



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 12:04 pm GMT

PDB ID : 3W3W
Title : Crystal structure of Kap121p bound to Ste12p
Authors : Kobayashi, J.; Matsuura, Y.
Deposited on : 2012-12-28
Resolution : 2.20 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 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 : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

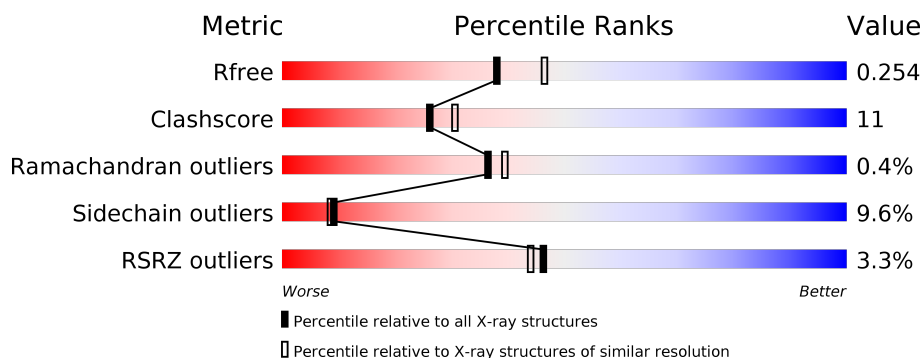
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1078	
2	B	69	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8039 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
1	A	1028	Total	C	N	O	S	0	0	0
			7850	5042	1263	1508	37			

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 Protein STE12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	0
			88	57	16	15			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total	O	0	0
			99	99		
3	B	2	Total	O	0	0
			2	2		

SER
ALA
HIS
PRO
ASP
LYS
ASN
LYS
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.57Å 126.16Å 130.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.18 – 2.20 39.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (39.18-2.20) 95.5 (39.18-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.215 , 0.256 0.216 , 0.254	Depositor DCC
R_{free} test set	3185 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8039	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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

