Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 05:25 PM EDT

PDB ID	:	3W3U
Title	:	Crystal structure of Kap121p mutant R349A/Q350A/D353A/E396A/N430K /D438A/N477A
Authors	:	Kobayashi, J.; Matsuura, Y.
Deposited on	:	2012-12-28
Resolution	:	2.60 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:

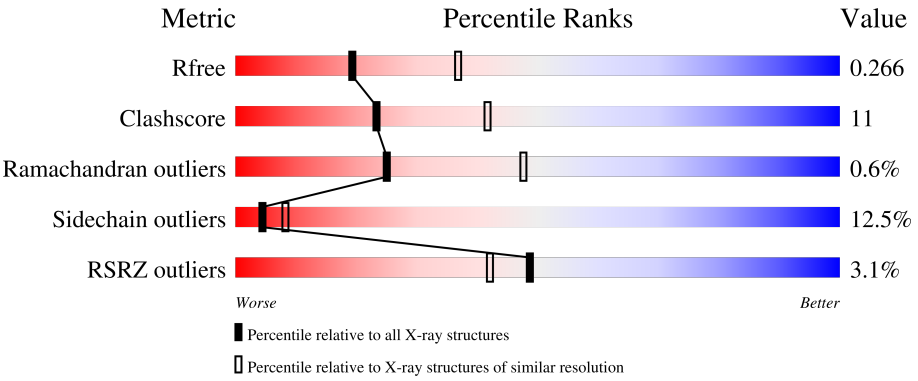
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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% 70% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7849 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	1030	7849	5043	1260	1510	36	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

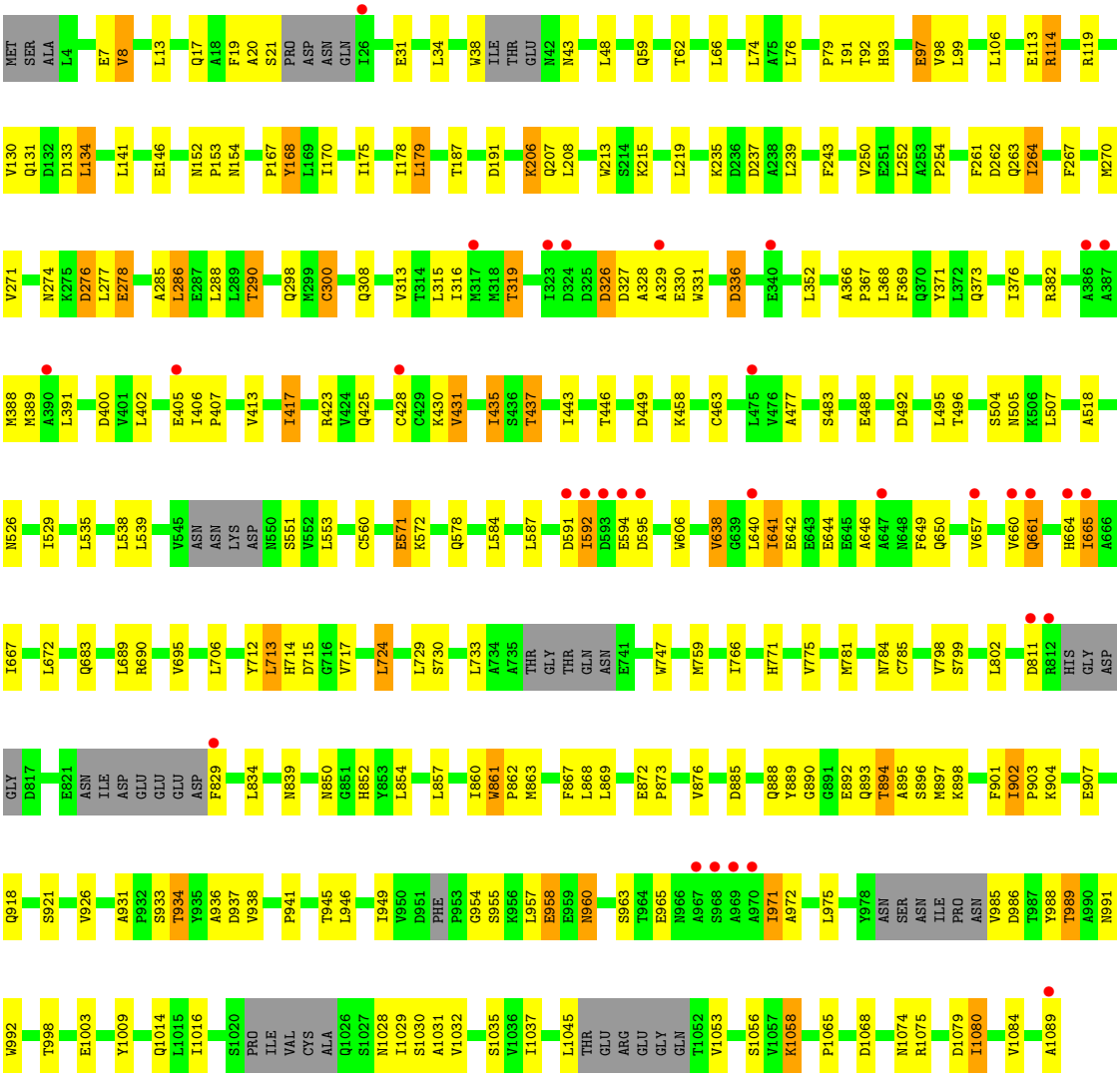
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P32337
A	?	-	SER	deletion	UNP P32337
A	?	-	SER	deletion	UNP P32337
A	?	-	LYS	deletion	UNP P32337
A	?	-	LEU	deletion	UNP P32337
A	?	-	MET	deletion	UNP P32337
A	?	-	ILE	deletion	UNP P32337
A	?	-	MET	deletion	UNP P32337
A	?	-	SER	deletion	UNP P32337
A	?	-	LYS	deletion	UNP P32337
A	?	-	ASN	deletion	UNP P32337
A	349	ALA	ARG	engineered mutation	UNP P32337
A	350	ALA	GLN	engineered mutation	UNP P32337
A	353	ALA	ASP	engineered mutation	UNP P32337
A	396	ALA	GLU	engineered mutation	UNP P32337
A	430	LYS	ASN	engineered mutation	UNP P32337
A	438	ALA	ASP	engineered mutation	UNP P32337
A	477	ALA	ASN	engineered mutation	UNP P32337

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-3

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.38Å 124.20Å 85.03Å 90.00° 116.73° 90.00°	Depositor
Resolution (Å)	26.54 – 2.60 26.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (26.54-2.60) 97.7 (26.53-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.222 , 0.267 0.221 , 0.266	Depositor DCC
R_{free} test set	2165 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	65.7	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7849	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.66	0/7988	0.86	8/10884 (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	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	300	CYS	N-CA-CB	-13.87	85.64	110.60
