Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2023 – 03:54 PM EDT

PDB ID	:	1JEQ
Title	:	Crystal Structure of the Ku Heterodimer
Authors	:	Walker, J.R.; Corpina, R.A.; Goldberg, J.
Deposited on	:	2001-06-18
Resolution	:	2.70 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:

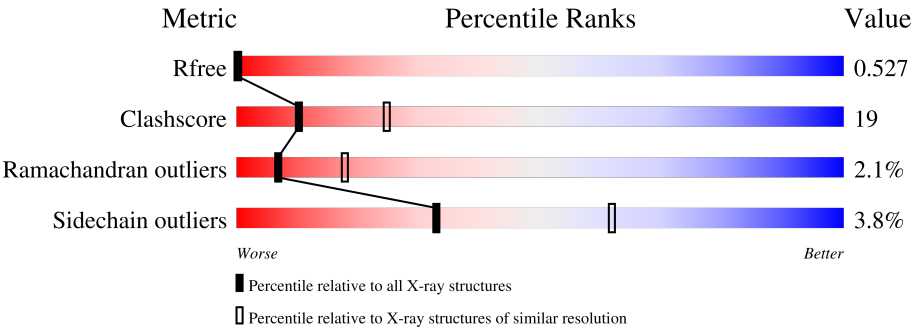
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	609	50% 38% · 10%
2	B	565	60% 30% · 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8633 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 KU70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	4419	2830	748	821	20	0	0	0

- Molecule 2 is a protein called KU80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	520	4172	2673	700	776	23	0	0	0

- Molecule 3 is water.

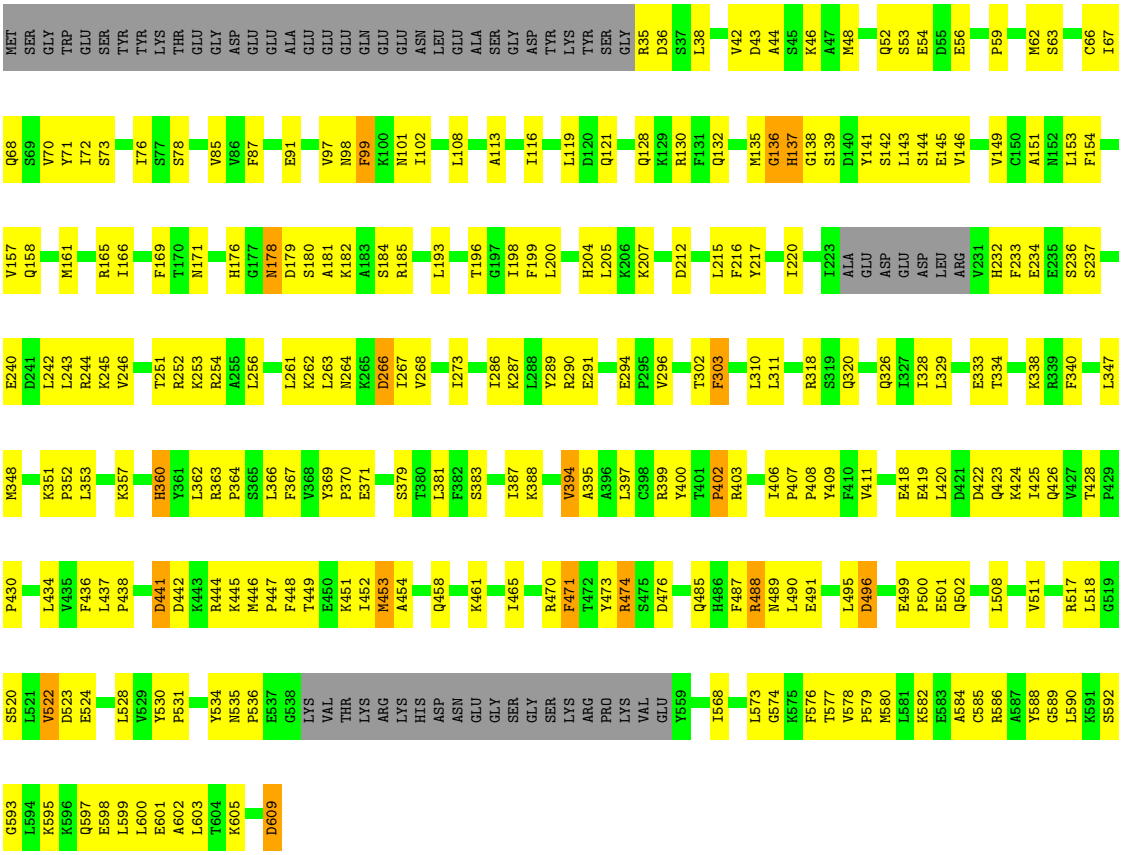
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	21	21	21	0	0
3	B	21	Total	O	0	0
			21	21		

3 Residue-property plots (i)

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.

