



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:56 PM UTC

PDB ID : 3W3Y / pdb_00003w3y
Title : Crystal structure of Kap121p bound to Nup53p
Authors : Kobayashi, J.; Matsuura, Y.
Deposited on : 2012-12-28
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

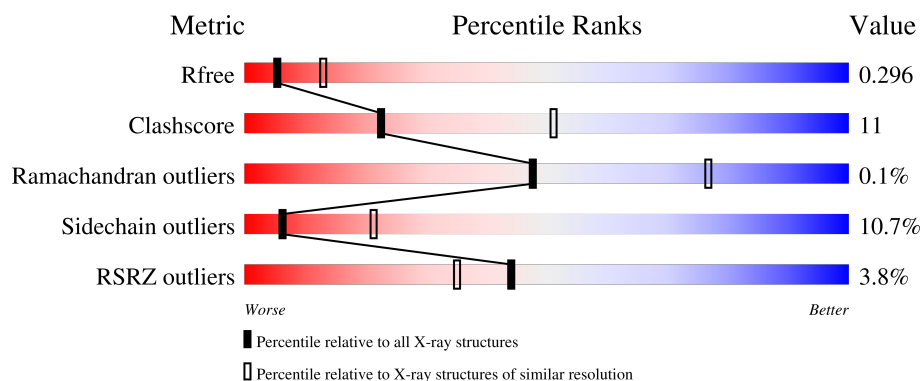
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1078	
2	B	48	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7862 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-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1026	7799	5011	1250	1501	37	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P32337
A	?	-	SER	deletion	UNP P32337
A	?	-	SER	deletion	UNP P32337
A	?	-	LYS	deletion	UNP P32337
A	?	-	LEU	deletion	UNP P32337
A	?	-	MET	deletion	UNP P32337
A	?	-	ILE	deletion	UNP P32337
A	?	-	MET	deletion	UNP P32337
A	?	-	SER	deletion	UNP P32337
A	?	-	LYS	deletion	UNP P32337
A	?	-	ASN	deletion	UNP P32337

