90
1:B:357:ILE:HB	2:B:641:HOH:O	1.72	0.88
1:B:409:ARG:HD2	1:B:413:ARG:HH12	1.37	0.88
1:B:224:LYS:H	1:B:303:GLN:NE2	1.72	0.87
1:A:305:THR:HG22	1:A:307:LEU:HG	1.57	0.86
1:B:103:ILE:HD12	1:B:316:ASN:HA	1.57	0.86
1:A:470:ARG:HH22	1:A:494:THR:CB	1.89	0.85
1:A:74:ILE:HA	1:A:78:GLN:HE21	1.40	0.84
1:B:409:ARG:HD2	1:B:413:ARG:NH1	1.92	0.83
1:A:74:ILE:HA	1:A:78:GLN:NE2	1.94	0.82
1:B:444:GLN:HA	1:B:447:GLN:HE21	1.43	0.82
1:A:201:TYR:CE2	1:A:317:THR:HG23	2.14	0.82
1:B:128:ILE:HG12	1:B:140:ASN:ND2	1.94	0.81
1:B:171:PHE:HA	1:B:174:TYR:CD1	2.15	0.81
1:B:305:THR:CG2	1:B:307:LEU:HG	2.11	0.80
1:A:170:ASN:HD22	1:A:173:LYS:HB2	1.46	0.79
1:A:470:ARG:CZ	1:A:494:THR:HB	2.13	0.78
1:B:409:ARG:CD	1:B:413:ARG:NH1	2.45	0.78
1:B:305:THR:HG22	1:B:306:THR:N	1.92	0.78
1:A:83:GLN:HG2	1:A:381:ALA:HB2	1.66	0.76
1:B:305:THR:HG21	1:B:307:LEU:HG	1.68	0.76
1:A:348:ASP:HA	1:A:372:THR:HB	1.68	0.76
1:B:417:SER:HB2	1:B:512:ARG:NH1	2.00	0.76
1:B:372:THR:HG22	1:B:375:GLU:H	1.51	0.75
1:B:366:LYS:HB3	2:B:681:HOH:O	1.86	0.74
1:A:298:ARG:HH21	1:A:330:ASN:ND2	1.86	0.74
1:B:409:ARG:HD2	1:B:413:ARG:HH22	1.53	0.73
1:B:409:ARG:HD2	1:B:413:ARG:NH2	2.04	0.73
1:A:366:LYS:HD3	2:A:702:HOH:O	1.90	0.71
1:B:106:ILE:HD11	1:B:185:LEU:CD1	2.20	0.70
1:B:291:GLN:O	1:B:295:LYS:HG3	1.92	0.70
1:B:305:THR:CG2	1:B:306:THR:H	1.96	0.70
1:B:409:ARG:HH11	1:B:413:ARG:HH12	1.38	0.70
1:B:418:VAL:HG23	1:B:442:LEU:HD13	1.72	0.70
1:A:170:ASN:HD21	1:A:173:LYS:CG	2.04	0.70
1:A:277:PRO:HB2	1:A:279:ILE:HG23	1.74	0.69
1:A:443:ALA:O	1:A:445:ASP:N	2.24	0.69
1:B:154:GLY:HA2	1:B:157:ALA:HB3	1.73	0.69
1:A:470:ARG:NH1	1:A:494:THR:HB	2.08	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LYS:HA	1:B:329:PRO:O	1.93	0.69
1:A:170:ASN:ND2	1:A:173:LYS:CB	2.54	0.68
1:B:112:TYR:O	1:B:115:VAL:HG22	1.93	0.68
1:B:464:ASN:O	1:B:465:PHE:HB2	1.92	0.68
1:B:115:VAL:HG21	1:B:174:TYR:CE2	2.28	0.68
1:B:409:ARG:HD2	1:B:413:ARG:CZ	2.23	0.68
1:B:310:SER:CB	1:B:328:LYS:HG2	2.23	0.68
1:B:409:ARG:HD3	1:B:413:ARG:HH12	1.57	0.67
1:A:305:THR:O	1:A:306:THR:HB	1.93	0.67
