



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 PM GMT

PDB ID : 3VSK  
Title : Crystal structure of penicillin-binding protein 3 (PBP3) from methicillin-resistant *Staphylococcus aureus* in the apo form.  
Authors : Yoshida, H.; Tame, J.R.; Park, S.Y.  
Deposited on : 2012-04-25  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

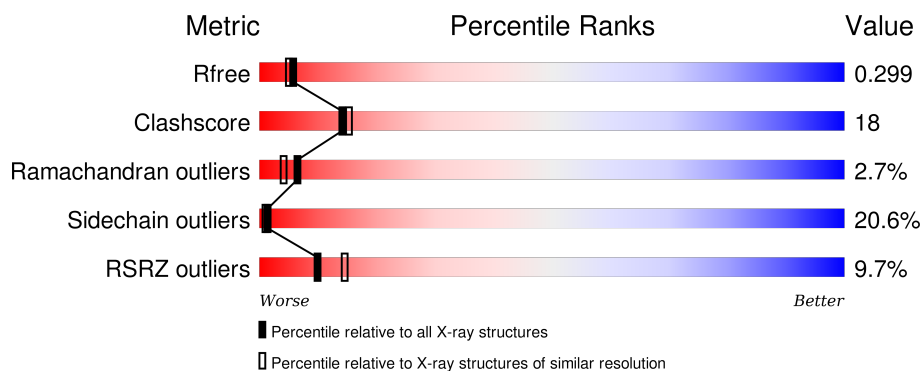
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	646	
1	B	646	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10150 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 Penicillin-binding protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	631	Total	C	N	O	S	0	0	0
			4943	3105	852	967	19			
1	B	631	Total	C	N	O	S	0	0	0
			4947	3107	853	968	19			

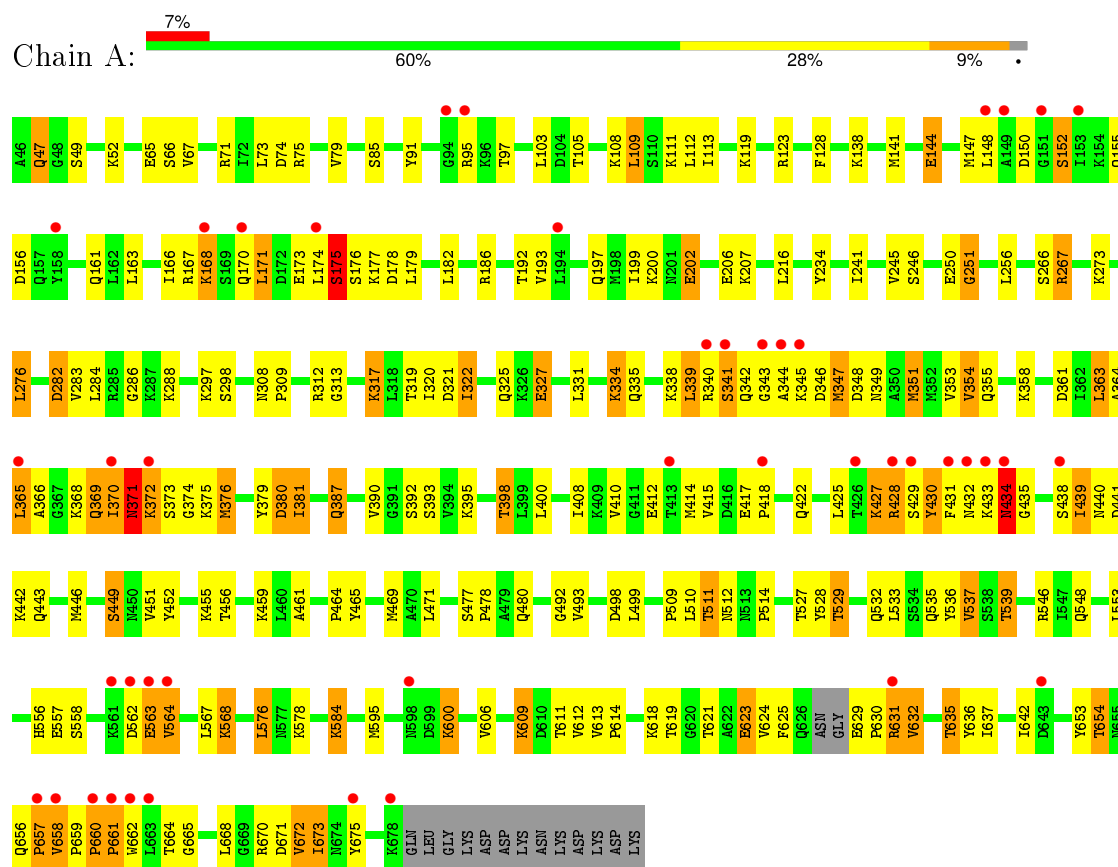
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	141	Total	O	0	0
			141	141		
2	B	119	Total	O	0	0
			119	119		

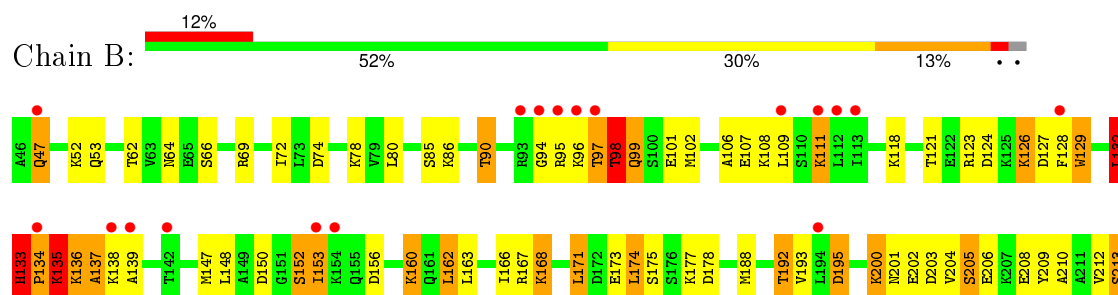
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Penicillin-binding protein 3



#### • Molecule 1: Penicillin-binding protein 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.42Å 143.42Å 189.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.90 – 2.30 46.35 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (40.90-2.30) 96.8 (46.35-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.261 , 0.300 0.257 , 0.299	Depositor DCC
$R_{free}$ test set	4270 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 85105 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	0/5025	0.71	0/6769
1	B	0.47	0/5028	0.70	1/6772 (0.0%)
All	All	0.48	0/10053	0.71	1/13541 (0.0%)