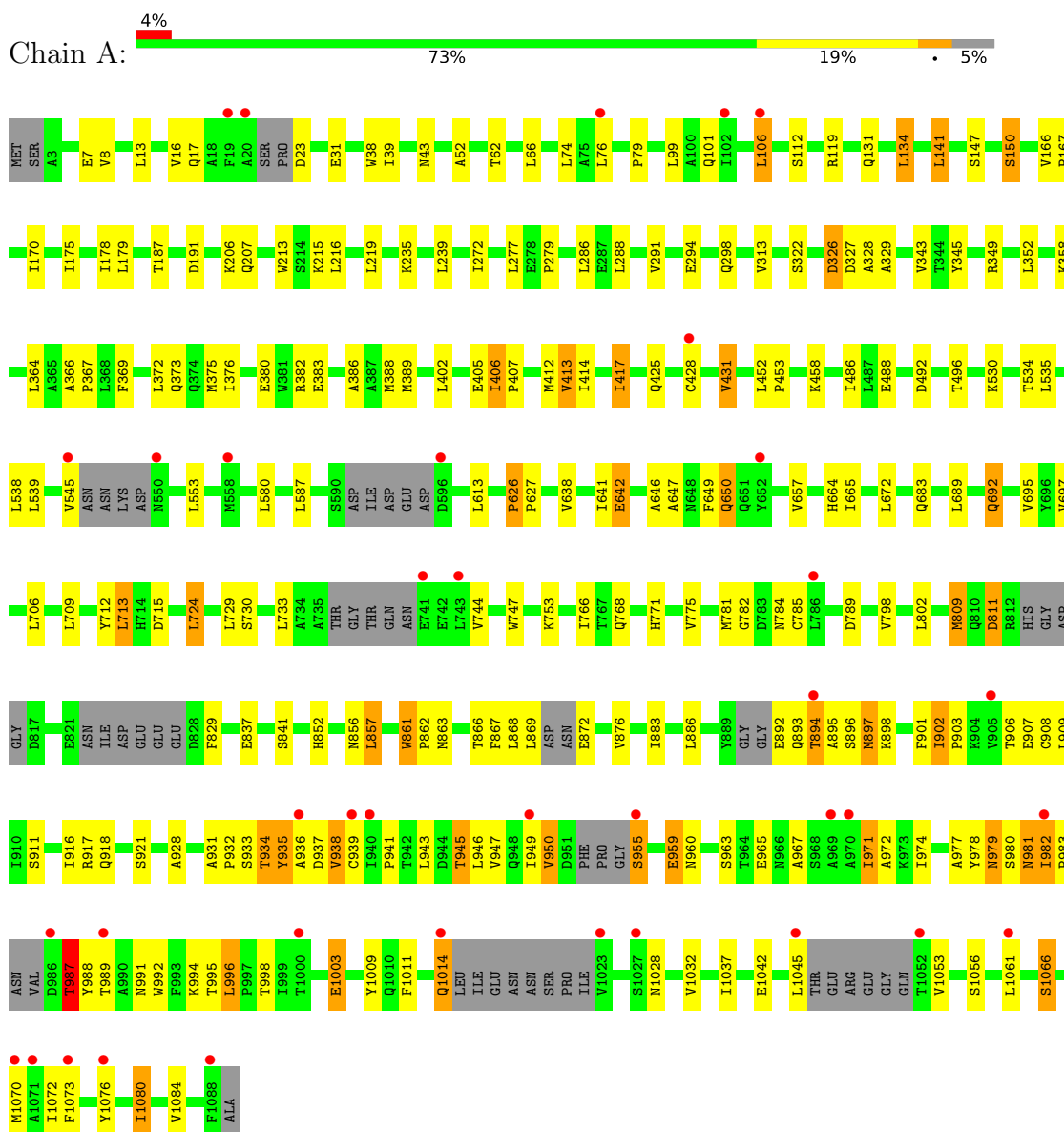
- Molecule 2 is a protein called Nucleoporin NUP53.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	8	63	40	11	12	0	0	0

3 Residue-property plots

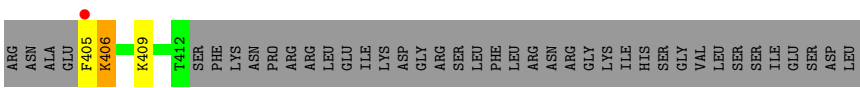
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-3



• Molecule 2: Nucleoporin NUP53





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.33Å 131.44Å 131.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.33 – 2.80 30.33 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.33-2.80) 94.6 (30.33-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.251 , 0.297 0.249 , 0.296	Depositor DCC
R_{free} test set	1633 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.039 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7862	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.74	0/7935	1.07	19/10822 (0.2%)
2	B	0.83	0/63	1.28	0/82
All	All	0.74	0/7998	1.08	19/10904 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	646	ALA	N-CA-C	15.45	131.93	112.92
1	A	647	ALA	N-CA-C	-10.51	100.95	113.88
1	A	979	ASN	N-CA-C	9.42	122.51	111.02
1	A	987	THR	N-CA-C	-7.58	102.02	111.11
1	A	646	ALA	CB-CA-C	-7.29	98.25	110.56
1	A	982	ILE	N-CA-C	6.75	115.24	107.89
1	A	279	PRO	N-CA-C	6.48	118.60	110.70
1	A	364	LEU	N-CA-C	6.10	120.88	113.38
1	A	935	TYR	N-CA-C	5.85	121.99	114.56
1	A	697	VAL	N-CA-C	5.76	116.41	110.36
1	A	936	ALA	N-CA-C	5.70	122.93	110.80
1	A	431	VAL	CB-CA-C	-5.46	104.68	112.22
1	A	326	ASP	N-CA-C	5.38	117.90	111.71
1	A	406	ILE	N-CA-CB	-5.36	103.70	111.21
1	A	646	ALA	CA-C-O	-5.34	113.31	119.56
1	A	626	PRO	N-CA-C	5.17	117.01	110.70
1	A	782	GLY	N-CA-C	5.17	118.94	111.24
1	A	829	PHE	N-CA-C	-5.16	105.73	112.23
1	A	343	VAL	N-CA-C	5.12	115.34	110.53