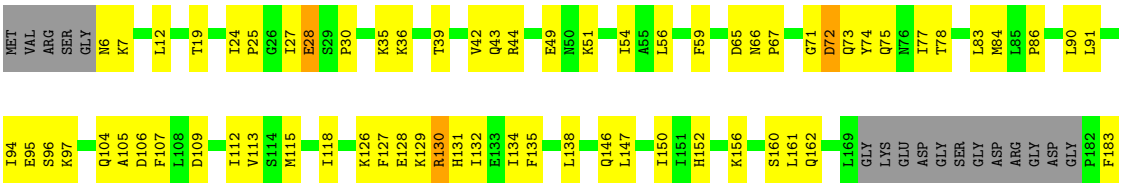
- Molecule 1: KU70

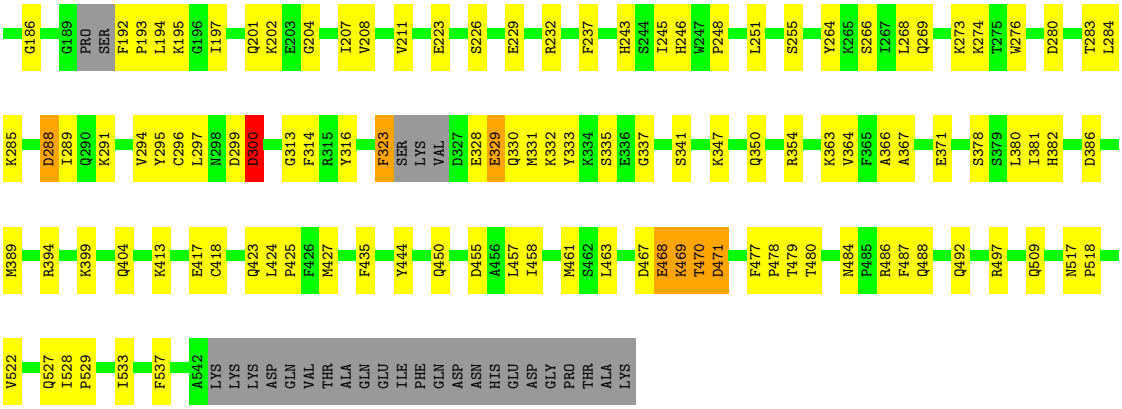
Chain A:



- Molecule 2: KU80

Chain B:




G186
G189 PRO SER F192 P193 L194 K195 G196 I197
Q201 K202 E203 G204
I207 V208
V211
E223
S226
E229
R232
F237
H243 S244 I245 H246 W247 P248
L251
S255
Y264 K265 S266 I267 L268 Q269
K273 K274 T275 W276
D280
T283 L284
K285
D288 I289 Q290 K291
V294 Y295 C296 L297 N298 D299 D300
G313 F314 R315 Y316
F323 SER LYS VAL D327 E328 E329 Q330 M331 K332 Y333 K334 S335 E336 G337
S341
K347
Q350
R354
K363 V364 F365 A366 A367
E371
S378 S379 L380 I381 H382
D386
M389
R394
K399
Q404
K413
E417 C418
Q423 L424 P425 F426 M427
F435
Y444
Q450
D455 A456 L457 I458
M461 S462 L463
D467 E468 K469 T470 D471
F477 P478 T479 T480
N484 P485 R486 F487 Q488
Q492
R497
Q509
N517 P518
V522
Q527 I528 P529
I533
F537
A542 LYS LYS LYS ASP GLN VAL THR ALA GLN GLU ILE PHE GLN ASP ASN HIS GLU ASP GLY PRO THR ALA LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.21Å 86.19Å 203.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.70 74.61 – 1.22	Depositor EDS
% Data completeness (in resolution range)	80.8 (19.89-2.70) 11.8 (74.61-1.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	21.45 (at 1.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.283 0.522 , 0.527	Depositor DCC
R_{free} test set	2430 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	7.1	Xtriage
Anisotropy	1.902	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 12.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.56	EDS
Total number of atoms	8633	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.42	0/4504	0.65	0/6061
2	B	0.43	0/4256	0.66	0/5739
All	All	0.42	0/8760	0.66	0/11800

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	4419	0	4512	222	0
2	B	4172	0	4209	142	0
3	A	21	0	0	1	0
3	B	21	0	0	2	0
All	All	8633	0	8721	326	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 19.

