



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:02 PM BST

PDB ID : 6AHO  
Title : Crystal structure of Kap114p  
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Deposited on : 2018-08-20  
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](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 : 2.13.1  
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) : 2.13.1

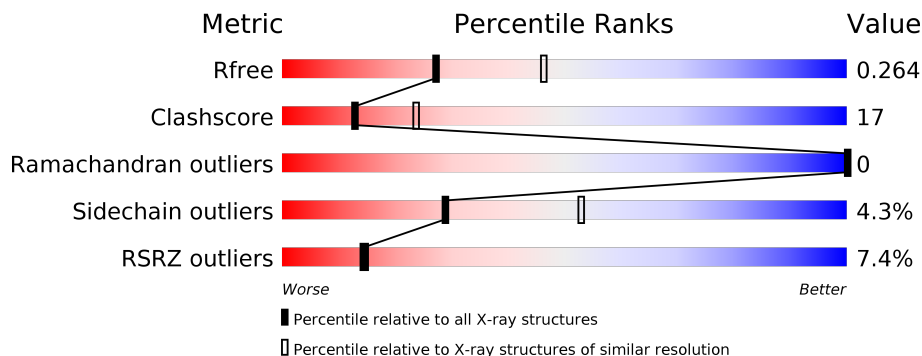
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	1009	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7294 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 Importin subunit beta-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	916	7294	4681	1175	1406	32	0	0	0

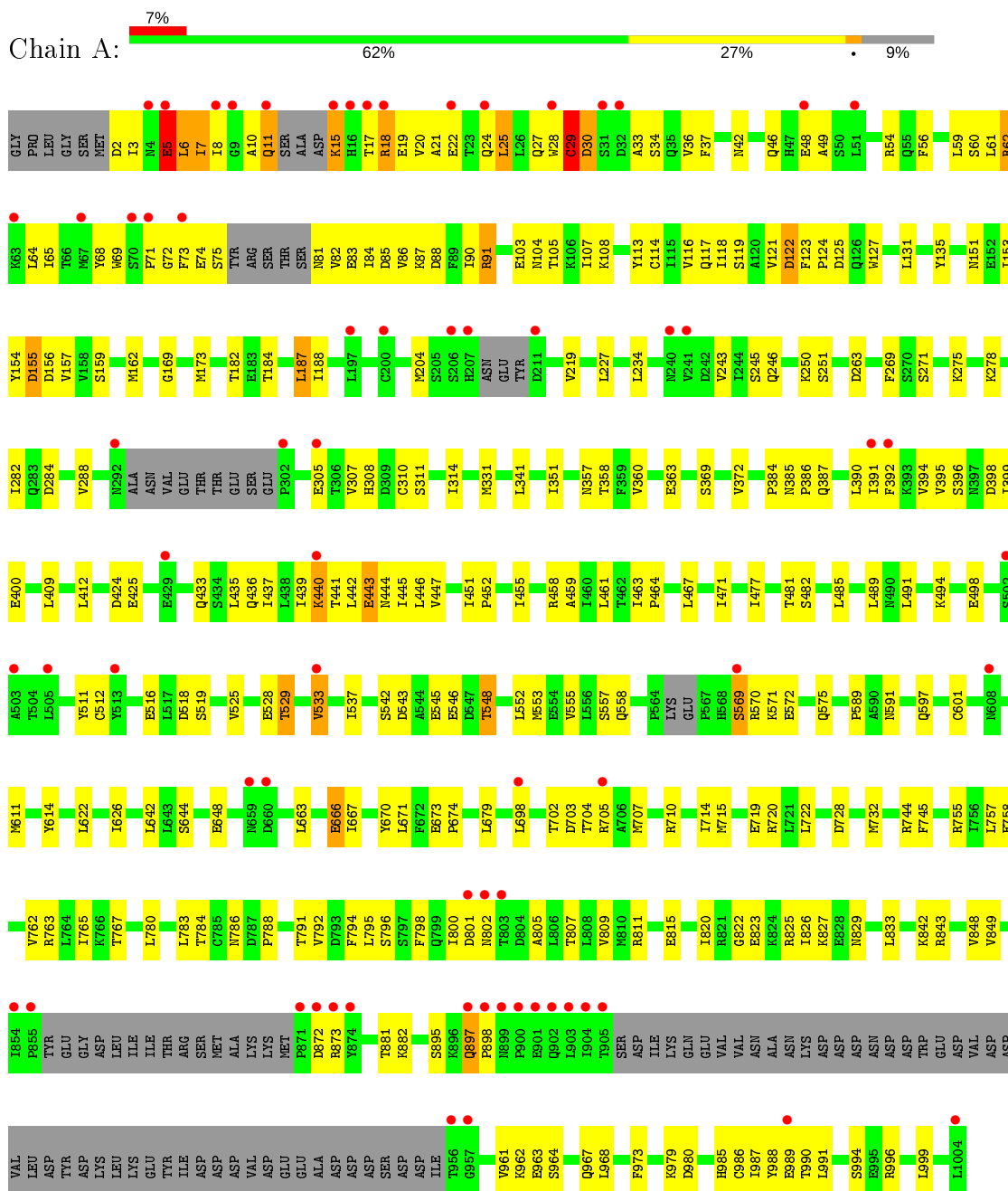
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P53067
A	-3	PRO	-	expression tag	UNP P53067
A	-2	LEU	-	expression tag	UNP P53067
A	-1	GLY	-	expression tag	UNP P53067
A	0	SER	-	expression tag	UNP P53067

