



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:45 pm BST

PDB ID : 3TJ0  
Title : Crystal Structure of Influenza B Virus Nucleoprotein  
Authors : Ng, A.K.L.; Zhang, H.; Liu, J.; Au, S.W.N.; Wang, J.; Shaw, P.C.  
Deposited on : 2011-08-23  
Resolution : 3.23 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

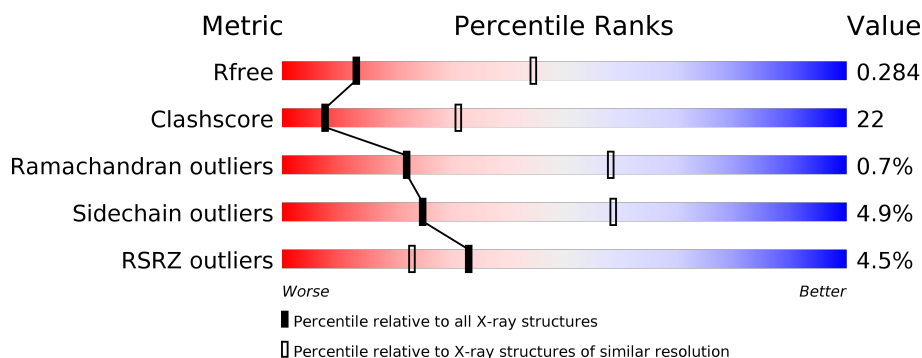
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.23 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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 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  $\leq 5\%$ . 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	562	<div> <div>4%</div> <div> <div></div> <div>49%</div> <div>30%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	562	<div> <div>4%</div> <div> <div></div> <div>49%</div> <div>28%</div> <div>•</div> <div>19%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7022 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3519	2223	618	648	30			
1	B	457	Total	C	N	O	S	0	0	0
			3503	2213	613	647	30			

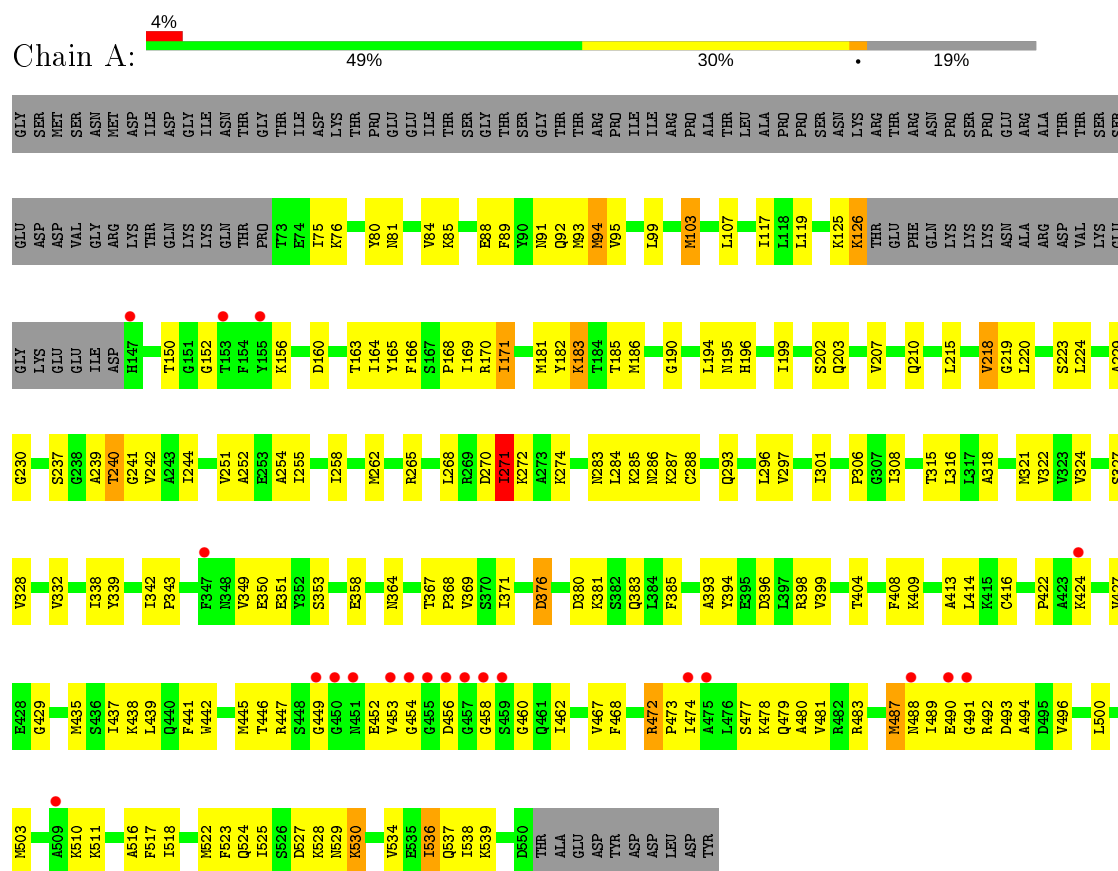
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP C4LQ26
A	0	SER	-	EXPRESSION TAG	UNP C4LQ26
A	142	LYS	ARG	SEE REMARK 999	UNP C4LQ26
A	537	GLN	PRO	SEE REMARK 999	UNP C4LQ26
B	-1	GLY	-	EXPRESSION TAG	UNP C4LQ26
B	0	SER	-	EXPRESSION TAG	UNP C4LQ26
B	142	LYS	ARG	SEE REMARK 999	UNP C4LQ26
B	537	GLN	PRO	SEE REMARK 999	UNP C4LQ26