1:A:214:TRP:O	1:A:219:ARG:NH1	2.28	0.67
1:B:444:GLN:HA	1:B:447:GLN:NE2	2.09	0.67
1:B:469:THR:O	1:B:470:ARG:HD3	1.95	0.67
1:B:111:PHE:O	1:B:115:VAL:HG13	1.94	0.67
1:B:363:LYS:C	2:B:681:HOH:O	2.31	0.67
1:A:170:ASN:HD21	1:A:173:LYS:CB	2.08	0.66
1:B:154:GLY:O	1:B:158:LYS:N	2.29	0.66
1:B:213:ASN:HB2	2:B:698:HOH:O	1.94	0.65
1:A:470:ARG:NH2	1:A:491:LEU:HA	2.12	0.65
1:B:211:ARG:HD3	1:B:288:THR:HA	1.77	0.65
1:A:195:MET:HB2	1:A:199:GLU:HG3	1.78	0.65
1:B:141:TYR:CZ	1:B:329:PRO:HG3	2.31	0.65
1:B:461:LYS:HB3	1:B:508:LEU:HB3	1.77	0.64
1:B:154:GLY:HA3	1:B:166:ILE:HD11	1.79	0.64
1:A:418:VAL:HG12	1:A:419:GLU:N	2.13	0.64
1:B:154:GLY:O	1:B:158:LYS:HB2	1.98	0.64
1:B:171:PHE:HA	1:B:174:TYR:HD1	1.59	0.64
1:A:456:VAL:HG12	1:A:456:VAL:O	1.96	0.64
1:B:106:ILE:CD1	1:B:185:LEU:HD11	2.27	0.64
1:A:75:THR:C	1:A:77:GLN:H	2.01	0.63
1:A:279:ILE:HG13	1:A:279:ILE:O	1.99	0.63
1:A:74:ILE:CA	1:A:78:GLN:HE21	2.09	0.63
1:B:325:ASP:HA	1:B:328:LYS:HG3	1.80	0.63
1:B:372:THR:CG2	1:B:374:THR:H	2.12	0.63
1:B:504:LEU:HB3	1:B:506:LEU:HD22	1.81	0.63
1:B:130:VAL:HG12	1:B:169:PRO:HG3	1.80	0.63
1:B:413:ARG:CZ	1:B:416:MET:HE1	2.28	0.63
1:A:170:ASN:HD21	1:A:173:LYS:HB2	1.64	0.62
1:B:413:ARG:NH1	1:B:416:MET:CE	2.62	0.62
1:A:305:THR:HG22	1:A:307:LEU:CG	2.29	0.62
1:B:112:TYR:HE1	2:B:608:HOH:O	1.83	0.62
1:B:310:SER:HA	1:B:331:GLY:O	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:HIS:HD2	1:A:324:SER:OG	1.83	0.61
1:A:451:LEU:N	1:A:483:GLU:HG2	2.15	0.61
1:A:454:ARG:CB	1:A:515:SER:CB	2.78	0.61
1:A:499:ASP:C	1:A:501:PRO:HD2	2.20	0.61
1:A:470:ARG:HH12	1:A:494:THR:HB	1.67	0.60
1:A:415:SER:HB2	1:A:512:ARG:HH11	1.67	0.60
1:A:362:GLU:O	1:A:366:LYS:HG3	2.02	0.59
1:B:153:PRO:HB2	1:B:155:PHE:CD2	2.37	0.59
1:B:224:LYS:H	1:B:303:GLN:HE21	1.48	0.59
1:B:224:LYS:N	1:B:303:GLN:HE21	1.99	0.59
1:A:170:ASN:HD21	1:A:173:LYS:HG3	1.67	0.59
1:B:170:ASN:H	1:B:170:ASN:HD22	1.47	0.59
1:B:115:VAL:HG12	1:B:307:LEU:HD11	1.85	0.59
1:B:413:ARG:HG2	2:B:627:HOH:O	2.02	0.59
1:A:306:THR:HG22	2:A:544:HOH:O	2.03	0.58
