



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:56 PM UTC

PDB ID : 1JEY / pdb_00001jey
Title : Crystal Structure of the Ku heterodimer bound to DNA
Authors : Walker, J.R.; Corpina, R.A.; Goldberg, J.
Deposited on : 2001-06-19
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

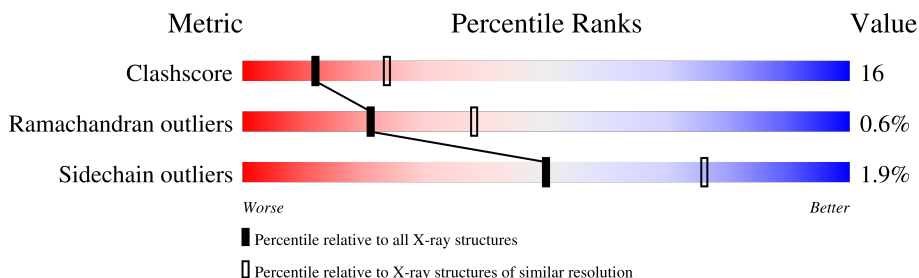
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	21	24% 62% 14%
2	D	34	21% 71% 9%
3	A	609	57% 22% • 19%
4	B	565	65% 27% • 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9472 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 DNA chain called DNA (5'-D(*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*GP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	18	Total	C	N	O	P	0	0	0
			368	179	58	114	17			

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	31	Total	C	N	O	P	0	0	0
			625	300	117	178	30			

- Molecule 3 is a protein called Ku70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	493	Total	C	N	O	S	0	0	0
			3982	2550	675	739	18			

- Molecule 4 is a protein called Ku80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	530	Total	C	N	O	S	0	0	0
			4242	2717	714	788	23			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	O	0	0
			2	2		
5	D	2	Total	O	0	0
			2	2		
5	A	142	Total	O	0	0
			142	142		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	109	Total 109	O 109	0	0

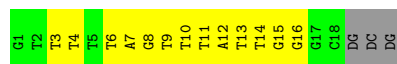
3 Residue-property plots

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. 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. 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.

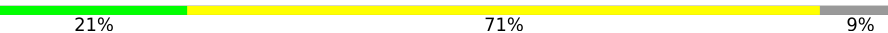
Note EDS was not executed.

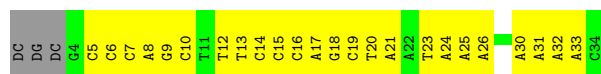
- Molecule 1: DNA (5'-D(*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*GP*CP*GP*CP*G)-3')

Chain C: 



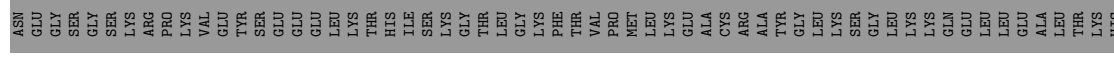
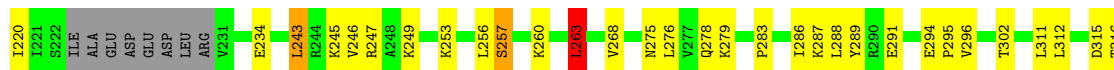
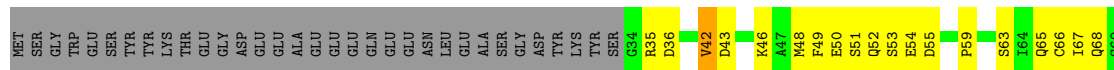
- Molecule 2: DNA (34-MER)

Chain D: 