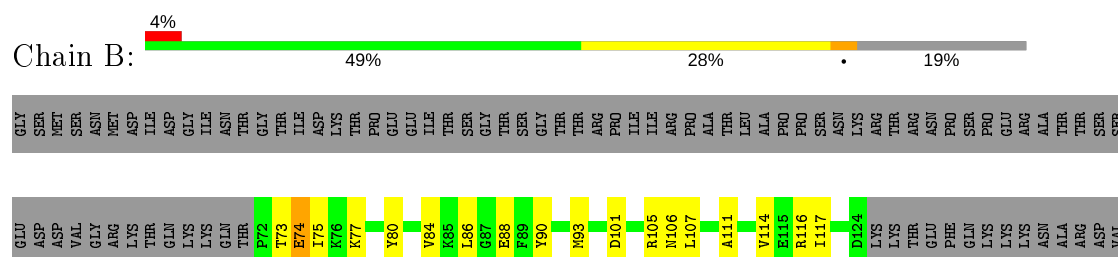
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Nucleoprotein



#### • Molecule 1: Nucleoprotein





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.95Å 123.34Å 198.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 3.23 49.52 – 3.23	Depositor EDS
% Data completeness (in resolution range)	93.0 (47.05-3.23) 92.8 (49.52-3.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.58 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.245 , 0.291 0.240 , 0.284	Depositor DCC
$R_{free}$ test set	1023 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	1.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7022	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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, 0.333 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	0.22	0/3572	0.42	0/4791
1	B	0.22	0/3556	0.42	0/4772
All	All	0.22	0/7128	0.42	0/9563

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	2
1	B	0	4
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	VAL	Peptide
1	A	487	MET	Peptide
1	B	347	PHE	Peptide
1	B	348	ASN	Peptide
1	B	449	GLY	Peptide
1	B	538	ILE	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	3519	0	3626	168	0
1	B	3503	0	3603	148	0
All	All	7022	0	7229	314	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 22.

