Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:05 PM GMT

PDB ID	:	3W3T
Title	:	Crystal structure of Kap121p
Authors	:	Kobayashi, J.; Matsuura, Y.
Deposited on	:	2012-12-28
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		12
Ramachandran outliers		0.3%
Sidechain outliers		13.2%
RSRZ outliers		2.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▊ Percentile relative to X-ray structures of similar resolution
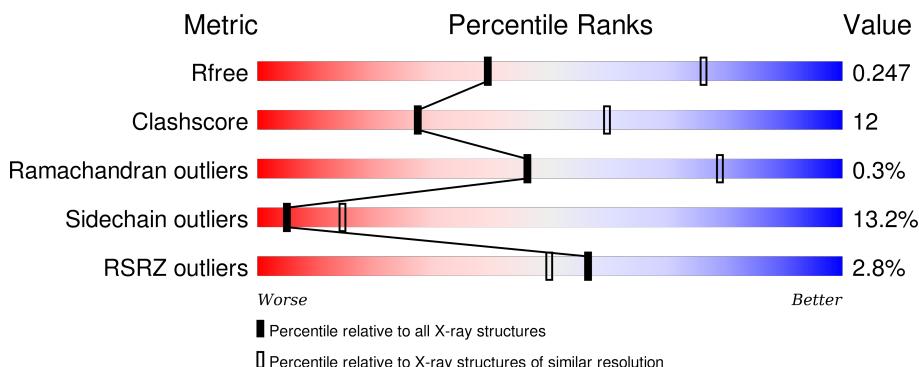
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 >=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 <=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	3% 72% 19% • 5%
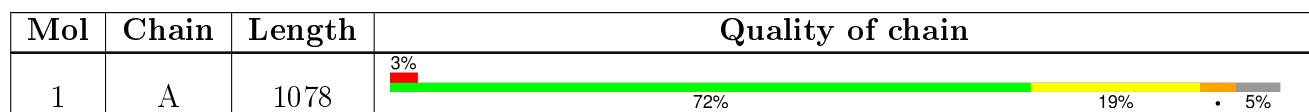
2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7845 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	1025	7845	5035	1263	1511	36	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

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: Importin subunit beta-3
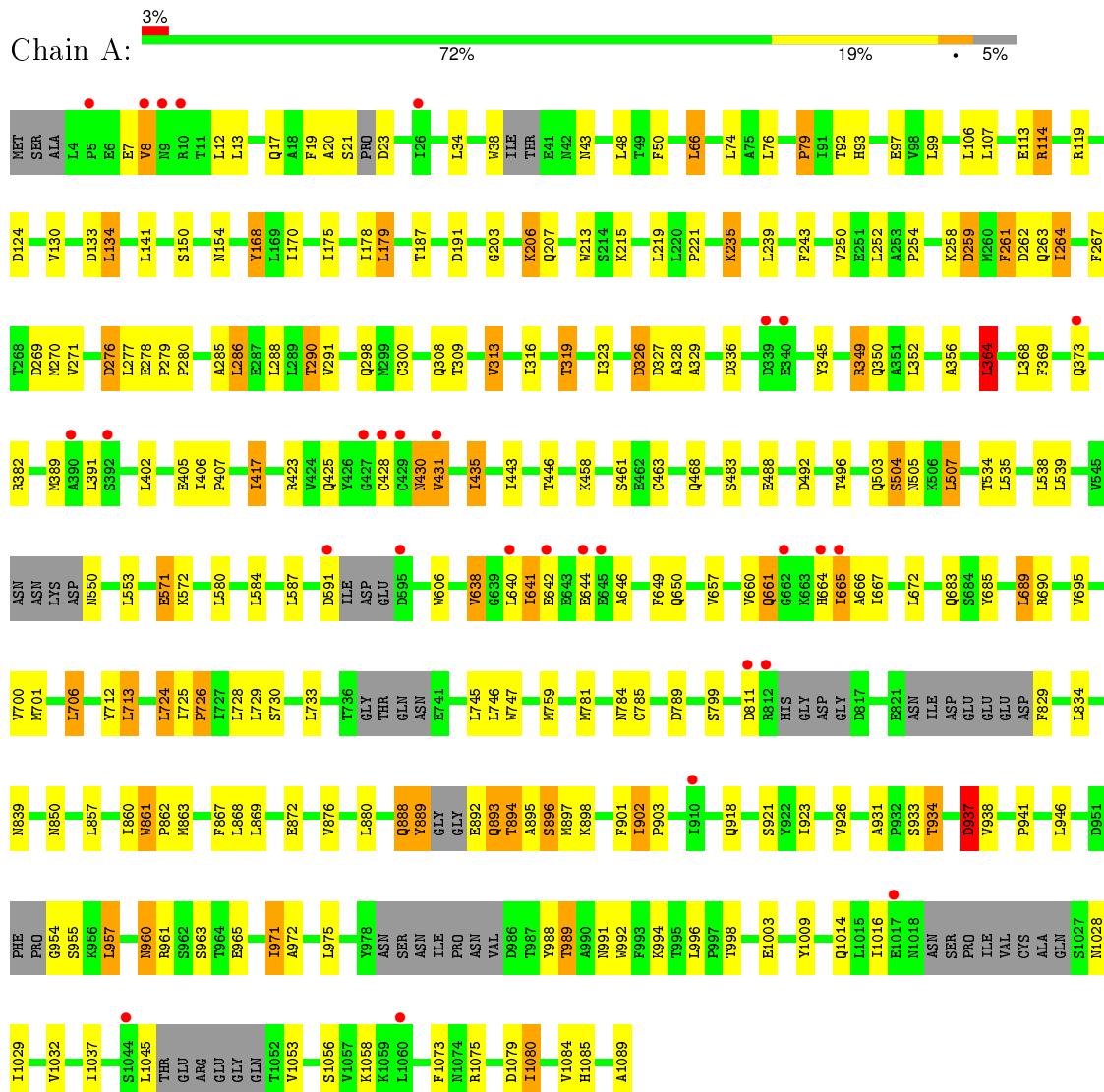
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.77Å 124.39Å 85.19Å 90.00° 117.02° 90.00°	Depositor
Resolution (Å)	28.32 – 2.90 28.30 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.32-2.90) 99.7 (28.30-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.201 , 0.247 0.200 , 0.247	Depositor DCC
R_{free} test set	1621 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	79.5	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 45.3	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 31923 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7845	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.63	0/7981	0.86	14/10869 (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	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	646	ALA	N-CA-C	11.72	142.65	111.00
1	A	957	LEU	CB-CA-C	10.18	129.54	110.20
1	A	1075	ARG	N-CA-CB	-8.24	95.77	110.60
1	A	1073	PHE	CB-CA-C	-8.11	94.18	110.40
1	A	300	CYS	N-CA-CB	-7.97	96.26	110.60
1	A	76	LEU	CA-CB-CG	7.08	131.59	115.30
1	A	646	ALA	CB-CA-C	-6.54	100.29	110.10
1	A	364	LEU	CB-CG-CD2	-6.30	100.29	111.00
1	A	937	ASP	CB-CA-C	-5.49	99.41	110.40
1	A	124	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	957	LEU	N-CA-C	-5.33	96.61	111.00
1	A	79	PRO	CA-C-N	-5.33	105.48	117.20
1	A	364	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	364	LEU	N-CA-C	5.12	124.82	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	ASP	Peptide
1	A	79	PRO	Mainchain

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	7845	0	7740	185	0
All	All	7845	0	7740	185	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 12.