All (326) 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:446:MET:HE1	2:B:363:LYS:HD2	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:TYR:O	1:A:536:PRO:HD3	1.65	0.96
1:A:178:ASN:H	1:A:178:ASN:HD22	1.13	0.94
1:A:588:TYR:HB2	1:A:590:LEU:HD22	1.57	0.87
1:A:326:GLN:NE2	1:A:328:ILE:HD11	1.91	0.86
1:A:485:GLN:HE21	1:A:489:ASN:HD21	1.26	0.83
2:B:404:GLN:HG2	2:B:423:GLN:NE2	1.94	0.82
2:B:313:GLY:HA2	2:B:323:PHE:H	1.45	0.81
1:A:403:ARG:HE	1:A:406:ILE:HD11	1.48	0.77
1:A:446:MET:CE	2:B:363:LYS:HD2	2.15	0.76
2:B:112:ILE:HA	2:B:115:MET:HE3	1.68	0.76
1:A:520:SER:O	1:A:524:GLU:HG3	1.86	0.76
1:A:500:PRO:HG2	1:A:502:GLN:HE22	1.51	0.75
2:B:226:SER:OG	2:B:229:GLU:HG2	1.87	0.74
1:A:485:GLN:NE2	1:A:489:ASN:HD21	1.87	0.73
2:B:273:LYS:HG3	2:B:274:LYS:N	2.05	0.71
2:B:77:ILE:HG21	2:B:113:VAL:HG21	1.72	0.71
1:A:178:ASN:HD22	1:A:178:ASN:N	1.84	0.71
1:A:296:VAL:HG11	2:B:295:TYR:HB3	1.73	0.71
2:B:28:GLU:OE2	2:B:36:LYS:HE3	1.91	0.71
1:A:500:PRO:HG2	1:A:502:GLN:NE2	2.06	0.70
1:A:178:ASN:H	1:A:178:ASN:ND2	1.88	0.69
2:B:469:LYS:O	2:B:471:ASP:N	2.25	0.69
2:B:457:LEU:HD22	2:B:533:ILE:HD12	1.74	0.69
1:A:328:ILE:O	1:A:329:LEU:HD23	1.93	0.69
1:A:157:VAL:HG11	1:A:161:MET:SD	2.33	0.68
2:B:467:ASP:CG	2:B:468:GLU:H	1.97	0.68
1:A:592:SER:HB2	1:A:599:LEU:HD21	1.75	0.68
2:B:273:LYS:HG3	2:B:274:LYS:H	1.58	0.67
1:A:348:MET:CE	2:B:518:PRO:HD3	2.25	0.67
1:A:142:SER:OG	1:A:145:GLU:HG3	1.94	0.67
1:A:585:CYS:HA	1:A:590:LEU:HD21	1.76	0.67
1:A:488:ARG:HG2	1:A:501:GLU:O	1.95	0.67
1:A:593:GLY:HA3	1:A:598:GLU:OE1	1.96	0.66
1:A:534:TYR:HD2	1:A:536:PRO:HG3	1.61	0.66
1:A:143:LEU:H	1:A:176:HIS:HE1	1.43	0.65
1:A:454:ALA:HB2	2:B:378:SER:HB3	1.79	0.65
2:B:35:LYS:HE3	2:B:94:ILE:O	1.96	0.65
1:A:242:LEU:O	1:A:246:VAL:HG23	1.97	0.64
1:A:451:LYS:HE2	1:A:453:MET:SD	2.36	0.64
2:B:152:HIS:CE1	2:B:156:LYS:HE3	2.32	0.64
1:A:320:GLN:HG3	2:B:276:TRP:CE3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LYS:HE3	2:B:455:ASP:HB2	1.79	0.64
2:B:207:ILE:O	2:B:211:VAL:HG23	1.97	0.64
1:A:251:THR:HG22	1:A:252:ARG:N	2.11	0.63
1:A:490:LEU:HD21	2:B:314:PHE:HB2	1.81	0.63
2:B:115:MET:HE2	2:B:150:ILE:HG23	1.80	0.63
1:A:574:GLY:HA2	1:A:600:LEU:HD21	1.80	0.63
1:A:592:SER:HB2	1:A:599:LEU:CD2	2.28	0.63
1:A:151:ALA:HB2	1:A:193:LEU:HD21	1.79	0.63
2:B:528:ILE:HB	2:B:529:PRO:HD3	1.81	0.62
2:B:24:ILE:HG23	2:B:25:PRO:HD2	1.80	0.62
1:A:444:ARG:NH1	2:B:268:LEU:O	2.32	0.62
2:B:27:ILE:HG23	2:B:183:PHE:CD2	2.34	0.62
2:B:54:ILE:HD12	2:B:86:PRO:HB3	1.82	0.62
1:A:52:GLN:O	1:A:54:GLU:HG3	2.00	0.62
2:B:115:MET:CE	2:B:150:ILE:HG23	2.30	0.61
1:A:142:SER:HA	1:A:176:HIS:CE1	2.35	0.61
1:A:534:TYR:CD2	1:A:536:PRO:HG3	2.35	0.61
1:A:157:VAL:HG11	1:A:161:MET:CE	2.31	0.61
1:A:252:ARG:N	1:A:252:ARG:HD2	2.16	0.61
1:A:326:GLN:HE21	1:A:328:ILE:HD11	1.64	0.60
1:A:302:THR:OG1	2:B:291:LYS:HG2	2.02	0.60