1:B:409:ARG:HH11	1:B:413:ARG:NH1	2.01	0.58
1:B:101:ASN:ND2	1:B:405:THR:HB	2.17	0.58
1:A:328:LYS:CB	1:A:329:PRO:CD	2.79	0.58
1:B:299:PHE:O	1:B:303:GLN:HB2	2.04	0.58
1:A:351:ILE:HD13	1:A:365:LEU:HD13	1.85	0.58
1:B:409:ARG:HD3	1:B:413:ARG:NH1	2.14	0.57
1:B:305:THR:HG22	1:B:307:LEU:HG	1.86	0.57
1:B:447:GLN:HG3	1:B:447:GLN:O	2.04	0.57
1:B:413:ARG:NH1	1:B:416:MET:HE1	2.20	0.57
1:B:201:TYR:C	1:B:202:LEU:HD12	2.24	0.57
1:B:306:THR:O	1:B:306:THR:HG22	2.05	0.57
1:B:354:VAL:O	1:B:354:VAL:HG12	2.02	0.57
1:A:94:GLU:HG2	1:A:339:ARG:HH22	1.70	0.57
1:A:470:ARG:NH2	1:A:494:THR:CB	2.56	0.56
1:A:328:LYS:O	1:A:329:PRO:C	2.43	0.56
1:A:75:THR:O	1:A:77:GLN:N	2.25	0.56
1:B:224:LYS:N	1:B:303:GLN:NE2	2.47	0.56
1:B:415:SER:HA	1:B:516:PHE:CE1	2.40	0.56
1:A:318:MET:HE2	1:A:319:LEU:HA	1.88	0.56
1:A:97:ARG:HA	2:A:559:HOH:O	2.04	0.56
1:B:136:LEU:HG	1:B:152:MET:O	2.05	0.56
1:A:355:SER:HA	2:A:636:HOH:O	2.06	0.55
1:A:435:CYS:SG	1:A:488:ALA:HB1	2.46	0.55
1:B:211:ARG:HH22	1:B:296:GLU:CD	2.10	0.55
1:B:427:LYS:HD2	1:B:430:GLU:HG3	1.89	0.55
1:B:508:LEU:HD22	1:B:509:MET:H	1.70	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ALA:HB1	1:B:496:ILE:HD13	1.89	0.55
1:A:371:ILE:HG23	2:A:580:HOH:O	2.06	0.55
1:B:409:ARG:HB2	1:B:413:ARG:CZ	2.37	0.55
1:B:437:GLU:O	1:B:441:GLU:HB2	2.07	0.55
1:B:496:ILE:HG12	1:B:504:LEU:CD1	2.36	0.55
1:A:472:SER:C	1:A:475:SER:H	2.10	0.55
1:B:138:THR:HG22	1:B:139:SER:N	2.22	0.55
1:A:358:GLY:HA3	2:A:638:HOH:O	2.07	0.54
1:B:115:VAL:HG21	1:B:174:TYR:CD2	2.42	0.54
1:B:115:VAL:CG2	1:B:174:TYR:HE2	2.20	0.54
1:A:75:THR:C	1:A:77:GLN:N	2.61	0.54
1:B:139:SER:HB2	1:B:143:ALA:HB3	1.89	0.54
1:B:154:GLY:HA3	1:B:166:ILE:CD1	2.38	0.54
1:B:223:ILE:HD11	1:B:284:VAL:HG23	1.89	0.54
1:A:470:ARG:HA	2:A:595:HOH:O	2.07	0.54
1:B:500:PHE:CG	1:B:501:PRO:HA	2.42	0.54
1:A:211:ARG:HD3	1:A:288:THR:HA	1.90	0.54
1:A:442:LEU:HD12	1:A:484:ILE:HG21	1.90	0.54
1:B:119:ASP:OD1	1:B:173:LYS:HE2	2.08	0.54
1:A:328:LYS:CB	1:A:329:PRO:HD3	2.30	0.54
1:A:419:GLU:CG	1:A:508:LEU:HD21	2.37	0.54