1	A	1075	ARG	N-CA-CB	-9.18	94.08	110.60
1	A	646	ALA	N-CA-C	6.99	129.86	111.00
1	A	646	ALA	CB-CA-C	-6.89	99.77	110.10
1	A	936	ALA	N-CA-CB	-6.76	100.63	110.10
1	A	76	LEU	CA-CB-CG	5.60	128.17	115.30
1	A	330	GLU	C-N-CA	-5.21	108.69	121.70
1	A	400	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	7849	0	7756	177	0
All	All	7849	0	7756	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:898:LYS:NZ	1:A:937:ASP:OD2	1.83	1.10
1:A:1058:LYS:HD3	1:A:1089:ALA:HB3	1.34	1.05
1:A:406:ILE:HG23	1:A:407:PRO:HD3	1.40	1.04
1:A:892:GLU:HG2	1:A:934:THR:CG2	1.90	1.00
1:A:890:GLY:O	1:A:893:GLN:HB3	1.63	0.97
1:A:898:LYS:NZ	1:A:937:ASP:CG	2.19	0.95
1:A:898:LYS:NZ	1:A:937:ASP:OD1	2.03	0.91
1:A:898:LYS:HZ3	1:A:937:ASP:CG	1.75	0.90
1:A:650:GLN:HG2	1:A:657:VAL:HG22	1.53	0.89
1:A:898:LYS:O	1:A:902:ILE:HG13	1.79	0.82
1:A:571:GLU:CD	1:A:572:LYS:H	1.83	0.82
1:A:571:GLU:HG2	1:A:572:LYS:N	1.95	0.81
1:A:571:GLU:OE1	1:A:572:LYS:N	2.12	0.81
1:A:571:GLU:CG	1:A:572:LYS:N	2.46	0.78
1:A:898:LYS:CG	1:A:902:ILE:HD11	2.14	0.78
1:A:898:LYS:HG3	1:A:902:ILE:HD11	1.66	0.77
1:A:406:ILE:CG2	1:A:407:PRO:HD3	2.15	0.75
1:A:191:ASP:OD2	1:A:235:LYS:HG2	1.87	0.75
1:A:888:GLN:HB3	1:A:889:TYR:CD2	2.22	0.74
1:A:892:GLU:HG2	1:A:934:THR:HG22	1.71	0.70
1:A:898:LYS:O	1:A:902:ILE:CG1	2.39	0.70
1:A:571:GLU:OE1	1:A:572:LYS:HB2	1.92	0.69
1:A:872:GLU:OE1	1:A:873:PRO:HD2	1.92	0.69
1:A:592:ILE:HG23	1:A:594:GLU:O	1.93	0.68
1:A:893:GLN:CG	1:A:893:GLN:O	2.42	0.67
1:A:985:VAL:HG23	1:A:986:ASP:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:MET:HA	1:A:389:MET:CE	2.25	0.67
1:A:892:GLU:CG	1:A:934:THR:CG2	2.72	0.66
1:A:683:GLN:HB2	1:A:724:LEU:HD13	1.76	0.65
1:A:902:ILE:N	1:A:903:PRO:HD2	2.11	0.65
1:A:504:SER:OG	1:A:505:ASN:N	2.30	0.65
1:A:892:GLU:CB	1:A:934:THR:HG21	2.27	0.65
1:A:898:LYS:HG3	1:A:902:ILE:CD1	2.27	0.64
1:A:492:ASP:O	1:A:496:THR:HG23	1.98	0.63
1:A:747:TRP:HE1	1:A:785:CYS:HB2	1.64	0.62
1:A:1009:TYR:HB3	1:A:1053:VAL:HG21	1.81	0.62
1:A:369:PHE:O	1:A:373:GLN:HG2	1.99	0.62
1:A:965:GLU:HG2	1:A:998:THR:HG23	1.82	0.62
1:A:286:LEU:O	1:A:290:THR:HG23	2.00	0.61
1:A:20:ALA:O	1:A:21:SER:HB2	2.01	0.60
1:A:640:LEU:HA	1:A:665:ILE:HG22	1.81	0.60
