



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:40 AM UTC

PDB ID : 3W3T / pdb_00003w3t
Title : Crystal structure of Kap121p
Authors : Kobayashi, J.; Matsuura, Y.
Deposited on : 2012-12-28
Resolution : 2.90 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

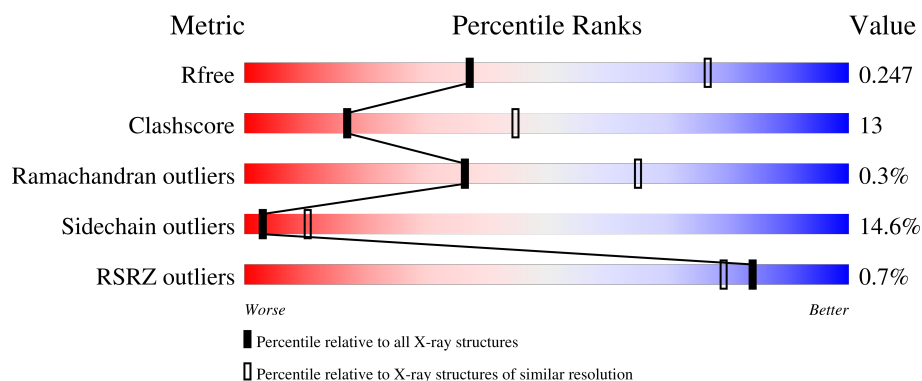
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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 Entry composition

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
1	A	1025	Total	C	N	O	S	0	0	0
			7845	5035	1263	1511	36			

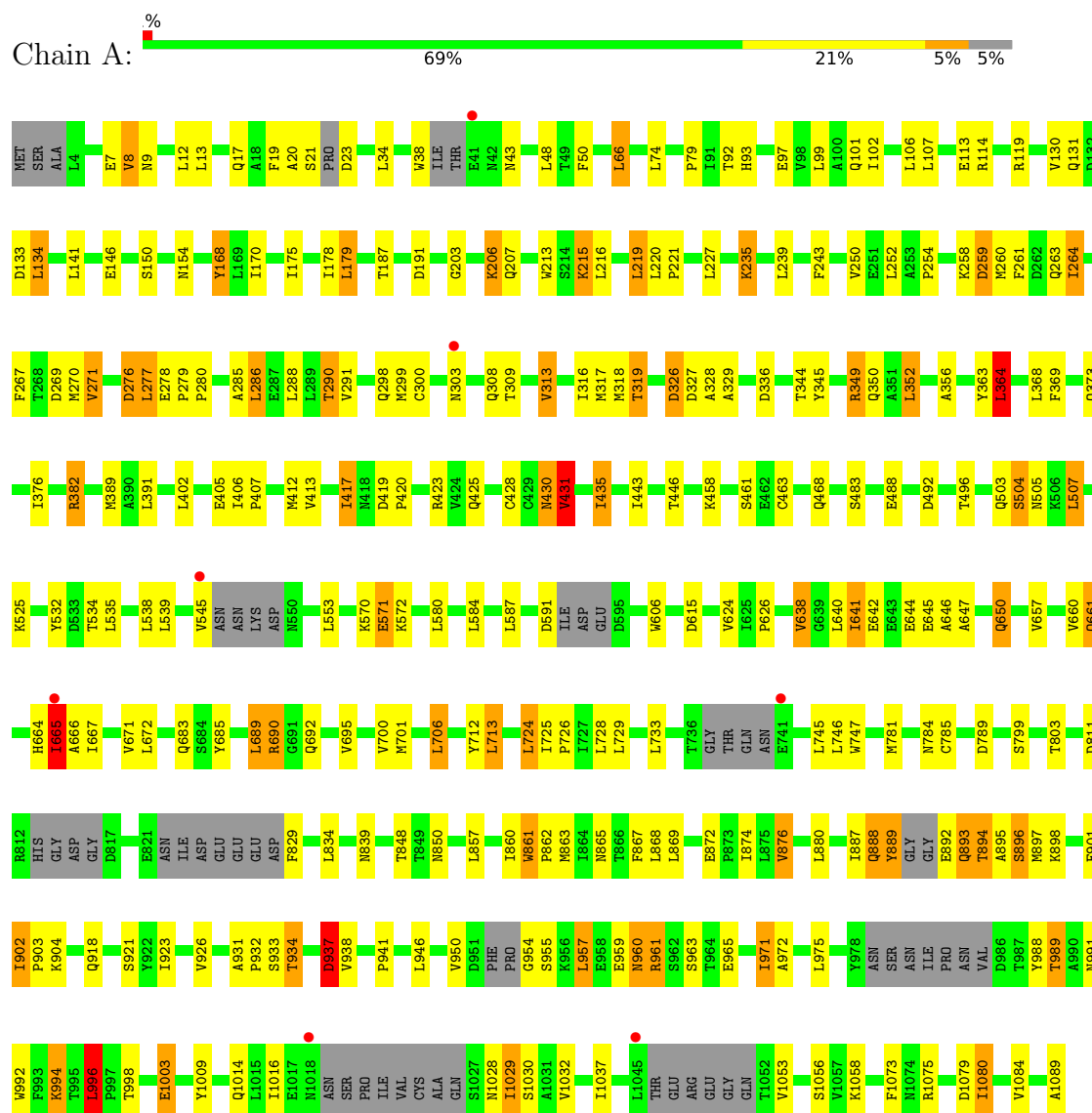
There are 11 discrepancies between the modelled and reference sequences:

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, 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



4 Data and refinement statistics

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 28.32 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.32-2.90) 99.6 (28.32-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.06%)	wwPDB-VP
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 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	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.*

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	0.87	0/7981	1.23	40/10869 (0.4%)

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 (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	646	ALA	N-CA-C	28.78	142.65	111.28
1	A	1073	PHE	CB-CA-C	-10.53	94.18	111.13
1	A	647	ALA	N-CA-C	-10.40	98.00	112.45
1	A	1073	PHE	CA-C-N	10.16	133.89	120.28
1	A	1073	PHE	C-N-CA	10.16	133.89	120.28
1	A	300	CYS	N-CA-CB	-9.36	96.26	110.20
1	A	1075	ARG	N-CA-CB	-9.36	95.77	110.28
1	A	364	LEU	N-CA-C	9.25	124.82	113.17
1	A	957	LEU	N-CA-C	-8.98	96.61	110.17
1	A	957	LEU	CB-CA-C	8.97	129.54	111.60
1	A	215	LYS	N-CA-C	-7.62	104.51	113.88
1	A	887	ILE	N-CA-C	7.25	118.89	110.62
1	A	937	ASP	N-CA-C	7.11	120.07	111.82
1	A	431	VAL	CB-CA-C	-6.99	103.02	111.97
1	A	303	ASN	N-CA-C	6.96	119.76	108.41
1	A	665	ILE	N-CA-C	6.80	117.33	108.35
1	A	299	MET	N-CA-C	6.65	119.38	111.33
1	A	626	PRO	CA-C-N	-6.39	112.42	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	626	PRO	C-N-CA	-6.39	112.42	119.19
1	A	932	PRO	CB-CA-C	-6.36	103.02	112.55
1	A	646	ALA	CB-CA-C	-6.33	100.29	110.79
1	A	645	GLU	CA-C-N	6.16	128.53	120.28
1	A	645	GLU	C-N-CA	6.16	128.53	120.28
1	A	959	GLU	N-CA-C	6.15	118.77	111.33
1	A	1029	ILE	N-CA-C	5.95	117.40	110.62
1	A	937	ASP	CB-CA-C	-5.86	99.41	110.67
1	A	260	MET	N-CA-C	-5.61	105.64	112.88
1	A	227	LEU	CA-C-N	-5.58	113.87	119.56
1	A	227	LEU	C-N-CA	-5.58	113.87	119.56
1	A	961	ARG	N-CA-C	-5.57	105.75	112.54
1	A	932	PRO	N-CA-C	5.50	120.77	113.40
1	A	570	LYS	N-CA-C	5.50	116.95	111.07
1	A	363	TYR	N-CA-C	5.32	117.89	111.40
1	A	277	LEU	N-CA-C	-5.17	101.84	110.17
1	A	865	ASN	N-CA-C	5.17	116.60	111.07
1	A	996	LEU	N-CA-C	-5.17	102.64	110.39
1	A	876	VAL	N-CA-C	-5.08	105.89	110.82
1	A	271	VAL	CB-CA-C	-5.07	105.44	112.24
1	A	525	LYS	CB-CA-C	-5.05	110.73	116.54
1	A	9	ASN	N-CA-C	5.04	117.17	111.02

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 ⓘ

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	198	0
All	All	7845	0	7740	198	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 13.