1:A:461:LYS:HG3	1:A:528:LEU:HD12	1.83	0.60
1:A:597:GLN:O	1:A:601:GLU:HG3	2.01	0.60
1:A:522:VAL:HG12	1:A:523:ASP:N	2.15	0.59
1:A:522:VAL:HB	3:A:630:HOH:O	2.02	0.59
1:A:590:LEU:HD23	1:A:590:LEU:H	1.67	0.59
2:B:364:VAL:O	2:B:418:CYS:HB2	2.03	0.59
2:B:131:HIS:ND1	2:B:160:SER:OG	2.33	0.58
1:A:578:VAL:HG22	1:A:579:PRO:HD3	1.85	0.58
1:A:302:THR:HG22	1:A:311:LEU:HD12	1.85	0.58
1:A:367:PHE:HZ	1:A:430:PRO:O	1.87	0.58
1:A:348:MET:HE1	2:B:518:PRO:HD3	1.86	0.57
1:A:68:GLN:O	1:A:72:ILE:HG13	2.03	0.57
2:B:313:GLY:CA	2:B:323:PHE:H	2.17	0.57
1:A:72:ILE:O	1:A:76:ILE:HG12	2.05	0.57
1:A:102:ILE:HG12	1:A:146:VAL:HG22	1.86	0.57
2:B:468:GLU:O	2:B:470:THR:N	2.36	0.57
1:A:534:TYR:C	1:A:536:PRO:HD3	2.24	0.57
1:A:363:ARG:NH1	1:A:364:PRO:O	2.37	0.57
1:A:72:ILE:HG12	1:A:116:ILE:HD13	1.87	0.57
2:B:65:ASP:HB3	2:B:78:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LYS:HG3	1:A:528:LEU:CD1	2.34	0.56
1:A:400:TYR:CE2	1:A:402:PRO:HG3	2.40	0.56
1:A:585:CYS:HA	1:A:590:LEU:CD2	2.35	0.56
2:B:7:LYS:HD2	2:B:127:PHE:CE2	2.40	0.56
2:B:194:LEU:O	2:B:202:LYS:HE2	2.04	0.56
1:A:182:LYS:HG2	1:A:185:ARG:NH2	2.20	0.56
1:A:44:ALA:O	1:A:137:HIS:HB2	2.07	0.55
2:B:246:HIS:CD2	2:B:248:PRO:HG3	2.42	0.55
1:A:54:GLU:C	1:A:56:GLU:H	2.09	0.55
2:B:39:THR:O	2:B:43:GLN:HG3	2.05	0.55
1:A:145:GLU:O	1:A:149:VAL:HG23	2.06	0.55
1:A:578:VAL:CG2	1:A:579:PRO:HD3	2.37	0.55
1:A:302:THR:O	1:A:310:LEU:HD12	2.06	0.55
1:A:363:ARG:HB2	1:A:364:PRO:HD2	1.89	0.54
1:A:420:LEU:HD23	1:A:426:GLN:HA	1.88	0.54
1:A:363:ARG:NH1	1:A:436:PHE:CE1	2.75	0.54
1:A:584:ALA:HB3	1:A:603:LEU:HD11	1.88	0.54
1:A:212:ASP:HB3	1:A:215:LEU:HG	1.89	0.54
1:A:333:GLU:OE2	2:B:497:ARG:NH2	2.39	0.54
2:B:112:ILE:HD11	2:B:146:GLN:HB3	1.88	0.54
1:A:46:LYS:HA	1:A:137:HIS:HD2	1.73	0.54
1:A:43:ASP:O	1:A:48:MET:HG3	2.07	0.54
1:A:445:LYS:HG2	1:A:446:MET:N	2.23	0.54
2:B:266:SER:HB2	2:B:363:LYS:HG3	1.88	0.54
2:B:280:ASP:HB2	2:B:289:ILE:HD11	1.89	0.54
2:B:294:VAL:HG12	2:B:295:TYR:N	2.23	0.54
2:B:323:PHE:CE2	2:B:328:GLU:HB3	2.43	0.54
1:A:113:ALA:HB1	1:A:495:LEU:HG	1.90	0.53
1:A:216:PHE:CZ	1:A:220:ILE:HD11	2.43	0.53
1:A:294:GLU:OE1	2:B:297:LEU:HD22	2.07	0.53
2:B:59:PHE:HB2	2:B:105:ALA:HB3	1.88	0.53
2:B:44:ARG:HG2	2:B:237:PHE:CE2	2.44	0.53
1:A:232:HIS:ND1	1:A:233:PHE:N	2.56	0.53
2:B:12:LEU:O	2:B:56:LEU:HD12	2.08	0.53
2:B:232:ARG:HG3	2:B:232:ARG:HH11	1.73	0.53
1:A:352:PRO:HA	1:A:394:VAL:HG23	1.91	0.53
2:B:131:HIS:CE1	2:B:162:GLN:HG3	2.44	0.53
1:A:42:VAL:HB	1:A:87:PHE:CD2	2.43	0.53
1:A:452:ILE:HD13	2:B:371:GLU:HG3	1.91	0.53
1:A:251:THR:CG2	1:A:252:ARG:N	2.72	0.53
2:B:223:GLU:HA	2:B:223:GLU:OE1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:ASN:HB3	2:B:487:PHE:CE1	2.44	0.52
1:A:66:CYS:O	1:A:70:VAL:HG23	2.09	0.52
2:B:193:PRO:C	2:B:195:LYS:H	2.12	0.52
1:A:488:ARG:NE	1:A:488:ARG:HA	2.24	0.52