1:A:650:GLN:CG	1:A:657:VAL:HG22	2.30	0.60
1:A:571:GLU:OE1	1:A:572:LYS:CB	2.50	0.59
1:A:316:ILE:O	1:A:319:THR:HB	2.02	0.59
1:A:437:THR:HG22	1:A:477:ALA:HB1	1.83	0.59
1:A:571:GLU:CG	1:A:572:LYS:H	2.15	0.59
1:A:946:LEU:HB3	1:A:971:ILE:HG22	1.84	0.59
1:A:861:TRP:NE1	1:A:897:MET:CE	2.66	0.58
1:A:388:MET:SD	1:A:413:VAL:HG22	2.44	0.58
1:A:19:PHE:CE1	1:A:34:LEU:HD12	2.39	0.58
1:A:888:GLN:HB3	1:A:889:TYR:CE2	2.39	0.58
1:A:946:LEU:HD13	1:A:971:ILE:HG22	1.86	0.58
1:A:975:LEU:HD22	1:A:989:THR:HG22	1.85	0.58
1:A:988:TYR:HA	1:A:991:ASN:HD22	1.69	0.58
1:A:872:GLU:O	1:A:876:VAL:HG23	2.04	0.57
1:A:431:VAL:HG12	1:A:435:ILE:HD13	1.86	0.57
1:A:892:GLU:HG2	1:A:934:THR:HG23	1.84	0.57
1:A:937:ASP:O	1:A:941:PRO:HG2	2.05	0.57
1:A:13:LEU:O	1:A:17:GLN:HG3	2.04	0.57
1:A:640:LEU:HD23	1:A:665:ILE:CG2	2.34	0.56
1:A:892:GLU:HB3	1:A:934:THR:HG21	1.86	0.56
1:A:660:VAL:C	1:A:661:GLN:HG2	2.25	0.56
1:A:1058:LYS:HD3	1:A:1089:ALA:CB	2.22	0.56
1:A:771:HIS:O	1:A:775:VAL:HG23	2.05	0.56
1:A:130:VAL:HG12	1:A:168:TYR:HE2	1.71	0.56
1:A:892:GLU:HG3	1:A:931:ALA:HA	1.88	0.55
1:A:898:LYS:HG2	1:A:902:ILE:HD11	1.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLU:HG2	1:A:8:VAL:H	1.72	0.54
1:A:98:VAL:O	1:A:99:LEU:C	2.45	0.54
1:A:286:LEU:O	1:A:290:THR:CG2	2.55	0.54
1:A:861:TRP:CD1	1:A:897:MET:CE	2.90	0.54
1:A:1037:ILE:HD12	1:A:1084:VAL:HG22	1.88	0.54
1:A:895:ALA:O	1:A:896:SER:C	2.46	0.54
1:A:175:ILE:HG13	1:A:179:LEU:HD22	1.88	0.54
1:A:1003:GLU:H	1:A:1003:GLU:CD	2.11	0.54
1:A:417:ILE:HD12	1:A:458:LYS:HG2	1.91	0.53
1:A:972:ALA:HB2	1:A:992:TRP:NE1	2.24	0.53
1:A:638:VAL:HG23	1:A:667:ILE:HG22	1.91	0.53
1:A:389:MET:HE1	1:A:430:LYS:HB3	1.89	0.53
1:A:417:ILE:HG12	1:A:428:CYS:SG	2.49	0.52
1:A:131:GLN:HB3	1:A:134:LEU:HB2	1.91	0.52
1:A:389:MET:HA	1:A:389:MET:HE2	1.92	0.52
1:A:861:TRP:CD1	1:A:897:MET:HE2	2.45	0.52
1:A:898:LYS:O	1:A:902:ILE:CD1	2.57	0.52
1:A:261:PHE:HA	1:A:264:ILE:HD11	1.91	0.52
1:A:747:TRP:CD1	1:A:781:MET:HG3	2.44	0.52
1:A:954:GLY:O	1:A:960:ASN:ND2	2.43	0.52
1:A:170:ILE:HG23	1:A:178:ILE:HG12	1.92	0.51
1:A:1028:ASN:O	1:A:1032:VAL:HG23	2.11	0.51
1:A:328:ALA:O	1:A:329:ALA:C	2.47	0.51
1:A:945:THR:O	1:A:949:ILE:HG13	2.10	0.51