### 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 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: Importin subunit beta-5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.62Å 116.62Å 189.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.97-2.50) 98.7 (19.97-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.50Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.211 , 0.263 0.212 , 0.264	Depositor DCC
$R_{free}$ test set	1986 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtrriage
Anisotropy	0.588	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 62.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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 i

### 5.1 Standard geometry i

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	0.51	2/7407 (0.0%)	0.69	9/10036 (0.1%)

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	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	CYS	CB-SG	-6.80	1.70	1.82
1	A	5	GLU	CD-OE1	-5.96	1.19	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LEU	CA-CB-CG	-13.48	84.30	115.30
1	A	6	LEU	CB-CG-CD2	-10.33	93.44	111.00
1	A	6	LEU	CA-CB-CG	8.01	133.73	115.30
1	A	91	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	18	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	122	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	122	ASP	C-N-CA	-5.43	108.11	121.70
1	A	7	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	A	121	VAL	CA-CB-CG1	-5.13	103.20	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	440	LYS	Peptide
1	A	545	GLU	Peptide
1	A	897	GLN	Peptide

## 5.2 Too-close contacts [i](#)

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	7294	0	7413	243	0
All	All	7294	0	7413	243	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 17.

All (243) 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:62:ARG:HH21	1:A:117:GLN:NE2	1.14	1.43
1:A:62:ARG:NH2	1:A:117:GLN:NE2	1.79	1.30
1:A:19:GLU:OE1	1:A:22:GLU:HG2	1.47	1.13
1:A:288:VAL:HG13	1:A:307:VAL:HG23	1.35	1.06
1:A:988:TYR:HA	1:A:991:LEU:HD13	1.43	0.98