1:A:128:GLN:O	1:A:132:GLN:HG2	2.10	0.52
1:A:351:LYS:C	1:A:394:VAL:HG22	2.30	0.52
1:A:199:PHE:N	1:A:199:PHE:CD1	2.77	0.52
1:A:171:ASN:HB3	1:A:205:LEU:HB2	1.92	0.51
1:A:200:LEU:C	1:A:200:LEU:HD23	2.30	0.51
1:A:38:LEU:HB2	1:A:252:ARG:HH22	1.75	0.51
1:A:348:MET:HE3	2:B:518:PRO:HD3	1.92	0.51
2:B:72:ASP:HA	2:B:75:GLN:NE2	2.24	0.51
2:B:27:ILE:HG23	2:B:183:PHE:CE2	2.46	0.51
1:A:447:PRO:HG3	2:B:243:HIS:CD2	2.45	0.51
2:B:134:ILE:HD11	2:B:161:LEU:HD11	1.91	0.51
2:B:450:GLN:HB3	2:B:537:PHE:CZ	2.46	0.51
1:A:59:PRO:HA	1:A:62:MET:HE2	1.93	0.50
1:A:588:TYR:HB2	1:A:590:LEU:CD2	2.38	0.50
1:A:296:VAL:HG13	2:B:296:CYS:O	2.11	0.50
1:A:296:VAL:CG1	2:B:295:TYR:HB3	2.40	0.50
1:A:488:ARG:HD3	1:A:501:GLU:OE2	2.12	0.50
1:A:157:VAL:HG11	1:A:161:MET:HE2	1.93	0.50
1:A:76:ILE:HD12	1:A:487:PHE:CD1	2.47	0.50
2:B:49:GLU:O	2:B:51:LYS:HE2	2.12	0.50
2:B:478:PRO:O	2:B:480:THR:N	2.45	0.50
1:A:261:LEU:C	1:A:261:LEU:HD23	2.32	0.49
1:A:199:PHE:N	1:A:199:PHE:HD1	2.10	0.49
1:A:369:TYR:CG	1:A:370:PRO:HD2	2.47	0.49
2:B:251:LEU:C	2:B:251:LEU:HD23	2.32	0.49
1:A:348:MET:HE1	2:B:517:ASN:HA	1.94	0.49
2:B:118:ILE:HD13	2:B:130:ARG:HB3	1.94	0.49
1:A:438:PRO:HB2	1:A:442:ASP:HB2	1.93	0.49
1:A:266:ASP:O	1:A:268:VAL:HG23	2.13	0.49
1:A:35:ARG:O	1:A:161:MET:HA	2.13	0.49
1:A:328:ILE:C	1:A:329:LEU:HD23	2.34	0.49
1:A:178:ASN:N	1:A:178:ASN:ND2	2.55	0.48
1:A:240:GLU:O	1:A:244:ARG:HG3	2.13	0.48
2:B:192:PHE:CD1	2:B:192:PHE:N	2.81	0.48
1:A:397:LEU:HD12	1:A:411:VAL:O	2.13	0.48
1:A:428:THR:HG23	2:B:354:ARG:CZ	2.44	0.48
1:A:97:VAL:O	1:A:97:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:HB2	1:A:500:PRO:HD2	1.96	0.48
2:B:19:THR:HG23	2:B:104:GLN:NE2	2.28	0.47
1:A:48:MET:HA	1:A:59:PRO:HG2	1.95	0.47
1:A:362:LEU:O	1:A:362:LEU:HG	2.14	0.47
2:B:49:GLU:OE2	2:B:274:LYS:NZ	2.47	0.47
2:B:232:ARG:HG3	2:B:232:ARG:NH1	2.30	0.47
2:B:467:ASP:CG	2:B:468:GLU:N	2.67	0.47
2:B:295:TYR:N	2:B:295:TYR:CD1	2.81	0.47
2:B:299:ASP:O	2:B:300:ASP:O	2.32	0.47
2:B:463:LEU:HD23	2:B:522:VAL:HG21	1.95	0.47
1:A:434:LEU:C	1:A:434:LEU:HD23	2.34	0.47
2:B:488:GLN:HG2	3:B:573:HOH:O	2.15	0.47
1:A:165:ARG:HA	1:A:199:PHE:O	2.15	0.47
1:A:264:ASN:C	1:A:264:ASN:OD1	2.52	0.47
1:A:347:LEU:CD2	2:B:461:MET:HE3	2.45	0.47
1:A:357:LYS:O	1:A:360:HIS:HB2	2.14	0.47
1:A:403:ARG:CG	1:A:406:ILE:HD12	2.45	0.47
2:B:186:GLY:O	2:B:232:ARG:HD3	2.15	0.47
1:A:362:LEU:HD11	2:B:269:GLN:HB2	1.97	0.46
1:A:371:GLU:OE1	1:A:371:GLU:HA	2.16	0.46
1:A:171:ASN:O	1:A:207:LYS:HD2	2.15	0.46
1:A:132:GLN:OE1	1:A:137:HIS:CE1	2.69	0.46
1:A:605:LYS:HG3	1:A:609:ASP:HB3	1.95	0.46
2:B:42:VAL:HG12	2:B:91:LEU:HD21	1.98	0.46
1:A:179:ASP:O	1:A:181:ALA:N	2.48	0.46
2:B:288:ASP:N	2:B:288:ASP:OD1	2.49	0.46
1:A:36:ASP:OD2	1:A:252:ARG:HD3	2.16	0.46
2:B:329:GLU:C	2:B:331:MET:H	2.18	0.46
1:A:441:ASP:O	1:A:444:ARG:NH1	2.49	0.46
1:A:383:SER:O	1:A:387:ILE:HG13	2.16	0.46
