



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:53 PM UTC

PDB ID : 3W3W / pdb_00003w3w
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 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

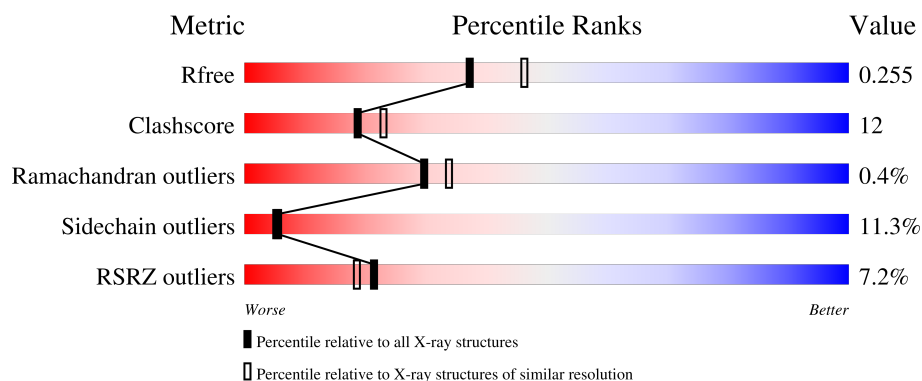
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	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
			Total	C	N	O	S			
1	A	1028	7850	5042	1263	1508	37	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

- Molecule 2 is a protein called Protein STE12.

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

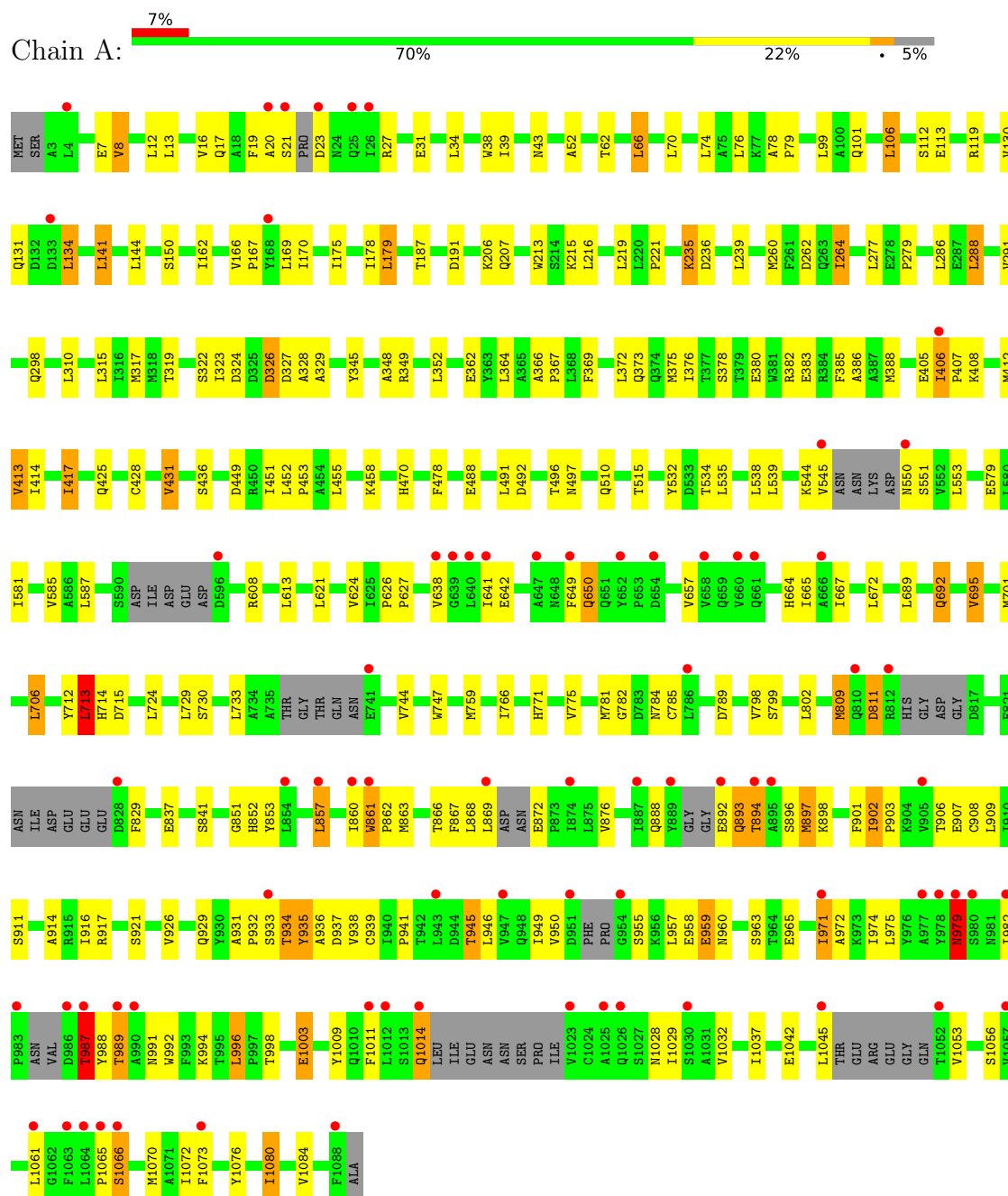
- Molecule 3 is water.