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.92	0.51
1:A:893:GLN:O	1:A:893:GLN:HG2	2.11	0.51
1:A:458:LYS:HE3	1:A:463:CYS:SG	2.50	0.51
1:A:327:ASP:O	1:A:328:ALA:HB3	2.12	0.50
1:A:988:TYR:O	1:A:991:ASN:HB2	2.12	0.50
1:A:985:VAL:HG23	1:A:986:ASP:N	2.24	0.50
1:A:715:ASP:HB2	1:A:766:ILE:HD11	1.93	0.50
1:A:261:PHE:HA	1:A:264:ILE:CD1	2.42	0.50
1:A:640:LEU:HD23	1:A:665:ILE:HG21	1.94	0.50
1:A:898:LYS:O	1:A:902:ILE:HD11	2.11	0.49
1:A:1080:ILE:O	1:A:1080:ILE:HD12	2.12	0.49
1:A:641:ILE:HG12	1:A:642:GLU:H	1.77	0.49
1:A:971:ILE:HD11	1:A:992:TRP:HB2	1.94	0.49
1:A:747:TRP:CG	1:A:781:MET:HG3	2.48	0.49
1:A:243:PHE:CE2	1:A:285:ALA:HB2	2.48	0.48
1:A:918:GLN:HB2	1:A:963:SER:HA	1.96	0.48
1:A:417:ILE:O	1:A:425:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:GLN:O	1:A:893:GLN:HG3	2.12	0.48
1:A:902:ILE:HG21	1:A:938:VAL:HG11	1.95	0.48
1:A:38:TRP:CE3	1:A:43:ASN:HB3	2.48	0.48
1:A:641:ILE:HG22	1:A:664:HIS:O	2.12	0.48
1:A:863:MET:CE	1:A:867:PHE:CE2	2.97	0.48
1:A:957:LEU:O	1:A:958:GLU:C	2.52	0.48
1:A:712:TYR:CD1	1:A:713:LEU:HD13	2.48	0.47
1:A:261:PHE:O	1:A:264:ILE:HD12	2.13	0.47
1:A:861:TRP:NE1	1:A:897:MET:HE2	2.29	0.47
1:A:278:GLU:H	1:A:278:GLU:HG2	1.37	0.47
1:A:650:GLN:HG2	1:A:657:VAL:CG2	2.36	0.47
1:A:584:LEU:HD13	1:A:606:TRP:CD2	2.51	0.46
1:A:861:TRP:CD1	1:A:897:MET:HE1	2.50	0.46
1:A:897:MET:O	1:A:898:LYS:C	2.54	0.46
1:A:799:SER:HB2	1:A:860:ILE:CG2	2.45	0.46
1:A:267:PHE:O	1:A:271:VAL:HG23	2.16	0.46
1:A:328:ALA:O	1:A:331:TRP:N	2.49	0.46
1:A:901:PHE:C	1:A:901:PHE:CD2	2.89	0.46
1:A:435:ILE:HG23	1:A:443:ILE:CD1	2.47	0.45
1:A:114:ARG:HA	1:A:114:ARG:HD2	1.77	0.45
1:A:119:ARG:HD2	1:A:154:ASN:OD1	2.16	0.45
1:A:747:TRP:NE1	1:A:785:CYS:HB2	2.31	0.45
1:A:274:ASN:OD1	1:A:276:ASP:HB2	2.17	0.45
1:A:854:LEU:HD11	1:A:890:GLY:HA2	1.97	0.45
1:A:690:ARG:HE	1:A:690:ARG:HB2	1.38	0.45
1:A:366:ALA:HB3	1:A:367:PRO:CD	2.47	0.44
1:A:1014:GLN:C	1:A:1016:ILE:H	2.19	0.44
1:A:888:GLN:HE21	1:A:888:GLN:HB2	1.60	0.44
1:A:584:LEU:HD13	1:A:606:TRP:CE2	2.52	0.44
1:A:799:SER:HB2	1:A:860:ILE:HG21	1.99	0.44
1:A:20:ALA:O	1:A:21:SER:CB	2.66	0.44
1:A:894:THR:O	1:A:897:MET:N	2.47	0.43