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	7799	0	7659	159	0
2	B	63	0	66	5	0
All	All	7862	0	7725	164	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 11.

All (164) 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)
2:B:405:PHE:HD1	2:B:406:LYS:HB2	1.09	1.13
1:A:406:ILE:HG23	1:A:407:PRO:HD3	1.13	1.11
1:A:892:GLU:HB3	1:A:934:THR:HG21	1.44	0.99
1:A:965:GLU:HG2	1:A:998:THR:HG23	1.44	0.99
1:A:902:ILE:N	1:A:903:PRO:HD2	1.78	0.97
2:B:405:PHE:CD1	2:B:406:LYS:HB2	2.00	0.96
1:A:638:VAL:HG23	1:A:665:ILE:CG2	1.97	0.93
1:A:892:GLU:CD	1:A:934:THR:HG22	1.96	0.91
1:A:406:ILE:CG2	1:A:407:PRO:HD3	2.00	0.90
1:A:534:THR:O	1:A:538:LEU:HD13	1.79	0.82
1:A:987:THR:HG23	1:A:991:ASN:HD21	1.44	0.82
1:A:894:THR:O	1:A:897:MET:HG3	1.80	0.81
1:A:414:ILE:O	1:A:417:ILE:HG22	1.82	0.79
1:A:892:GLU:CG	1:A:934:THR:CG2	2.61	0.79
1:A:988:TYR:HA	1:A:991:ASN:HD22	1.46	0.79
1:A:932:PRO:O	1:A:978:TYR:OH	2.00	0.78
1:A:980:SER:C	1:A:981:ASN:HD22	1.93	0.77
1:A:406:ILE:HG23	1:A:407:PRO:CD	2.05	0.76
1:A:965:GLU:CG	1:A:998:THR:HG23	2.15	0.76
1:A:932:PRO:O	1:A:978:TYR:CE1	2.40	0.75
1:A:638:VAL:CG2	1:A:665:ILE:CG2	2.65	0.74
1:A:892:GLU:CG	1:A:934:THR:HG22	2.17	0.74
1:A:892:GLU:CB	1:A:934:THR:HG21	2.16	0.73
1:A:892:GLU:HG2	1:A:934:THR:CG2	2.18	0.73
1:A:892:GLU:HB3	1:A:934:THR:CG2	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PHE:O	1:A:373:GLN:HG2	1.89	0.72
1:A:650:GLN:HG2	1:A:657:VAL:HG22	1.71	0.71
1:A:641:ILE:HG23	1:A:664:HIS:HB3	1.71	0.71
1:A:902:ILE:N	1:A:903:PRO:CD	2.52	0.71
1:A:987:THR:HG23	1:A:991:ASN:ND2	2.04	0.71
1:A:946:LEU:HD13	1:A:971:ILE:HG22	1.72	0.71
1:A:946:LEU:CD1	1:A:971:ILE:HG22	2.22	0.69
2:B:405:PHE:HE1	2:B:406:LYS:HE2	1.56	0.69
1:A:638:VAL:HG23	1:A:665:ILE:HG22	1.74	0.69
1:A:987:THR:HG22	1:A:988:TYR:N	2.09	0.67
1:A:902:ILE:HG21	1:A:938:VAL:HG11	1.77	0.67
1:A:641:ILE:HG22	1:A:664:HIS:O	1.96	0.65
1:A:16:VAL:HG23	1:A:66:LEU:HD12	1.79	0.65