All (185) 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:861:TRP:NE1	1:A:897:MET:HE1	1.52	1.23
1:A:898:LYS:NZ	1:A:937:ASP:OD1	1.70	1.22
1:A:19:PHE:HB3	1:A:66:LEU:HD21	1.24	1.14
1:A:892:GLU:HB3	1:A:934:THR:HG21	1.32	1.11
1:A:861:TRP:NE1	1:A:897:MET:CE	2.17	1.07
1:A:406:ILE:HG23	1:A:407:PRO:HD3	1.42	1.01
1:A:957:LEU:O	1:A:961:ARG:HB2	1.64	0.97
1:A:861:TRP:CE2	1:A:897:MET:HE2	1.99	0.96
1:A:892:GLU:CB	1:A:934:THR:HG21	1.96	0.94
1:A:861:TRP:CD1	1:A:897:MET:HE1	2.06	0.89
1:A:892:GLU:HB3	1:A:934:THR:CG2	2.01	0.88
1:A:892:GLU:CG	1:A:934:THR:CG2	2.53	0.86
1:A:19:PHE:CB	1:A:66:LEU:HD21	2.07	0.84
1:A:861:TRP:CE2	1:A:897:MET:CE	2.61	0.80
1:A:898:LYS:O	1:A:902:ILE:HG13	1.82	0.80
1:A:861:TRP:HE1	1:A:897:MET:HE1	1.43	0.78
1:A:892:GLU:CB	1:A:934:THR:CG2	2.61	0.77
1:A:892:GLU:HG2	1:A:934:THR:CG2	2.16	0.76
1:A:19:PHE:HB3	1:A:66:LEU:CD2	2.13	0.76
1:A:571:GLU:OE1	1:A:572:LYS:N	2.17	0.76
1:A:892:GLU:CD	1:A:934:THR:HG22	2.07	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:LYS:O	1:A:902:ILE:CG1	2.35	0.75
1:A:861:TRP:CD1	1:A:897:MET:CE	2.70	0.73
1:A:571:GLU:CD	1:A:572:LYS:H	1.91	0.73
1:A:406:ILE:CG2	1:A:407:PRO:HD3	2.17	0.73
1:A:430:ASN:C	1:A:430:ASN:HD22	1.92	0.72
1:A:893:GLN:HG2	1:A:893:GLN:O	1.90	0.71
1:A:937:ASP:O	1:A:941:PRO:HG2	1.90	0.71
1:A:650:GLN:HG2	1:A:657:VAL:HG22	1.72	0.70
1:A:1058:LYS:HD3	1:A:1089:ALA:HB3	1.73	0.70
1:A:888:GLN:HB3	1:A:889:TYR:CE2	2.27	0.69
1:A:888:GLN:HB3	1:A:889:TYR:CD2	2.29	0.67
1:A:683:GLN:HB2	1:A:724:LEU:HD13	1.76	0.67
1:A:571:GLU:CG	1:A:572:LYS:N	2.58	0.67
1:A:892:GLU:CG	1:A:934:THR:HG22	2.26	0.66
1:A:863:MET:CE	1:A:867:PHE:CE2	2.78	0.66
1:A:747:TRP:HE1	1:A:785:CYS:HB2	1.61	0.66
1:A:571:GLU:HG2	1:A:572:LYS:N	2.10	0.66
1:A:389:MET:CE	1:A:389:MET:HA	2.26	0.65
1:A:504:SER:OG	1:A:505:ASN:N	2.31	0.63
1:A:19:PHE:HE1	1:A:34:LEU:HD12	1.62	0.63
1:A:369:PHE:O	1:A:373:GLN:HG2	1.98	0.63
1:A:336:ASP:C	1:A:336:ASP:OD2	2.37	0.63
1:A:19:PHE:CE1	1:A:34:LEU:HD12	2.34	0.61
1:A:747:TRP:CD1	1:A:781:MET:HG3	2.36	0.61
1:A:937:ASP:OD2	1:A:937:ASP:N	2.32	0.60
1:A:988:TYR:HA	1:A:991:ASN:HD22	1.66	0.60
1:A:892:GLU:HG2	1:A:934:THR:HG23	1.83	0.60
1:A:895:ALA:O	1:A:896:SER:C	2.37	0.60
1:A:191:ASP:OD2	1:A:235:LYS:HG2	2.02	0.60