1:A:377:TYR:HB2	1:A:399:SER:HB2	1.89	0.53
1:B:372:THR:HG23	1:B:374:THR:H	1.72	0.53
1:B:440:SER:C	1:B:442:LEU:H	2.11	0.53
1:B:149:ARG:H	1:B:152:MET:HE1	1.74	0.53
1:B:98:ASN:HB3	1:B:405:THR:HG21	1.91	0.53
1:B:499:ASP:O	1:B:502:HIS:HB2	2.07	0.53
1:B:420:ARG:O	1:B:508:LEU:HD22	2.07	0.53
1:B:75:THR:N	2:B:645:HOH:O	2.42	0.53
1:B:105:HIS:HD2	1:B:324:SER:OG	1.92	0.53
1:A:102:THR:HA	2:A:711:HOH:O	2.08	0.52
1:A:446:LEU:O	1:A:447:GLN:CB	2.57	0.52
1:B:287:GLY:HA3	1:B:292:GLU:HG3	1.92	0.52
1:A:141:TYR:CZ	1:A:329:PRO:HG3	2.44	0.52
1:B:119:ASP:O	1:B:121:PRO:HD3	2.09	0.52
1:B:507:ARG:HH11	1:B:507:ARG:HG2	1.74	0.52
1:A:434:LEU:O	1:A:438:LEU:HB2	2.10	0.52
1:B:224:LYS:H	1:B:303:GLN:HE22	1.51	0.52
1:B:301:ILE:O	1:B:305:THR:HB	2.09	0.52
1:B:508:LEU:HD22	1:B:509:MET:N	2.25	0.51
1:B:112:TYR:HD1	2:B:552:HOH:O	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:LYS:HD3	1:B:470:ARG:HH21	1.75	0.51
1:B:134:SER:O	1:B:135:MET:HG3	2.10	0.51
1:B:223:ILE:HG22	1:B:224:LYS:N	2.25	0.51
1:A:298:ARG:NH2	1:A:330:ASN:O	2.44	0.51
1:A:305:THR:HG21	1:A:307:LEU:HD12	1.92	0.51
1:B:372:THR:HG22	1:B:374:THR:N	2.26	0.51
1:A:470:ARG:NH1	1:A:495:GLU:HG2	2.26	0.50
1:B:152:MET:CE	1:B:157:ALA:HB2	2.41	0.50
1:A:215:PRO:HD2	1:A:218:LYS:HD3	1.93	0.50
1:A:242:SER:O	1:A:246:ARG:HG3	2.11	0.50
1:A:418:VAL:HG12	1:A:419:GLU:H	1.76	0.50
1:A:457:THR:HA	1:A:471:ALA:HB2	1.93	0.50
1:B:163:GLN:CD	1:B:163:GLN:H	2.14	0.50
1:B:128:ILE:HG12	1:B:140:ASN:HD22	1.74	0.50
1:B:367:ALA:N	2:B:681:HOH:O	2.33	0.50
1:B:366:LYS:N	2:B:681:HOH:O	2.44	0.50
1:B:179:LYS:O	1:B:183:GLU:HG3	2.11	0.50
1:B:416:MET:HB3	1:B:442:LEU:HD11	1.94	0.49
1:A:418:VAL:HG23	1:A:442:LEU:HD21	1.95	0.49
1:A:278:GLN:HG3	1:A:278:GLN:O	2.12	0.49
1:B:115:VAL:HG21	1:B:174:TYR:HE2	1.71	0.49
1:B:152:MET:HE2	1:B:157:ALA:HB2	1.94	0.49
1:A:442:LEU:HD12	1:A:484:ILE:HD13	1.94	0.49
1:A:498:ALA:C	1:A:500:PHE:N	2.63	0.49
1:B:463:VAL:CG2	1:B:505:ARG:HB3	2.42	0.49
1:B:340:GLN:HG2	2:B:535:HOH:O	2.12	0.49
1:B:516:PHE:O	1:B:517:PRO:C	2.51	0.49