1:A:1066:SER:O	1:A:1070:MET:HG2	1.96	0.65
1:A:861:TRP:NE1	1:A:897:MET:HE2	2.11	0.65
1:A:937:ASP:O	1:A:941:PRO:HG2	1.97	0.64
1:A:901:PHE:C	1:A:903:PRO:HD2	2.22	0.63
1:A:131:GLN:HB3	1:A:134:LEU:HB2	1.80	0.63
1:A:893:GLN:HG2	1:A:893:GLN:O	1.98	0.63
1:A:861:TRP:HE1	1:A:897:MET:CE	2.12	0.62
1:A:892:GLU:CB	1:A:934:THR:CG2	2.76	0.61
1:A:492:ASP:O	1:A:496:THR:HG23	2.00	0.61
1:A:1080:ILE:O	1:A:1080:ILE:HD12	2.01	0.60
1:A:932:PRO:O	1:A:978:TYR:CZ	2.54	0.60
1:A:294:GLU:HG2	1:A:358:LYS:HE3	1.82	0.60
1:A:898:LYS:O	1:A:902:ILE:CG1	2.50	0.60
1:A:980:SER:C	1:A:981:ASN:ND2	2.59	0.59
1:A:366:ALA:HB3	1:A:367:PRO:CD	2.32	0.59
1:A:987:THR:CG2	1:A:988:TYR:N	2.64	0.59
1:A:898:LYS:O	1:A:902:ILE:HG12	2.01	0.59
1:A:932:PRO:O	1:A:978:TYR:HE1	1.81	0.59
1:A:712:TYR:CD1	1:A:713:LEU:HD13	2.38	0.58
1:A:971:ILE:HD11	1:A:992:TRP:HB2	1.86	0.58
1:A:987:THR:CG2	1:A:991:ASN:HD21	2.15	0.58
1:A:638:VAL:CG2	1:A:665:ILE:HG23	2.34	0.58
1:A:715:ASP:HB2	1:A:766:ILE:HD11	1.86	0.58
1:A:191:ASP:OD2	1:A:235:LYS:HG2	2.05	0.57
1:A:945:THR:O	1:A:949:ILE:HG13	2.04	0.57
1:A:1028:ASN:O	1:A:1032:VAL:HG23	2.05	0.57
1:A:345:TYR:O	1:A:349:ARG:HG3	2.05	0.56
1:A:7:GLU:HG2	1:A:8:VAL:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:GLN:CG	1:A:657:VAL:HG22	2.35	0.56
1:A:170:ILE:HG23	1:A:178:ILE:HG12	1.87	0.56
1:A:1003:GLU:H	1:A:1003:GLU:CD	2.14	0.55
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.89	0.54
1:A:328:ALA:O	1:A:329:ALA:C	2.50	0.53
1:A:695:VAL:O	1:A:695:VAL:HG22	2.08	0.53
1:A:932:PRO:HB3	1:A:977:ALA:HB1	1.90	0.53
1:A:369:PHE:CD1	1:A:412:MET:HE1	2.44	0.53
1:A:893:GLN:O	1:A:893:GLN:CG	2.56	0.52
1:A:388:MET:SD	1:A:413:VAL:HG22	2.50	0.52
1:A:167:PRO:HG3	1:A:207:GLN:HG2	1.92	0.52
1:A:76:LEU:O	1:A:79:PRO:HB3	2.10	0.51
1:A:1061:LEU:HD21	1:A:1072:ILE:HD12	1.92	0.51
1:A:1009:TYR:HB3	1:A:1053:VAL:HG21	1.93	0.51
1:A:375:MET:HE2	1:A:383:GLU:O	2.11	0.51