1:A:898:LYS:CG	1:A:902:ILE:HD11	2.32	0.59
1:A:258:LYS:O	1:A:259:ASP:OD1	2.21	0.59
1:A:417:ILE:HG12	1:A:428:CYS:SG	2.42	0.58
1:A:902:ILE:N	1:A:903:PRO:HD2	2.18	0.58
1:A:316:ILE:O	1:A:319:THR:HB	2.03	0.58
1:A:889:TYR:N	1:A:889:TYR:CD2	2.70	0.58
1:A:492:ASP:O	1:A:496:THR:HG23	2.03	0.58
1:A:389:MET:HE1	1:A:389:MET:HA	1.85	0.58
1:A:650:GLN:CG	1:A:657:VAL:HG22	2.34	0.57
1:A:892:GLU:CG	1:A:931:ALA:HA	2.34	0.57
1:A:937:ASP:O	1:A:941:PRO:CG	2.53	0.56
1:A:892:GLU:HG2	1:A:931:ALA:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:GLU:HG2	1:A:998:THR:HG23	1.88	0.56
1:A:20:ALA:O	1:A:21:SER:HB2	2.05	0.56
1:A:389:MET:HE3	1:A:430:ASN:HB3	1.87	0.56
1:A:345:TYR:O	1:A:349:ARG:HG2	2.05	0.56
1:A:267:PHE:O	1:A:271:VAL:HG23	2.05	0.56
1:A:175:ILE:HG13	1:A:179:LEU:HD22	1.88	0.56
1:A:946:LEU:HD13	1:A:971:ILE:HG22	1.88	0.56
1:A:872:GLU:O	1:A:876:VAL:HG23	2.07	0.55
1:A:431:VAL:HG12	1:A:435:ILE:HD13	1.88	0.55
1:A:660:VAL:C	1:A:661:GLN:HG2	2.27	0.55
1:A:286:LEU:HD22	1:A:290:THR:HG22	1.90	0.54
1:A:7:GLU:HG2	1:A:8:VAL:H	1.71	0.54
1:A:898:LYS:HG3	1:A:902:ILE:CD1	2.38	0.54
1:A:893:GLN:CG	1:A:893:GLN:O	2.56	0.54
1:A:328:ALA:O	1:A:329:ALA:C	2.46	0.54
1:A:276:ASP:OD2	1:A:276:ASP:N	2.39	0.54
1:A:954:GLY:O	1:A:960:ASN:ND2	2.42	0.53
1:A:584:LEU:HD13	1:A:606:TRP:CD2	2.44	0.52
1:A:898:LYS:HG2	1:A:902:ILE:HD11	1.91	0.52
1:A:286:LEU:O	1:A:290:THR:HG23	2.11	0.51
1:A:747:TRP:CG	1:A:781:MET:HG3	2.45	0.51
1:A:897:MET:O	1:A:898:LYS:C	2.47	0.51
1:A:898:LYS:HG3	1:A:902:ILE:HD11	1.92	0.50
1:A:641:ILE:HG12	1:A:642:GLU:H	1.76	0.50
1:A:975:LEU:HD22	1:A:989:THR:HG22	1.94	0.50
1:A:640:LEU:HA	1:A:665:ILE:HG22	1.94	0.50
1:A:458:LYS:HE3	1:A:463:CYS:SG	2.52	0.49
1:A:326:ASP:OD1	1:A:382:ARG:NH1	2.45	0.49
1:A:327:ASP:O	1:A:328:ALA:HB3	2.11	0.49
1:A:892:GLU:HG2	1:A:931:ALA:CA	2.42	0.49
1:A:431:VAL:O	1:A:435:ILE:HB	2.12	0.49
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.94	0.49
1:A:261:PHE:HA	1:A:264:ILE:HD11	1.94	0.49
1:A:430:ASN:ND2	1:A:430:ASN:C	2.64	0.49
1:A:13:LEU:O	1:A:17:GLN:HG3	2.13	0.49
1:A:701:MET:HG2	1:A:746:LEU:HD22	1.94	0.48
1:A:1009:TYR:HB3	1:A:1053:VAL:HG21	1.93	0.48
1:A:571:GLU:OE1	1:A:572:LYS:CB	2.60	0.48
1:A:571:GLU:OE1	1:A:572:LYS:HB2	2.13	0.48