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	0.78	2/7986 (0.0%)	0.91	11/10880 (0.1%)
2	B	0.87	0/89	1.01	0/119
All	All	0.79	2/8075 (0.0%)	0.91	11/10999 (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
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	CYS	CB-SG	-5.30	1.73	1.81
1	A	400	ASP	CB-CG	5.16	1.62	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	ASP	CB-CG-OD2	7.96	125.46	118.30
1	A	364	LEU	CB-CG-CD1	-7.61	98.06	111.00
1	A	936	ALA	N-CA-C	6.60	128.81	111.00
1	A	237	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	979	ASN	N-CA-C	5.79	126.62	111.00
1	A	724	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	74	LEU	CB-CG-CD1	5.56	120.45	111.00
1	A	256	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	260	MET	CG-SD-CE	5.23	108.57	100.20
1	A	431	VAL	CB-CA-C	-5.14	101.63	111.40
1	A	76	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	616	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	7850	0	7758	172	0
2	B	88	0	96	7	0
3	A	99	0	0	7	0
3	B	2	0	0	2	0
All	All	8039	0	7854	177	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 (177) 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:892:GLU:HB3	1:A:934:THR:HG21	1.37	1.06
1:A:406:ILE:HG23	1:A:407:PRO:HD3	1.09	1.03
1:A:902:ILE:N	1:A:903:PRO:HD2	1.73	1.02
1:A:406:ILE:CG2	1:A:407:PRO:HD3	1.97	0.95
1:A:638:VAL:HG23	1:A:665:ILE:CG2	1.99	0.92
1:A:534:THR:O	1:A:538:LEU:HD13	1.71	0.90
1:A:892:GLU:CG	1:A:934:THR:CG2	2.50	0.90
1:A:892:GLU:CD	1:A:934:THR:HG22	1.92	0.89
1:A:892:GLU:CB	1:A:934:THR:HG21	2.04	0.88
1:A:406:ILE:HG23	1:A:407:PRO:CD	2.01	0.87
1:A:894:THR:O	1:A:897:MET:HG3	1.75	0.86
1:A:965:GLU:HG2	1:A:998:THR:HG23	1.58	0.85
1:A:414:ILE:O	1:A:417:ILE:HG22	1.77	0.84
1:A:892:GLU:HG2	1:A:934:THR:CG2	2.07	0.84
1:A:988:TYR:HA	1:A:991:ASN:HD22	1.43	0.81
1:A:641:ILE:HG23	1:A:664:HIS:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:ILE:N	1:A:903:PRO:CD	2.47	0.78
1:A:987:THR:HG22	1:A:988:TYR:N	1.98	0.78
1:A:892:GLU:HB3	1:A:934:THR:CG2	2.12	0.78
1:A:987:THR:HG23	1:A:991:ASN:HD21	1.49	0.78
1:A:861:TRP:HE1	1:A:897:MET:HE1	1.47	0.77
1:A:638:VAL:CG2	1:A:665:ILE:CG2	2.64	0.75
1:A:902:ILE:HG21	1:A:938:VAL:HG11	1.67	0.75
1:A:892:GLU:CG	1:A:934:THR:HG22	2.16	0.75
1:A:898:LYS:HG3	1:A:902:ILE:HD11	1.68	0.74
1:A:638:VAL:HG23	1:A:665:ILE:HG22	1.69	0.74
3:A:1102:HOH:O	2:B:611:LYS:HE2	1.87	0.74
1:A:837:GLU:HG2	3:A:1174:HOH:O	1.89	0.73
1:A:861:TRP:HE1	1:A:897:MET:CE	2.02	0.73
1:A:369:PHE:O	1:A:373:GLN:HG2	1.89	0.72
1:A:987:THR:HG23	1:A:991:ASN:ND2	2.05	0.71
1:A:1009:TYR:HB3	1:A:1053:VAL:HG21	1.71	0.71
1:A:641:ILE:HG22	1:A:664:HIS:O	1.91	0.70
1:A:892:GLU:CB	1:A:934:THR:CG2	2.70	0.70
1:A:131:GLN:HB3	1:A:134:LEU:HB2	1.72	0.70
1:A:937:ASP:O	1:A:941:PRO:HG2	1.93	0.69
1:A:975:LEU:HD22	1:A:989:THR:HG22	1.73	0.69
1:A:650:GLN:HG2	1:A:657:VAL:HG22	1.75	0.68
1:A:1066:SER:O	1:A:1070:MET:HG2	1.95	0.67
2:B:613:LEU:HD13	3:B:701:HOH:O	1.94	0.66
1:A:987:THR:CG2	1:A:991:ASN:HD21	2.08	0.66
1:A:20:ALA:O	1:A:21:SER:HB2	1.96	0.66
2:B:615:ILE:HG22	2:B:615:ILE:O	1.97	0.65
1:A:987:THR:CG2	1:A:988:TYR:N	2.58	0.65
