



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:53 pm BST

PDB ID : 3W3V
Title : Crystal structure of Kap121p mutant D353K/E396K/D438K
Authors : Kobayashi, J.; Matsuura, Y.
Deposited on : 2012-12-28
Resolution : 3.20 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	:	2.11
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)	:	2.11

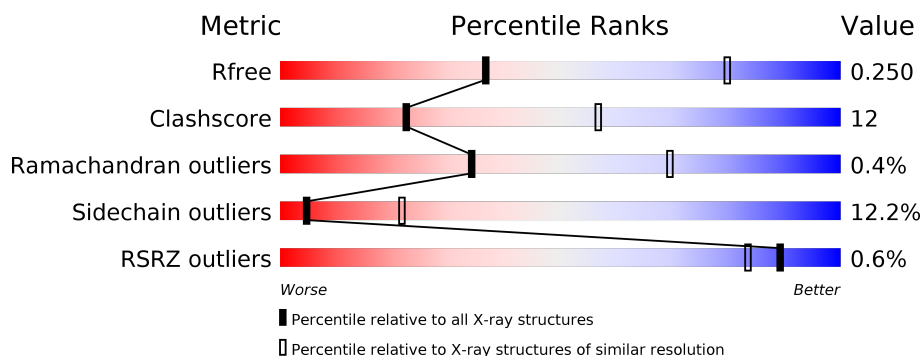
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7841 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	1025	Total	C	N	O	S	0	0	0
			7841	5036	1266	1503	36			

There are 14 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	353	LYS	ASP	ENGINEERED MUTATION	UNP P32337
A	396	LYS	GLU	ENGINEERED MUTATION	UNP P32337
A	438	LYS	ASP	ENGINEERED MUTATION	UNP P32337

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

Chain A:

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.79Å 122.31Å 84.67Å 90.00° 116.08° 90.00°	Depositor
Resolution (Å)	25.55 – 3.20 25.55 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.55-3.20) 99.7 (25.55-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.17Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.203 , 0.252 0.201 , 0.250	Depositor DCC
R_{free} test set	1186 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7841	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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	0.52	0/7977	0.75	4/10861 (0.0%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	76	LEU	CA-CB-CG	6.82	130.98	115.30
1	A	364	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	79	PRO	CA-C-N	-5.65	104.77	117.20
1	A	364	LEU	CB-CG-CD2	-5.12	102.29	111.00