1:A:62:ARG:NH2	1:A:117:GLN:HE21	1.56	0.96
1:A:19:GLU:OE1	1:A:22:GLU:CG	2.23	0.86
1:A:288:VAL:HG13	1:A:307:VAL:CG2	2.06	0.85
1:A:62:ARG:NH2	1:A:117:GLN:HE22	1.58	0.81
1:A:443:GLU:OE2	1:A:443:GLU:N	2.13	0.81
1:A:409:LEU:HD23	1:A:455:ILE:HD11	1.63	0.80
1:A:153:ILE:HG23	1:A:157:VAL:HG22	1.63	0.80
1:A:557:SER:HG	1:A:601:CYS:HG	1.12	0.80
1:A:153:ILE:HG23	1:A:157:VAL:CG2	2.11	0.79
1:A:987:ILE:O	1:A:991:LEU:CD1	2.31	0.78
1:A:7:ILE:HG21	1:A:56:PHE:CE2	2.19	0.77
1:A:61:LEU:CD1	1:A:65:ILE:HD11	2.15	0.77
1:A:6:LEU:HD21	1:A:25:LEU:HD22	1.67	0.77
1:A:62:ARG:CZ	1:A:117:GLN:NE2	2.48	0.76
1:A:21:ALA:HA	1:A:24:GLN:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:ILE:HD11	1:A:825:ARG:HB3	1.68	0.76
1:A:798:PHE:CE2	1:A:800:ILE:HD11	2.20	0.75
1:A:719:GLU:OE1	1:A:755:ARG:NH2	2.17	0.75
1:A:807:THR:HG22	1:A:811:ARG:HD2	1.69	0.74
1:A:155:ASP:OD1	1:A:155:ASP:N	2.21	0.72
1:A:69:TRP:NE1	1:A:122:ASP:OD2	2.22	0.72
1:A:881:THR:HG22	1:A:987:ILE:HG12	1.72	0.71
1:A:62:ARG:HH21	1:A:117:GLN:HE22	0.72	0.71
1:A:988:TYR:CA	1:A:991:LEU:HD13	2.18	0.71
1:A:964:SER:HB3	1:A:967:GLN:HG3	1.73	0.70
1:A:20:VAL:O	1:A:24:GLN:HB2	1.92	0.70
1:A:829:ASN:O	1:A:833:LEU:HD12	1.92	0.70
1:A:512:CYS:HB3	1:A:558:GLN:OE1	1.91	0.69
1:A:444:ASN:HA	1:A:447:VAL:HG22	1.72	0.69
1:A:985:HIS:O	1:A:989:GLU:HG2	1.94	0.68
1:A:3:ILE:HA	1:A:6:LEU:HD13	1.76	0.67
1:A:794:PHE:HD2	1:A:795:LEU:HD12	1.60	0.67
1:A:424:ASP:OD1	1:A:425:GLU:N	2.28	0.67
1:A:59:LEU:HA	1:A:62:ARG:HB3	1.76	0.66
1:A:62:ARG:CZ	1:A:117:GLN:HE21	2.08	0.66
1:A:467:LEU:HD13	1:A:481:THR:HG22	1.77	0.66
1:A:784:THR:HG22	1:A:791:THR:HG21	1.77	0.66
1:A:24:GLN:O	1:A:27:GLN:HB2	1.95	0.66
1:A:2:ASP:OD1	1:A:6:LEU:HD12	1.96	0.66
1:A:159:SER:H	1:A:162:MET:HE3	1.61	0.65
1:A:6:LEU:HD23	1:A:7:ILE:HD12	1.78	0.65
1:A:962:LYS:N	1:A:962:LYS:HD2	2.11	0.65
1:A:29:CYS:SG	1:A:68:TYR:CZ	2.89	0.65
1:A:83:GLU:OE2	1:A:86:VAL:HG23	1.97	0.65
1:A:6:LEU:HD21	1:A:25:LEU:CD2	2.26	0.65
1:A:765:ILE:HD11	1:A:800:ILE:HG21	1.79	0.65
1:A:987:ILE:O	1:A:991:LEU:HD13	1.96	0.65
1:A:988:TYR:CE1	1:A:996:ARG:HG3	2.32	0.65