1:A:898:LYS:O	1:A:902:ILE:HG12	1.98	0.64
1:A:345:TYR:CZ	1:A:349:ARG:HD2	2.32	0.63
2:B:616:LYS:O	2:B:617:THR:HG23	1.97	0.63
1:A:167:PRO:HG3	1:A:207:GLN:HG2	1.81	0.63
1:A:901:PHE:C	1:A:903:PRO:HD2	2.18	0.62
1:A:715:ASP:HB2	1:A:766:ILE:HD11	1.82	0.62
1:A:898:LYS:O	1:A:902:ILE:CG1	2.47	0.62
1:A:492:ASP:O	1:A:496:THR:HG23	1.98	0.61
1:A:971:ILE:HD11	1:A:992:TRP:HB2	1.82	0.61
1:A:695:VAL:O	1:A:695:VAL:HG22	2.00	0.60
1:A:712:TYR:CD1	1:A:713:LEU:HD13	2.36	0.60
1:A:16:VAL:HG23	1:A:66:LEU:HD12	1.84	0.59
1:A:366:ALA:HB3	1:A:367:PRO:CD	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:TRP:NE1	1:A:897:MET:CE	2.66	0.58
1:A:417:ILE:HG13	1:A:458:LYS:HD3	1.86	0.58
1:A:626:PRO:HB2	1:A:627:PRO:HD3	1.86	0.57
1:A:892:GLU:HG2	1:A:934:THR:HG23	1.82	0.57
1:A:144:LEU:HD21	1:A:162:ILE:HD12	1.87	0.57
1:A:1080:ILE:HD12	1:A:1080:ILE:O	2.05	0.56
1:A:893:GLN:CG	1:A:893:GLN:O	2.53	0.56
1:A:20:ALA:O	1:A:21:SER:CB	2.54	0.56
1:A:372:LEU:O	1:A:376:ILE:HG12	2.06	0.56
1:A:1037:ILE:HD12	1:A:1084:VAL:HG22	1.88	0.56
1:A:945:THR:O	1:A:949:ILE:HG13	2.06	0.56
1:A:264:ILE:HD11	1:A:288:LEU:CD1	2.36	0.56
1:A:650:GLN:CG	1:A:657:VAL:HG22	2.34	0.56
1:A:638:VAL:CG2	1:A:665:ILE:HG23	2.36	0.56
1:A:892:GLU:OE1	1:A:933:SER:OG	2.16	0.55
1:A:362:GLU:HB2	3:A:1194:HOH:O	2.07	0.55
1:A:914:ALA:O	1:A:963:SER:OG	2.21	0.55
1:A:972:ALA:HB2	1:A:992:TRP:NE1	2.21	0.55
1:A:191:ASP:OD2	1:A:235:LYS:HG2	2.07	0.55
1:A:857:LEU:HD12	1:A:857:LEU:O	2.06	0.55
1:A:1028:ASN:O	1:A:1032:VAL:HG23	2.07	0.55
1:A:76:LEU:O	1:A:79:PRO:HB3	2.07	0.54
1:A:388:MET:SD	1:A:413:VAL:HG22	2.47	0.54
1:A:408:LYS:HB2	3:A:1144:HOH:O	2.08	0.54
1:A:328:ALA:O	1:A:329:ALA:C	2.43	0.53
1:A:417:ILE:O	1:A:425:GLN:HG2	2.07	0.53
1:A:13:LEU:O	1:A:17:GLN:HG3	2.09	0.53
1:A:362:GLU:HB2	3:A:1110:HOH:O	2.08	0.53
1:A:515:THR:HG21	2:B:607:ALA:HB3	1.91	0.52
1:A:322:SER:O	1:A:382:ARG:NH2	2.42	0.52
1:A:327:ASP:O	1:A:328:ALA:HB3	2.09	0.52
1:A:747:TRP:HE1	1:A:785:CYS:HB2	1.75	0.52
1:A:366:ALA:HB3	1:A:367:PRO:HD3	1.91	0.52
1:A:987:THR:HG22	1:A:988:TYR:H	1.75	0.52
1:A:911:SER:O	1:A:917:ARG:HD3	2.11	0.51
1:A:1003:GLU:CD	1:A:1003:GLU:H	2.13	0.51
1:A:747:TRP:CG	1:A:781:MET:HG3	2.46	0.50
1:A:934:THR:O	1:A:934:THR:OG1	2.29	0.50
1:A:7:GLU:HG2	1:A:8:VAL:H	1.77	0.50
1:A:861:TRP:N	1:A:862:PRO:HD2	2.27	0.50
1:A:908:CYS:HB3	1:A:916:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:O	1:A:264:ILE:HG13	2.11	0.49
1:A:906:THR:HA	1:A:909:LEU:HD12	1.94	0.49
1:A:112:SER:O	1:A:119:ARG:NH2	2.45	0.49
1:A:987:THR:CG2	1:A:991:ASN:ND2	2.72	0.49
1:A:996:LEU:N	1:A:996:LEU:HD23	2.27	0.49
1:A:893:GLN:HG2	1:A:893:GLN:O	2.13	0.48
1:A:939:CYS:HB3	1:A:974:ILE:HG12	1.95	0.48
1:A:809:MET:C	1:A:811:ASP:H	2.16	0.48
1:A:170:ILE:HG23	1:A:178:ILE:HG12	1.96	0.48
1:A:898:LYS:NZ	1:A:937:ASP:OD1	2.43	0.48
2:B:613:LEU:CD1	3:B:701:HOH:O	2.56	0.47
1:A:39:ILE:HG22	1:A:39:ILE:O	2.14	0.47
1:A:933:SER:C	1:A:935:TYR:H	2.18	0.47
1:A:375:MET:CE	1:A:386:ALA:HB3	2.44	0.47
1:A:436:SER:HB3	1:A:478:PHE:HA	1.97	0.47
1:A:1076:TYR:CG	1:A:1080:ILE:HD11	2.51	0.46
1:A:413:VAL:HG13	1:A:428:CYS:SG	2.55	0.46
1:A:326:ASP:OD1	1:A:382:ARG:NH1	2.47	0.46
1:A:175:ILE:HG13	1:A:179:LEU:HD22	1.97	0.46