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

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	7841	0	7757	181	0
All	All	7841	0	7757	181	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 (181) 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:19:PHE:HB3	1:A:66:LEU:HD21	1.26	1.15
1:A:898:LYS:NZ	1:A:937:ASP:OD1	1.84	1.10
1:A:861:TRP:NE1	1:A:897:MET:HE1	1.80	0.95
1:A:892:GLU:HB3	1:A:934:THR:HG21	1.49	0.93
1:A:406:ILE:HG23	1:A:407:PRO:HD3	1.50	0.91
1:A:861:TRP:CD1	1:A:897:MET:HE1	2.07	0.89
1:A:861:TRP:CE2	1:A:897:MET:HE2	2.07	0.88
1:A:19:PHE:CB	1:A:66:LEU:HD21	2.08	0.84
1:A:892:GLU:CB	1:A:934:THR:HG21	2.08	0.83
1:A:861:TRP:NE1	1:A:897:MET:CE	2.40	0.83
1:A:957:LEU:O	1:A:961:ARG:HB2	1.78	0.82
1:A:893:GLN:HG2	1:A:893:GLN:O	1.80	0.79
1:A:892:GLU:HB3	1:A:934:THR:CG2	2.14	0.77
1:A:898:LYS:O	1:A:902:ILE:HG13	1.84	0.77
1:A:892:GLU:CD	1:A:934:THR:HG22	2.05	0.77
1:A:892:GLU:CG	1:A:934:THR:CG2	2.62	0.76
1:A:389:MET:CE	1:A:389:MET:HA	2.16	0.76
1:A:898:LYS:O	1:A:902:ILE:CG1	2.35	0.74
1:A:650:GLN:HG2	1:A:657:VAL:HG22	1.70	0.73
1:A:406:ILE:CG2	1:A:407:PRO:HD3	2.20	0.72
1:A:937:ASP:O	1:A:941:PRO:HG2	1.90	0.71
1:A:861:TRP:CE2	1:A:897:MET:CE	2.73	0.71
1:A:571:GLU:OE1	1:A:572:LYS:N	2.19	0.70
1:A:1058:LYS:HD3	1:A:1089:ALA:HB3	1.73	0.69
1:A:571:GLU:CD	1:A:572:LYS:H	1.97	0.68
1:A:888:GLN:HB3	1:A:889:TYR:CD2	2.29	0.68
1:A:888:GLN:HB3	1:A:889:TYR:CE2	2.28	0.68
1:A:898:LYS:HG2	1:A:902:ILE:HD11	1.77	0.67
1:A:892:GLU:CB	1:A:934:THR:CG2	2.71	0.67
1:A:430:ASN:C	1:A:430:ASN:HD22	1.97	0.67
1:A:19:PHE:HE1	1:A:34:LEU:HD12	1.60	0.67
1:A:892:GLU:HG2	1:A:934:THR:CG2	2.24	0.66
1:A:434:GLN:NE2	1:A:438:LYS:HE2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:MET:CE	1:A:867:PHE:CE2	2.80	0.64
1:A:369:PHE:O	1:A:373:GLN:HG2	1.98	0.63
1:A:892:GLU:CG	1:A:934:THR:HG22	2.26	0.63
1:A:861:TRP:CD1	1:A:897:MET:CE	2.82	0.62
1:A:683:GLN:HB2	1:A:724:LEU:HD13	1.81	0.61
1:A:175:ILE:HG13	1:A:179:LEU:HD22	1.81	0.61
1:A:19:PHE:CE1	1:A:34:LEU:HD12	2.35	0.61
1:A:988:TYR:HA	1:A:991:ASN:HD22	1.65	0.61
1:A:571:GLU:CG	1:A:572:LYS:N	2.63	0.60
1:A:19:PHE:HB3	1:A:66:LEU:CD2	2.16	0.60
1:A:389:MET:HE2	1:A:389:MET:HA	1.83	0.59
1:A:369:PHE:HE2	1:A:402:LEU:HD21	1.67	0.59
1:A:267:PHE:O	1:A:271:VAL:HG23	2.03	0.59
1:A:946:LEU:HD13	1:A:971:ILE:HG22	1.85	0.59
1:A:902:ILE:N	1:A:903:PRO:HD2	2.18	0.58
1:A:504:SER:OG	1:A:505:ASN:N	2.37	0.58
1:A:701:MET:HG2	1:A:746:LEU:HD22	1.85	0.57
1:A:889:TYR:N	1:A:889:TYR:CD2	2.72	0.57
1:A:571:GLU:HG2	1:A:572:LYS:N	2.18	0.57
1:A:20:ALA:O	1:A:21:SER:HB2	2.05	0.57
1:A:336:ASP:C	1:A:336:ASP:OD2	2.43	0.57
1:A:38:TRP:CE3	1:A:43:ASN:HB3	2.40	0.57
1:A:892:GLU:HG2	1:A:931:ALA:HA	1.87	0.56
1:A:286:LEU:HD22	1:A:290:THR:HG22	1.88	0.56
1:A:389:MET:HE1	1:A:430:ASN:HB3	1.86	0.56