1:A:626:PRO:HB2	1:A:627:PRO:HD3	1.91	0.51
1:A:892:GLU:OE1	1:A:933:SER:OG	2.26	0.50
1:A:417:ILE:HG13	1:A:458:LYS:HD3	1.94	0.50
1:A:902:ILE:CG2	1:A:938:VAL:HG11	2.41	0.50
1:A:1037:ILE:HD12	1:A:1084:VAL:HG22	1.93	0.50
1:A:911:SER:O	1:A:917:ARG:HD3	2.11	0.50
1:A:372:LEU:O	1:A:376:ILE:HG12	2.12	0.50
1:A:861:TRP:N	1:A:862:PRO:HD2	2.26	0.49
1:A:747:TRP:HE1	1:A:785:CYS:HB2	1.77	0.49
1:A:861:TRP:NE1	1:A:897:MET:CE	2.73	0.49
1:A:809:MET:C	1:A:811:ASP:H	2.19	0.49
1:A:417:ILE:O	1:A:425:GLN:HG2	2.12	0.49
1:A:933:SER:C	1:A:935:TYR:H	2.21	0.49
1:A:996:LEU:N	1:A:996:LEU:HD23	2.28	0.49
1:A:112:SER:O	1:A:119:ARG:NH2	2.45	0.48
1:A:66:LEU:C	1:A:66:LEU:HD13	2.38	0.48
1:A:965:GLU:CD	1:A:998:THR:HG23	2.39	0.48
1:A:992:TRP:O	1:A:995:THR:OG1	2.28	0.48
1:A:906:THR:HA	1:A:909:LEU:HD12	1.96	0.48
1:A:747:TRP:CG	1:A:781:MET:HG3	2.49	0.47
1:A:939:CYS:HB3	1:A:974:ILE:HG12	1.95	0.47
1:A:641:ILE:HG22	1:A:664:HIS:C	2.39	0.47
1:A:327:ASP:O	1:A:328:ALA:HB3	2.15	0.47
1:A:934:THR:O	1:A:934:THR:OG1	2.31	0.47
1:A:775:VAL:HG22	1:A:841:SER:HA	1.95	0.46
1:A:959:GLU:CD	1:A:959:GLU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:SER:O	1:A:382:ARG:NH2	2.49	0.46
1:A:366:ALA:HB3	1:A:367:PRO:HD3	1.97	0.46
1:A:683:GLN:HB2	1:A:724:LEU:HD13	1.97	0.46
1:A:857:LEU:O	1:A:857:LEU:HD12	2.15	0.46
1:A:928:ALA:O	1:A:977:ALA:HB2	2.17	0.45
1:A:413:VAL:HG13	1:A:428:CYS:SG	2.57	0.45
1:A:946:LEU:HD12	1:A:971:ILE:HG22	1.99	0.45
1:A:798:VAL:O	1:A:802:LEU:HG	2.16	0.45
1:A:898:LYS:O	1:A:902:ILE:HG13	2.17	0.45
1:A:771:HIS:O	1:A:775:VAL:HG23	2.17	0.45
1:A:13:LEU:O	1:A:17:GLN:HG3	2.17	0.44
1:A:950:VAL:O	1:A:955:SER:OG	2.35	0.44
1:A:1080:ILE:HD12	1:A:1080:ILE:C	2.42	0.44
1:A:987:THR:HG22	1:A:988:TYR:H	1.81	0.44
1:A:417:ILE:CG1	1:A:458:LYS:HD3	2.48	0.43
1:A:972:ALA:HB1	1:A:1011:PHE:CD2	2.53	0.43
1:A:52:ALA:HB1	1:A:106:LEU:HD13	2.00	0.43
1:A:213:TRP:C	1:A:215:LYS:H	2.25	0.43
1:A:918:GLN:HB2	1:A:963:SER:OG	2.18	0.43