1:A:902:ILE:N	1:A:903:PRO:CD	2.81	0.43
1:A:902:ILE:CG2	1:A:938:VAL:HG11	2.47	0.43
1:A:93:HIS:O	1:A:93:HIS:CG	2.71	0.43
1:A:872:GLU:CD	1:A:873:PRO:HD2	2.37	0.43
1:A:946:LEU:HB3	1:A:971:ILE:CG2	2.48	0.43
1:A:250:VAL:O	1:A:254:PRO:HD3	2.18	0.43
1:A:495:LEU:HA	1:A:495:LEU:HD23	1.76	0.43
1:A:507:LEU:HA	1:A:507:LEU:HD23	1.82	0.43
1:A:431:VAL:O	1:A:435:ILE:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:HD22	1:A:290:THR:HG22	2.01	0.43
1:A:326:ASP:OD1	1:A:382:ARG:NH1	2.52	0.43
1:A:641:ILE:HG12	1:A:642:GLU:N	2.34	0.43
1:A:369:PHE:CE2	1:A:402:LEU:HD21	2.54	0.43
1:A:213:TRP:C	1:A:215:LYS:H	2.22	0.42
1:A:274:ASN:C	1:A:276:ASP:H	2.22	0.42
1:A:97:GLU:H	1:A:97:GLU:HG2	1.53	0.42
1:A:714:HIS:ND1	1:A:717:VAL:HG23	2.35	0.42
1:A:1031:ALA:O	1:A:1035:SER:HB3	2.20	0.42
1:A:861:TRP:N	1:A:862:PRO:HD2	2.34	0.42
1:A:1065:PRO:HG2	1:A:1068:ASP:HB2	2.02	0.42
1:A:902:ILE:HG13	1:A:902:ILE:H	1.35	0.42
1:A:904:LYS:O	1:A:907:GLU:HB2	2.20	0.42
1:A:965:GLU:CG	1:A:998:THR:HG23	2.49	0.41
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.91	0.41
1:A:206:LYS:HB3	1:A:252:LEU:HD11	2.03	0.41
1:A:526:ASN:O	1:A:529:ILE:HG22	2.20	0.41
1:A:406:ILE:HG23	1:A:407:PRO:CD	2.28	0.41
1:A:167:PRO:HB2	1:A:208:LEU:CD1	2.51	0.41
1:A:152:ASN:HA	1:A:153:PRO:HD2	1.90	0.41
1:A:892:GLU:CG	1:A:934:THR:HG21	2.48	0.41
1:A:594:GLU:HA	1:A:595:ASP:C	2.40	0.41
1:A:829:PHE:CD2	1:A:829:PHE:N	2.89	0.41
1:A:518:ALA:HB2	1:A:560:CYS:HA	2.03	0.40
1:A:315:LEU:CD1	1:A:371:TYR:HB3	2.52	0.40
1:A:798:VAL:O	1:A:802:LEU:HG	2.21	0.40
1:A:885:ASP:O	1:A:889:TYR:HD2	2.04	0.40
1:A:892:GLU:CB	1:A:934:THR:CG2	2.95	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	1008/1078 (94%)	955 (95%)	47 (5%)	6 (1%)	25 47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ILE
1	A	1074	ASN
1	A	8	VAL
1	A	336	ASP
1	A	591	ASP
1	A	958	GLU

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	841/931 (90%)	736 (88%)	105 (12%)	4 8

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	59	GLN
1	A	62	THR
1	A	66	LEU
1	A	74	LEU
1	A	92	THR
1	A	97	GLU
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	146	GLU
1	A	168	TYR

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	187	THR