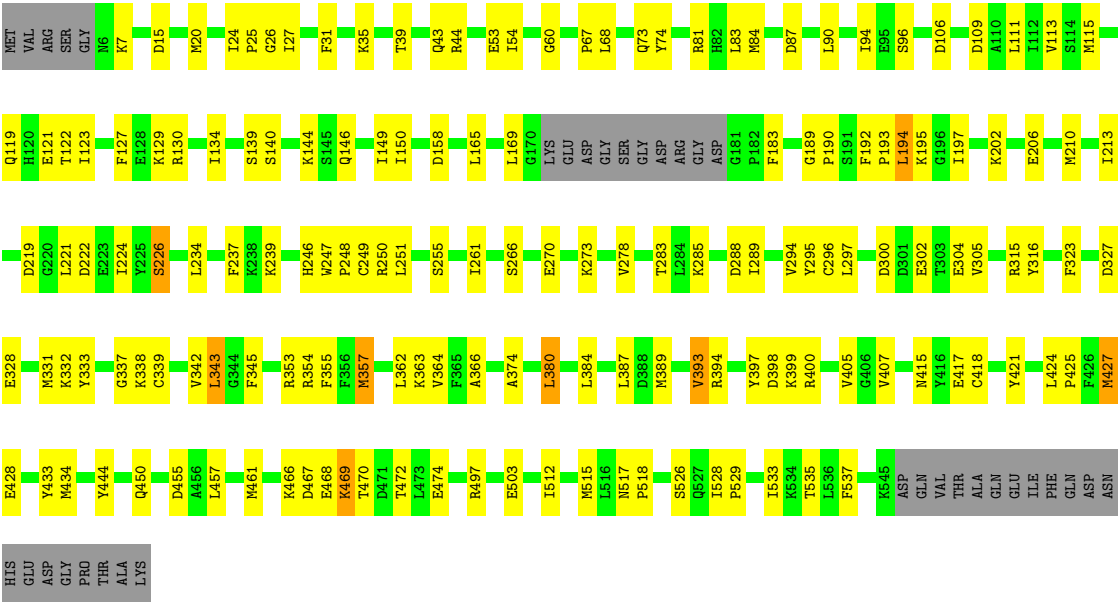


- Molecule 3: Ku70

Chain A: 



● Molecule 4: Ku80



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, α , β , γ	83.92Å 126.31Å 126.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.74 – 2.50	Depositor
% Data completeness (in resolution range)	97.8 (24.74-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9472	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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	C	0.32	0/410	0.72	0/633
2	D	0.32	0/701	0.65	0/1077
3	A	0.44	0/4060	0.96	14/5468 (0.3%)
4	B	0.43	0/4329	0.92	12/5838 (0.2%)
All	All	0.42	0/9500	0.91	26/13016 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	529	VAL	N-CA-C	9.34	119.00	111.62
3	A	401	THR	CA-C-N	8.75	128.76	119.05
3	A	401	THR	C-N-CA	8.75	128.76	119.05
3	A	488	ARG	N-CA-C	-7.44	103.17	111.28
3	A	263	LEU	N-CA-C	-7.25	103.10	112.23
4	B	405	VAL	N-CA-C	-7.10	98.23	108.53
3	A	55	ASP	N-CA-C	-6.98	104.68	112.57
3	A	174	ASN	CA-C-N	6.65	126.15	119.24
3	A	174	ASN	C-N-CA	6.65	126.15	119.24
4	B	60	GLY	N-CA-C	-6.34	106.18	115.63
3	A	439	PHE	N-CA-C	-6.33	102.36	110.53
4	B	140	SER	N-CA-C	6.29	119.77	110.46
3	A	89	GLY	N-CA-C	-6.14	106.61	115.27
3	A	342	ASP	N-CA-C	-6.09	101.25	110.39
4	B	393	VAL	N-CA-C	6.06	117.65	108.80
4	B	444	TYR	N-CA-C	5.83	119.71	112.59
4	B	54	ILE	N-CA-C	5.72	116.36	108.12
3	A	42	VAL	N-CA-C	5.72	116.17	108.17
3	A	321	ILE	N-CA-C	5.71	116.08	107.80
4	B	96	SER	N-CA-C	5.38	119.61	112.72
3	A	206	LYS	N-CA-C	5.36	117.64	110.35
4	B	122	THR	N-CA-C	-5.29	106.80	113.20
4	B	226	SER	N-CA-C	-5.24	101.98	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	234	LEU	N-CA-C	-5.22	106.22	112.59
4	B	343	LEU	N-CA-C	-5.16	107.12	113.41
4	B	139	SER	N-CA-C	5.08	116.90	111.36

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	C	368	0	210	22	0
2	D	625	0	349	42	0
3	A	3982	0	4064	119	0
4	B	4242	0	4294	131	0
5	A	142	0	0	7	0
5	B	109	0	0	6	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	9472	0	8917	284	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 16.