All (314) 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:285:LYS:HB2	1:B:297:VAL:HG11	1.33	1.08
1:A:156:LYS:HD2	1:A:169:ILE:HD11	1.47	0.94
1:A:215:LEU:O	1:A:219:GLY:HA2	1.69	0.93
1:A:328:VAL:H	1:A:449:GLY:H	1.09	0.93
1:A:285:LYS:HB2	1:A:297:VAL:HG11	1.54	0.89
1:B:296:LEU:HD13	1:B:500:LEU:HD12	1.51	0.88
1:A:453:VAL:HG12	1:A:454:GLY:H	1.45	0.81
1:A:328:VAL:N	1:A:449:GLY:H	1.79	0.81
1:A:328:VAL:H	1:A:449:GLY:N	1.79	0.80
1:A:364:ASN:HD21	1:A:439:LEU:H	1.28	0.80
1:A:364:ASN:HB3	1:B:526:SER:HB2	1.65	0.78
1:A:536:ILE:HG13	1:A:537:GLN:H	1.48	0.77
1:A:332:VAL:HG23	1:A:445:MET:HE1	1.67	0.76
1:B:318:ALA:HA	1:B:321:MET:HE2	1.69	0.75
1:B:171:ILE:HD13	1:B:171:ILE:H	1.51	0.75
1:B:403:LEU:HD23	1:B:522:MET:HE3	1.69	0.74
1:A:75:ILE:H	1:A:75:ILE:HD12	1.53	0.73
1:B:155:TYR:OH	1:B:421:VAL:HG21	1.89	0.73
1:B:347:PHE:HD2	1:B:348:ASN:O	1.72	0.72
1:B:447:ARG:HD3	1:B:447:ARG:H	1.54	0.71
1:B:518:ILE:HD13	1:B:518:ILE:H	1.55	0.71
1:A:296:LEU:HA	1:A:496:VAL:HG11	1.71	0.71
1:B:207:VAL:HG22	1:B:393:ALA:HB2	1.71	0.71
1:B:402:ALA:HB2	1:B:538:ILE:HG22	1.72	0.71
1:A:308:ILE:H	1:A:308:ILE:HD12	1.55	0.70
1:B:346:GLY:C	1:B:347:PHE:CD1	2.64	0.70
1:B:511:LYS:HD3	1:B:511:LYS:H	1.56	0.70
1:A:536:ILE:O	1:A:537:GLN:HB2	1.92	0.70
1:A:380:ASP:HB3	1:A:414:LEU:HG	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:SER:O	1:B:224:LEU:HB2	1.91	0.69
1:A:125:LYS:O	1:A:126:LYS:HB2	1.91	0.69
1:B:93:MET:HG2	1:B:114:VAL:HG13	1.73	0.69
1:A:268:LEU:HD21	1:A:306:PRO:HD2	1.73	0.69
1:A:487:MET:SD	1:A:488:ASN:HB2	2.33	0.68
1:A:285:LYS:HA	1:A:288:CYS:HB2	1.75	0.68
1:B:489:ILE:HG23	1:B:490:GLU:H	1.59	0.68
1:A:453:VAL:HB	1:A:516:ALA:HA	1.78	0.65
1:A:223:SER:O	1:A:224:LEU:HB2	1.96	0.65
1:A:404:THR:HG1	1:A:408:PHE:HE2	1.45	0.65
1:B:467:VAL:HG23	1:B:468:PHE:H	1.61	0.64
1:A:163:THR:HG22	1:A:164:ILE:H	1.63	0.64
1:B:515:ASN:HB3	1:B:518:ILE:HG23	1.79	0.64
1:B:151:GLY:HA3	1:B:172:THR:HG22	1.78	0.63
1:A:364:ASN:ND2	1:A:439:LEU:H	1.95	0.63
1:A:283:ASN:O	1:A:286:ASN:HB2	1.99	0.63
1:A:353:SER:H	1:A:358:GLU:HB2	1.64	0.63
1:B:199:ILE:HG23	1:B:244:ILE:HG21	1.79	0.63
1:B:284:LEU:O	1:B:285:LYS:HB3	1.98	0.63
1:B:422:PRO:HB2	1:B:424:LYS:HG2	1.79	0.63
1:A:349:VAL:HG12	1:A:350:GLU:H	1.64	0.62
1:B:347:PHE:CD2	1:B:348:ASN:HA	2.34	0.62
1:A:467:VAL:HG23	1:A:468:PHE:H	1.62	0.61
1:B:285:LYS:HA	1:B:288:CYS:HB2	1.82	0.61
1:B:296:LEU:HA	1:B:496:VAL:HG11	1.82	0.61
1:A:170:ARG:O	1:A:170:ARG:HG3	2.01	0.61
1:A:165:TYR:HB3	1:A:429:GLY:HA2	1.82	0.61
1:A:171:ILE:HD13	1:A:171:ILE:H	1.64	0.60
1:B:357:TYR:HB2	1:B:442:TRP:CH2	2.37	0.60
1:A:446:THR:OG1	1:A:447:ARG:HG2	2.01	0.60
1:B:117:ILE:HG21	1:B:173:PHE:HE1	1.67	0.60
1:A:364:ASN:HA	1:A:438:LYS:HD2	1.84	0.60
1:A:453:VAL:HG21	1:A:517:PHE:H	1.66	0.60
1:A:524:GLN:HG2	1:A:527:ASP:CB	2.32	0.59