1	A	206	LYS
1	A	207	GLN
1	A	219	LEU
1	A	237	ASP
1	A	239	LEU
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	298	GLN
1	A	300	CYS
1	A	308	GLN
1	A	313	VAL
1	A	319	THR
1	A	326	ASP
1	A	336	ASP
1	A	352	LEU
1	A	368	LEU
1	A	376	ILE
1	A	391	LEU
1	A	405	GLU
1	A	417	ILE
1	A	423	ARG
1	A	431	VAL
1	A	435	ILE
1	A	437	THR
1	A	446	THR
1	A	449	ASP
1	A	483	SER
1	A	488	GLU
1	A	535	LEU
1	A	538	LEU
1	A	539	LEU
1	A	551	SER

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Mol	Chain	Res	Type
1	A	553	LEU
1	A	571	GLU
1	A	578	GLN
1	A	587	LEU
1	A	592	ILE
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	729	LEU
1	A	730	SER
1	A	733	LEU
1	A	759	MET
1	A	784	ASN
1	A	811	ASP
1	A	834	LEU
1	A	839	ASN
1	A	850	ASN
1	A	852	HIS
1	A	857	LEU
1	A	861	TRP
1	A	868	LEU
1	A	869	LEU
1	A	894	THR
1	A	902	ILE
1	A	921	SER
1	A	926	VAL
1	A	933	SER
1	A	934	THR
1	A	955	SER
1	A	960	ASN
1	A	971	ILE
1	A	989	THR
1	A	1029	ILE

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Mol	Chain	Res	Type
1	A	1030	SER
1	A	1045	LEU
1	A	1056	SER
1	A	1058	LYS
1	A	1079	ASP
1	A	1080	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	142	GLN
1	A	207	GLN
1	A	303	ASN
1	A	374	GLN
1	A	448	HIS
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
1	A	960	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 monosaccharides 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^{th} 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	1030/1078 (95%)	-0.09	32 (3%) 49 42	46, 73, 112, 212	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	ILE	6.7
1	A	593	ASP	6.2
1	A	594	GLU	5.2
1	A	592	ILE	4.7
1	A	829	PHE	4.6
1	A	664	HIS	4.2
1	A	340	GLU	3.8
1	A	591	ASP	3.7
1	A	1089	ALA	3.1
1	A	475	LEU	3.0
1	A	428	CYS	3.0
1	A	811	ASP	2.9
1	A	661	GLN	2.9
1	A	324	ASP	2.9
1	A	595	ASP	2.9
1	A	970	ALA	2.7
1	A	386	ALA	2.7
1	A	665	ILE	2.7
1	A	323	ILE	2.7
1	A	647	ALA	2.7
1	A	969	ALA	2.6
1	A	387	ALA	2.6
1	A	968	SER	2.4
1	A	390	ALA	2.4
1	A	640	LEU	2.4
1	A	660	VAL	2.4
1	A	812	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	ALA	2.2
1	A	657	VAL	2.1
1	A	317	MET	2.1
1	A	405	GLU	2.0
1	A	967	ALA	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.