1:A:972:ALA:HB2	1:A:992:TRP:NE1	2.27	0.48
1:A:996:LEU:N	1:A:996:LEU:HD23	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:LEU:HD13	1:A:606:TRP:CE2	2.48	0.48
1:A:965:GLU:CG	1:A:998:THR:HG23	2.44	0.48
1:A:888:GLN:HE21	1:A:888:GLN:HB2	1.50	0.48
1:A:417:ILE:O	1:A:425:GLN:HG2	2.14	0.48
1:A:261:PHE:O	1:A:264:ILE:HD12	2.13	0.48
1:A:946:LEU:HB3	1:A:971:ILE:HG22	1.94	0.47
1:A:286:LEU:O	1:A:290:THR:CG2	2.61	0.47
1:A:258:LYS:O	1:A:259:ASP:CG	2.53	0.47
1:A:712:TYR:CD1	1:A:713:LEU:HD13	2.50	0.47
1:A:640:LEU:HD23	1:A:665:ILE:CG2	2.45	0.47
1:A:799:SER:HB2	1:A:860:ILE:HG21	1.97	0.47
1:A:206:LYS:HB3	1:A:252:LEU:HD11	1.96	0.47
1:A:1014:GLN:C	1:A:1016:ILE:H	2.18	0.47
1:A:571:GLU:CG	1:A:572:LYS:H	2.25	0.47
1:A:988:TYR:O	1:A:991:ASN:HB2	2.15	0.47
1:A:261:PHE:HA	1:A:264:ILE:CD1	2.45	0.46
1:A:279:PRO:N	1:A:280:PRO:CD	2.78	0.46
1:A:356:ALA:HA	1:A:364:LEU:HD11	1.96	0.46
1:A:638:VAL:HG23	1:A:667:ILE:HG22	1.97	0.46
1:A:326:ASP:CG	1:A:382:ARG:NH1	2.69	0.46
1:A:863:MET:CE	1:A:867:PHE:HE2	2.28	0.46
1:A:664:HIS:O	1:A:665:ILE:HG23	2.15	0.46
1:A:1003:GLU:CD	1:A:1003:GLU:H	2.19	0.46
1:A:937:ASP:O	1:A:941:PRO:CD	2.65	0.46
1:A:901:PHE:CD2	1:A:901:PHE:C	2.89	0.45
1:A:1058:LYS:CD	1:A:1089:ALA:HB3	2.42	0.45
1:A:657:VAL:HG12	1:A:666:ALA:HA	1.98	0.45
1:A:747:TRP:NE1	1:A:785:CYS:HB2	2.29	0.45
1:A:93:HIS:O	1:A:93:HIS:CG	2.70	0.45
1:A:326:ASP:CG	1:A:382:ARG:HH11	2.20	0.45
1:A:1080:ILE:HD12	1:A:1080:ILE:O	2.17	0.45
1:A:130:VAL:HG12	1:A:168:TYR:HE2	1.82	0.45
1:A:1028:ASN:O	1:A:1032:VAL:HG23	2.17	0.45
1:A:861:TRP:N	1:A:862:PRO:HD2	2.32	0.45
1:A:898:LYS:O	1:A:902:ILE:CD1	2.65	0.44
1:A:1037:ILE:HD12	1:A:1084:VAL:HG22	1.99	0.44
1:A:38:TRP:CE3	1:A:43:ASN:HB3	2.52	0.44
1:A:119:ARG:HD2	1:A:154:ASN:OD1	2.17	0.44
1:A:895:ALA:C	1:A:897:MET:N	2.68	0.44
1:A:829:PHE:N	1:A:829:PHE:CD2	2.86	0.44
1:A:898:LYS:O	1:A:902:ILE:HD11	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ILE:HD12	1:A:458:LYS:HG2	2.00	0.44
1:A:700:VAL:HG12	1:A:728:LEU:HD11	2.00	0.43
1:A:406:ILE:HG23	1:A:407:PRO:CD	2.30	0.43
1:A:902:ILE:HG13	1:A:902:ILE:H	1.34	0.43
1:A:946:LEU:CD1	1:A:971:ILE:HG22	2.48	0.43
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.83	0.43
1:A:971:ILE:HD11	1:A:992:TRP:HB2	2.00	0.43