1:A:352:ARG:NH2	2:A:555:HOH:O	2.46	0.49
1:A:379:GLN:O	1:A:383:LEU:HG	2.12	0.49
1:B:170:ASN:N	1:B:170:ASN:HD22	2.07	0.49
1:B:306:THR:CG2	1:B:306:THR:O	2.60	0.49
1:A:394:TYR:O	1:A:398:ILE:HG12	2.12	0.48
1:A:75:THR:H	1:A:78:GLN:NE2	2.11	0.48
1:A:141:TYR:O	1:A:145:ARG:HG3	2.12	0.48
1:B:103:ILE:HD12	1:B:316:ASN:CA	2.35	0.48
1:B:289:SER:O	1:B:293:VAL:HG23	2.14	0.48
1:B:118:ARG:NH1	1:B:177:VAL:HG22	2.28	0.48
1:A:445:ASP:C	1:A:447:GLN:H	2.17	0.48
1:A:415:SER:HB3	2:A:675:HOH:O	2.14	0.47
1:B:419:GLU:HG2	1:B:510:GLY:HA3	1.97	0.47
1:A:211:ARG:HH22	1:A:296:GLU:CD	2.17	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:MET:HG2	2:A:615:HOH:O	2.14	0.47
1:A:338:ASN:OD1	1:A:338:ASN:O	2.32	0.47
1:A:163:GLN:N	1:A:163:GLN:OE1	2.34	0.47
1:A:361:THR:HA	1:A:364:MET:HE3	1.96	0.47
1:A:361:THR:HA	1:A:364:MET:CE	2.45	0.47
1:B:317:THR:HG21	2:B:550:HOH:O	2.15	0.47
1:A:313:ILE:HB	1:A:334:GLN:HB2	1.96	0.47
1:A:500:PHE:N	1:A:501:PRO:HD2	2.30	0.47
1:A:414:LYS:O	1:A:514:SER:HA	2.15	0.47
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.80	0.47
1:B:154:GLY:O	1:B:158:LYS:CB	2.63	0.47
1:B:307:LEU:N	1:B:307:LEU:HD23	2.30	0.47
1:B:352:ARG:HH11	1:B:352:ARG:HG2	1.80	0.47
1:B:484:ILE:CB	2:B:532:HOH:O	2.62	0.47
1:A:130:VAL:CG1	1:A:169:PRO:HG3	2.44	0.46
1:A:305:THR:O	1:A:306:THR:CB	2.60	0.46
1:B:472:SER:HB2	1:B:487:ILE:CG2	2.44	0.46
1:B:77:GLN:OE1	1:B:80:ARG:NH1	2.48	0.46
1:A:113:ALA:H	1:A:138:THR:HG21	1.81	0.46
1:B:170:ASN:ND2	1:B:170:ASN:N	2.63	0.46
1:B:352:ARG:HG2	1:B:352:ARG:NH1	2.30	0.46
1:B:453:GLY:O	1:B:477:VAL:HA	2.15	0.46
1:A:278:GLN:HE21	1:A:280:LEU:HD21	1.81	0.46
1:A:188:TYR:CE1	1:A:297:ILE:HG12	2.51	0.46
1:A:432:TYR:OH	1:A:493:LYS:HA	2.16	0.46
1:B:476:SER:O	1:B:477:VAL:CB	2.63	0.46
1:A:418:VAL:CG1	1:A:419:GLU:N	2.79	0.46
1:B:409:ARG:HB2	1:B:413:ARG:NH2	2.30	0.46
1:B:372:THR:CG2	1:B:374:THR:HB	2.45	0.46
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.81	0.46
1:A:351:ILE:HB	1:A:371:ILE:O	2.15	0.46
1:B:170:ASN:ND2	1:B:170:ASN:H	2.12	0.46
1:B:310:SER:HB3	1:B:328:LYS:HG2	1.96	0.46