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	8
1	B	0	19
All	All	0	27

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	622	ALA	N-CA-C	5.49	125.81	111.00

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	GLY	Peptide
1	A	371	ASN	Peptide
1	A	430	TYR	Peptide
1	A	434	ASN	Peptide
1	A	563	GLU	Peptide
1	A	657	PRO	Peptide
1	A	658	VAL	Peptide
1	A	660	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	132	LEU	Peptide
1	B	133	HIS	Peptide
1	B	218	LYS	Peptide
1	B	219	LEU	Peptide
1	B	345	LYS	Peptide
1	B	346	ASP	Peptide
1	B	371	ASN	Peptide
1	B	372	LYS	Peptide
1	B	412	GLU	Peptide
1	B	425	LEU	Peptide
1	B	428	ARG	Peptide
1	B	560	ASN	Peptide
1	B	561	LYS	Peptide
1	B	562	ASP	Peptide
1	B	612	VAL	Peptide
1	B	621	THR	Peptide
1	B	624	VAL	Peptide
1	B	640	ALA	Peptide
1	B	96	LYS	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	4943	0	4992	155	0
1	B	4947	0	4994	224	0
2	A	141	0	0	3	0
2	B	119	0	0	9	0
All	All	10150	0	9986	362	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 18.

All (362) 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:339:LEU:CD2	1:B:663:LEU:HD22	1.65	1.25
1:B:339:LEU:HD22	1:B:663:LEU:CD2	1.68	1.21
1:B:339:LEU:HD22	1:B:663:LEU:HD22	1.00	0.99
1:B:441:ASP:HA	2:B:819:HOH:O	1.64	0.95
1:B:324:LEU:HD23	1:B:363:LEU:HD12	1.51	0.92
1:A:408:ILE:HG21	1:A:456:THR:HG22	1.52	0.90
1:B:339:LEU:CD2	1:B:663:LEU:CD2	2.39	0.90
1:A:529:THR:HG22	1:A:532:GLN:H	1.37	0.87
1:B:658:VAL:HG21	1:B:663:LEU:HD12	1.67	0.76
1:A:354:VAL:H	1:A:364:ALA:HB2	1.52	0.75
1:A:428:ARG:HE	1:A:451:VAL:HB	1.52	0.73
1:B:339:LEU:HD21	1:B:663:LEU:HD22	1.69	0.72
1:B:129:TRP:HB3	1:B:136:LYS:HE3	1.71	0.71
1:A:428:ARG:NH2	1:A:449:SER:OG	2.23	0.71
1:A:320:ILE:HG12	1:A:363:LEU:HA	1.73	0.70
1:B:52:LYS:HD2	1:B:66:SER:HB3	1.73	0.69
1:B:200:LYS:HD2	1:B:202:GLU:HG2	1.74	0.69
1:A:353:VAL:HA	1:A:364:ALA:HB1	1.74	0.69
1:B:238:LEU:HD22	1:B:325:GLN:HG2	1.75	0.69
1:B:336:ILE:HD13	1:B:369:GLN:HE21	1.57	0.68
1:B:594:LYS:HE3	1:B:642:ILE:HG23	1.74	0.68
1:B:657:PRO:HG2	1:B:658:VAL:HG13	1.75	0.68
1:B:444:ALA:CB	2:B:819:HOH:O	2.41	0.68
1:B:247:THR:HG22	1:B:250:GLU:H	1.58	0.68
1:A:91:TYR:HB2	1:A:199:ILE:HD11	1.76	0.67
1:B:598:ASN:ND2	1:B:610:ASP:OD2	2.24	0.67
1:A:71:ARG:HH22	1:A:563:GLU:HA	1.58	0.67
1:A:344:ALA:HA	2:A:830:HOH:O	1.93	0.67
1:A:246:SER:HB2	1:A:250:GLU:HG3	1.77	0.67
1:B:47:GLN:NE2	1:B:560:ASN:O	2.27	0.67
1:A:390:VAL:HG21	1:A:533:LEU:HD21	1.75	0.66
1:B:390:VAL:O	1:B:622:ALA:HB3	1.96	0.66
1:A:427:LYS:HD3	1:A:432:ASN:HB3	1.78	0.65
1:B:444:ALA:HB3	2:B:819:HOH:O	1.95	0.65
1:A:347:MET:HE2	1:A:656:GLN:HE21	1.62	0.65
1:A:49:SER:HB2	1:A:65:GLU:HB3	1.80	0.64
1:B:108:LYS:O	1:B:111:LYS:HG2	1.98	0.64
1:A:345:LYS:O	1:A:371:ASN:HB3	1.97	0.64
1:B:392:SER:OG	1:B:618:LYS:NZ	2.31	0.64
1:A:375:LYS:HG3	1:B:512:ASN:HD22	1.63	0.64
1:B:331:LEU:HD13	1:B:671:ASP:HB3	1.78	0.63
1:A:370:ILE:HD13	1:B:513:ASN:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:N	2:A:733:HOH:O	2.31	0.63
1:A:273:LYS:HZ2	1:B:484:ARG:HH12	1.46	0.62
1:A:241:ILE:HD13	1:A:381:ILE:HG22	1.80	0.62
1:B:612:VAL:O	1:B:614:PRO:HD3	1.98	0.62
1:A:250:GLU:OE2	1:B:484:ARG:NH1	2.33	0.62
1:A:395:LYS:HA	1:A:398:THR:HG23	1.82	0.62
1:B:215:GLN:HA	1:B:218:LYS:HG3	1.82	0.62
1:B:329:GLU:HG2	1:B:365:LEU:HD22	1.81	0.62
1:B:395:LYS:HE2	1:B:522:ILE:HG22	1.82	0.61
1:A:660:PRO:O	1:A:662:TRP:N	2.33	0.61
1:B:447:HIS:HA	1:B:600:LYS:HE3	1.82	0.61
1:A:630:PRO:O	1:A:631:ARG:NH1	2.33	0.61
1:B:354:VAL:HG13	1:B:363:LEU:HB3	1.82	0.61
1:A:349:ASN:HB2	1:A:654:THR:HG23	1.83	0.61
1:A:327:GLU:HG3	1:A:675:TYR:CZ	2.34	0.61
1:B:641:PRO:HD2	1:B:646:LYS:H	1.66	0.61
1:B:370:ILE:HD11	1:B:375:LYS:HG3	1.83	0.61
1:A:52:LYS:HD3	1:A:66:SER:HB3	1.83	0.61
1:A:535:GLN:O	1:A:539:THR:HG22	2.01	0.60
1:B:321:ASP:HB3	1:B:324:LEU:HB2	1.84	0.60
1:B:594:LYS:NZ	1:B:639:TYR:OH	2.34	0.60
1:B:611:THR:H	1:B:613:VAL:HG22	1.67	0.60
1:A:537:VAL:HG21	1:A:637:ILE:HB	1.84	0.60
1:A:365:LEU:HD11	1:A:380:ASP:HB3	1.82	0.60
1:A:276:LEU:HD13	1:A:499:LEU:HD21	1.84	0.60
1:B:674:ASN:N	1:B:674:ASN:OD1	2.35	0.59
1:B:205:SER:HB2	1:B:208:GLU:HB2	1.84	0.59
1:A:273:LYS:HZ2	1:B:484:ARG:HH22	1.51	0.59
1:A:428:ARG:NE	1:A:451:VAL:HB	2.18	0.59
1:B:339:LEU:HD22	1:B:663:LEU:HD21	1.75	0.59