1:A:37:PHE:HB3	1:A:90:ILE:HD11	1.77	0.65
1:A:243:VAL:HA	1:A:246:GLN:HB2	1.79	0.64
1:A:11:GLN:O	1:A:18:ARG:NH1	2.31	0.64
1:A:5:GLU:HA	1:A:8:ILE:HB	1.78	0.64
1:A:34:SER:OG	1:A:83:GLU:N	2.30	0.63
1:A:42:ASN:O	1:A:46:GLN:HG2	1.98	0.63
1:A:707:MET:HB3	1:A:745:PHE:HZ	1.64	0.63
1:A:795:LEU:HD23	1:A:809:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG21	1:A:56:PHE:HE2	1.63	0.61
1:A:963:GLU:HB3	1:A:967:GLN:HB2	1.83	0.61
1:A:65:ILE:HG23	1:A:69:TRP:CE3	2.36	0.61
1:A:765:ILE:CD1	1:A:800:ILE:HG21	2.32	0.60
1:A:622:LEU:O	1:A:626:ILE:HD12	2.02	0.60
1:A:7:ILE:CD1	1:A:25:LEU:HD13	2.31	0.59
1:A:182:THR:HG22	1:A:184:THR:H	1.68	0.59
1:A:780:LEU:O	1:A:784:THR:HG23	2.03	0.59
1:A:69:TRP:CZ2	1:A:87:LYS:HB2	2.38	0.58
1:A:131:LEU:O	1:A:135:TYR:HD1	1.86	0.58
1:A:61:LEU:HD13	1:A:65:ILE:HD11	1.86	0.58
1:A:84:ILE:HG13	1:A:87:LYS:HE3	1.85	0.58
1:A:84:ILE:O	1:A:87:LYS:HG2	2.03	0.58
1:A:87:LYS:HG3	1:A:88:ASP:N	2.17	0.58
1:A:477:ILE:O	1:A:481:THR:HG23	2.04	0.58
1:A:56:PHE:CZ	1:A:60:SER:HB3	2.39	0.58
1:A:103:GLU:HG3	1:A:104:ASN:H	1.69	0.58
1:A:91:ARG:HD3	1:A:127:TRP:CE2	2.38	0.58
1:A:436:GLN:O	1:A:440:LYS:HB2	2.04	0.58
1:A:446:LEU:HB3	1:A:491:LEU:HD11	1.86	0.57
1:A:516:GLU:HG2	1:A:518:ASP:OD1	2.05	0.57
1:A:644:SER:O	1:A:648:GLU:HG3	2.05	0.57
1:A:897:GLN:HB3	1:A:898:PRO:HD3	1.86	0.57
1:A:61:LEU:HD12	1:A:65:ILE:HD11	1.87	0.56
1:A:987:ILE:O	1:A:991:LEU:HD12	2.03	0.56
1:A:433:GLN:O	1:A:437:ILE:HG13	2.06	0.56
1:A:188:ILE:H	1:A:188:ILE:HD12	1.70	0.56
1:A:62:ARG:HA	1:A:65:ILE:HD12	1.87	0.55
1:A:91:ARG:HD3	1:A:127:TRP:CD2	2.41	0.55
1:A:341:LEU:HB3	1:A:372:VAL:HG11	1.89	0.55
1:A:153:ILE:HG23	1:A:157:VAL:HG21	1.87	0.55
1:A:187:LEU:CD2	1:A:245:SER:HB3	2.36	0.55
1:A:703:ASP:OD1	1:A:704:THR:N	2.40	0.55
1:A:698:LEU:O	1:A:702:THR:HG23	2.07	0.55
1:A:849:VAL:HG21	1:A:882:LYS:HG2	1.89	0.55
1:A:21:ALA:HB1	1:A:25:LEU:HD12	1.88	0.54
1:A:7:ILE:HG13	1:A:10:ALA:HB3	1.89	0.54
1:A:60:SER:O	1:A:64:LEU:HD23	2.07	0.54
1:A:895:SER:O	1:A:897:GLN:HG3	2.08	0.54
1:A:204:MET:CE	1:A:219:VAL:HA	2.37	0.54