All (284) 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)
4:B:457:LEU:HD11	4:B:461:MET:HE3	1.38	1.05
4:B:115:MET:HE1	4:B:150:ILE:HG23	1.38	1.01
3:A:65:GLN:HG2	3:A:123:LYS:HE3	1.42	1.00
3:A:161:MET:HE3	3:A:164:LYS:HE2	1.49	0.92
3:A:68:GLN:HE22	3:A:123:LYS:HD2	1.36	0.91
1:C:8:DG:H2''	1:C:9:DT:H5''	1.53	0.88
3:A:469:LEU:HD13	3:A:514:MET:HE2	1.57	0.85
2:D:20:DT:H2''	2:D:21:DA:H5'	1.59	0.83
4:B:24:ILE:HB	4:B:27:ILE:HB	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:31:PHE:CE2	4:B:35:LYS:HE2	2.14	0.82
3:A:363:ARG:HG3	3:A:363:ARG:HH11	1.46	0.81
2:D:16:DC:H1'	2:D:17:DA:H5'	1.62	0.80
4:B:111:LEU:HD13	4:B:134:ILE:HD11	1.68	0.76
4:B:337:GLY:HA2	4:B:399:LYS:HA	1.67	0.75
4:B:450:GLN:HB3	4:B:537:PHE:CZ	2.21	0.75
3:A:451:LYS:HE3	4:B:417:GLU:CG	2.17	0.74
3:A:68:GLN:NE2	3:A:123:LYS:HD2	2.03	0.73
2:D:20:DT:H2''	2:D:21:DA:C5'	2.19	0.73
2:D:14:DC:H4'	2:D:15:DC:OP1	1.89	0.72
3:A:175:PRO:HG3	5:A:611:HOH:O	1.90	0.72
4:B:249:CYS:C	4:B:250:ARG:HD2	2.15	0.71
4:B:328:GLU:O	4:B:332:LYS:HB2	1.91	0.71
4:B:467:ASP:HB3	4:B:474:GLU:HG3	1.71	0.71
1:C:12:DA:H2''	1:C:13:DT:C6	2.26	0.71
3:A:348:MET:HE1	4:B:517:ASN:HA	1.71	0.69
4:B:90:LEU:O	4:B:94:ILE:HG12	1.92	0.69
3:A:72:ILE:HG12	3:A:116:ILE:HD13	1.75	0.69
1:C:8:DG:C2'	1:C:9:DT:H5''	2.23	0.69
3:A:507:THR:O	4:B:394:ARG:HD2	1.93	0.69
3:A:509:PRO:HG3	4:B:343:LEU:HD23	1.75	0.69
3:A:46:LYS:HE2	3:A:50:GLU:OE2	1.94	0.68
4:B:81:ARG:HH22	4:B:87:ASP:CG	2.03	0.67
4:B:111:LEU:HG	4:B:115:MET:HE2	1.75	0.67
2:D:19:DC:H2''	2:D:20:DT:H72	1.76	0.67
3:A:348:MET:HE3	4:B:518:PRO:HD3	1.76	0.67
2:D:33:DA:H5''	3:A:257:SER:HA	1.78	0.66
4:B:111:LEU:HG	4:B:115:MET:CE	2.26	0.65
2:D:15:DC:H5''	2:D:16:DC:C6	2.32	0.65
1:C:3:DT:H2''	1:C:4:DT:H71	1.80	0.64
2:D:19:DC:H2''	2:D:20:DT:C7	2.27	0.64
4:B:53:GLU:HG3	4:B:127:PHE:CZ	2.32	0.64
2:D:9:DG:H2''	2:D:10:DC:C6	2.33	0.64
2:D:6:DC:H2''	2:D:7:DC:C5	2.33	0.63
4:B:130:ARG:HH21	4:B:158:ASP:HB3	1.62	0.63
1:C:9:DT:H2''	1:C:10:DT:O5'	1.98	0.63
3:A:348:MET:CE	4:B:518:PRO:HD3	2.28	0.63
1:C:6:DT:H2''	1:C:7:DA:C8	2.34	0.63
4:B:53:GLU:OE2	4:B:84:MET:HA	1.99	0.63
1:C:9:DT:H2'	1:C:10:DT:H71	1.81	0.62
2:D:25:DA:H2''	2:D:26:DA:H5'	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:206:GLU:O	4:B:210:MET:HG3	2.00	0.62