1:B:340:ARG:HA	1:B:372:LYS:NZ	2.18	0.59
1:B:324:LEU:O	1:B:363:LEU:HD11	2.03	0.58
1:A:344:ALA:HB1	1:A:347:MET:HB2	1.84	0.58
1:B:658:VAL:HB	1:B:662:TRP:HE1	1.68	0.58
1:A:632:VAL:N	1:A:656:GLN:O	2.36	0.58
1:A:455:LYS:O	1:A:459:LYS:HG3	2.03	0.58
1:B:123:ARG:HD2	1:B:127:ASP:OD2	2.03	0.58
1:B:641:PRO:HD3	1:B:677:PHE:CZ	2.38	0.58
1:A:369:GLN:HB3	1:A:376:MET:HG2	1.85	0.58
1:B:347:MET:HE2	1:B:656:GLN:HE21	1.68	0.58
1:B:345:LYS:O	1:B:371:ASN:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:GLN:HB3	1:A:658:VAL:HG13	1.86	0.57
1:B:215:GLN:NE2	1:B:215:GLN:H	2.03	0.57
1:B:134:PRO:HB3	1:B:138:LYS:HB2	1.87	0.57
1:B:283:VAL:HG11	1:B:555:ILE:HD13	1.87	0.57
1:B:72:ILE:HD11	1:B:284:LEU:HD11	1.86	0.57
1:A:175:SER:O	1:A:175:SER:OG	2.21	0.57
1:A:600:LYS:H	1:A:600:LYS:HE3	1.69	0.57
1:B:214:GLN:CA	2:B:789:HOH:O	2.52	0.56
1:B:380:ASP:N	1:B:380:ASP:OD1	2.36	0.56
1:B:94:GLY:HA3	1:B:193:VAL:HG13	1.87	0.56
1:B:336:ILE:HD13	1:B:369:GLN:NE2	2.19	0.56
1:B:340:ARG:HG3	1:B:372:LYS:HG2	1.87	0.56
1:A:414:MET:HG2	1:A:415:VAL:H	1.69	0.56
1:B:150:ASP:OD1	1:B:152:SER:HB3	2.06	0.56
1:B:629:GLU:HG3	1:B:631:ARG:HH12	1.69	0.56
1:B:419:LEU:HB3	1:B:465:TYR:CZ	2.41	0.56
1:B:215:GLN:HE21	1:B:215:GLN:H	1.52	0.56
1:B:417:GLU:HB3	1:B:419:LEU:HG	1.87	0.56
1:A:477:SER:HB3	1:A:478:PRO:HD3	1.87	0.56
1:B:358:LYS:HG3	1:B:359:ASN:N	2.20	0.56
1:B:640:ALA:HB3	1:B:647:LEU:HB3	1.87	0.55
1:B:422:GLN:NE2	1:B:468:GLY:O	2.34	0.55
1:B:126:LYS:O	1:B:129:TRP:HB2	2.06	0.55
1:B:624:VAL:HG23	1:B:632:VAL:HA	1.89	0.55
1:A:509:PRO:HB2	1:B:368:LYS:HE2	1.88	0.55
1:B:205:SER:CB	1:B:208:GLU:HB2	2.37	0.54
1:A:428:ARG:HH11	1:A:430:TYR:HE1	1.56	0.54
1:B:416:ASP:HB3	1:B:451:VAL:HG11	1.89	0.54
1:B:74:ASP:OD1	1:B:78:LYS:N	2.36	0.54
1:A:461:ALA:HA	1:A:478:PRO:HG3	1.89	0.54
1:B:641:PRO:HD3	1:B:677:PHE:CE1	2.42	0.54
1:B:662:TRP:HD1	1:B:663:LEU:H	1.55	0.54
1:B:214:GLN:OE1	1:B:215:GLN:NE2	2.40	0.54
1:B:617:GLY:HA2	1:B:638:GLY:HA2	1.90	0.54
1:A:618:LYS:HD2	1:A:619:THR:H	1.73	0.54
1:A:273:LYS:HZ2	1:B:484:ARG:NH1	2.06	0.53
1:A:171:LEU:HA	1:A:174:LEU:HD13	1.90	0.53
1:B:215:GLN:N	1:B:215:GLN:HE21	2.07	0.53
1:B:416:ASP:N	1:B:416:ASP:OD1	2.41	0.53
1:B:148:LEU:HD23	1:B:153:ILE:O	2.08	0.53
1:B:325:GLN:HA	1:B:363:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:NZ	1:B:484:ARG:HH22	2.07	0.53
1:B:417:GLU:O	1:B:419:LEU:N	2.39	0.53
1:A:659:PRO:HD2	1:A:662:TRP:HZ2	1.74	0.53
1:A:325:GLN:OE1	1:A:365:LEU:HB2	2.08	0.53
1:A:393:SER:OG	1:A:635:THR:HG22	2.08	0.53
1:A:368:LYS:HD3	1:B:509:PRO:HD2	1.89	0.53
1:A:512:ASN:HD22	1:B:375:LYS:HE3	1.74	0.53
1:A:387:GLN:HG2	1:A:527:THR:CB	2.39	0.53
1:A:387:GLN:HG2	1:A:527:THR:OG1	2.09	0.53
1:A:339:LEU:HG	1:A:342:GLN:H	1.73	0.52
1:B:600:LYS:HG2	1:B:603:THR:N	2.24	0.52
1:A:335:GLN:HG2	1:A:668:LEU:HB2	1.92	0.52
1:A:141:MET:HE1	1:A:144:GLU:HG3	1.90	0.52
1:B:358:LYS:HG3	1:B:359:ASN:H	1.75	0.52
1:B:359:ASN:HA	1:B:550:HIS:NE2	2.24	0.52
1:B:404:GLN:NE2	1:B:580:ASN:OD1	2.43	0.51
1:B:156:ASP:OD2	1:B:160:LYS:NZ	2.37	0.51
1:A:512:ASN:O	1:A:514:PRO:HD3	2.09	0.51
1:A:174:LEU:O	1:A:176:SER:N	2.43	0.51
1:A:351:MET:HA	1:A:366:ALA:CB	2.41	0.51
1:B:597:PHE:CE2	1:B:617:GLY:HA3	2.46	0.51
1:A:557:GLU:OE1	1:A:558:SER:N	2.28	0.51
1:A:375:LYS:HG3	1:B:512:ASN:ND2	2.26	0.51
1:A:327:GLU:HG3	1:A:675:TYR:CE1	2.46	0.51
1:A:108:LYS:HD2	1:A:111:LYS:HD2	1.93	0.51
1:B:343:GLY:O	1:B:657:PRO:HG3	2.10	0.51
1:B:314:GLN:HB3	1:B:556:HIS:O	2.11	0.51
1:A:653:TYR:CE2	1:A:665:GLY:HA3	2.46	0.50
1:A:371:ASN:O	1:A:372:LYS:HB2	2.12	0.50
1:A:415:VAL:HG12	1:A:438:SER:OG	2.12	0.50
1:B:657:PRO:O	1:B:659:PRO:HD3	2.11	0.50
1:A:65:GLU:O	1:A:288:LYS:HB2	2.11	0.50
1:B:247:THR:HG22	1:B:250:GLU:HG3	1.94	0.50
1:B:410:VAL:HG13	1:B:585:GLU:HG3	1.93	0.50
1:A:273:LYS:HZ2	1:B:484:ARG:NH2	2.09	0.50
1:B:312:ARG:NH1	1:B:562:ASP:OD1	2.41	0.50
1:A:390:VAL:HG11	1:A:528:TYR:HD2	1.76	0.50
1:B:290:GLU:HG2	1:B:307:LEU:HD12	1.93	0.50
1:A:428:ARG:HH12	1:A:449:SER:HB2	1.77	0.50
1:A:365:LEU:HD13	1:A:366:ALA:H	1.76	0.50
1:A:351:MET:HA	1:A:366:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ASN:HB2	1:B:654:THR:OG1	2.12	0.50
1:B:434:ASN:HB3	1:B:436:HIS:NE2	2.27	0.50
1:A:341:SER:C	1:A:343:GLY:H	2.15	0.49
1:B:212:VAL:O	1:B:214:GLN:HG3	2.12	0.49
1:A:614:PRO:HB2	1:A:642:ILE:HD13	1.93	0.49