All (198) 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:OD1	1.70	1.22
1:A:19:PHE:HB3	1:A:66:LEU:HD21	1.24	1.14
1:A:861:TRP:NE1	1:A:897:MET:HE1	1.65	1.11
1:A:892:GLU:HB3	1:A:934:THR:HG21	1.32	1.11
1:A:861:TRP:CE2	1:A:897:MET:HE2	1.86	1.08
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:389:MET:HE2	1:A:389:MET:HA	1.47	0.97
1:A:957:LEU:O	1:A:961:ARG:HB2	1.64	0.97
1:A:892:GLU:CB	1:A:934:THR:HG21	1.96	0.94
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:861:TRP:CD1	1:A:897:MET:HE1	2.10	0.86
1:A:19:PHE:CB	1:A:66:LEU:HD21	2.07	0.84
1:A:898:LYS:O	1:A:902:ILE:HG13	1.82	0.80
1:A:892:GLU:CD	1:A:934:THR:HG22	2.07	0.80
1:A:571:GLU:CD	1:A:572:LYS:H	1.91	0.78
1:A:892:GLU:CB	1:A:934:THR:CG2	2.61	0.77
1:A:430:ASN:C	1:A:430:ASN:HD22	1.92	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: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:406:ILE:CG2	1:A:407:PRO:HD3	2.17	0.73
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:336:ASP:OD2	1:A:336:ASP:C	2.37	0.67
1:A:683:GLN:HB2	1:A:724:LEU:HD13	1.76	0.67
1:A:888:GLN:HB3	1:A:889:TYR:CD2	2.29	0.67
1:A:571:GLU:CG	1:A:572:LYS:N	2.58	0.67
1:A:863:MET:CE	1:A:867:PHE:CE2	2.78	0.66
1:A:892:GLU:CG	1:A:934:THR:HG22	2.26	0.66
1:A:747:TRP:HE1	1:A:785:CYS:HB2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:GLU:HG2	1:A:572:LYS:N	2.10	0.66
1:A:895:ALA:O	1:A:896:SER:C	2.37	0.65
1:A:504:SER:OG	1:A:505:ASN:N	2.31	0.63
1:A:861:TRP:HE1	1:A:897:MET:HE1	1.57	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: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:861:TRP:CE2	1:A:897:MET:CE	2.61	0.60
1:A:988:TYR:HA	1:A:991:ASN:HD22	1.66	0.60
1:A:389:MET:HA	1:A:389:MET:CE	2.26	0.60
1:A:892:GLU:HG2	1:A:934:THR:HG23	1.83	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:328:ALA:O	1:A:329:ALA:C	2.46	0.58
1:A:316:ILE:O	1:A:319:THR:HB	2.03	0.58
1:A:902:ILE:N	1:A:903:PRO:HD2	2.18	0.58
1:A:889:TYR:CD2	1:A:889:TYR:N	2.70	0.58
1:A:492:ASP:O	1:A:496:THR:HG23	2.03	0.58
1:A:660:VAL:C	1:A:661:GLN:HG2	2.27	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:892:GLU:HG2	1:A:931:ALA:HA	1.86	0.56
1:A:937:ASP:O	1:A:941:PRO:CG	2.53	0.56
1:A:20:ALA:O	1:A:21:SER:HB2	2.05	0.56
1:A:965:GLU:HG2	1:A:998:THR:HG23	1.88	0.56
1:A:345:TYR:O	1:A:349:ARG:HG2	2.05	0.56
1:A:389:MET:HE2	1:A:389:MET:CA	2.30	0.56
1:A:175:ILE:HG13	1:A:179:LEU:HD22	1.88	0.56
1:A:267:PHE:O	1:A:271:VAL:HG23	2.05	0.56
1:A:946:LEU:HD13	1:A:971:ILE:HG22	1.88	0.56
1:A:897:MET:O	1:A:898:LYS:C	2.47	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: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:O	1:A:893:GLN:CG	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:258:LYS:O	1:A:259:ASP:CG	2.53	0.52
1:A:571:GLU:CD	1:A:572:LYS:N	2.66	0.51
1:A:286:LEU:O	1:A:290:THR:HG23	2.11	0.51
1:A:1014:GLN:C	1:A:1016:ILE:H	2.18	0.51
1:A:747:TRP:CG	1:A:781:MET:HG3	2.45	0.51
1:A:326:ASP:CG	1:A:382:ARG:NH1	2.69	0.51
1:A:1003:GLU:H	1:A:1003:GLU:CD	2.19	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:326:ASP:CG	1:A:382:ARG:HH11	2.20	0.49
1:A:901:PHE:C	1:A:901:PHE:CD2	2.89	0.49
1:A:327:ASP:O	1:A:328:ALA:HB3	2.11	0.49
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.94	0.49
1:A:431:VAL:O	1:A:435:ILE:HB	2.12	0.49
1:A:892:GLU:HG2	1:A:931:ALA:CA	2.42	0.49