1:A:364:ASN:HD21	1:A:439:LEU:N	1.99	0.59
1:A:284:LEU:O	1:A:285:LYS:HB3	2.02	0.59
1:A:318:ALA:HA	1:A:321:MET:HE2	1.84	0.59
1:B:276:ALA:O	1:B:279:LYS:HG2	2.03	0.58
1:B:296:LEU:HD22	1:B:317:LEU:HB2	1.86	0.58
1:B:422:PRO:HG2	1:B:425:GLU:HG2	1.85	0.58
1:A:364:ASN:OD1	1:A:525:ILE:HG21	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:VAL:CG2	1:A:517:PHE:H	2.16	0.58
1:A:117:ILE:HG23	1:A:150:THR:HG23	1.86	0.58
1:B:296:LEU:HD21	1:B:313:ASP:HB3	1.86	0.58
1:B:156:LYS:HB2	1:B:156:LYS:NZ	2.19	0.57
1:A:218:VAL:HG11	1:A:252:ALA:HA	1.86	0.57
1:A:91:ASN:O	1:A:95:VAL:HG23	2.05	0.57
1:B:489:ILE:HG23	1:B:490:GLU:N	2.18	0.57
1:A:528:LYS:O	1:A:529:ASN:HB2	2.04	0.57
1:B:462:ILE:HG23	1:B:477:SER:HB3	1.86	0.57
1:B:237:SER:OG	1:B:241:GLY:HA3	2.05	0.56
1:B:148:ASN:N	1:B:175:LYS:HZ1	2.04	0.56
1:A:516:ALA:O	1:A:517:PHE:HB2	2.05	0.56
1:A:94:MET:HE1	1:A:99:LEU:HD12	1.87	0.56
1:B:537:GLN:HG3	1:B:538:ILE:H	1.70	0.56
1:B:366:ALA:C	1:B:368:PRO:HD3	2.27	0.55
1:B:522:MET:O	1:B:534:VAL:HG12	2.07	0.55
1:B:101:ASP:O	1:B:105:ARG:HG2	2.07	0.55
1:A:422:PRO:HB2	1:A:424:LYS:HG2	1.89	0.55
1:A:328:VAL:HB	1:A:449:GLY:HA3	1.89	0.55
1:A:524:GLN:HG2	1:A:527:ASP:HB2	1.89	0.55
1:B:74:GLU:HG2	1:B:74:GLU:O	2.06	0.55
1:A:107:LEU:HD11	1:A:371:ILE:HG12	1.89	0.54
1:A:195:ASN:O	1:A:199:ILE:HG13	2.07	0.54
1:A:338:ILE:HD11	1:A:368:PRO:HG3	1.88	0.54
1:A:409:LYS:HB2	1:A:414:LEU:HD12	1.89	0.54
1:B:467:VAL:HG23	1:B:468:PHE:N	2.22	0.54
1:B:297:VAL:O	1:B:301:ILE:HG13	2.07	0.54
1:A:103:MET:HG3	1:A:166:PHE:HZ	1.72	0.54
1:B:169:ILE:HG22	1:B:171:ILE:HG23	1.90	0.54
1:A:376:ASP:OD1	1:A:416:CYS:HB2	2.07	0.54
1:B:474:ILE:O	1:B:474:ILE:HG22	2.08	0.54
1:A:462:ILE:HG13	1:A:477:SER:HB3	1.89	0.54
1:B:293:GLN:HE22	1:B:324:VAL:HB	1.73	0.53
1:B:170:ARG:O	1:B:170:ARG:HG3	2.08	0.53
1:B:478:LYS:O	1:B:481:VAL:HG22	2.09	0.53
1:A:182:TYR:O	1:A:186:MET:HB2	2.08	0.53
1:B:504:MET:O	1:B:508:MET:HG2	2.07	0.53
1:A:107:LEU:HA	1:A:369:VAL:O	2.08	0.53
1:A:285:LYS:O	1:A:285:LYS:HG2	2.09	0.53
1:A:316:LEU:HG	1:A:500:LEU:HD12	1.90	0.53
1:A:491:GLY:O	1:A:492:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:VAL:O	1:B:350:GLU:HB3	2.07	0.53
1:A:332:VAL:HG23	1:A:445:MET:CE	2.38	0.53
1:A:262:MET:HG2	1:A:265:ARG:HH12	1.74	0.53
1:B:347:PHE:CD2	1:B:348:ASN:CA	2.92	0.52
1:A:480:ALA:O	1:A:483:ARG:HB3	2.09	0.52
1:B:347:PHE:CD2	1:B:348:ASN:O	2.60	0.52
1:A:199:ILE:HG23	1:A:244:ILE:HG21	1.91	0.52
1:A:453:VAL:HG12	1:A:454:GLY:N	2.19	0.52
1:B:186:MET:HG2	1:B:190:GLY:HA2	1.92	0.52
1:B:347:PHE:HD2	1:B:348:ASN:CA	2.23	0.52
1:B:528:LYS:HG2	1:B:529:ASN:H	1.73	0.52
1:A:446:THR:O	1:A:447:ARG:C	2.49	0.51
1:A:510:LYS:NZ	1:A:511:LYS:HE2	2.25	0.51
1:B:411:ARG:HG2	1:B:546:PHE:CE2	2.45	0.51
1:B:447:ARG:N	1:B:447:ARG:HD3	2.25	0.51
1:B:355:VAL:HG23	1:B:445:MET:HB2	1.93	0.51