1:A:661:PRO:HG2	1:A:662:TRP:CZ3	2.47	0.49
1:B:489:VAL:HG12	1:B:539:THR:HG21	1.94	0.49
1:B:247:THR:CG2	1:B:250:GLU:H	2.24	0.49
1:A:537:VAL:CG2	1:A:637:ILE:HB	2.41	0.49
1:A:584:LYS:HE3	1:A:584:LYS:H	1.77	0.49
1:A:492:GLY:H	1:A:532:GLN:NE2	2.10	0.49
1:A:512:ASN:ND2	1:B:375:LYS:HE3	2.28	0.49
1:A:668:LEU:O	1:A:672:VAL:HG13	2.13	0.49
1:B:366:ALA:HB3	1:B:379:TYR:O	2.12	0.49
1:A:578:LYS:H	1:B:254:LYS:NZ	2.11	0.49
1:B:340:ARG:HA	1:B:372:LYS:HE2	1.95	0.49
1:A:150:ASP:HB3	1:A:152:SER:H	1.78	0.48
1:B:214:GLN:N	2:B:789:HOH:O	2.45	0.48
1:B:263:LYS:HB2	1:B:265:TYR:HD1	1.77	0.48
1:A:308:ASN:OD1	1:A:309:PRO:HD2	2.13	0.48
1:B:162:LEU:HD22	1:B:166:ILE:HD11	1.95	0.48
1:B:62:THR:HG1	1:B:292:LYS:HZ2	1.57	0.48
1:A:141:MET:CE	1:A:144:GLU:HG3	2.44	0.48
1:A:624:VAL:HG22	1:A:625:PHE:H	1.78	0.48
1:B:623:GLU:HA	1:B:632:VAL:HG23	1.96	0.48
1:B:412:GLU:HG3	1:B:413:THR:H	1.78	0.48
1:A:347:MET:CE	1:A:656:GLN:HE21	2.27	0.48
1:B:419:LEU:HD13	1:B:465:TYR:CE2	2.49	0.48
1:A:251:GLY:HA3	1:A:267:ARG:O	2.14	0.48
1:B:106:ALA:HB2	1:B:188:MET:SD	2.54	0.48
1:B:335:GLN:O	1:B:335:GLN:NE2	2.46	0.47
1:A:631:ARG:NH2	1:A:657:PRO:HB3	2.29	0.47
1:B:337:LYS:HA	1:B:340:ARG:HB2	1.96	0.47
1:B:488:GLN:O	1:B:546:ARG:HD3	2.13	0.47
1:B:612:VAL:HG21	1:B:674:ASN:HB3	1.95	0.47
1:A:670:ARG:O	1:A:673:ILE:HG22	2.14	0.47
1:A:578:LYS:O	1:B:254:LYS:HE3	2.15	0.47
1:B:445:LEU:O	1:B:618:LYS:HE2	2.15	0.47
1:B:454:PHE:HE1	1:B:522:ILE:HG12	1.79	0.47
1:A:170:GLN:O	1:A:173:GLU:HG2	2.15	0.47
1:A:387:GLN:HG2	1:A:527:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:OG1	1:B:99:GLN:N	2.47	0.47
1:B:340:ARG:HA	1:B:372:LYS:CE	2.44	0.47
1:A:171:LEU:HD12	1:A:174:LEU:HD22	1.97	0.47
1:B:253:PRO:HG2	1:B:273:LYS:HG2	1.97	0.47
1:A:73:LEU:HD22	1:A:79:VAL:HA	1.96	0.47
1:A:623:GLU:HA	1:A:632:VAL:HG22	1.97	0.47
1:B:282:ASP:HB2	2:B:723:HOH:O	2.14	0.47
1:B:441:ASP:OD1	1:B:441:ASP:N	2.48	0.46
1:A:372:LYS:HD3	1:A:372:LYS:HA	1.47	0.46
1:A:370:ILE:HG13	1:A:370:ILE:H	1.30	0.46
1:A:148:LEU:HD11	1:A:155:GLN:NE2	2.30	0.46
1:B:629:GLU:HG3	1:B:631:ARG:NH1	2.30	0.46
1:B:663:LEU:C	1:B:665:GLY:H	2.18	0.46
1:A:408:ILE:CG2	1:A:456:THR:HG22	2.33	0.46
1:B:329:GLU:CD	1:B:365:LEU:HD13	2.36	0.46
1:A:661:PRO:HG2	1:A:662:TRP:CE3	2.50	0.46
1:B:127:ASP:C	1:B:129:TRP:H	2.20	0.46
1:B:668:LEU:O	1:B:672:VAL:HG13	2.16	0.46
1:B:192:THR:HG23	1:B:195:ASP:HB3	1.97	0.46
1:A:464:PRO:O	1:B:123:ARG:NH2	2.47	0.46
1:B:215:GLN:HA	1:B:218:LYS:CG	2.46	0.46
1:B:69:ARG:NH2	1:B:277:GLU:OE1	2.39	0.46
1:B:344:ALA:HB1	1:B:347:MET:HB2	1.98	0.45
1:B:585:GLU:O	1:B:589:ILE:HD13	2.16	0.45
1:B:171:LEU:O	1:B:174:LEU:HB2	2.17	0.45
1:B:625:PHE:HA	1:B:630:PRO:HA	1.99	0.45
1:B:86:LYS:HD2	1:B:201:ASN:HB3	1.97	0.45
1:B:53:GLN:HB3	1:B:64:ASN:HB2	1.97	0.45
1:B:98:THR:HG23	1:B:101:GLU:HG2	1.97	0.45
1:B:437:VAL:HB	1:B:438:SER:H	1.56	0.45
1:B:444:ALA:HB2	2:B:819:HOH:O	2.08	0.45
1:A:348:ASP:OD1	1:A:654:THR:OG1	2.33	0.45
1:B:215:GLN:HB2	1:B:222:VAL:CG2	2.46	0.45
1:A:331:LEU:HD22	1:A:671:ASP:HB3	1.98	0.45
1:B:597:PHE:CZ	1:B:617:GLY:HA3	2.51	0.45
1:A:67:VAL:HG23	1:A:286:GLY:HA3	1.99	0.45
1:B:362:ILE:HG12	1:B:362:ILE:H	1.62	0.45
1:B:446:MET:HB3	1:B:596:ALA:HA	1.98	0.45
1:B:204:VAL:HG22	1:B:208:GLU:HB3	1.99	0.45
1:B:348:ASP:OD1	1:B:348:ASP:N	2.45	0.45
1:B:129:TRP:HE3	1:B:136:LYS:HG3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:HD22	1:B:581:ASN:CG	2.37	0.45
1:B:137:ALA:O	1:B:139:ALA:N	2.50	0.45
1:A:529:THR:HG21	2:A:730:HOH:O	2.17	0.44
1:B:133:HIS:CE1	1:B:135:LYS:HB2	2.52	0.44
1:B:359:ASN:CG	1:B:359:ASN:O	2.55	0.44
1:A:339:LEU:HD12	1:A:342:GLN:HB2	1.98	0.44
1:A:430:TYR:CZ	1:A:431:PHE:CE2	3.05	0.44
1:B:664:THR:O	1:B:667:ASP:N	2.49	0.44
1:A:317:LYS:HD3	1:A:556:HIS:NE2	2.32	0.44
1:B:132:LEU:O	1:B:135:LYS:HB3	2.17	0.44
1:B:582:THR:HG23	1:B:584:LYS:H	1.82	0.44
1:A:349:ASN:HB2	1:A:654:THR:CG2	2.47	0.44
1:B:664:THR:O	1:B:667:ASP:HB2	2.18	0.44
1:B:147:MET:HB3	1:B:153:ILE:HB	2.00	0.44
1:B:466:TYR:O	1:B:469:MET:HB3	2.18	0.44
1:A:439:ILE:HG21	1:A:452:TYR:HD2	1.83	0.44
1:B:428:ARG:HB3	1:B:429:SER:H	1.50	0.44
1:B:331:LEU:HD23	1:B:331:LEU:HA	1.80	0.44
1:B:263:LYS:HB2	1:B:265:TYR:CD1	2.53	0.44
1:B:334:LYS:O	1:B:338:LYS:N	2.47	0.44
1:B:369:GLN:N	1:B:369:GLN:OE1	2.51	0.43