4:B:528:ILE:HB	4:B:529:PRO:HD3	1.80	0.62
3:A:283:PRO:HB2	5:A:687:HOH:O	2.00	0.62
3:A:157:VAL:HG11	3:A:161:MET:SD	2.40	0.62
2:D:8:DA:H2''	2:D:9:DG:OP2	2.00	0.61
3:A:451:LYS:HE3	4:B:417:GLU:HG3	1.83	0.61
2:D:17:DA:H2''	2:D:18:DG:C8	2.36	0.61
3:A:311:LEU:HD13	4:B:289:ILE:HD12	1.82	0.61
3:A:287:LYS:HD3	4:B:295:TYR:CE2	2.36	0.61
3:A:400:TYR:CZ	3:A:402:PRO:HG3	2.36	0.61
2:D:20:DT:OP2	2:D:20:DT:H2'	2.01	0.60
4:B:457:LEU:HD22	4:B:533:ILE:CD1	2.31	0.60
4:B:497:ARG:NH1	4:B:503:GLU:O	2.34	0.60
2:D:16:DC:C1'	2:D:17:DA:H5'	2.30	0.60
1:C:3:DT:C2'	1:C:4:DT:H71	2.32	0.59
4:B:53:GLU:HG3	4:B:127:PHE:CE2	2.37	0.59
4:B:24:ILE:HG21	4:B:27:ILE:HD12	1.82	0.59
3:A:529:VAL:HG12	3:A:530:TYR:CD2	2.37	0.59
4:B:192:PHE:HD1	4:B:192:PHE:H	1.51	0.59
4:B:362:LEU:HB2	4:B:421:TYR:HB3	1.83	0.59
4:B:457:LEU:CD1	4:B:461:MET:HE3	2.22	0.58
3:A:279:LYS:HE3	5:A:735:HOH:O	2.03	0.58
3:A:296:VAL:HG13	4:B:296:CYS:O	2.04	0.58
4:B:193:PRO:C	4:B:195:LYS:H	2.11	0.58
4:B:304:GLU:HG2	4:B:305:VAL:N	2.18	0.58
4:B:39:THR:O	4:B:43:GLN:HG3	2.03	0.58
4:B:106:ASP:HB3	4:B:109:ASP:HB2	1.85	0.57
1:C:12:DA:H2''	1:C:13:DT:H71	1.86	0.57
3:A:363:ARG:HG3	3:A:363:ARG:NH1	2.18	0.57
4:B:468:GLU:O	4:B:470:THR:HG23	2.04	0.57
3:A:36:ASP:OD1	3:A:162:SER:HB2	2.05	0.57
2:D:18:DG:H2''	2:D:19:DC:C6	2.40	0.56
2:D:25:DA:H1'	2:D:26:DA:H5''	1.86	0.56
3:A:161:MET:CE	3:A:164:LYS:HE2	2.30	0.56
2:D:13:DT:O2	2:D:14:DC:N4	2.38	0.56
1:C:12:DA:H2''	1:C:13:DT:C5	2.41	0.56
3:A:289:TYR:CE2	3:A:291:GLU:HB2	2.40	0.56
3:A:387:ILE:O	3:A:391:GLU:HG3	2.05	0.56
3:A:157:VAL:HG13	3:A:157:VAL:O	2.05	0.55
3:A:363:ARG:NH1	3:A:364:PRO:O	2.39	0.55
4:B:239:LYS:HE3	5:B:624:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:216:PHE:CZ	3:A:220:ILE:HD11	2.42	0.55
2:D:19:DC:H2'	2:D:19:DC:OP2	2.07	0.55
3:A:154:PHE:O	3:A:157:VAL:HG12	2.06	0.55
3:A:253:LYS:HE2	4:B:434:MET:O	2.07	0.55
2:D:15:DC:H5''	2:D:16:DC:C5	2.42	0.55
3:A:191:GLY:HA2	3:A:194:ARG:NH1	2.22	0.55
3:A:400:TYR:CE2	3:A:402:PRO:HG3	2.42	0.55
2:D:16:DC:C2'	2:D:17:DA:H5'	2.37	0.54
3:A:48:MET:HA	3:A:59:PRO:HG2	1.89	0.54
3:A:276:LEU:HD12	5:B:642:HOH:O	2.06	0.54
3:A:65:GLN:HG2	3:A:123:LYS:CE	2.28	0.54