1:A:46:GLN:HB3	1:A:48:GLU:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD13	1:A:65:ILE:CG1	2.38	0.54
1:A:663:LEU:HB2	1:A:702:THR:HG22	1.90	0.54
1:A:548:THR:O	1:A:552:LEU:HG	2.07	0.53
1:A:452:PRO:O	1:A:455:ILE:HG22	2.07	0.53
1:A:73:PHE:CD1	1:A:73:PHE:O	2.61	0.53
1:A:105:THR:HA	1:A:108:LYS:HE3	1.89	0.53
1:A:83:GLU:OE2	1:A:86:VAL:N	2.39	0.53
1:A:7:ILE:HD11	1:A:25:LEU:HD13	1.89	0.53
1:A:360:VAL:HG11	1:A:548:THR:HB	1.90	0.53
1:A:153:ILE:CG2	1:A:157:VAL:HG22	2.37	0.52
1:A:801:ASP:O	1:A:802:ASN:ND2	2.41	0.52
1:A:62:ARG:NE	1:A:117:GLN:NE2	2.57	0.52
1:A:37:PHE:HB3	1:A:90:ILE:CD1	2.40	0.52
1:A:5:GLU:O	1:A:8:ILE:HG22	2.10	0.52
1:A:385:ASN:ND2	1:A:424:ASP:OD1	2.42	0.52
1:A:557:SER:OG	1:A:601:CYS:SG	2.38	0.52
1:A:2:ASP:HB3	1:A:3:ILE:HD12	1.92	0.51
1:A:571:LYS:O	1:A:575:GLN:HG3	2.10	0.51
1:A:2:ASP:O	1:A:6:LEU:HB2	2.10	0.51
1:A:572:GLU:N	1:A:572:GLU:OE2	2.35	0.51
1:A:464:PRO:HG3	1:A:511:TYR:CE2	2.45	0.51
1:A:187:LEU:HD21	1:A:245:SER:HB3	1.92	0.51
1:A:46:GLN:HB3	1:A:48:GLU:HG3	1.92	0.51
1:A:441:THR:O	1:A:445:ILE:HD13	2.11	0.51
1:A:104:ASN:HB3	1:A:107:ILE:HG12	1.93	0.51
1:A:7:ILE:CG2	1:A:7:ILE:O	2.59	0.51
1:A:811:ARG:NH1	1:A:848:VAL:O	2.43	0.51
1:A:21:ALA:HB1	1:A:25:LEU:CD1	2.40	0.50
1:A:446:LEU:HD11	1:A:463:ILE:HD11	1.92	0.50
1:A:807:THR:O	1:A:811:ARG:HG3	2.10	0.50
1:A:311:SER:HA	1:A:314:ILE:HD12	1.92	0.50
1:A:485:LEU:O	1:A:489:LEU:HD22	2.12	0.50
1:A:65:ILE:HG21	1:A:118:ILE:CD1	2.42	0.50
1:A:980:ASP:CG	1:A:985:HIS:HD1	2.15	0.50
1:A:529:THR:O	1:A:533:VAL:HG13	2.12	0.49
1:A:811:ARG:O	1:A:815:GLU:HG3	2.12	0.49
1:A:987:ILE:HG22	1:A:991:LEU:HD11	1.94	0.49
1:A:74:GLU:N	1:A:74:GLU:OE2	2.46	0.49
1:A:614:TYR:CE2	1:A:667:ILE:HD11	2.47	0.49
1:A:569:SER:O	1:A:570:ARG:HG2	2.13	0.48
1:A:973:PHE:CD1	1:A:999:LEU:HD21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:CYS:SG	1:A:30:ASP:N	2.86	0.48
1:A:823:GLU:HG2	1:A:827:LYS:HE3	1.95	0.48
1:A:271:SER:O	1:A:275:LYS:HG3	2.13	0.48
1:A:351:ILE:CG2	1:A:358:THR:HG21	2.43	0.48
1:A:673:GLU:HG3	1:A:674:PRO:HD3	1.95	0.48
1:A:250:LYS:HE2	1:A:284:ASP:CG	2.34	0.48
1:A:707:MET:HE2	1:A:714:ILE:HD11	1.96	0.48