1:A:533:LEU:HB3	1:A:637:ILE:HG21	2.00	0.43
1:A:511:THR:OG1	1:A:512:ASN:N	2.51	0.43
1:B:370:ILE:O	1:B:373:SER:N	2.45	0.43
1:A:144:GLU:HA	1:A:147:MET:HB2	1.99	0.43
1:B:213:SER:OG	1:B:213:SER:O	2.36	0.43
1:B:439:ILE:O	1:B:439:ILE:HD12	2.18	0.43
1:A:418:PRO:HG2	1:A:433:LYS:O	2.18	0.43
1:B:90:THR:HG22	1:B:223:ASN:HB2	2.00	0.43
1:A:529:THR:HG22	1:A:532:GLN:N	2.19	0.43
1:A:371:ASN:HA	1:A:374:GLY:N	2.33	0.43
1:A:175:SER:O	1:A:178:ASP:N	2.50	0.43
1:A:442:LYS:HB3	1:A:595:MET:SD	2.59	0.43
1:B:392:SER:HB3	1:B:619:THR:O	2.18	0.43
1:A:425:LEU:HD22	1:A:427:LYS:HE2	2.01	0.43
1:A:636:TYR:OH	1:A:665:GLY:N	2.44	0.43
1:B:351:MET:O	1:B:651:ILE:HA	2.18	0.43
1:B:678:LYS:H	1:B:678:LYS:HD2	1.83	0.43
1:B:167:ARG:HA	1:B:167:ARG:HD2	1.87	0.43
1:B:663:LEU:HA	1:B:663:LEU:HD23	1.76	0.43
1:B:216:LEU:HD12	1:B:217:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:THR:O	1:B:124:ASP:HB2	2.19	0.43
1:B:420:HIS:HA	1:B:426:THR:O	2.19	0.43
1:A:173:GLU:C	1:A:175:SER:N	2.72	0.43
1:B:336:ILE:HD11	1:B:376:MET:SD	2.58	0.43
1:B:167:ARG:NH1	1:B:168:LYS:HE2	2.34	0.43
1:B:348:ASP:O	1:B:368:LYS:HA	2.19	0.42
1:B:209:TYR:OH	1:B:224:THR:HG23	2.19	0.42
1:B:214:GLN:H	1:B:214:GLN:HG3	1.44	0.42
1:B:673:ILE:O	1:B:677:PHE:HD2	2.01	0.42
1:B:465:TYR:CZ	1:B:467:SER:HA	2.54	0.42
1:B:247:THR:O	1:B:250:GLU:HB2	2.19	0.42
1:A:631:ARG:HG3	1:A:657:PRO:HA	2.00	0.42
1:A:284:LEU:O	1:A:313:GLY:HA3	2.18	0.42
1:B:404:GLN:HG3	1:B:581:ASN:ND2	2.35	0.42
1:A:578:LYS:H	1:B:254:LYS:HZ2	1.67	0.42
1:B:214:GLN:HA	2:B:789:HOH:O	2.19	0.42
1:A:119:LYS:HB3	1:A:186:ARG:NH1	2.35	0.42
1:B:175:SER:O	1:B:178:ASP:HB2	2.20	0.42
1:A:381:ILE:H	1:A:381:ILE:HD13	1.85	0.42
1:B:370:ILE:O	1:B:373:SER:OG	2.29	0.42
1:A:365:LEU:HD21	1:A:380:ASP:HB3	2.02	0.42
1:B:80:LEU:HD21	1:B:322:ILE:HG12	2.02	0.42
1:B:441:ASP:CA	2:B:819:HOH:O	2.42	0.42
1:A:440:ASN:OD1	1:A:443:GLN:HG3	2.20	0.42
1:B:660:PRO:HD2	1:B:662:TRP:CZ2	2.54	0.42
1:A:533:LEU:HB3	1:A:637:ILE:CG2	2.50	0.42
1:B:611:THR:OG1	1:B:670:ARG:HD2	2.20	0.42
1:A:584:LYS:N	1:A:584:LYS:HE3	2.34	0.42
1:A:465:TYR:HA	1:A:469:MET:SD	2.60	0.42
1:B:325:GLN:HA	1:B:363:LEU:CD2	2.49	0.42
1:A:321:ASP:H	1:A:363:LEU:HD23	1.84	0.41
1:A:390:VAL:HG23	1:A:635:THR:HG21	2.02	0.41
1:B:510:LEU:HD21	1:B:516:ASN:HB2	2.02	0.41
1:B:622:ALA:O	1:B:632:VAL:HG22	2.20	0.41
1:A:392:SER:HB3	1:A:395:LYS:HD2	2.02	0.41
1:A:567:LEU:HD12	1:A:568:LYS:N	2.35	0.41
1:A:434:ASN:HB2	1:A:435:GLY:H	1.67	0.41
1:B:129:TRP:CE3	1:B:136:LYS:HG3	2.55	0.41
1:A:498:ASP:OD1	1:A:498:ASP:N	2.52	0.41
1:A:234:TYR:CG	1:A:322:ILE:HD12	2.55	0.41
1:B:129:TRP:HZ2	1:B:173:GLU:OE2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:LEU:HG	1:B:380:ASP:OD1	2.19	0.41
1:B:400:LEU:HA	1:B:400:LEU:HD23	1.89	0.41
1:B:174:LEU:HD12	1:B:174:LEU:HA	1.82	0.41
1:B:625:PHE:CD1	1:B:626:GLN:N	2.88	0.41
1:A:433:LYS:HD3	1:A:433:LYS:HA	1.88	0.41
1:A:75:ARG:HD2	1:A:319:THR:O	2.20	0.41
1:B:328:VAL:HG21	1:B:363:LEU:HD13	2.01	0.41
1:B:408:ILE:CG2	1:B:412:GLU:HB3	2.51	0.41
1:B:446:MET:HG2	1:B:446:MET:H	1.47	0.41
1:A:600:LYS:H	1:A:600:LYS:CE	2.31	0.41
1:B:516:ASN:HB3	1:B:525:TYR:CD1	2.55	0.41
1:B:255:GLU:H	1:B:255:GLU:HG3	1.54	0.41
1:B:328:VAL:O	1:B:332:LEU:N	2.51	0.41
1:B:395:LYS:HB3	1:B:453:MET:HE3	2.01	0.41
1:A:539:THR:HB	1:A:546:ARG:HA	2.02	0.41
1:B:417:GLU:HA	1:B:418:PRO:HD3	1.90	0.41
1:B:416:ASP:HA	1:B:451:VAL:HG21	2.02	0.41
1:B:431:PHE:CE1	1:B:436:HIS:CD2	3.08	0.41
1:A:168:LYS:HG2	1:A:168:LYS:H	1.42	0.41
1:A:334:LYS:O	1:A:338:LYS:N	2.53	0.41
1:A:128:PHE:CG	1:A:182:LEU:HD13	2.56	0.41
1:A:548:GLN:HB2	1:A:576:LEU:HD11	2.03	0.41
1:B:646:LYS:HA	1:B:646:LYS:HD3	1.95	0.40
1:B:615:THR:HG21	1:B:673:ILE:HG21	2.02	0.40
1:A:200:LYS:HE2	1:A:202:GLU:HB2	2.02	0.40
1:A:600:LYS:H	1:A:600:LYS:CD	2.32	0.40
1:B:357:PRO:HG3	1:B:538:SER:OG	2.22	0.40
1:A:91:TYR:O	1:A:197:GLN:N	2.51	0.40
1:B:510:LEU:HD23	1:B:510:LEU:HA	1.75	0.40
1:A:105:THR:O	1:A:109:LEU:HB2	2.22	0.40
1:B:126:LYS:HG3	1:B:166:ILE:HG21	2.04	0.40
1:B:97:THR:HA	1:B:101:GLU:OE2	2.21	0.40
1:A:355:GLN:HB2	1:A:361:ASP:O	2.22	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	627/646 (97%)	551 (88%)	66 (10%)	10 (2%)	12	11
1	B	625/646 (97%)	539 (86%)	62 (10%)	24 (4%)	4	2
All	All	1252/1292 (97%)	1090 (87%)	128 (10%)	34 (3%)	6	4