1:A:287:LYS:HE2	1:A:327:SER:O	2.10	0.51
1:A:169:ILE:HG22	1:A:171:ILE:HG23	1.93	0.51
1:A:523:PHE:CZ	1:A:530:LYS:HB3	2.46	0.51
1:A:538:ILE:O	1:A:538:ILE:HD12	2.10	0.51
1:B:342:ILE:HB	1:B:343:PRO:HD3	1.93	0.51
1:B:117:ILE:HG21	1:B:173:PHE:CE1	2.45	0.51
1:A:293:GLN:O	1:A:297:VAL:HG12	2.10	0.51
1:B:163:THR:HG22	1:B:164:ILE:N	2.26	0.51
1:A:202:SER:OG	1:A:230:GLY:HA2	2.11	0.50
1:A:493:ASP:O	1:A:494:ALA:HB2	2.12	0.50
1:A:342:ILE:HB	1:A:343:PRO:HD3	1.93	0.50
1:A:107:LEU:HD12	1:A:369:VAL:O	2.12	0.50
1:B:528:LYS:HG2	1:B:529:ASN:N	2.27	0.50
1:A:183:LYS:NZ	1:A:190:GLY:HA3	2.27	0.50
1:B:318:ALA:HA	1:B:321:MET:CE	2.40	0.50
1:B:373:ARG:NH2	1:B:417:LYS:HB3	2.27	0.50
1:A:409:LYS:HB3	1:A:413:ALA:HB3	1.92	0.50
1:A:458:GLY:C	1:A:460:GLY:H	2.14	0.50
1:B:117:ILE:HD11	1:B:152:GLY:H	1.76	0.50
1:A:152:GLY:O	1:A:170:ARG:HA	2.12	0.50
1:A:89:PHE:O	1:A:93:MET:HB2	2.12	0.50
1:A:237:SER:HB2	1:A:241:GLY:HA3	1.95	0.49
1:B:239:ALA:O	1:B:242:VAL:HG12	2.12	0.49
1:B:247:GLY:HA3	1:B:321:MET:SD	2.52	0.49
1:B:528:LYS:C	1:B:530:LYS:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:MET:O	1:A:487:MET:HG3	2.11	0.49
1:A:237:SER:OG	1:A:241:GLY:HA3	2.11	0.49
1:A:536:ILE:HG13	1:A:537:GLN:N	2.23	0.49
1:B:357:TYR:HD1	1:B:442:TRP:CE2	2.31	0.49
1:B:237:SER:O	1:B:240:THR:HG23	2.12	0.49
1:B:529:ASN:HB2	1:B:531:THR:HG23	1.95	0.49
1:A:88:GLU:O	1:A:92:GLN:HG2	2.13	0.49
1:A:125:LYS:O	1:A:126:LYS:CB	2.61	0.48
1:A:318:ALA:HA	1:A:321:MET:CE	2.43	0.48
1:A:297:VAL:O	1:A:301:ILE:HG13	2.13	0.48
1:A:220:LEU:HD23	1:A:315:THR:HG23	1.95	0.48
1:B:195:ASN:O	1:B:199:ILE:HG13	2.13	0.48
1:A:237:SER:CB	1:A:241:GLY:HA3	2.43	0.48
1:B:447:ARG:H	1:B:447:ARG:HH11	1.60	0.48
1:A:383:GLN:HA	1:A:437:ILE:HD12	1.96	0.48
1:A:224:LEU:HD12	1:A:322:VAL:HG21	1.96	0.48
1:A:396:ASP:HB3	1:A:399:VAL:HG23	1.95	0.48
1:B:525:ILE:HD12	1:B:526:SER:N	2.28	0.48
1:B:411:ARG:HG2	1:B:546:PHE:CZ	2.49	0.48
1:B:107:LEU:HD21	1:B:371:ILE:HD11	1.95	0.48
1:B:251:VAL:O	1:B:255:ILE:HG13	2.14	0.48
1:B:258:ILE:O	1:B:262:MET:HG2	2.13	0.48
1:B:111:ALA:HB2	1:B:337:SER:HB3	1.95	0.48
1:B:153:THR:HA	1:B:170:ARG:HA	1.95	0.48
1:A:169:ILE:CG2	1:A:171:ILE:HG23	2.44	0.47
1:B:253:GLU:HA	1:B:256:ARG:HD3	1.95	0.47
1:A:349:VAL:HG12	1:A:350:GLU:N	2.29	0.47
1:A:165:TYR:HB3	1:A:429:GLY:CA	2.44	0.47
1:B:162:LYS:HD2	1:B:163:THR:N	2.30	0.47
1:B:196:HIS:CE1	1:B:333:VAL:HG13	2.49	0.47
1:A:81:ASN:O	1:A:85:LYS:HG3	2.15	0.47
1:B:285:LYS:CB	1:B:297:VAL:HG11	2.25	0.47
1:A:321:MET:HA	1:A:324:VAL:O	2.14	0.47
1:A:367:THR:N	1:A:368:PRO:HD3	2.29	0.47
1:B:267:LEU:C	1:B:268:LEU:HD12	2.35	0.47
1:B:162:LYS:HD2	1:B:163:THR:H	1.80	0.47
1:A:210:GLN:HE21	1:A:210:GLN:HA	1.79	0.47
1:A:467:VAL:HG23	1:A:468:PHE:N	2.26	0.47
1:B:169:ILE:CG2	1:B:171:ILE:HG23	2.44	0.47
1:B:84:VAL:O	1:B:88:GLU:HG3	2.14	0.47