1:A:386:PRO:O	1:A:390:LEU:HG	2.13	0.48
1:A:21:ALA:HA	1:A:24:GLN:CB	2.39	0.48
1:A:395:VAL:O	1:A:399:ILE:HG13	2.14	0.48
1:A:445:ILE:HG21	1:A:459:ALA:CB	2.43	0.48
1:A:7:ILE:O	1:A:7:ILE:HG22	2.14	0.47
1:A:91:ARG:HB3	1:A:127:TRP:CZ2	2.49	0.47
1:A:10:ALA:HB2	1:A:21:ALA:HB3	1.95	0.47
1:A:62:ARG:HE	1:A:117:GLN:NE2	2.11	0.47
1:A:61:LEU:HD12	1:A:114:CYS:SG	2.54	0.47
1:A:400:GLU:OE1	1:A:441:THR:HG21	2.14	0.47
1:A:805:ALA:O	1:A:809:VAL:HG23	2.15	0.47
1:A:707:MET:HB3	1:A:745:PHE:CZ	2.47	0.47
1:A:34:SER:O	1:A:86:VAL:HG11	2.14	0.47
1:A:61:LEU:HD13	1:A:65:ILE:CD1	2.44	0.47
1:A:988:TYR:HA	1:A:991:LEU:CD1	2.29	0.47
1:A:351:ILE:HG22	1:A:358:THR:HG21	1.97	0.46
1:A:822:GLY:O	1:A:826:ILE:HG13	2.15	0.46
1:A:87:LYS:O	1:A:91:ARG:HG3	2.16	0.46
1:A:546:GLU:HG3	1:A:591:ASN:HD22	1.80	0.46
1:A:34:SER:HA	1:A:82:VAL:HG23	1.97	0.46
1:A:17:THR:O	1:A:20:VAL:HG22	2.15	0.46
1:A:398:ASP:HB3	1:A:412:LEU:HD11	1.98	0.46
1:A:153:ILE:CG2	1:A:157:VAL:CG2	2.90	0.45
1:A:390:LEU:O	1:A:394:VAL:HG23	2.15	0.45
1:A:7:ILE:HD12	1:A:25:LEU:HD13	1.97	0.45
1:A:103:GLU:O	1:A:108:LYS:HE2	2.17	0.45
1:A:471:ILE:HG13	1:A:477:ILE:HG12	1.98	0.45
1:A:792:VAL:O	1:A:796:SER:HB3	2.16	0.45
1:A:961:VAL:HG11	1:A:968:LEU:HD11	1.99	0.45
1:A:62:ARG:HD3	1:A:113:TYR:HB3	1.98	0.45
1:A:49:ALA:HB3	1:A:54:ARG:HG3	1.98	0.45
1:A:679:LEU:O	1:A:720:ARG:NH1	2.50	0.45
1:A:7:ILE:HG23	1:A:10:ALA:HB3	1.99	0.45
1:A:722:LEU:O	1:A:763:ARG:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:MET:CG	1:A:597:GLN:HB2	2.48	0.44
1:A:61:LEU:HD13	1:A:65:ILE:HG13	1.99	0.44
1:A:33:ALA:HB3	1:A:81:ASN:O	2.17	0.44
1:A:788:PRO:O	1:A:792:VAL:HG23	2.17	0.44
1:A:451:ILE:HG13	1:A:455:ILE:HG23	2.00	0.44
1:A:65:ILE:HG21	1:A:118:ILE:HD13	2.00	0.44
1:A:385:ASN:N	1:A:386:PRO:HD2	2.33	0.44
1:A:537:ILE:HD11	1:A:555:VAL:HG12	1.99	0.43
1:A:409:LEU:CD2	1:A:455:ILE:HD11	2.40	0.43
1:A:3:ILE:HG13	1:A:6:LEU:HD13	1.99	0.43
1:A:715:MET:O	1:A:719:GLU:HG3	2.17	0.43
1:A:873:ARG:HG2	1:A:873:ARG:HH11	1.83	0.43
1:A:15:LYS:HG3	1:A:18:ARG:HG3	2.00	0.43
1:A:546:GLU:HG3	1:A:591:ASN:ND2	2.33	0.43