1:A:492:ASP:O	1:A:496:THR:HG23	2.06	0.56
1:A:438:LYS:HD3	1:A:438:LYS:N	2.21	0.55
1:A:747:TRP:CD1	1:A:781:MET:HG3	2.41	0.55
1:A:747:TRP:HE1	1:A:785:CYS:HB2	1.72	0.55
1:A:584:LEU:HD13	1:A:606:TRP:CD2	2.41	0.55
1:A:640:LEU:HD23	1:A:665:ILE:CG2	2.37	0.55
1:A:975:LEU:HD22	1:A:989:THR:HG22	1.88	0.54
1:A:276:ASP:OD2	1:A:276:ASP:N	2.40	0.54
1:A:316:ILE:O	1:A:319:THR:HB	2.08	0.54
1:A:345:TYR:O	1:A:349:ARG:HG2	2.08	0.54
1:A:898:LYS:CG	1:A:902:ILE:HD11	2.36	0.54
1:A:191:ASP:OD2	1:A:235:LYS:HG2	2.07	0.54
1:A:892:GLU:CG	1:A:931:ALA:HA	2.38	0.54
1:A:954:GLY:O	1:A:960:ASN:ND2	2.40	0.54
1:A:650:GLN:CG	1:A:657:VAL:HG22	2.35	0.54
1:A:937:ASP:N	1:A:937:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:VAL:HG12	1:A:728:LEU:HD11	1.91	0.53
1:A:434:GLN:HE22	1:A:438:LYS:HE2	1.72	0.53
1:A:641:ILE:HG12	1:A:642:GLU:H	1.73	0.53
1:A:937:ASP:O	1:A:941:PRO:CG	2.57	0.53
1:A:895:ALA:O	1:A:896:SER:C	2.46	0.52
1:A:130:VAL:HG12	1:A:168:TYR:HE2	1.75	0.52
1:A:286:LEU:O	1:A:290:THR:HG23	2.10	0.52
1:A:458:LYS:HE3	1:A:463:CYS:SG	2.49	0.52
1:A:438:LYS:CD	1:A:438:LYS:N	2.73	0.51
1:A:660:VAL:C	1:A:661:GLN:HG2	2.30	0.51
1:A:972:ALA:HB2	1:A:992:TRP:NE1	2.26	0.51
1:A:584:LEU:HD13	1:A:606:TRP:CE2	2.46	0.51
1:A:747:TRP:CG	1:A:781:MET:HG3	2.46	0.50
1:A:946:LEU:CD1	1:A:971:ILE:HG22	2.41	0.50
1:A:206:LYS:HB3	1:A:252:LEU:HD11	1.94	0.50
1:A:258:LYS:O	1:A:259:ASP:OD1	2.29	0.50
1:A:278:GLU:HB2	1:A:280:PRO:HD2	1.92	0.50
1:A:417:ILE:HG12	1:A:428:CYS:SG	2.51	0.50
1:A:709:LEU:HD12	1:A:753:LYS:HG2	1.94	0.50
1:A:417:ILE:O	1:A:425:GLN:HG2	2.12	0.49
1:A:971:ILE:HD11	1:A:992:TRP:HB2	1.93	0.49
1:A:872:GLU:O	1:A:876:VAL:HG23	2.12	0.49
1:A:366:ALA:HB3	1:A:367:PRO:CD	2.43	0.49
1:A:712:TYR:CD1	1:A:713:LEU:HD13	2.48	0.49
1:A:7:GLU:HG2	1:A:8:VAL:H	1.77	0.49
1:A:897:MET:O	1:A:898:LYS:C	2.50	0.49
1:A:286:LEU:O	1:A:290:THR:CG2	2.61	0.48
1:A:918:GLN:HB2	1:A:963:SER:HA	1.95	0.48
1:A:799:SER:HB2	1:A:860:ILE:HG21	1.94	0.48
1:A:988:TYR:O	1:A:991:ASN:HB2	2.14	0.48
1:A:261:PHE:O	1:A:264:ILE:HD12	2.14	0.47
1:A:327:ASP:O	1:A:328:ALA:HB3	2.14	0.47
1:A:863:MET:HE1	1:A:867:PHE:CE2	2.48	0.47
1:A:431:VAL:HG12	1:A:435:ILE:HD13	1.95	0.47
1:A:435:ILE:HG23	1:A:443:ILE:CD1	2.45	0.47
1:A:326:ASP:OD1	1:A:382:ARG:NH1	2.48	0.47
1:A:279:PRO:N	1:A:280:PRO:HD2	2.29	0.47
1:A:119:ARG:HD2	1:A:154:ASN:OD1	2.15	0.47
1:A:640:LEU:HA	1:A:665:ILE:HG22	1.97	0.47
1:A:213:TRP:C	1:A:215:LYS:H	2.18	0.46
1:A:880:LEU:O	1:A:923:ILE:HD11	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PHE:HA	1:A:264:ILE:HD11	1.97	0.46
1:A:571:GLU:OE1	1:A:572:LYS:HB2	2.16	0.46
1:A:1003:GLU:CD	1:A:1003:GLU:H	2.18	0.46
1:A:1058:LYS:CD	1:A:1089:ALA:HB3	2.43	0.46
1:A:431:VAL:O	1:A:435:ILE:HB	2.15	0.46
1:A:435:ILE:HG13	1:A:439:PHE:CE2	2.50	0.46
1:A:657:VAL:HG12	1:A:666:ALA:HA	1.96	0.46