1:A:446:THR:C	1:A:447:ARG:HG2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:HIS:HE1	1:B:339:TYR:CE1	2.32	0.47
1:B:75:ILE:HD12	1:B:75:ILE:H	1.80	0.47
1:A:196:HIS:HE1	1:A:339:TYR:OH	1.97	0.47
1:B:373:ARG:HB2	1:B:376:ASP:OD2	2.15	0.47
1:B:293:GLN:NE2	1:B:324:VAL:HB	2.29	0.46
1:A:524:GLN:CD	1:B:347:PHE:CE1	2.88	0.46
1:A:524:GLN:OE1	1:A:524:GLN:N	2.48	0.46
1:B:86:LEU:HD22	1:B:197:ILE:HD11	1.97	0.46
1:B:346:GLY:O	1:B:347:PHE:CD1	2.67	0.46
1:B:233:ILE:HD12	1:B:244:ILE:HD11	1.97	0.46
1:B:80:TYR:HA	1:B:352:TYR:HB3	1.96	0.46
1:B:183:LYS:NZ	1:B:190:GLY:HA3	2.30	0.46
1:B:107:LEU:HD12	1:B:369:VAL:O	2.16	0.46
1:B:523:PHE:HE1	1:B:533:PRO:HG3	1.81	0.46
1:A:537:GLN:HG3	1:A:538:ILE:N	2.31	0.46
1:A:404:THR:OG1	1:A:408:PHE:HE2	1.96	0.46
1:B:402:ALA:HB2	1:B:538:ILE:CG2	2.41	0.46
1:A:522:MET:HG3	1:A:534:VAL:HB	1.97	0.46
1:B:462:ILE:O	1:B:462:ILE:HG22	2.16	0.46
1:B:249:THR:O	1:B:253:GLU:HG3	2.16	0.46
1:B:356:GLY:O	1:B:360:MET:HG2	2.16	0.46
1:A:328:VAL:H	1:A:449:GLY:CA	2.28	0.45
1:B:347:PHE:HD2	1:B:348:ASN:C	2.19	0.45
1:A:237:SER:O	1:A:240:THR:HG23	2.16	0.45
1:A:94:MET:CE	1:A:99:LEU:HD12	2.45	0.45
1:B:203:GLN:O	1:B:207:VAL:HG23	2.16	0.45
1:A:364:ASN:HD22	1:A:438:LYS:HD2	1.81	0.45
1:B:518:ILE:H	1:B:518:ILE:CD1	2.21	0.45
1:A:383:GLN:HG3	1:A:408:PHE:CD1	2.51	0.45
1:B:221:ASP:HB3	1:B:222:PRO:HD2	1.97	0.45
1:B:440:GLN:O	1:B:525:ILE:HG13	2.17	0.45
1:A:308:ILE:HD12	1:A:308:ILE:N	2.27	0.45
1:B:230:GLY:O	1:B:233:ILE:HG22	2.16	0.45
1:B:294:LYS:HZ3	1:B:294:LYS:HB3	1.82	0.45
1:B:285:LYS:HG2	1:B:285:LYS:O	2.17	0.45
1:A:186:MET:HG2	1:A:190:GLY:HA2	1.99	0.45
1:B:346:GLY:C	1:B:347:PHE:CG	2.90	0.45
1:A:207:VAL:CG2	1:A:393:ALA:HB2	2.47	0.44
1:A:241:GLY:O	1:A:244:ILE:HG12	2.17	0.44
1:B:267:LEU:O	1:B:268:LEU:HD12	2.17	0.44
1:B:90:TYR:HB2	1:B:336:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:TRP:HH2	1:A:530:LYS:HD2	1.83	0.44
1:A:119:LEU:HD23	1:A:194:LEU:HD22	1.98	0.44
1:A:199:ILE:HG23	1:A:244:ILE:HD13	1.99	0.44
1:A:199:ILE:O	1:A:203:GLN:HG3	2.18	0.44
1:A:489:ILE:HG13	1:A:490:GLU:H	1.83	0.44
1:A:439:LEU:HB3	1:A:441:PHE:O	2.18	0.44
1:B:116:ARG:HD3	1:B:116:ARG:HA	1.82	0.44
1:B:196:HIS:HE1	1:B:339:TYR:HE1	1.65	0.44
1:B:424:LYS:HB3	1:B:424:LYS:HE2	1.79	0.44
1:A:207:VAL:HG22	1:A:393:ALA:HB2	2.00	0.44
1:B:268:LEU:HA	1:B:274:LYS:HD3	1.99	0.43
1:B:511:LYS:CD	1:B:511:LYS:H	2.23	0.43
1:A:385:PHE:CG	1:A:435:MET:HG3	2.53	0.43
1:B:349:VAL:HG12	1:B:349:VAL:O	2.19	0.43
1:A:489:ILE:CG2	1:A:492:ARG:HH12	2.31	0.43
1:A:524:GLN:HG2	1:A:527:ASP:HB3	2.00	0.43
1:B:453:VAL:HG22	1:B:518:ILE:HD11	2.00	0.43
1:B:158:VAL:O	1:B:165:TYR:HB2	2.18	0.43
1:B:90:TYR:CE1	1:B:111:ALA:HA	2.52	0.43
1:A:472:ARG:HG2	1:A:474:ILE:H	1.83	0.43
1:A:446:THR:OG1	1:A:447:ARG:CZ	2.67	0.43
1:B:242:VAL:HG23	1:B:245:LYS:HD2	2.01	0.43