1:A:363:GLU:OE1	1:A:461:LEU:HD13	2.19	0.43
1:A:758:GLU:O	1:A:762:VAL:HG13	2.19	0.43
1:A:440:LYS:HA	1:A:443:GLU:CD	2.39	0.43
1:A:498:GLU:OE2	1:A:543:ASP:HB2	2.18	0.43
1:A:123:PHE:O	1:A:124:PRO:C	2.56	0.43
1:A:251:SER:HB3	1:A:310:CYS:HA	2.01	0.43
1:A:442:LEU:O	1:A:446:LEU:HD12	2.18	0.43
1:A:71:PRO:HA	1:A:72:GLY:HA3	1.83	0.43
1:A:87:LYS:HD2	1:A:91:ARG:NH2	2.34	0.43
1:A:525:VAL:O	1:A:528:GLU:HG2	2.19	0.43
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.80	0.42
1:A:728:ASP:O	1:A:732:MET:HG3	2.19	0.42
1:A:986:CYS:O	1:A:990:THR:HG23	2.19	0.42
1:A:439:ILE:O	1:A:443:GLU:OE2	2.37	0.42
1:A:59:LEU:HA	1:A:62:ARG:CB	2.48	0.42
1:A:444:ASN:HA	1:A:447:VAL:CG2	2.47	0.42
1:A:452:PRO:HD2	1:A:455:ILE:HG21	2.00	0.42
1:A:71:PRO:HG3	1:A:75:SER:OG	2.19	0.42
1:A:707:MET:HE3	1:A:710:ARG:HB2	2.02	0.42
1:A:796:SER:OG	1:A:843:ARG:HD2	2.19	0.42
1:A:973:PHE:CG	1:A:999:LEU:HD21	2.55	0.42
1:A:278:LYS:O	1:A:282:ILE:HG13	2.19	0.42
1:A:103:GLU:HG3	1:A:104:ASN:N	2.33	0.42
1:A:3:ILE:HD11	1:A:28:TRP:HH2	1.85	0.42
1:A:169:GLY:O	1:A:173:MET:HG2	2.20	0.41
1:A:384:PRO:HG2	1:A:387:GLN:OE1	2.20	0.41
1:A:386:PRO:HG2	1:A:387:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:O	1:A:36:VAL:HG12	2.21	0.41
1:A:435:LEU:O	1:A:439:ILE:HG12	2.20	0.41
1:A:823:GLU:CG	1:A:827:LYS:HE3	2.49	0.41
1:A:392:PHE:O	1:A:396:SER:OG	2.22	0.41
1:A:666:GLU:OE1	1:A:666:GLU:N	2.51	0.41
1:A:116:VAL:O	1:A:119:SER:OG	2.39	0.41
1:A:744:ARG:HH11	1:A:744:ARG:HG3	1.85	0.41
1:A:757:LEU:HG	1:A:783:LEU:HD13	2.03	0.41
1:A:33:ALA:HA	1:A:36:VAL:HG12	2.03	0.41
1:A:83:GLU:CD	1:A:85:ASP:H	2.23	0.41
1:A:872:ASP:OD1	1:A:872:ASP:N	2.51	0.41
1:A:3:ILE:H	1:A:3:ILE:HD12	1.86	0.41
1:A:622:LEU:HD13	1:A:671:LEU:HD13	2.03	0.41
1:A:357:ASN:HA	1:A:548:THR:HG21	2.03	0.41
1:A:204:MET:HE2	1:A:219:VAL:HA	2.03	0.40
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.86	0.40
1:A:589:PRO:HB3	1:A:642:LEU:HD13	2.04	0.40
1:A:331:MET:SD	1:A:391:ILE:HD12	2.62	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	900/1009 (89%)	851 (95%)	49 (5%)	0	<b>100</b> <b>100</b>