1:A:892:GLU:OE1	1:A:933:SER:N	2.50	0.43
1:A:685:TYR:O	1:A:689:LEU:HB2	2.18	0.43
1:A:863:MET:HE1	1:A:867:PHE:HE2	1.82	0.43
1:A:503:GLN:O	1:A:504:SER:O	2.36	0.43
1:A:706:LEU:HA	1:A:706:LEU:HD12	1.91	0.43
1:A:250:VAL:O	1:A:254:PRO:HD3	2.17	0.43
1:A:690:ARG:HE	1:A:690:ARG:HB2	1.25	0.43
1:A:641:ILE:HG12	1:A:642:GLU:N	2.34	0.43
1:A:349:ARG:H	1:A:349:ARG:HG2	1.53	0.42
1:A:894:THR:O	1:A:895:ALA:C	2.57	0.42
1:A:435:ILE:HG23	1:A:443:ILE:CD1	2.49	0.42
1:A:895:ALA:O	1:A:897:MET:N	2.52	0.42
1:A:863:MET:HE1	1:A:867:PHE:CE2	2.53	0.42
1:A:213:TRP:C	1:A:215:LYS:H	2.22	0.42
1:A:350:GLN:HE21	1:A:350:GLN:HB2	1.67	0.42
1:A:725:ILE:HB	1:A:726:PRO:HD3	2.02	0.41
1:A:243:PHE:CE2	1:A:285:ALA:HB2	2.55	0.41
1:A:918:GLN:HB2	1:A:963:SER:HA	2.02	0.41
1:A:461:SER:HA	1:A:468:GLN:NE2	2.36	0.41
1:A:170:ILE:HG23	1:A:178:ILE:HG12	2.03	0.41
1:A:326:ASP:HA	1:A:382:ARG:NH1	2.36	0.41
1:A:203:GLY:HA2	1:A:206:LYS:HG2	2.03	0.41
1:A:880:LEU:O	1:A:923:ILE:HD11	2.21	0.41
1:A:269:ASP:OD1	1:A:309:THR:HG23	2.20	0.41
1:A:745:LEU:HD12	1:A:745:LEU:HA	1.89	0.41
1:A:503:GLN:O	1:A:504:SER:C	2.58	0.41
1:A:369:PHE:CE2	1:A:402:LEU:HD21	2.55	0.41
1:A:114:ARG:HA	1:A:114:ARG:HD2	1.77	0.41
1:A:323:ILE:HG13	1:A:323:ILE:O	2.21	0.40
1:A:507:LEU:HA	1:A:507:LEU:HD23	1.87	0.40
1:A:107:LEU:HA	1:A:107:LEU:HD12	1.95	0.40
1:A:309:THR:O	1:A:313:VAL:HB	2.22	0.40
1:A:12:LEU:HB3	1:A:50:PHE:CE2	2.57	0.40
1:A:889:TYR:HD2	1:A:889:TYR:N	2.20	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	999/1078 (93%)	958 (96%)	38 (4%)	3 (0%)	46	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	504	SER
1	A	994	LYS

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	844/937 (90%)	733 (87%)	111 (13%)	5	14

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	66	LEU
1	A	74	LEU
1	A	92	THR
1	A	97	GLU

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Mol	Chain	Res	Type
1	A	106	LEU
1	A	113	GLU
1	A	114	ARG
1	A	133	ASP
1	A	134	LEU
1	A	141	LEU
1	A	150	SER
1	A	168	TYR
1	A	179	LEU
1	A	187	THR
1	A	206	LYS
1	A	207	GLN
1	A	219	LEU
1	A	221	PRO
1	A	235	LYS
1	A	239	LEU
1	A	261	PHE
1	A	262	ASP
1	A	263	GLN
1	A	264	ILE
1	A	270	MET
1	A	276	ASP
1	A	277	LEU
1	A	278	GLU
1	A	286	LEU
1	A	288	LEU