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	SER
1	A	175	SER
1	A	609	LYS
1	B	133	HIS
1	B	134	PRO
1	B	210	ALA
1	B	430	TYR
1	B	640	ALA
1	A	373	SER
1	A	439	ILE
1	B	98	THR
1	B	99	GLN
1	B	390	VAL
1	B	437	VAL
1	B	558	SER
1	B	663	LEU
1	B	664	THR
1	B	665	GLY
1	B	128	PHE
1	B	213	SER
1	B	358	LYS
1	A	371	ASN
1	B	135	LYS
1	B	137	ALA
1	B	275	TYR

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Mol	Chain	Res	Type
1	B	429	SER
1	A	282	ASP
1	B	136	LYS
1	B	641	PRO
1	A	606	VAL
1	B	624	VAL
1	B	659	PRO
1	A	564	VAL
1	A	661	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	546/559 (98%)	443 (81%)	103 (19%)	2	1
1	B	547/559 (98%)	425 (78%)	122 (22%)	1	1
All	All	1093/1118 (98%)	868 (79%)	225 (21%)	1	1

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	74	ASP
1	A	85	SER
1	A	95	ARG
1	A	97	THR
1	A	103	LEU
1	A	109	LEU
1	A	112	LEU
1	A	113	ILE
1	A	123	ARG
1	A	138	LYS
1	A	144	GLU
1	A	156	ASP
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	163	LEU
1	A	166	ILE
1	A	167	ARG
1	A	168	LYS
1	A	171	LEU
1	A	175	SER
1	A	177	LYS
1	A	179	LEU
1	A	192	THR
1	A	193	VAL
1	A	202	GLU
1	A	206	GLU
1	A	207	LYS
1	A	216	LEU
1	A	245	VAL
1	A	256	LEU
1	A	266	SER
1	A	267	ARG
1	A	276	LEU
1	A	282	ASP
1	A	283	VAL
1	A	297	LYS
1	A	298	SER
1	A	312	ARG
1	A	317	LYS
1	A	322	ILE
1	A	327	GLU
1	A	334	LYS
1	A	339	LEU
1	A	340	ARG
1	A	341	SER
1	A	346	ASP
1	A	347	MET
1	A	351	MET
1	A	354	VAL
1	A	358	LYS
1	A	363	LEU
1	A	365	LEU
1	A	369	GLN
1	A	370	ILE
1	A	372	LYS
1	A	376	MET