3:A:388:LYS:HE3	4:B:455:ASP:HB2	1.89	0.54
4:B:248:PRO:O	4:B:338:LYS:HE2	2.07	0.54
4:B:266:SER:OG	4:B:363:LYS:HG3	2.08	0.53
3:A:316:THR:HG23	3:A:318:ARG:HH12	1.74	0.53
1:C:10:DT:H2''	1:C:11:DT:C6	2.44	0.53
4:B:115:MET:CE	4:B:150:ILE:HG23	2.26	0.53
3:A:350:PHE:HB3	3:A:394:VAL:CG1	2.38	0.53
2:D:12:DT:H2''	2:D:13:DT:OP1	2.09	0.53
3:A:296:VAL:HG11	4:B:295:TYR:HB3	1.90	0.53
2:D:17:DA:H2''	2:D:18:DG:H8	1.74	0.53
3:A:311:LEU:CD1	4:B:289:ILE:HD12	2.38	0.52
4:B:270:GLU:OE2	4:B:273:LYS:NZ	2.42	0.52
1:C:14:DT:H5''	4:B:400:ARG:HB2	1.90	0.52
3:A:423:GLN:O	3:A:424:LYS:HB2	2.10	0.52
3:A:143:LEU:H	3:A:176:HIS:HE1	1.56	0.52
4:B:283:THR:O	4:B:285:LYS:HG2	2.10	0.52
3:A:420:LEU:HD23	3:A:426:GLN:HA	1.92	0.52
4:B:251:LEU:HB2	4:B:261:ILE:HD13	1.91	0.51
4:B:467:ASP:CG	4:B:468:GLU:H	2.17	0.51
4:B:250:ARG:HD2	4:B:250:ARG:N	2.25	0.51
3:A:418:GLU:HB2	3:A:430:PRO:HB3	1.93	0.51
3:A:43:ASP:O	3:A:48:MET:HG3	2.11	0.51
1:C:3:DT:H5''	3:A:80:ARG:NH1	2.26	0.51
1:C:11:DT:H2''	1:C:12:DA:C8	2.46	0.51
3:A:70:VAL:O	3:A:74:LYS:HG2	2.11	0.51
3:A:72:ILE:O	3:A:76:ILE:HG12	2.11	0.51
4:B:194:LEU:O	4:B:202:LYS:HE2	2.10	0.51
4:B:354:ARG:NH1	5:B:642:HOH:O	2.43	0.50
4:B:512:ILE:O	4:B:515:MET:HG2	2.11	0.50
3:A:75:ILE:HD12	3:A:116:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:DC:H2''	2:D:20:DT:C5	2.47	0.50
4:B:31:PHE:HE2	4:B:35:LYS:HE2	1.71	0.50
4:B:247:TRP:NE1	4:B:338:LYS:HE3	2.26	0.50
3:A:51:SER:O	3:A:52:GLN:HB2	2.12	0.50
3:A:287:LYS:HD3	4:B:295:TYR:HE2	1.74	0.50
4:B:294:VAL:HG12	4:B:295:TYR:N	2.26	0.50
4:B:461:MET:HG2	4:B:526:SER:HB3	1.93	0.50
3:A:42:VAL:HB	3:A:87:PHE:CD2	2.47	0.49
2:D:14:DC:C4'	2:D:15:DC:OP1	2.59	0.49
1:C:12:DA:C2'	1:C:13:DT:H71	2.41	0.49
3:A:402:PRO:HD2	3:A:406:ILE:HD13	1.94	0.49
1:C:6:DT:H2''	1:C:7:DA:N7	2.27	0.49
3:A:176:HIS:HD2	5:A:667:HOH:O	1.96	0.49
3:A:286:ILE:HD12	4:B:315:ARG:HG3	1.93	0.49
4:B:294:VAL:HG11	4:B:304:GLU:OE2	2.13	0.49
2:D:25:DA:H2''	2:D:26:DA:C5'	2.42	0.49
4:B:193:PRO:C	4:B:195:LYS:N	2.71	0.48
3:A:363:ARG:HB2	3:A:364:PRO:HD2	1.96	0.48
4:B:338:LYS:HG3	4:B:397:TYR:O	2.14	0.48
2:D:16:DC:H2''	2:D:17:DA:H5'	1.96	0.48
4:B:304:GLU:HG2	4:B:305:VAL:H	1.79	0.48
3:A:243:LEU:HD22	3:A:247:ARG:NE	2.28	0.48