2:B:484:ASN:C	2:B:486:ARG:H	2.19	0.46
1:A:253:LYS:HD3	2:B:435:PHE:CE2	2.51	0.46
1:A:234:GLU:HG2	1:A:424:LYS:HG2	1.98	0.46
1:A:135:MET:O	1:A:136:GLY:C	2.52	0.45
1:A:217:TYR:HA	1:A:220:ILE:HB	1.99	0.45
2:B:77:ILE:HD11	2:B:109:ASP:HB3	1.98	0.45
2:B:106:ASP:HB3	2:B:109:ASP:HB2	1.98	0.45
2:B:323:PHE:CD2	2:B:328:GLU:HB3	2.52	0.45
2:B:424:LEU:HB3	2:B:425:PRO:HD2	1.98	0.45
1:A:179:ASP:C	1:A:181:ALA:H	2.19	0.45
1:A:318:ARG:O	1:A:328:ILE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ILE:C	1:A:199:PHE:HD1	2.20	0.45
2:B:283:THR:O	2:B:284:LEU:HB2	2.17	0.45
1:A:121:GLN:OE1	1:A:130:ARG:NH1	2.49	0.45
2:B:109:ASP:O	2:B:113:VAL:HG23	2.16	0.45
1:A:196:THR:O	1:A:196:THR:HG22	2.16	0.45
1:A:252:ARG:O	1:A:254:ARG:HG3	2.17	0.45
2:B:477:PHE:N	2:B:478:PRO:HD3	2.32	0.45
1:A:303:PHE:HA	1:A:311:LEU:HG	1.98	0.45
1:A:458:GLN:NE2	1:A:528:LEU:O	2.43	0.45
2:B:83:LEU:O	2:B:84:MET:HB3	2.17	0.45
1:A:56:GLU:HG2	1:A:237:SER:O	2.16	0.45
1:A:264:ASN:OD1	1:A:266:ASP:N	2.49	0.45
2:B:90:LEU:O	2:B:94:ILE:HG12	2.17	0.45
1:A:573:LEU:O	1:A:576:PHE:HB2	2.17	0.44
1:A:91:GLU:N	1:A:136:GLY:O	2.51	0.44
1:A:71:TYR:OH	1:A:85:VAL:HG23	2.18	0.44
2:B:138:LEU:O	2:B:201:GLN:HA	2.17	0.44
1:A:448:PHE:CD2	1:A:448:PHE:N	2.86	0.44
2:B:7:LYS:HE3	2:B:126:LYS:O	2.16	0.44
1:A:302:THR:HA	2:B:291:LYS:HA	2.00	0.44
1:A:262:LYS:HG2	1:A:268:VAL:HG22	2.00	0.44
1:A:578:VAL:N	1:A:579:PRO:CD	2.81	0.44
1:A:59:PRO:HA	1:A:62:MET:CE	2.48	0.44
1:A:470:ARG:O	1:A:471:PHE:HB3	2.18	0.44
1:A:465:ILE:HG23	1:A:518:LEU:CD2	2.47	0.44
1:A:584:ALA:CB	1:A:603:LEU:HD11	2.48	0.44
1:A:595:LYS:HB2	1:A:598:GLU:HG3	2.00	0.44
2:B:66:ASN:HA	2:B:67:PRO:HD3	1.88	0.44
2:B:337:GLY:HA2	2:B:399:LYS:HA	2.00	0.44
1:A:154:PHE:CD1	1:A:198:ILE:HD13	2.53	0.43
1:A:363:ARG:HG3	1:A:363:ARG:HH11	1.83	0.43
1:A:256:LEU:N	1:A:273:ILE:O	2.41	0.43
1:A:379:SER:HB2	2:B:444:TYR:CD2	2.53	0.43
1:A:445:LYS:CG	1:A:446:MET:N	2.81	0.43
2:B:332:LYS:HG2	2:B:333:TYR:N	2.33	0.43
1:A:347:LEU:HD21	2:B:461:MET:HE3	2.00	0.43
1:A:151:ALA:CB	1:A:193:LEU:HD21	2.48	0.43
1:A:388:LYS:HB3	2:B:458:ILE:HD12	2.01	0.43
1:A:473:TYR:CZ	2:B:424:LEU:HD13	2.53	0.43
2:B:131:HIS:HE1	2:B:162:GLN:HG3	1.82	0.43
1:A:289:TYR:O	1:A:291:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ARG:CZ	2:B:389:MET:HE3	2.49	0.43
1:A:149:VAL:O	1:A:153:LEU:HG	2.19	0.43
1:A:353:LEU:CD2	1:A:395:ALA:HB2	2.49	0.43
1:A:437:LEU:HD23	3:B:579:HOH:O	2.19	0.43
2:B:6:ASN:N	2:B:128:GLU:OE1	2.51	0.43
1:A:338:LYS:O	1:A:340:PHE:HD1	2.02	0.43
1:A:108:LEU:HD11	1:A:154:PHE:CD2	2.53	0.42
1:A:158:GLN:OE1	1:A:158:GLN:N	2.52	0.42
1:A:511:VAL:HG11	2:B:255:SER:HB3	2.00	0.42
1:A:216:PHE:CZ	1:A:220:ILE:CD1	3.02	0.42
1:A:399:ARG:HG2	1:A:408:PRO:HB2	2.01	0.42
2:B:73:GLN:O	2:B:74:TYR:C	2.55	0.42
2:B:134:ILE:HD12	2:B:134:ILE:N	2.35	0.42
1:A:142:SER:HB3	1:A:182:LYS:HD3	2.02	0.42