1:A:52:ALA:HB1	1:A:106:LEU:HD13	1.97	0.46
1:A:641:ILE:CG2	1:A:664:HIS:HB3	2.40	0.46
1:A:695:VAL:CG2	1:A:695:VAL:O	2.62	0.46
1:A:771:HIS:O	1:A:775:VAL:HG23	2.16	0.46
1:A:175:ILE:HA	1:A:178:ILE:HG22	1.98	0.46
1:A:692:GLN:HG2	1:A:692:GLN:H	1.55	0.46
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.96	0.46
1:A:130:VAL:HG11	1:A:169:LEU:HD21	1.98	0.46
1:A:417:ILE:CG1	1:A:458:LYS:HD3	2.46	0.45
1:A:898:LYS:NZ	1:A:937:ASP:OD2	2.49	0.45
1:A:264:ILE:HD11	1:A:288:LEU:HD11	1.99	0.45
1:A:375:MET:HE1	1:A:386:ALA:HB3	1.98	0.45
1:A:888:GLN:HE21	1:A:888:GLN:HB2	1.61	0.45
1:A:898:LYS:HG3	1:A:902:ILE:CD1	2.42	0.45
1:A:66:LEU:CD1	1:A:70:LEU:HD12	2.47	0.45
1:A:641:ILE:HG22	1:A:664:HIS:C	2.37	0.45
1:A:799:SER:HB2	1:A:860:ILE:CG2	2.47	0.44
1:A:1061:LEU:HD21	1:A:1072:ILE:HD12	1.98	0.44
1:A:714:HIS:CE1	3:A:1123:HOH:O	2.71	0.44
1:A:863:MET:CE	1:A:867:PHE:HE2	2.31	0.43
1:A:775:VAL:HG22	1:A:841:SER:HA	2.00	0.43
1:A:406:ILE:CG2	1:A:407:PRO:CD	2.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:MET:O	1:A:898:LYS:C	2.57	0.43
1:A:861:TRP:NE1	1:A:897:MET:HE2	2.33	0.43
1:A:902:ILE:H	1:A:903:PRO:HD2	1.72	0.43
1:A:13:LEU:HG	1:A:17:GLN:OE1	2.18	0.43
1:A:898:LYS:O	1:A:902:ILE:HG13	2.16	0.43
1:A:317:MET:HB2	1:A:348:ALA:HB2	2.01	0.43
1:A:38:TRP:CE3	1:A:43:ASN:HB3	2.54	0.43
1:A:608:ARG:NH2	3:A:1178:HOH:O	2.52	0.42
1:A:66:LEU:C	1:A:66:LEU:HD13	2.38	0.42
1:A:417:ILE:HD11	1:A:458:LYS:HG2	2.01	0.42
1:A:851:GLY:O	1:A:853:TYR:N	2.52	0.42
1:A:1073:PHE:HA	1:A:1076:TYR:CD2	2.54	0.42
1:A:747:TRP:CD1	1:A:781:MET:HG3	2.54	0.42
1:A:946:LEU:HD13	1:A:971:ILE:HG22	2.02	0.42
1:A:872:GLU:O	1:A:876:VAL:HG23	2.20	0.41
1:A:897:MET:HG3	1:A:897:MET:H	1.65	0.41
1:A:452:LEU:HB2	1:A:453:PRO:HD3	2.01	0.41
1:A:131:GLN:CB	1:A:134:LEU:HD22	2.51	0.41
1:A:66:LEU:HD13	1:A:66:LEU:O	2.21	0.41
1:A:544:LYS:HE2	1:A:579:GLU:OE2	2.19	0.41
1:A:221:PRO:HB3	1:A:260:MET:SD	2.60	0.41
1:A:979:ASN:H	1:A:979:ASN:ND2	2.19	0.41
1:A:1011:PHE:HA	1:A:1014:GLN:HG3	2.03	0.41
1:A:19:PHE:CZ	1:A:34:LEU:HD23	2.56	0.41
1:A:78:ALA:HB3	1:A:79:PRO:CA	2.50	0.41
1:A:946:LEU:CD1	1:A:971:ILE:HG22	2.50	0.41
1:A:988:TYR:O	1:A:991:ASN:HB2	2.21	0.41
1:A:798:VAL:O	1:A:802:LEU:HG	2.21	0.41
1:A:799:SER:HB2	1:A:860:ILE:HG21	2.03	0.41
1:A:323:ILE:O	1:A:324:ASP:HB2	2.21	0.40
1:A:315:LEU:O	1:A:319:THR:HG23	2.20	0.40
1:A:470:HIS:NE2	2:B:609:ILE:HD12	2.36	0.40
1:A:581:ILE:O	1:A:585:VAL:HG23	2.21	0.40
1:A:78:ALA:N	1:A:79:PRO:HA	2.35	0.40
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.91	0.40
1:A:141:LEU:HA	1:A:141:LEU:HD12	1.69	0.40
1:A:310:LEU:C	1:A:310:LEU:HD13	2.42	0.40
1:A:701:MET:HG3	1:A:706:LEU:HD22	2.04	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	1002/1078 (93%)	953 (95%)	45 (4%)	4 (0%)	36	39
2	B	10/69 (14%)	8 (80%)	2 (20%)	0	100	100
All	All	1012/1147 (88%)	961 (95%)	47 (5%)	4 (0%)	36	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	852	HIS
1	A	8	VAL
1	A	695	VAL
1	A	1065	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	845/937 (90%)	764 (90%)	81 (10%)	9	8
2	B	10/59 (17%)	9 (90%)	1 (10%)	8	7
All	All	855/996 (86%)	773 (90%)	82 (10%)	9	8