3:A:317:LYS:HE2	3:A:330:GLU:OE2	2.14	0.48
2:D:32:DA:H2''	2:D:33:DA:C8	2.49	0.48
3:A:263:LEU:N	3:A:263:LEU:HD23	2.29	0.48
2:D:6:DC:H2''	2:D:7:DC:H5	1.79	0.47
2:D:16:DC:H2''	2:D:17:DA:C5'	2.43	0.47
4:B:355:PHE:O	4:B:425:PRO:HD3	2.14	0.47
4:B:357:MET:SD	4:B:425:PRO:HB3	2.54	0.47
2:D:14:DC:OP2	2:D:14:DC:H2'	2.15	0.47
4:B:461:MET:HE2	4:B:526:SER:HB2	1.95	0.47
3:A:401:THR:HG23	3:A:406:ILE:CG2	2.45	0.47
4:B:338:LYS:O	4:B:339:CYS:HB3	2.12	0.47
2:D:5:DC:H2''	2:D:6:DC:C6	2.49	0.47
2:D:23:DT:H2''	2:D:24:DA:C8	2.48	0.47
3:A:433:GLN:HE22	4:B:353:ARG:HG3	1.78	0.47
4:B:73:GLN:O	4:B:74:TYR:C	2.57	0.47
4:B:115:MET:O	4:B:119:GLN:HG3	2.14	0.47
4:B:165:LEU:O	4:B:226:SER:HA	2.14	0.47
4:B:457:LEU:HD22	4:B:533:ILE:HD12	1.96	0.47
2:D:7:DC:H2''	2:D:8:DA:O5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:121:GLU:C	4:B:123:ILE:H	2.22	0.47
4:B:366:ALA:HB2	4:B:374:ALA:HA	1.96	0.47
2:D:20:DT:OP2	2:D:20:DT:H6	1.98	0.46
4:B:68:LEU:HD12	4:B:113:VAL:HG22	1.97	0.46
3:A:289:TYR:HE2	3:A:291:GLU:HB2	1.79	0.46
3:A:316:THR:OG1	4:B:278:VAL:HG12	2.15	0.46
1:C:3:DT:H2''	1:C:4:DT:C6	2.50	0.46
2:D:20:DT:H2''	2:D:21:DA:O5'	2.16	0.46
3:A:363:ARG:NH1	3:A:436:PHE:CE1	2.84	0.46
3:A:462:MET:HG2	4:B:380:LEU:HA	1.97	0.46
3:A:49:PHE:HD2	3:A:128:GLN:HG3	1.80	0.46
3:A:294:GLU:OE1	4:B:297:LEU:HD22	2.15	0.46
4:B:15:ASP:O	4:B:20:MET:HG3	2.16	0.46
4:B:169:LEU:HD22	4:B:224:ILE:HD12	1.98	0.46
4:B:466:LYS:HA	4:B:472:THR:O	2.16	0.46
4:B:53:GLU:CB	4:B:83:LEU:HD22	2.46	0.46
1:C:12:DA:H2''	1:C:13:DT:C7	2.45	0.45
4:B:246:HIS:NE2	4:B:248:PRO:HG3	2.31	0.45
4:B:342:VAL:HA	4:B:393:VAL:HG12	1.98	0.45
3:A:234:GLU:O	3:A:245:LYS:NZ	2.47	0.45
4:B:144:LYS:HE2	5:B:649:HOH:O	2.15	0.45
4:B:146:GLN:O	4:B:150:ILE:HG13	2.16	0.45
3:A:397:LEU:HD12	3:A:411:VAL:O	2.16	0.45
3:A:434:LEU:C	3:A:434:LEU:HD23	2.41	0.45
4:B:219:ASP:O	4:B:222:ASP:HB2	2.17	0.45
3:A:312:LEU:HB2	3:A:315:ASP:OD2	2.16	0.45
3:A:402:PRO:HD2	3:A:406:ILE:HG21	1.99	0.45
4:B:24:ILE:O	4:B:26:GLY:N	2.50	0.44
4:B:129:LYS:HD3	4:B:239:LYS:O	2.17	0.44
4:B:357:MET:HE2	4:B:357:MET:HA	1.98	0.44
4:B:364:VAL:O	4:B:418:CYS:HB2	2.16	0.44
1:C:15:DG:OP1	4:B:398:ASP:HB2	2.16	0.44
5:A:714:HOH:O	4:B:433:TYR:HE1	2.01	0.44