1:A:420:LEU:CD2	1:A:426:GLN:HA	2.49	0.42
2:B:347:LYS:HB2	2:B:350:GLN:HG3	2.01	0.42
1:A:366:LEU:HB2	1:A:434:LEU:HB3	2.02	0.42
1:A:447:PRO:HD3	2:B:243:HIS:CD2	2.54	0.42
1:A:508:LEU:HD23	2:B:394:ARG:NE	2.34	0.42
1:A:263:LEU:HD22	1:A:347:LEU:HD22	2.02	0.42
1:A:418:GLU:CG	1:A:419:GLU:N	2.82	0.42
2:B:193:PRO:C	2:B:195:LYS:N	2.72	0.42
1:A:403:ARG:HG3	1:A:406:ILE:HD12	2.01	0.42
1:A:577:THR:OG1	1:A:580:MET:HG3	2.19	0.42
1:A:196:THR:O	1:A:196:THR:CG2	2.67	0.42
2:B:135:PHE:CD1	2:B:135:PHE:N	2.87	0.42
2:B:147:LEU:HA	2:B:150:ILE:HD12	2.00	0.42
2:B:413:LYS:HD3	2:B:413:LYS:HA	1.82	0.42
1:A:340:PHE:HB2	1:A:408:PRO:HD3	2.02	0.42
1:A:204:HIS:ND1	1:A:204:HIS:N	2.66	0.41
1:A:67:ILE:HG22	1:A:119:LEU:HD13	2.02	0.41
1:A:141:TYR:CD1	1:A:141:TYR:C	2.93	0.41
1:A:251:THR:CG2	1:A:252:ARG:H	2.33	0.41
1:A:568:ILE:HG12	1:A:573:LEU:HD22	2.02	0.41
2:B:146:GLN:HB2	2:B:150:ILE:HD11	2.02	0.41
2:B:204:GLY:O	2:B:208:VAL:HG23	2.20	0.41
2:B:335:SER:C	2:B:337:GLY:H	2.23	0.41
1:A:99:PHE:HD2	1:A:99:PHE:HA	1.72	0.41
1:A:233:PHE:CD2	1:A:245:LYS:HG2	2.56	0.41
1:A:236:SER:OG	1:A:245:LYS:HD2	2.20	0.41
1:A:406:ILE:HA	1:A:407:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASP:OD1	1:A:423:GLN:HG2	2.20	0.41
2:B:128:GLU:C	2:B:129:LYS:HG3	2.40	0.41
2:B:381:ILE:HD11	2:B:418:CYS:HA	2.03	0.41
1:A:329:LEU:HD22	2:B:497:ARG:HE	1.85	0.41
2:B:19:THR:H	2:B:104:GLN:HE22	1.66	0.41
2:B:71:GLY:O	2:B:73:GLN:HG3	2.21	0.41
2:B:283:THR:HB	2:B:285:LYS:HG2	2.00	0.41
1:A:63:SER:HG	1:A:169:PHE:HD2	1.68	0.41
1:A:490:LEU:HA	1:A:490:LEU:HD12	1.74	0.41
2:B:197:ILE:HD11	2:B:202:LYS:HG2	2.02	0.41
1:A:423:GLN:HB2	1:A:425:ILE:HG13	2.03	0.41
1:A:451:LYS:HE3	2:B:417:GLU:CD	2.41	0.41
1:A:451:LYS:HE3	2:B:417:GLU:CG	2.51	0.41
1:A:511:VAL:CG1	2:B:255:SER:HB3	2.51	0.41
2:B:382:HIS:NE2	2:B:417:GLU:OE2	2.49	0.41
1:A:465:ILE:HG23	1:A:518:LEU:HD21	2.02	0.41
1:A:491:GLU:HG3	2:B:316:TYR:CE2	2.56	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.81	0.41
1:A:585:CYS:O	1:A:590:LEU:HD23	2.21	0.41
2:B:245:ILE:HG22	2:B:246:HIS:N	2.36	0.41
2:B:492:GLN:NE2	2:B:509:GLN:HG3	2.36	0.41
2:B:528:ILE:O	2:B:529:PRO:C	2.58	0.41
2:B:132:ILE:HB	2:B:161:LEU:CD1	2.51	0.41
2:B:294:VAL:HG12	2:B:295:TYR:H	1.85	0.41
1:A:142:SER:HA	1:A:176:HIS:NE2	2.36	0.40
1:A:447:PRO:CD	2:B:243:HIS:CD2	3.04	0.40
1:A:474:ARG:HG2	1:A:476:ASP:OD1	2.21	0.40
2:B:246:HIS:HB3	2:B:264:TYR:CE2	2.57	0.40
1:A:101:ASN:ND2	1:A:139:SER:HB3	2.36	0.40
1:A:166:ILE:O	1:A:200:LEU:HA	2.22	0.40
1:A:318:ARG:HG3	1:A:334:THR:HG21	2.04	0.40
1:A:582:LYS:O	1:A:586:ARG:HG3	2.21	0.40
2:B:366:ALA:O	2:B:367:ALA:C	2.60	0.40
1:A:530:TYR:O	1:A:531:PRO:C	2.59	0.40
1:A:286:ILE:HG22	1:A:287:LYS:N	2.37	0.40
1:A:326:GLN:HE21	1:A:328:ILE:CD1	2.33	0.40
1:A:442:ASP:HA	1:A:444:ARG:NH1	2.37	0.40
1:A:495:LEU:O	1:A:496:ASP:C	2.60	0.40