1:A:261:PHE:HA	1:A:264:ILE:HD11	1.94	0.49
1:A:13:LEU:O	1:A:17:GLN:HG3	2.13	0.49
1:A:861:TRP:CZ2	1:A:897:MET:HE2	2.42	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
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:286:LEU:O	1:A:290:THR:CG2	2.61	0.47
1:A:946:LEU:HB3	1:A:971:ILE:HG22	1.94	0.47
1:A:389:MET:HE1	1:A:430:ASN:HB3	1.96	0.47
1:A:895:ALA:C	1:A:897:MET:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:TYR:CD1	1:A:713:LEU:HD13	2.50	0.47
1:A:894:THR:O	1:A:895:ALA:C	2.57	0.47
1:A:206:LYS:HB3	1:A:252:LEU:HD11	1.96	0.47
1:A:213:TRP:C	1:A:215:LYS:H	2.22	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: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:863:MET:HE1	1:A:867:PHE:HE2	1.80	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:664:HIS:O	1:A:665:ILE:HG23	2.15	0.46
1:A:863:MET:CE	1:A:867:PHE:HE2	2.28	0.46
1:A:317:MET:HE2	1:A:344:THR:HB	1.97	0.46
1:A:937:ASP:O	1:A:941:PRO:CD	2.65	0.46
1:A:503:GLN:O	1:A:504:SER:C	2.58	0.45
1:A:318:MET:HE1	1:A:352:LEU:HD12	1.98	0.45
1:A:369:PHE:CD1	1:A:412:MET:HE1	2.52	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:93:HIS:O	1:A:93:HIS:CG	2.70	0.45
1:A:747:TRP:NE1	1:A:785:CYS:HB2	2.29	0.45
1:A:130:VAL:HG12	1:A:168:TYR:HE2	1.82	0.45
1:A:1080:ILE:O	1:A:1080:ILE:HD12	2.17	0.45
1:A:318:MET:HE2	1:A:349:ARG:HA	1.99	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:38:TRP:CE3	1:A:43:ASN:HB3	2.52	0.44
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:119:ARG:HD2	1:A:154:ASN:OD1	2.17	0.44
1:A:829:PHE:CD2	1:A:829:PHE:N	2.86	0.44
1:A:417:ILE:HD12	1:A:458:LYS:HG2	2.00	0.44
1:A:898:LYS:O	1:A:902:ILE:HD11	2.18	0.44
1:A:894:THR:C	1:A:896:SER:N	2.75	0.44
1:A:700:VAL:HG12	1:A:728:LEU:HD11	2.00	0.43
1:A:1014:GLN:C	1:A:1016:ILE:N	2.75	0.43
1:A:406:ILE:HG23	1:A:407:PRO:CD	2.30	0.43
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:971:ILE:HD11	1:A:992:TRP:HB2	2.00	0.43
1:A:685:TYR:O	1:A:689:LEU:HB2	2.18	0.43
1:A:892:GLU:OE1	1:A:933:SER:N	2.50	0.43
1:A:503:GLN:O	1:A:504:SER:O	2.36	0.43
1:A:706:LEU:HD12	1:A:706:LEU:HA	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:532:TYR:CD2	1:A:532:TYR:C	2.97	0.43
1:A:641:ILE:HG12	1:A:642:GLU:N	2.34	0.43
1:A:349:ARG:HG2	1:A:349:ARG:H	1.53	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:350:GLN:HE21	1:A:350:GLN:HB2	1.67	0.42
1:A:898:LYS:NZ	1:A:937:ASP:CG	2.66	0.42
1:A:615:ASP:CG	1:A:692:GLN:HE21	2.28	0.42
1:A:725:ILE:HB	1:A:726:PRO:HD3	2.02	0.41
1:A:430:ASN:C	1:A:430:ASN:ND2	2.64	0.41
1:A:243:PHE:CE2	1:A:285:ALA:HB2	2.55	0.41
1:A:461:SER:HA	1:A:468:GLN:NE2	2.36	0.41
1:A:918:GLN:HB2	1:A:963:SER:HA	2.02	0.41
1:A:170:ILE:HG23	1:A:178:ILE:HG12	2.03	0.41
1:A:203:GLY:HA2	1:A:206:LYS:HG2	2.03	0.41
1:A:326:ASP:HA	1:A:382:ARG:NH1	2.36	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:880:LEU:O	1:A:923:ILE:HD11	2.21	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:419:ASP:O	1:A:420:PRO:C	2.64	0.40
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.95	0.40
1:A:219:LEU:O	1:A:220:LEU:C	2.64	0.40
1:A:507:LEU:HD23	1:A:507:LEU:HA	1.87	0.40
1:A:12:LEU:HB3	1:A:50:PHE:CE2	2.57	0.40
1:A:309:THR:O	1:A:313:VAL:HB	2.22	0.40
1:A:503:GLN:C	1:A:504:SER:O	2.63	0.40
1:A:889:TYR:N	1:A:889:TYR:HD2	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%)	36 65