1:A:446:THR:HG23	1:A:446:THR:O	2.18	0.43
1:B:202:SER:OG	1:B:230:GLY:HA2	2.19	0.43
1:B:353:SER:H	1:B:358:GLU:HB2	1.84	0.43
1:B:349:VAL:O	1:B:350:GLU:CB	2.67	0.43
1:A:103:MET:HA	1:A:103:MET:CE	2.48	0.42
1:A:462:ILE:HD12	1:A:462:ILE:HA	1.81	0.42
1:A:524:GLN:HE21	1:A:527:ASP:HB2	1.84	0.42
1:A:80:TYR:O	1:A:84:VAL:HG23	2.19	0.42
1:B:522:MET:HG3	1:B:534:VAL:CG1	2.50	0.42
1:A:442:TRP:CH2	1:A:530:LYS:HD2	2.54	0.42
1:A:76:LYS:HB3	1:A:351:GLU:HB2	2.00	0.42
1:A:524:GLN:CD	1:A:524:GLN:N	2.72	0.42
1:A:75:ILE:N	1:A:75:ILE:HD12	2.27	0.42
1:B:481:VAL:HA	1:B:484:MET:HE2	2.01	0.42
1:B:410:PRO:O	1:B:414:LEU:HB2	2.20	0.42
1:A:239:ALA:HA	1:A:242:VAL:HG12	2.02	0.42
1:B:273:ALA:HA	1:B:276:ALA:HB3	2.00	0.42
1:B:283:ASN:O	1:B:286:ASN:HB2	2.20	0.42
1:B:457:GLY:HA3	1:B:480:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:THR:O	1:B:73:THR:HG22	2.20	0.42
1:B:256:ARG:O	1:B:260:ARG:HG3	2.20	0.42
1:B:346:GLY:O	1:B:347:PHE:CG	2.72	0.42
1:B:77:LYS:O	1:B:80:TYR:HB3	2.19	0.42
1:A:383:GLN:HE22	1:A:409:LYS:H	1.67	0.41
1:A:456:ASP:HB3	1:A:479:GLN:HG3	2.02	0.41
1:B:530:LYS:HD3	1:B:530:LYS:N	2.35	0.41
1:A:170:ARG:O	1:A:170:ARG:CG	2.67	0.41
1:A:251:VAL:O	1:A:255:ILE:HG13	2.20	0.41
1:A:229:ALA:HB2	1:A:394:TYR:CE2	2.55	0.41
1:A:398:ARG:HD3	1:A:539:LYS:O	2.20	0.41
1:A:528:LYS:O	1:A:529:ASN:CB	2.68	0.41
1:B:106:ASN:ND2	1:B:367:THR:HG23	2.35	0.41
1:B:218:VAL:HG13	1:B:220:LEU:HG	2.03	0.41
1:A:270:ASP:C	1:A:272:LYS:H	2.23	0.41
1:A:376:ASP:OD1	1:A:381:LYS:HD3	2.20	0.41
1:A:452:GLU:CD	1:A:452:GLU:N	2.74	0.41
1:A:478:LYS:O	1:A:481:VAL:HG22	2.21	0.41
1:B:153:THR:HG23	1:B:170:ARG:HB2	2.02	0.41
1:B:198:MET:HE3	1:B:237:SER:HB3	2.03	0.41
1:A:262:MET:HA	1:A:265:ARG:HH22	1.86	0.41
1:A:270:ASP:O	1:A:271:ILE:HG22	2.21	0.41
1:A:296:LEU:CA	1:A:496:VAL:HG11	2.47	0.41
1:B:270:ASP:OD1	1:B:272:LYS:HB3	2.21	0.41
1:A:223:SER:O	1:A:224:LEU:CB	2.64	0.41
1:A:271:ILE:HA	1:A:274:LYS:HB3	2.03	0.41
1:A:472:ARG:HA	1:A:473:PRO:HD3	1.86	0.41
1:A:254:ALA:O	1:A:258:ILE:HG13	2.20	0.40
1:A:284:LEU:O	1:A:285:LYS:CB	2.69	0.40
1:A:220:LEU:CD2	1:A:315:THR:HG23	2.51	0.40
1:A:163:THR:HG22	1:A:164:ILE:N	2.33	0.40
1:A:308:ILE:H	1:A:308:ILE:CD1	2.30	0.40
1:B:447:ARG:H	1:B:447:ARG:CD	2.26	0.40
1:A:181:MET:O	1:A:185:THR:HG22	2.21	0.40
1:A:489:ILE:HG22	1:A:492:ARG:HH12	1.86	0.40
1:B:372:LEU:HD11	1:B:433:ALA:HB2	2.03	0.40
1:B:492:ARG:O	1:B:493:ASP:HB2	2.22	0.40
1:A:168:PRO:HD3	1:A:427:VAL:O	2.21	0.40
1:A:537:GLN:CG	1:A:538:ILE:N	2.85	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	454/562 (81%)	413 (91%)	39 (9%)	2 (0%)	34	68
1	B	453/562 (81%)	409 (90%)	40 (9%)	4 (1%)	17	52
All	All	907/1124 (81%)	822 (91%)	79 (9%)	6 (1%)	22	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	ILE
1	B	271	ILE
1	B	347	PHE
1	B	511	LYS
1	B	474	ILE
1	A	536	ILE