1:A:272:ILE:HG21	1:A:313:VAL:HB	2.01	0.43
1:A:641:ILE:HG12	1:A:642:GLU:N	2.32	0.43
1:A:1011:PHE:HA	1:A:1014:GLN:HG3	2.00	0.43
2:B:405:PHE:HD1	2:B:406:LYS:CB	2.02	0.43
1:A:897:MET:O	1:A:898:LYS:C	2.62	0.43
1:A:13:LEU:HG	1:A:17:GLN:OE1	2.19	0.43
1:A:638:VAL:HG23	1:A:665:ILE:HG23	1.89	0.43
1:A:7:GLU:HG2	1:A:8:VAL:N	2.33	0.43
2:B:405:PHE:CD1	2:B:406:LYS:N	2.86	0.43
1:A:872:GLU:O	1:A:876:VAL:HG23	2.18	0.42
1:A:375:MET:HE1	1:A:386:ALA:HB3	2.00	0.42
1:A:39:ILE:O	1:A:39:ILE:HG22	2.19	0.42
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.84	0.42
1:A:1073:PHE:HA	1:A:1076:TYR:CD2	2.54	0.42
1:A:406:ILE:CG2	1:A:407:PRO:CD	2.82	0.42
1:A:883:ILE:HA	1:A:886:LEU:HD12	2.02	0.42
1:A:892:GLU:HG2	1:A:934:THR:HG23	1.98	0.42
1:A:959:GLU:N	1:A:959:GLU:OE1	2.53	0.42
1:A:982:ILE:HA	1:A:983:PRO:HD2	1.92	0.42
1:A:895:ALA:C	1:A:897:MET:N	2.77	0.41
1:A:908:CYS:HB3	1:A:916:ILE:HG22	2.01	0.41
1:A:967:ALA:O	1:A:971:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLN:HG3	1:A:837:GLU:HG3	2.02	0.41
1:A:1076:TYR:CG	1:A:1080:ILE:HD11	2.55	0.41
1:A:931:ALA:HB1	1:A:934:THR:HG23	2.02	0.41
1:A:943:LEU:O	1:A:947:VAL:HG23	2.21	0.41
1:A:863:MET:CE	1:A:867:PHE:CE2	3.04	0.41
1:A:452:LEU:HB2	1:A:453:PRO:HD3	2.03	0.40
1:A:38:TRP:CE3	1:A:43:ASN:HB3	2.56	0.40
1:A:147:SER:O	1:A:150:SER:HB3	2.21	0.40
1:A:692:GLN:H	1:A:692:GLN:HG2	1.63	0.40
1:A:709:LEU:HD12	1:A:753:LYS:HG2	2.04	0.40
1:A:747:TRP:CD1	1:A:781:MET:HG3	2.56	0.40
1:A:175:ILE:HA	1:A:178:ILE:HG22	2.02	0.40
1:A:856:ASN:ND2	1:A:856:ASN:H	2.20	0.40
1:A:191:ASP:OD2	1:A:235:LYS:HE2	2.21	0.40
1:A:369:PHE:HE2	1:A:402:LEU:HD21	1.86	0.40
1:A:895:ALA:C	1:A:897:MET:H	2.30	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	1000/1078 (93%)	955 (96%)	44 (4%)	1 (0%)	48	77
2	B	6/48 (12%)	5 (83%)	1 (17%)	0	100	100
All	All	1006/1126 (89%)	960 (95%)	45 (4%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	852	HIS