There are no symmetry-related clashes.

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	542/609 (89%)	473 (87%)	56 (10%)	13 (2%)	6	15
2	B	512/565 (91%)	454 (89%)	49 (10%)	9 (2%)	8	21
All	All	1054/1174 (90%)	927 (88%)	105 (10%)	22 (2%)	7	18

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	180	SER
1	A	290	ARG
2	B	96	SER
2	B	97	LYS
2	B	300	ASP
2	B	470	THR
1	A	136	GLY
1	A	267	ILE
1	A	402	PRO
2	B	468	GLU
2	B	479	THR
2	B	527	GLN
2	B	469	LYS
1	A	137	HIS
1	A	138	GLY
1	A	522	VAL
1	A	98	ASN
1	A	535	ASN
1	A	602	ALA
2	B	95	GLU
1	A	589	GLY

5.3.2 Protein sidechains (i)

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	495/548 (90%)	473 (96%)	22 (4%)	28	56
2	B	469/505 (93%)	454 (97%)	15 (3%)	39	68
All	All	964/1053 (92%)	927 (96%)	37 (4%)	33	62

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	SER
1	A	78	SER
1	A	99	PHE
1	A	144	SER
1	A	178	ASN
1	A	184	SER
1	A	243	LEU
1	A	266	ASP
1	A	303	PHE
1	A	360	HIS
1	A	381	LEU
1	A	394	VAL
1	A	409	TYR
1	A	441	ASP
1	A	449	THR
1	A	453	MET
1	A	471	PHE
1	A	474	ARG
1	A	488	ARG
1	A	496	ASP
1	A	517	ARG
1	A	609	ASP
2	B	28	GLU
2	B	30	PRO
2	B	72	ASP
2	B	107	PHE
2	B	130	ARG

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Mol	Chain	Res	Type
2	B	288	ASP
2	B	300	ASP
2	B	323	PHE
2	B	329	GLU
2	B	330	GLN
2	B	341	SER
2	B	380	LEU
2	B	386	ASP
2	B	427	MET
2	B	471	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	176	HIS
1	A	178	ASN
1	A	326	GLN
1	A	433	GLN
1	A	485	GLN
1	A	502	GLN
2	B	43	GLN
2	B	75	GLN
2	B	104	GLN
2	B	152	HIS
2	B	423	GLN
2	B	452	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.