3:A:492:ALA:HB2	3:A:500:PRO:HA	1.98	0.44
4:B:345:PHE:CD2	4:B:384:LEU:HD21	2.53	0.44
2:D:30:DA:H2''	2:D:31:DA:OP2	2.18	0.44
3:A:66:CYS:SG	3:A:246:VAL:HG21	2.56	0.44
4:B:327:ASP:HB3	4:B:331:MET:HE3	1.98	0.44
1:C:8:DG:H2''	1:C:9:DT:C5'	2.34	0.44
3:A:369:TYR:CG	3:A:370:PRO:HD2	2.52	0.44
4:B:27:ILE:HG23	4:B:183:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:185:ARG:HG3	3:A:185:ARG:HH11	1.82	0.44
3:A:192:ASP:O	3:A:196:THR:HB	2.18	0.44
3:A:256:LEU:O	3:A:257:SER:HB3	2.18	0.44
3:A:350:PHE:HB3	3:A:394:VAL:HG11	1.98	0.44
3:A:260:LYS:HB3	3:A:268:VAL:CG1	2.48	0.43
3:A:531:PRO:C	3:A:533:ASP:N	2.76	0.43
4:B:123:ILE:HG23	4:B:123:ILE:O	2.18	0.43
4:B:467:ASP:CG	4:B:468:GLU:N	2.75	0.43
3:A:451:LYS:HE3	4:B:417:GLU:CD	2.43	0.43
3:A:508:LEU:HA	3:A:509:PRO:HD3	1.93	0.43
3:A:335:GLU:O	3:A:338:LYS:HB2	2.19	0.43
4:B:53:GLU:HG3	4:B:127:PHE:HZ	1.80	0.43
4:B:387:LEU:O	4:B:389:MET:HG3	2.17	0.43
4:B:44:ARG:HD2	4:B:237:PHE:CZ	2.54	0.42
2:D:8:DA:H3'	2:D:8:DA:P	2.59	0.42
3:A:53:SER:O	3:A:54:GLU:HG3	2.19	0.42
3:A:200:LEU:C	3:A:200:LEU:HD23	2.44	0.42
3:A:350:PHE:HB3	3:A:394:VAL:HG13	2.00	0.42
3:A:509:PRO:HG3	4:B:343:LEU:CD2	2.46	0.42
4:B:7:LYS:HD2	4:B:127:PHE:CE2	2.54	0.42
3:A:302:THR:HG22	3:A:311:LEU:HD12	2.01	0.42
3:A:403:ARG:O	3:A:406:ILE:HG22	2.20	0.42
3:A:461:LYS:HD3	3:A:461:LYS:HA	1.74	0.42
3:A:204:HIS:ND1	3:A:204:HIS:N	2.65	0.42
3:A:249:LYS:HE2	4:B:434:MET:CE	2.49	0.42
4:B:213:ILE:HD11	4:B:221:LEU:HD21	2.02	0.42
3:A:371:GLU:OE1	3:A:371:GLU:HA	2.19	0.42
4:B:251:LEU:C	4:B:251:LEU:HD23	2.44	0.42
2:D:13:DT:O4	2:D:19:DC:C5'	2.68	0.42
4:B:53:GLU:HB3	4:B:83:LEU:HD22	2.01	0.42
3:A:275:ASN:ND2	3:A:278:GLN:OE1	2.42	0.42
4:B:427:MET:HE2	4:B:428:GLU:HA	2.00	0.42
4:B:407:VAL:HB	4:B:424:LEU:HD11	2.01	0.42
4:B:468:GLU:O	4:B:469:LYS:C	2.62	0.42
2:D:19:DC:H2''	2:D:20:DT:C6	2.54	0.42
4:B:283:THR:HG21	4:B:288:ASP:OD2	2.20	0.42
3:A:340:PHE:HB2	3:A:408:PRO:HD3	2.00	0.41
3:A:370:PRO:HD3	3:A:382:PHE:CE2	2.55	0.41
4:B:149:ILE:HG13	5:B:609:HOH:O	2.21	0.41
1:C:15:DG:C6	1:C:16:DG:C6	3.08	0.41
3:A:75:ILE:HD13	4:B:316:TYR:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:315:ARG:NE	5:B:671:HOH:O	2.50	0.41
3:A:35:ARG:NH1	3:A:80:ARG:O	2.53	0.41