1:A:137:SER:O	1:A:150:ALA:CB	2.64	0.46
1:A:459:LYS:O	1:A:460:LEU:HD23	2.16	0.46
1:A:420:ARG:O	1:A:508:LEU:HD22	2.16	0.46
1:B:420:ARG:O	1:B:508:LEU:CD2	2.64	0.45
1:A:170:ASN:ND2	1:A:173:LYS:CG	2.74	0.45
1:A:478:VAL:O	1:A:479:SER:CB	2.65	0.45
1:A:498:ALA:O	1:A:499:ASP:HB2	2.16	0.45
1:B:112:TYR:HD2	1:B:174:TYR:CE1	2.35	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:SER:HA	1:B:481:ALA:HB2	1.97	0.45
1:B:516:PHE:CB	1:B:517:PRO:HD2	2.47	0.45
1:B:89:PHE:O	1:B:92:GLU:HB3	2.16	0.45
1:B:418:VAL:HG12	1:B:438:LEU:HD22	1.98	0.45
1:B:464:ASN:O	1:B:465:PHE:CB	2.63	0.45
1:B:496:ILE:HG12	1:B:504:LEU:HD12	1.98	0.45
1:A:220:ARG:HD3	1:A:285:VAL:CG2	2.46	0.45
1:B:496:ILE:HG12	1:B:504:LEU:HD11	1.97	0.45
1:B:374:THR:O	1:B:378:GLN:HG3	2.16	0.45
1:B:413:ARG:HD2	1:B:416:MET:HE3	1.98	0.45
1:A:248:ILE:HD12	1:A:249:SER:N	2.31	0.45
1:A:424:GLU:HA	1:A:506:LEU:O	2.16	0.45
1:B:500:PHE:CD1	1:B:501:PRO:HA	2.52	0.45
1:A:278:GLN:NE2	1:A:280:LEU:HD21	2.32	0.45
1:A:77:GLN:N	2:A:696:HOH:O	2.50	0.45
1:B:508:LEU:HD13	1:B:508:LEU:C	2.38	0.45
1:A:113:ALA:HB2	1:A:138:THR:HG22	1.98	0.45
1:B:468:LYS:HD3	1:B:470:ARG:NH2	2.32	0.45
1:A:334:GLN:HG2	1:A:335:ILE:N	2.32	0.44
1:A:499:ASP:O	1:A:502:HIS:N	2.50	0.44
1:A:323:CYS:SG	1:A:335:ILE:HG13	2.57	0.44
1:A:372:THR:OG1	1:A:375:GLU:HG3	2.17	0.44
1:A:443:ALA:CB	2:A:583:HOH:O	2.64	0.44
1:B:117:MET:CE	1:B:124:LYS:HA	2.47	0.44
1:B:423:SER:HA	1:B:507:ARG:HE	1.81	0.44
1:A:426:ASN:HD21	1:A:427:LYS:NZ	2.15	0.44
1:A:418:VAL:HG23	1:A:442:LEU:CD2	2.47	0.44
1:B:148:VAL:HA	1:B:152:MET:HE1	2.00	0.44
1:A:245:GLU:HA	1:A:248:ILE:HD11	2.00	0.44
1:B:424:GLU:OE1	1:B:426:ASN:OD1	2.35	0.44
1:A:305:THR:CG2	1:A:307:LEU:HD12	2.47	0.43
1:A:97:ARG:HG3	1:A:97:ARG:O	2.18	0.43
1:B:365:LEU:HB3	1:B:370:ILE:HB	1.99	0.43
1:B:188:TYR:OH	1:B:296:GLU:OE1	2.26	0.43
1:A:352:ARG:CZ	2:A:555:HOH:O	2.66	0.43
1:A:295:LYS:HG3	1:A:332:GLN:NE2	2.34	0.43
1:B:423:SER:O	1:B:424:GLU:C	2.56	0.43
1:B:460:LEU:O	1:B:467:VAL:HA	2.18	0.43
1:B:478:VAL:C	2:B:653:HOH:O	2.57	0.43