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Mol	Chain	Res	Type
1	A	379	TYR
1	A	380	ASP
1	A	381	ILE
1	A	387	GLN
1	A	398	THR
1	A	400	LEU
1	A	410	VAL
1	A	412	GLU
1	A	417	GLU
1	A	422	GLN
1	A	427	LYS
1	A	428	ARG
1	A	429	SER
1	A	434	ASN
1	A	441	ASP
1	A	446	MET
1	A	449	SER
1	A	471	LEU
1	A	480	GLN
1	A	493	VAL
1	A	510	LEU
1	A	511	THR
1	A	529	THR
1	A	536	TYR
1	A	537	VAL
1	A	539	THR
1	A	553	LEU
1	A	562	ASP
1	A	564	VAL
1	A	568	LYS
1	A	576	LEU
1	A	584	LYS
1	A	600	LYS
1	A	609	LYS
1	A	611	THR
1	A	612	VAL
1	A	613	VAL
1	A	621	THR
1	A	623	GLU
1	A	629	GLU
1	A	631	ARG
1	A	632	VAL

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Mol	Chain	Res	Type
1	A	635	THR
1	A	654	THR
1	A	664	THR
1	A	672	VAL
1	A	673	ILE
1	B	47	GLN
1	B	85	SER
1	B	90	THR
1	B	95	ARG
1	B	97	THR
1	B	98	THR
1	B	102	MET
1	B	107	GLU
1	B	109	LEU
1	B	111	LYS
1	B	118	LYS
1	B	126	LYS
1	B	129	TRP
1	B	132	LEU
1	B	133	HIS
1	B	135	LYS
1	B	152	SER
1	B	153	ILE
1	B	160	LYS
1	B	162	LEU
1	B	163	LEU
1	B	168	LYS
1	B	171	LEU
1	B	174	LEU
1	B	177	LYS
1	B	192	THR
1	B	195	ASP
1	B	200	LYS
1	B	203	ASP
1	B	205	SER
1	B	206	GLU
1	B	214	GLN
1	B	215	GLN
1	B	216	LEU
1	B	217	SER
1	B	218	LYS
1	B	236	ASP

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Mol	Chain	Res	Type
1	B	238	LEU
1	B	245	VAL
1	B	247	THR
1	B	255	GLU
1	B	261	LEU
1	B	267	ARG
1	B	287	LYS
1	B	298	SER
1	B	306	VAL
1	B	322	ILE
1	B	324	LEU
1	B	332	LEU
1	B	335	GLN
1	B	338	LYS
1	B	341	SER
1	B	346	ASP
1	B	347	MET
1	B	351	MET
1	B	354	VAL
1	B	356	ASN
1	B	358	LYS
1	B	359	ASN
1	B	361	ASP
1	B	362	ILE
1	B	363	LEU
1	B	365	LEU
1	B	372	LYS
1	B	373	SER
1	B	376	MET
1	B	380	ASP
1	B	387	GLN
1	B	390	VAL
1	B	393	SER
1	B	410	VAL
1	B	413	THR
1	B	414	MET
1	B	416	ASP
1	B	417	GLU
1	B	426	THR
1	B	427	LYS
1	B	428	ARG
1	B	430	TYR