### 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	380/472 (80%)	367 (97%)	13 (3%)	37	68
1	B	378/472 (80%)	354 (94%)	24 (6%)	18	50
All	All	758/944 (80%)	721 (95%)	37 (5%)	25	58

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



Mol	Chain	Res	Type
1	A	94	MET
1	A	103	MET
1	A	126	LYS
1	A	160	ASP
1	A	171	ILE
1	A	183	LYS
1	A	240	THR
1	A	271	ILE
1	A	376	ASP
1	A	472	ARG
1	A	503	MET
1	A	518	ILE
1	A	530	LYS
1	B	74	GLU
1	B	148	ASN
1	B	156	LYS
1	B	159	ARG
1	B	162	LYS
1	B	171	ILE
1	B	173	PHE
1	B	183	LYS
1	B	205	ASN
1	B	240	THR
1	B	267	LEU
1	B	271	ILE
1	B	287	LYS
1	B	322	VAL
1	B	367	THR
1	B	376	ASP
1	B	411	ARG
1	B	434	LEU
1	B	447	ARG
1	B	451	ASN
1	B	472	ARG
1	B	511	LYS
1	B	518	ILE
1	B	530	LYS

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	92	GLN
1	A	196	HIS

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Mol	Chain	Res	Type
1	A	203	GLN
1	A	210	GLN
1	A	364	ASN
1	A	426	GLN
1	B	196	HIS
1	B	344	GLN
1	B	515	ASN
1	B	537	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 ⓘ

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	458/562 (81%)	0.31	21 (4%) 32 22	53, 75, 123, 143	0
1	B	457/562 (81%)	0.25	20 (4%) 34 24	58, 82, 121, 165	0
All	All	915/1124 (81%)	0.28	41 (4%) 33 23	53, 78, 122, 165	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	457	GLY	6.2
1	A	490	GLU	4.4
1	A	453	VAL	4.1
1	A	509	ALA	4.0
1	B	535	GLU	3.7
1	A	488	ASN	3.6
1	A	456	ASP	3.6
1	A	459	SER	3.6
1	A	454	GLY	3.5
1	B	508	MET	3.5
1	B	490	GLU	3.5
1	A	147	HIS	3.5
1	A	491	GLY	3.3
1	A	449	GLY	3.0
1	A	451	ASN	3.0
1	B	493	ASP	3.0
1	A	424	LYS	2.9
1	A	455	GLY	2.8
1	B	489	ILE	2.8
1	B	451	ASN	2.6
1	B	454	GLY	2.6
1	B	509	ALA	2.6
1	A	458	GLY	2.5
1	B	536	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	153	THR	2.5
1	A	450	GLY	2.4
1	B	263	ALA	2.4
1	A	347	PHE	2.4
1	A	155	TYR	2.3
1	A	474	ILE	2.3
1	B	269	ARG	2.2
1	B	512	THR	2.2
1	B	551	THR	2.2
1	B	537	GLN	2.2
1	B	539	LYS	2.2
1	B	222	PRO	2.1
1	B	491	GLY	2.1
1	B	549	ARG	2.1
1	B	174	LEU	2.1
1	A	475	ALA	2.0
1	B	348	ASN	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.