1:A:638:VAL:HG23	1:A:667:ILE:HG22	1.98	0.46
1:A:170:ILE:HG23	1:A:178:ILE:HG12	1.99	0.45
1:A:328:ALA:O	1:A:329:ALA:C	2.54	0.45
1:A:114:ARG:HA	1:A:114:ARG:HD2	1.78	0.45
1:A:364:LEU:O	1:A:368:LEU:HB2	2.17	0.45
1:A:571:GLU:OE1	1:A:572:LYS:CB	2.64	0.45
1:A:323:ILE:O	1:A:323:ILE:HG13	2.17	0.45
1:A:892:GLU:HG2	1:A:931:ALA:CA	2.45	0.45
1:A:250:VAL:O	1:A:254:PRO:HD3	2.17	0.45
1:A:965:GLU:HG2	1:A:998:THR:HG23	1.99	0.45
1:A:528:PHE:HZ	1:A:535:LEU:HD13	1.82	0.44
1:A:366:ALA:HB3	1:A:367:PRO:HD3	1.99	0.44
1:A:1028:ASN:O	1:A:1032:VAL:HG23	2.17	0.44
1:A:1058:LYS:HD2	1:A:1089:ALA:H	1.82	0.44
1:A:258:LYS:O	1:A:259:ASP:CG	2.56	0.44
1:A:261:PHE:HA	1:A:264:ILE:CD1	2.48	0.44
1:A:1014:GLN:C	1:A:1016:ILE:H	2.21	0.44
1:A:901:PHE:O	1:A:905:VAL:HG23	2.18	0.44
1:A:690:ARG:HE	1:A:690:ARG:HB2	1.22	0.43
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.99	0.43
1:A:152:ASN:HA	1:A:153:PRO:HD2	1.84	0.43
1:A:914:ALA:O	1:A:963:SER:HB2	2.18	0.43
1:A:664:HIS:O	1:A:665:ILE:HG23	2.19	0.43
1:A:264:ILE:H	1:A:264:ILE:HG13	1.68	0.43
1:A:863:MET:HE1	1:A:867:PHE:HE2	1.84	0.43
1:A:996:LEU:N	1:A:996:LEU:HD23	2.33	0.43
1:A:1034:ASP:O	1:A:1038:GLN:HG2	2.19	0.43
1:A:178:ILE:HD12	1:A:178:ILE:HA	1.90	0.43
1:A:892:GLU:HG2	1:A:934:THR:HG23	2.00	0.43
1:A:901:PHE:CD2	1:A:901:PHE:C	2.92	0.42
1:A:799:SER:HB2	1:A:860:ILE:CG2	2.50	0.42
1:A:714:HIS:ND1	1:A:717:VAL:HG23	2.35	0.42
1:A:215:LYS:HE3	1:A:215:LYS:HB2	1.84	0.42
1:A:535:LEU:O	1:A:538:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:GLU:CG	1:A:998:THR:HG23	2.50	0.42
1:A:243:PHE:CE2	1:A:285:ALA:HB2	2.55	0.42
1:A:203:GLY:HA2	1:A:206:LYS:HG2	2.02	0.41
1:A:388:MET:SD	1:A:413:VAL:HG22	2.60	0.41
1:A:646:ALA:HB1	1:A:657:VAL:HG21	2.02	0.41
1:A:1080:ILE:HD12	1:A:1080:ILE:O	2.19	0.41
1:A:349:ARG:H	1:A:349:ARG:HG2	1.57	0.41
1:A:422:PRO:O	1:A:425:GLN:HB2	2.19	0.41
1:A:758:LEU:HA	1:A:758:LEU:HD23	1.86	0.41
1:A:269:ASP:OD1	1:A:309:THR:HG23	2.20	0.41
1:A:356:ALA:HA	1:A:364:LEU:HD11	2.02	0.41
1:A:1037:ILE:HD12	1:A:1084:VAL:HG22	2.01	0.41
1:A:488:GLU:HB3	1:A:489:PRO:CD	2.50	0.41
1:A:641:ILE:HG12	1:A:642:GLU:N	2.35	0.41
1:A:747:TRP:NE1	1:A:785:CYS:HB2	2.34	0.41
1:A:863:MET:CE	1:A:867:PHE:HE2	2.32	0.41
1:A:775:VAL:HG22	1:A:841:SER:HA	2.02	0.41
1:A:435:ILE:CG2	1:A:443:ILE:CD1	2.99	0.41
1:A:7:GLU:HG2	1:A:8:VAL:N	2.36	0.41
1:A:615:ASP:CG	1:A:692:GLN:HE21	2.23	0.40
1:A:861:TRP:N	1:A:862:PRO:HD2	2.35	0.40
1:A:389:MET:CE	1:A:389:MET:CA	2.95	0.40
1:A:771:HIS:O	1:A:775:VAL:HG23	2.21	0.40
1:A:946:LEU:HB3	1:A:971:ILE:HG22	2.03	0.40
1:A:503:GLN:O	1:A:504:SER:O	2.40	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	999/1078 (93%)	956 (96%)	39 (4%)	4 (0%)	34 69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ILE
1	A	504	SER
1	A	994	LYS
1	A	8	VAL