3:A:49:PHE:CD2	3:A:128:GLN:HG3	2.56	0.41
4:B:366:ALA:CB	4:B:374:ALA:HA	2.51	0.41
2:D:6:DC:H2"	2:D:7:DC:C6	2.56	0.41
3:A:288:LEU:HD23	3:A:295:PRO:HA	2.02	0.41
4:B:424:LEU:HD23	4:B:424:LEU:HA	1.84	0.41
3:A:53:SER:C	3:A:54:GLU:HG3	2.45	0.41
3:A:157:VAL:HG11	3:A:161:MET:HE2	2.02	0.41
3:A:449:THR:HB	5:A:733:HOH:O	2.19	0.41
2:D:9:DG:H2"	2:D:10:DC:C5	2.56	0.41
3:A:102:ILE:HD13	3:A:146:VAL:HA	2.03	0.41
3:A:287:LYS:CD	4:B:295:TYR:HE2	2.33	0.41
3:A:363:ARG:NH1	3:A:363:ARG:CG	2.81	0.41
4:B:189:GLY:N	4:B:190:PRO:HD2	2.35	0.41
4:B:294:VAL:HG12	4:B:295:TYR:H	1.86	0.40
4:B:469:LYS:HD3	4:B:469:LYS:HA	1.85	0.40
3:A:63:SER:O	3:A:67:ILE:HG13	2.21	0.40
4:B:67:PRO:O	4:B:68:LEU:HD23	2.22	0.40
4:B:194:LEU:O	4:B:197:ILE:HG12	2.22	0.40
4:B:323:PHE:HE2	4:B:331:MET:HE3	1.86	0.40
4:B:333:TYR:CD2	4:B:333:TYR:C	3.00	0.40
1:C:3:DT:H2"	1:C:4:DT:C7	2.50	0.40
3:A:51:SER:O	3:A:52:GLN:CB	2.69	0.40
3:A:422:ASP:OD1	3:A:423:GLN:HG2	2.20	0.40
3:A:95:ASN:HA	5:A:642:HOH:O	2.21	0.40
3:A:157:VAL:O	3:A:157:VAL:CG1	2.69	0.40
3:A:479:GLU:O	3:A:481:PRO:HD3	2.21	0.40
3:A:511:VAL:CG1	4:B:255:SER:HB3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	489/609 (80%)	466 (95%)	21 (4%)	2 (0%)	30	49
4	B	526/565 (93%)	486 (92%)	36 (7%)	4 (1%)	16	31
All	All	1015/1174 (86%)	952 (94%)	57 (6%)	6 (1%)	21	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	302	GLU
4	B	25	PRO
4	B	469	LYS
3	A	257	SER
4	B	194	LEU
3	A	511	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	
3	A	448/548 (82%)	436 (97%)	12 (3%)	39	67
4	B	477/505 (94%)	471 (99%)	6 (1%)	61	82
All	All	925/1053 (88%)	907 (98%)	18 (2%)	50	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	140	ASP
3	A	194	ARG
3	A	196	THR
3	A	204	HIS
3	A	243	LEU
3	A	263	LEU
3	A	381	LEU
3	A	394	VAL
3	A	409	TYR
3	A	467	GLU

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Mol	Chain	Res	Type
3	A	496	ASP
3	A	527	GLU
4	B	300	ASP
4	B	357	MET
4	B	380	LEU
4	B	415	ASN
4	B	427	MET
4	B	535	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
3	A	101	ASN
3	A	176	HIS
3	A	178	ASN
3	A	433	GLN
4	B	45	GLN
4	B	75	GLN
4	B	76	ASN
4	B	152	HIS
4	B	188	HIS
4	B	488	GLN
4	B	510	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.