1:A:294:VAL:HG12	1:A:332:GLN:OE1	2.19	0.43
1:B:371:ILE:O	1:B:371:ILE:HG22	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:O	1:A:150:ALA:HB1	2.19	0.43
1:B:119:ASP:C	1:B:121:PRO:HD3	2.39	0.43
1:B:422:PHE:CE2	1:B:434:LEU:HD21	2.54	0.43
1:A:249:SER:HA	1:A:252:LEU:HD12	2.00	0.43
1:B:413:ARG:NH1	1:B:416:MET:HE2	2.34	0.43
1:B:287:GLY:CA	1:B:292:GLU:HG3	2.49	0.42
1:A:163:GLN:NE2	2:A:701:HOH:O	2.50	0.42
1:A:381:ALA:HB3	2:A:710:HOH:O	2.17	0.42
1:B:220:ARG:NE	2:B:682:HOH:O	2.35	0.42
1:A:356:GLY:HA3	1:A:394:TYR:OH	2.19	0.42
1:A:445:ASP:C	1:A:447:GLN:N	2.72	0.42
1:A:470:ARG:HH12	1:A:494:THR:C	2.22	0.42
1:B:188:TYR:CE1	1:B:297:ILE:HG12	2.54	0.42
1:A:170:ASN:ND2	1:A:170:ASN:O	2.53	0.42
1:B:115:VAL:CG2	1:B:174:TYR:CE2	2.97	0.42
1:B:348:ASP:HA	2:B:680:HOH:O	2.18	0.42
1:B:144:ARG:C	1:B:146:PHE:N	2.73	0.42
1:B:354:VAL:O	2:B:641:HOH:O	2.21	0.42
1:B:357:ILE:HG23	1:B:361:THR:OG1	2.20	0.42
1:B:436:GLN:HB3	1:B:485:PHE:CE1	2.55	0.42
1:B:504:LEU:HB3	1:B:506:LEU:CD2	2.47	0.42
1:B:516:PHE:HB3	1:B:517:PRO:HD2	2.01	0.42
1:A:429:GLU:CD	1:A:429:GLU:H	2.23	0.42
1:B:106:ILE:HD13	1:B:185:LEU:HD21	2.01	0.42
1:B:415:SER:HA	1:B:516:PHE:HE1	1.84	0.42
1:B:310:SER:OG	1:B:328:LYS:HE3	2.19	0.42
1:A:237:GLU:H	1:A:237:GLU:CD	2.23	0.42
1:A:494:THR:O	1:A:494:THR:HG22	2.19	0.42
1:A:116:GLU:OE2	1:A:116:GLU:HA	2.19	0.42
1:A:418:VAL:HG11	1:A:441:GLU:OE1	2.20	0.42
1:B:372:THR:HG21	1:B:374:THR:HB	2.01	0.41
1:B:505:ARG:NH2	2:B:679:HOH:O	2.47	0.41
1:A:446:LEU:O	1:A:447:GLN:HB3	2.21	0.41
1:A:248:ILE:C	1:A:250:PRO:HD2	2.41	0.41
1:A:504:LEU:HG	1:A:506:LEU:HD21	2.02	0.41
1:B:150:ALA:O	1:B:151:ALA:HB3	2.21	0.41
1:A:97:ARG:NH1	2:A:557:HOH:O	2.52	0.41
1:A:373:CYS:O	1:A:376:LEU:HB3	2.21	0.41
1:A:75:THR:OG1	1:A:78:GLN:HG2	2.20	0.41
1:A:248:ILE:H	1:A:248:ILE:HG13	1.78	0.41
1:A:223:ILE:HA	1:A:299:PHE:HZ	1.86	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:TYR:CE2	1:B:300:ARG:HD2	2.56	0.41
1:A:224:LYS:HD2	2:A:691:HOH:O	2.20	0.41
1:A:356:GLY:N	2:A:636:HOH:O	2.37	0.41
1:B:336:LEU:HA	1:B:337:PRO:HD3	1.83	0.41