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%)	721 (85%)	123 (15%)	3 10

All (123) 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
1	A	101	GLN
1	A	102	ILE
1	A	106	LEU

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Mol	Chain	Res	Type
1	A	113	GLU
1	A	131	GLN
1	A	133	ASP
1	A	134	LEU
1	A	141	LEU
1	A	146	GLU
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	216	LEU
1	A	219	LEU
1	A	221	PRO
1	A	235	LYS
1	A	239	LEU
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	376	ILE
1	A	382	ARG
1	A	391	LEU
1	A	405	GLU
1	A	413	VAL
1	A	417	ILE

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Mol	Chain	Res	Type
1	A	423	ARG
1	A	430	ASN
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	545	VAL
1	A	553	LEU
1	A	571	GLU
1	A	580	LEU
1	A	587	LEU
1	A	591	ASP
1	A	624	VAL
1	A	638	VAL
1	A	641	ILE
1	A	644	GLU
1	A	650	GLN
1	A	661	GLN
1	A	665	ILE
1	A	671	VAL
1	A	672	LEU
1	A	689	LEU
1	A	690	ARG
1	A	695	VAL
1	A	706	LEU
1	A	713	LEU
1	A	724	LEU
1	A	729	LEU
1	A	733	LEU
1	A	784	ASN
1	A	789	ASP
1	A	803	THR
1	A	811	ASP
1	A	834	LEU
1	A	839	ASN
1	A	848	THR

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Mol	Chain	Res	Type
1	A	850	ASN
1	A	857	LEU
1	A	861	TRP
1	A	868	LEU
1	A	869	LEU
1	A	874	ILE
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	904	LYS
1	A	921	SER
1	A	926	VAL
1	A	934	THR
1	A	937	ASP
1	A	938	VAL
1	A	950	VAL
1	A	955	SER
1	A	960	ASN
1	A	971	ILE
1	A	989	THR
1	A	994	LYS
1	A	996	LEU
1	A	1003	GLU
1	A	1029	ILE
1	A	1030	SER
1	A	1056	SER
1	A	1079	ASP
1	A	1080	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) 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	308	GLN
1	A	350	GLN
1	A	373	GLN

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Mol	Chain	Res	Type
1	A	374	GLN
1	A	418	ASN
1	A	430	ASN
1	A	448	HIS
1	A	477	ASN
1	A	497	ASN
1	A	541	ASN
1	A	550	ASN
1	A	661	GLN
1	A	668	HIS
1	A	692	GLN
1	A	801	ASN
1	A	839	ASN
1	A	850	ASN
1	A	856	ASN
1	A	888	GLN
1	A	893	GLN
1	A	918	GLN
1	A	960	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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%)	-0.32	7 (0%) 84 79	44, 79, 124, 174	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	GLU	3.4
1	A	303	ASN	3.0
1	A	665	ILE	2.8
1	A	741	GLU	2.4
1	A	545	VAL	2.3
1	A	1045	LEU	2.1
1	A	1018	ASN	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 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.