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	843/937 (90%)	740 (88%)	103 (12%)	5 22

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	42	ASN
1	A	66	LEU
1	A	106	LEU
1	A	113	GLU
1	A	114	ARG
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	209	PRO
1	A	216	LEU
1	A	219	LEU
1	A	237	ASP
1	A	239	LEU
1	A	261	PHE
1	A	263	GLN

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Mol	Chain	Res	Type
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	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
1	A	431	VAL
1	A	435	ILE
1	A	438	LYS
1	A	446	THR
1	A	483	SER
1	A	534	THR
1	A	535	LEU
1	A	538	LEU
1	A	539	LEU
1	A	545	VAL
1	A	553	LEU
1	A	571	GLU
1	A	580	LEU
1	A	587	LEU
1	A	638	VAL
1	A	641	ILE
1	A	644	GLU
1	A	649	PHE
1	A	661	GLN
1	A	665	ILE

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Mol	Chain	Res	Type
1	A	672	LEU
1	A	689	LEU
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	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
1	A	869	LEU
1	A	888	GLN
1	A	889	TYR
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	957	LEU
1	A	960	ASN
1	A	971	ILE
1	A	989	THR
1	A	994	LYS
1	A	1045	LEU
1	A	1056	SER
1	A	1070	MET
1	A	1079	ASP
1	A	1080	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	142	GLN
1	A	207	GLN
1	A	303	ASN
1	A	350	GLN
1	A	430	ASN
1	A	434	GLN
1	A	477	ASN
1	A	541	ASN
1	A	550	ASN
1	A	661	GLN
1	A	683	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	966	ASN
1	A	991	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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 [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%)	-0.36	6 (0%) 89 83	59, 113, 156, 182	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	664	HIS	2.9
1	A	428	CYS	2.8
1	A	591	ASP	2.2
1	A	642	GLU	2.1
1	A	968	SER	2.1
1	A	400	ASP	2.1

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.