There are no Ramachandran outliers to report.

### 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	846/931 (91%)	810 (96%)	36 (4%)	29 53

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	11	GLN
1	A	15	LYS
1	A	29	CYS
1	A	30	ASP
1	A	62	ARG
1	A	125	ASP
1	A	151	ASN
1	A	154	TYR
1	A	155	ASP
1	A	156	ASP
1	A	187	LEU
1	A	263	ASP
1	A	269	PHE
1	A	305	GLU
1	A	308	HIS
1	A	369	SER
1	A	443	GLU
1	A	458	ARG
1	A	482	SER
1	A	494	LYS
1	A	519	SER
1	A	529	THR
1	A	533	VAL
1	A	542	SER
1	A	548	THR
1	A	569	SER
1	A	611	MET
1	A	666	GLU
1	A	670	TYR
1	A	705	ARG
1	A	767	THR
1	A	786	ASN
1	A	842	LYS

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Mol	Chain	Res	Type
1	A	979	LYS
1	A	994	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	129	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 monosaccharides 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	916/1009 (90%)	0.30	68 (7%) <b>14</b> <b>15</b>	54, 78, 129, 159	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	871	PRO	6.8
1	A	902	GLN	5.9
1	A	904	ILE	5.9
1	A	900	PRO	5.6
1	A	17	THR	5.4
1	A	73	PHE	5.1
1	A	854	ILE	5.0
1	A	855	PRO	4.9
1	A	32	ASP	4.6
1	A	16	HIS	4.5
1	A	905	THR	4.2
1	A	31	SER	4.2
1	A	872	ASP	4.0
1	A	897	GLN	3.8
1	A	5	GLU	3.8
1	A	873	ARG	3.8
1	A	608	ASN	3.7
1	A	8	ILE	3.7
1	A	898	PRO	3.7
1	A	48	GLU	3.7
1	A	11	GLN	3.6
1	A	659	ASN	3.6
1	A	899	ASN	3.6
1	A	1004	LEU	3.5
1	A	429	GLU	3.5
1	A	513	TYR	3.5
1	A	302	PRO	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	956	THR	3.5
1	A	292	ASN	3.3
1	A	24	GLN	3.3
1	A	803	THR	3.3
1	A	207	HIS	3.3
1	A	15	LYS	3.2
1	A	802	ASN	3.2
1	A	705	ARG	3.0
1	A	957	GLY	2.8
1	A	22	GLU	2.8
1	A	874	TYR	2.7
1	A	901	GLU	2.7
1	A	200	CYS	2.6
1	A	503	ALA	2.6
1	A	211	ASP	2.6
1	A	801	ASP	2.6
1	A	903	LEU	2.5
1	A	502	SER	2.5
1	A	28	TRP	2.5
1	A	440	LYS	2.5
1	A	533	VAL	2.4
1	A	18	ARG	2.4
1	A	240	ASN	2.4
1	A	569	SER	2.4
1	A	4	ASN	2.4
1	A	51	LEU	2.4
1	A	392	PHE	2.3
1	A	505	LEU	2.3
1	A	206	SER	2.3
1	A	241	VAL	2.3
1	A	660	ASP	2.3
1	A	70	SER	2.3
1	A	305	GLU	2.3
1	A	197	LEU	2.2
1	A	698	LEU	2.1
1	A	9	GLY	2.1
1	A	71	PRO	2.1
1	A	391	ILE	2.1
1	A	989	GLU	2.1
1	A	67	MET	2.0
1	A	63	LYS	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 monosaccharides 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.