1:A:457:THR:HA	1:A:471:ALA:CB	2.51	0.41
1:B:444:GLN:O	1:B:447:GLN:HG2	2.20	0.41
1:B:458:ILE:O	1:B:469:THR:HA	2.22	0.41
1:B:508:LEU:HD13	1:B:509:MET:N	2.35	0.41
1:A:436:GLN:HB2	1:A:485:PHE:CZ	2.56	0.40
1:A:419:GLU:HG3	1:A:508:LEU:HD21	2.03	0.40
1:B:223:ILE:O	1:B:224:LYS:CB	2.68	0.40
1:B:495:GLU:O	1:B:498:ALA:HB3	2.21	0.40
1:A:312:GLY:N	1:A:324:SER:HB3	2.36	0.40
1:B:381:ALA:HB3	2:B:577:HOH:O	2.21	0.40
1:B:427:LYS:C	1:B:429:GLU:N	2.73	0.40
1:B:141:TYR:CE1	1:B:329:PRO:HG3	2.55	0.40
1:A:495:GLU:HA	1:A:495:GLU:OE1	2.20	0.40
1:A:508:LEU:C	1:A:508:LEU:HD13	2.42	0.40
1:B:140:ASN:HB2	2:B:634:HOH:O	2.21	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	394/459 (86%)	356 (90%)	24 (6%)	14 (4%)	4	3
1	B	374/459 (82%)	340 (91%)	28 (8%)	6 (2%)	11	15
All	All	768/918 (84%)	696 (91%)	52 (7%)	20 (3%)	6	6

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	LYS
1	A	444	GLN
1	A	452	LYS
1	A	454	ARG
1	A	475	SER
1	A	478	VAL
1	B	329	PRO
1	B	330	ASN
1	B	503	PRO
1	A	445	ASP
1	A	455	THR
1	B	424	GLU
1	B	477	VAL
1	A	111	PHE
1	A	246	ARG
1	A	76	SER
1	A	337	PRO
1	A	500	PHE
1	B	451	LEU
1	A	329	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	341/412 (83%)	331 (97%)	10 (3%)	48	68
1	B	317/412 (77%)	308 (97%)	9 (3%)	49	70
All	All	658/824 (80%)	639 (97%)	19 (3%)	48	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	SER
1	A	98	ASN
1	A	220	ARG
1	A	318	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	330	ASN
1	A	338	ASN
1	A	339	ARG
1	A	340	GLN
1	A	352	ARG
1	A	393	HIS
1	B	85	GLN
1	B	156	ILE
1	B	163	GLN
1	B	170	ASN
1	B	372	THR
1	B	382	LEU
1	B	383	LEU
1	B	393	HIS
1	B	506	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	98	ASN
1	A	101	ASN
1	A	105	HIS
1	A	142	HIS
1	A	170	ASN
1	A	212	GLN
1	A	233	ASN
1	A	278	GLN
1	A	330	ASN
1	A	340	GLN
1	A	397	HIS
1	A	426	ASN
1	B	105	HIS
1	B	163	GLN
1	B	170	ASN
1	B	212	GLN
1	B	303	GLN
1	B	406	HIS
1	B	426	ASN
1	B	447	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

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.