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Mol	Chain	Res	Type
1	B	432	ASN
1	B	437	VAL
1	B	438	SER
1	B	446	MET
1	B	447	HIS
1	B	459	LYS
1	B	467	SER
1	B	471	LEU
1	B	473	SER
1	B	476	SER
1	B	480	GLN
1	B	486	LEU
1	B	488	GLN
1	B	506	GLN
1	B	508	GLU
1	B	510	LEU
1	B	513	ASN
1	B	553	LEU
1	B	557	GLU
1	B	561	LYS
1	B	563	GLU
1	B	564	VAL
1	B	582	THR
1	B	584	LYS
1	B	588	GLN
1	B	591	GLU
1	B	595	MET
1	B	597	PHE
1	B	598	ASN
1	B	599	ASP
1	B	603	THR
1	B	611	THR
1	B	612	VAL
1	B	619	THR
1	B	624	VAL
1	B	626	GLN
1	B	632	VAL
1	B	662	TRP
1	B	667	ASP
1	B	670	ARG
1	B	673	ILE
1	B	674	ASN

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Mol	Chain	Res	Type
1	B	678	LYS

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

Mol	Chain	Res	Type
1	A	50	HIS
1	A	155	GLN
1	A	215	GLN
1	A	355	GLN
1	A	369	GLN
1	A	656	GLN
1	B	215	GLN
1	B	404	GLN
1	B	480	GLN
1	B	488	GLN
1	B	513	ASN
1	B	627	ASN
1	B	656	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	631/646 (97%)	0.54	44 (6%) 19 27	30, 67, 127, 171	0
1	B	631/646 (97%)	0.80	78 (12%) 5 8	36, 77, 129, 165	0
All	All	1262/1292 (97%)	0.67	122 (9%) 10 14	30, 73, 128, 171	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	LEU	10.3
1	B	216	LEU	10.2
1	A	432	ASN	8.1
1	B	424	GLY	7.8
1	B	438	SER	7.7
1	A	174	LEU	7.4
1	B	432	ASN	7.3
1	B	217	SER	7.2
1	B	138	LYS	6.9
1	B	218	LYS	6.7
1	B	343	GLY	6.6
1	A	660	PRO	6.4
1	A	341	SER	6.3
1	B	661	PRO	6.2
1	B	423	GLY	6.0
1	A	343	GLY	5.7
1	B	677	PHE	5.6
1	A	151	GLY	5.5
1	B	437	VAL	5.4
1	B	421	PHE	5.3
1	A	562	ASP	5.3
1	B	96	LYS	5.3
1	B	601	ASP	5.2
1	B	339	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	611	THR	4.8
1	A	372	LYS	4.7
1	B	433	LYS	4.7
1	B	194	LEU	4.6
1	B	451	VAL	4.4
1	B	415	VAL	4.3
1	A	340	ARG	4.3
1	A	95	ARG	4.2
1	B	371	ASN	4.2
1	A	433	LYS	4.1
1	B	418	PRO	4.1
1	B	662	TRP	4.1
1	B	625	PHE	4.0
1	B	658	VAL	4.0
1	B	134	PRO	4.0
1	B	219	LEU	3.9
1	B	113	ILE	3.9
1	A	657	PRO	3.9
1	B	111	LYS	3.8
1	A	661	PRO	3.7
1	B	561	LYS	3.6
1	A	662	TRP	3.5
1	A	658	VAL	3.5
1	B	153	ILE	3.5
1	B	363	LEU	3.5
1	B	436	HIS	3.5
1	B	47	GLN	3.4
1	A	370	ILE	3.4
1	B	593	PHE	3.2
1	B	374	GLY	3.2
1	A	563	GLU	3.2
1	A	413	THR	3.2
1	A	153	ILE	3.2
1	A	663	LEU	3.2
1	A	561	LYS	3.1
1	A	631	ARG	3.0
1	A	675	TYR	3.0
1	B	596	ALA	3.0
1	B	112	LEU	3.0
1	B	428	ARG	2.9
1	B	439	ILE	2.9
1	B	154	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	434	ASN	2.8
1	B	626	GLN	2.8
1	A	429	SER	2.8
1	A	431	PHE	2.7
1	B	345	LYS	2.7
1	B	95	ARG	2.7
1	B	429	SER	2.7
1	B	465	TYR	2.7
1	B	109	LEU	2.7
1	B	643	ASP	2.7
1	A	564	VAL	2.7
1	A	345	LYS	2.6
1	B	94	GLY	2.6
1	B	657	PRO	2.6
1	B	341	SER	2.6
1	B	337	LYS	2.6
1	B	410	VAL	2.6
1	A	194	LEU	2.6
1	B	336	ILE	2.5
1	B	612	VAL	2.5
1	A	418	PRO	2.5
1	A	168	LYS	2.5
1	A	598	ASN	2.5
1	B	128	PHE	2.5
1	A	434	ASN	2.4
1	A	344	ALA	2.4
1	B	93	ARG	2.4
1	B	408	ILE	2.4
1	B	340	ARG	2.4
1	A	158	TYR	2.4
1	A	148	LEU	2.3
1	A	149	ALA	2.3
1	A	426	THR	2.3
1	B	97	THR	2.3
1	A	365	LEU	2.3
1	B	388	PHE	2.3
1	A	643	ASP	2.2
1	B	430	TYR	2.2
1	B	419	LEU	2.2
1	B	220	PRO	2.2
1	B	142	THR	2.2
1	B	454	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	372	LYS	2.2
1	B	440	ASN	2.2
1	B	640	ALA	2.2
1	A	94	GLY	2.1
1	B	660	PRO	2.1
1	A	428	ARG	2.1
1	A	170	GLN	2.1
1	B	139	ALA	2.1
1	B	584	LYS	2.1
1	A	678	LYS	2.1
1	B	307	LEU	2.0
1	B	458	LEU	2.0
1	B	608	PHE	2.0
1	A	438	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.