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	31	GLU

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Mol	Chain	Res	Type
1	A	62	THR
1	A	74	LEU
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	219	LEU
1	A	236	ASP
1	A	239	LEU
1	A	266	GLN
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	405	GLU
1	A	417	ILE
1	A	431	VAL
1	A	449	ASP
1	A	488	GLU
1	A	535	LEU
1	A	539	LEU
1	A	545	VAL
1	A	551	SER
1	A	553	LEU
1	A	587	LEU
1	A	613	LEU
1	A	642	GLU
1	A	649	PHE
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

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Mol	Chain	Res	Type
1	A	730	SER
1	A	733	LEU
1	A	744	VAL
1	A	759	MET
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	868	LEU
1	A	869	LEU
1	A	888	GLN
1	A	893	GLN
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	926	VAL
1	A	934	THR
1	A	945	THR
1	A	955	SER
1	A	959	GLU
1	A	960	ASN
1	A	971	ILE
1	A	979	ASN
1	A	987	THR
1	A	989	THR
1	A	996	LEU
1	A	1014	GLN
1	A	1029	ILE
1	A	1045	LEU
1	A	1056	SER
1	A	1066	SER
1	A	1080	ILE
2	B	613	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	303	ASN
1	A	430	ASN
1	A	541	ASN
1	A	856	ASN
1	A	888	GLN
1	A	893	GLN
1	A	979	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

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	1028/1078 (95%)	-0.00	34 (3%) 46 44	23, 48, 93, 131	0
2	B	12/69 (17%)	-0.39	0 100 100	27, 42, 66, 82	0
All	All	1040/1147 (90%)	-0.01	34 (3%) 46 44	23, 47, 93, 131	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	980	SER	8.5
1	A	638	VAL	5.2
1	A	666	ALA	4.7
1	A	26	ILE	4.5
1	A	660	VAL	4.2
1	A	1073	PHE	3.9
1	A	1025	ALA	3.8
1	A	640	LEU	3.7
1	A	1060	LEU	3.7
1	A	662	GLY	3.5
1	A	132	ASP	3.5
1	A	661	GLN	3.5
1	A	639	GLY	3.5
1	A	1023	VAL	3.4
1	A	990	ALA	3.4
1	A	987	THR	3.3
1	A	652	TYR	3.1
1	A	25	GLN	3.0
1	A	1061	LEU	2.8
1	A	665	ILE	2.8
1	A	979	ASN	2.8
1	A	658	VAL	2.7
1	A	1029	ILE	2.6
1	A	895	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1027	SER	2.5
1	A	981	ASN	2.4
1	A	1066	SER	2.3
1	A	933	SER	2.3
1	A	1011	PHE	2.2
1	A	951	ASP	2.2
1	A	894	THR	2.1
1	A	1057	VAL	2.1
1	A	641	ILE	2.0
1	A	982	ILE	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.