1	A	290	THR
1	A	291	VAL
1	A	298	GLN
1	A	308	GLN
1	A	313	VAL
1	A	319	THR
1	A	326	ASP
1	A	349	ARG
1	A	352	LEU
1	A	364	LEU
1	A	368	LEU
1	A	391	LEU
1	A	405	GLU
1	A	417	ILE
1	A	423	ARG
1	A	430	ASN

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Mol	Chain	Res	Type
1	A	431	VAL
1	A	435	ILE
1	A	446	THR
1	A	483	SER
1	A	488	GLU
1	A	507	LEU
1	A	534	THR
1	A	535	LEU
1	A	538	LEU
1	A	539	LEU
1	A	550	ASN
1	A	553	LEU
1	A	571	GLU
1	A	580	LEU
1	A	587	LEU
1	A	591	ASP
1	A	638	VAL
1	A	641	ILE
1	A	644	GLU
1	A	649	PHE
1	A	661	GLN
1	A	665	ILE
1	A	672	LEU
1	A	689	LEU
1	A	695	VAL
1	A	706	LEU
1	A	713	LEU
1	A	724	LEU
1	A	726	PRO
1	A	729	LEU
1	A	730	SER
1	A	733	LEU
1	A	759	MET
1	A	784	ASN
1	A	789	ASP
1	A	811	ASP
1	A	834	LEU
1	A	839	ASN
1	A	850	ASN
1	A	857	LEU
1	A	861	TRP
1	A	868	LEU

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Mol	Chain	Res	Type
1	A	869	LEU
1	A	888	GLN
1	A	889	TYR
1	A	893	GLN
1	A	894	THR
1	A	896	SER
1	A	902	ILE
1	A	921	SER
1	A	926	VAL
1	A	934	THR
1	A	937	ASP
1	A	938	VAL
1	A	955	SER
1	A	960	ASN
1	A	971	ILE
1	A	989	THR
1	A	1029	ILE
1	A	1045	LEU
1	A	1056	SER
1	A	1079	ASP
1	A	1080	ILE
1	A	1085	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	207	GLN
1	A	303	ASN
1	A	350	GLN
1	A	374	GLN
1	A	430	ASN
1	A	477	ASN
1	A	541	ASN
1	A	550	ASN
1	A	661	GLN
1	A	692	GLN
1	A	839	ASN
1	A	850	ASN
1	A	856	ASN
1	A	888	GLN
1	A	893	GLN

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Mol	Chain	Res	Type
1	A	960	ASN
1	A	966	ASN
1	A	991	ASN

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	1025/1078 (95%)	-0.21	29 (2%)	56	50	44, 80, 124, 174	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	ILE	6.1
1	A	664	HIS	4.3
1	A	428	CYS	3.6
1	A	340	GLU	3.3
1	A	9	ASN	3.0
1	A	26	ILE	3.0
1	A	1060	LEU	3.0
1	A	591	ASP	2.9
1	A	392	SER	2.9
1	A	595	ASP	2.8
1	A	431	VAL	2.8
1	A	339	ASP	2.7
1	A	642	GLU	2.6
1	A	910	ILE	2.5
1	A	811	ASP	2.4
1	A	427	GLY	2.3
1	A	1017	GLU	2.3
1	A	1044	SER	2.3
1	A	640	LEU	2.3
1	A	429	CYS	2.3
1	A	390	ALA	2.2
1	A	10	ARG	2.2
1	A	645	GLU	2.2
1	A	373	GLN	2.2
1	A	812	ARG	2.1
1	A	8	VAL	2.0
1	A	5	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	644	GLU	2.0
1	A	662	GLY	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.