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	834/937 (89%)	746 (89%)	88 (11%)	6	22
2	B	8/44 (18%)	6 (75%)	2 (25%)	0	2
All	All	842/981 (86%)	752 (89%)	90 (11%)	6	21

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	31	GLU
1	A	62	THR
1	A	74	LEU
1	A	101	GLN
1	A	106	LEU
1	A	134	LEU
1	A	141	LEU
1	A	150	SER
1	A	166	VAL
1	A	179	LEU
1	A	187	THR
1	A	206	LYS
1	A	216	LEU
1	A	219	LEU
1	A	239	LEU
1	A	277	LEU
1	A	286	LEU
1	A	288	LEU
1	A	291	VAL
1	A	298	GLN
1	A	326	ASP
1	A	352	LEU
1	A	380	GLU
1	A	389	MET
1	A	405	GLU
1	A	413	VAL

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Mol	Chain	Res	Type
1	A	417	ILE
1	A	431	VAL
1	A	486	ILE
1	A	488	GLU
1	A	530	LYS
1	A	535	LEU
1	A	539	LEU
1	A	545	VAL
1	A	553	LEU
1	A	580	LEU
1	A	587	LEU
1	A	613	LEU
1	A	642	GLU
1	A	649	PHE
1	A	650	GLN
1	A	672	LEU
1	A	689	LEU
1	A	692	GLN
1	A	706	LEU
1	A	713	LEU
1	A	724	LEU
1	A	729	LEU
1	A	730	SER
1	A	733	LEU
1	A	744	VAL
1	A	784	ASN
1	A	789	ASP
1	A	809	MET
1	A	811	ASP
1	A	857	LEU
1	A	861	TRP
1	A	866	THR
1	A	868	LEU
1	A	869	LEU
1	A	894	THR
1	A	896	SER
1	A	897	MET
1	A	902	ILE
1	A	907	GLU
1	A	921	SER
1	A	934	THR
1	A	938	VAL

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Mol	Chain	Res	Type
1	A	945	THR
1	A	950	VAL
1	A	955	SER
1	A	959	GLU
1	A	960	ASN
1	A	971	ILE
1	A	979	ASN
1	A	981	ASN
1	A	987	THR
1	A	989	THR
1	A	994	LYS
1	A	996	LEU
1	A	1003	GLU
1	A	1014	GLN
1	A	1042	GLU
1	A	1045	LEU
1	A	1056	SER
1	A	1066	SER
1	A	1080	ILE
2	B	406	LYS
2	B	409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	183	GLN
1	A	303	ASN
1	A	468	GLN
1	A	541	ASN
1	A	801	ASN
1	A	856	ASN
1	A	888	GLN
1	A	893	GLN
1	A	966	ASN
1	A	979	ASN
1	A	981	ASN
1	A	991	ASN
1	A	1041	ASN
1	A	1085	HIS

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	1026/1078 (95%)	0.22	38 (3%) 45 36	34, 81, 148, 204	0
2	B	8/48 (16%)	0.26	1 (12%) 8 6	47, 62, 89, 94	0
All	All	1034/1126 (91%)	0.22	39 (3%) 44 35	34, 81, 148, 204	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	786	LEU	4.2
1	A	1045	LEU	3.9
1	A	596	ASP	3.8
1	A	982	ILE	3.7
1	A	986	ASP	3.5
1	A	1073	PHE	3.5
1	A	1061	LEU	3.2
1	A	550	ASN	3.1
1	A	1088	PHE	3.0
1	A	652	TYR	3.0
1	A	1023	VAL	3.0
1	A	20	ALA	2.9
1	A	19	PHE	2.9
1	A	940	ILE	2.8
1	A	955	SER	2.8
1	A	102	ILE	2.8
1	A	1027	SER	2.7
1	A	545	VAL	2.7
1	A	1052	THR	2.7
1	A	970	ALA	2.6
1	A	905	VAL	2.5
1	A	1071	ALA	2.4
1	A	558	MET	2.4
1	A	1000	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1070	MET	2.2
1	A	936	ALA	2.2
2	B	405	PHE	2.2
1	A	949	ILE	2.2
1	A	894	THR	2.1
1	A	939	CYS	2.1
1	A	741	GLU	2.1
1	A	76	LEU	2.1
1	A	1076	TYR	2.1
1	A	106	LEU	2.1
1	A	969	ALA	2.1
1	A	1014	GLN	2.0
1	A	428	CYS	2.0
1	A	743	LEU	2.0
1	A	989	THR	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 oligosaccharides 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.