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

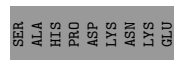
3 Residue-property plots

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



- Molecule 2: Protein STE12



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 , 0.255	Depositor DCC
R_{free} test set	3185 reflections (4.84%)	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 , 34.0	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	1.06	4/7986 (0.1%)	1.21	20/10880 (0.2%)
2	B	1.30	1/89 (1.1%)	1.26	0/119
All	All	1.06	5/8075 (0.1%)	1.21	20/10999 (0.2%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	621	LEU	N-CA	6.49	1.52	1.46
1	A	262	ASP	CA-C	-5.62	1.45	1.52
2	B	616	LYS	CA-C	5.19	1.59	1.52
1	A	455	LEU	N-CA	5.10	1.52	1.46
1	A	378	SER	C-O	5.04	1.30	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	979	ASN	N-CA-C	12.79	126.62	111.02
1	A	987	THR	N-CA-C	-9.05	101.39	111.07
1	A	936	ALA	N-CA-C	8.46	128.81	110.80
1	A	406	ILE	N-CA-CB	-8.00	100.01	111.21
1	A	431	VAL	CB-CA-C	-7.67	101.63	112.22
1	A	935	TYR	N-CA-C	6.98	123.55	114.75
1	A	782	GLY	N-CA-C	6.77	121.32	111.24
1	A	550	ASN	CA-C-N	6.15	128.43	120.44
1	A	550	ASN	C-N-CA	6.15	128.43	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	LEU	N-CA-C	5.95	120.69	113.38
1	A	279	PRO	N-CA-C	5.73	117.69	110.70
1	A	491	LEU	N-CA-C	5.69	117.16	111.07
1	A	497	ASN	N-CA-C	5.29	116.73	111.07
1	A	829	PHE	N-CA-C	-5.27	105.58	112.23
1	A	510	GLN	CA-C-N	5.21	127.21	120.44
1	A	510	GLN	C-N-CA	5.21	127.21	120.44
1	A	982	ILE	N-CA-C	5.12	114.09	108.05
1	A	713	LEU	N-CA-C	5.09	119.47	113.16
1	A	451	ILE	N-CA-C	5.05	115.28	110.53
1	A	27	ARG	N-CA-C	5.04	116.85	111.36

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	183	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	188	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 (188) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:892:GLU:CD	1:A:934:THR:HG22	1.92	0.93
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: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
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:NE1	1:A:897:MET:HE2	1.99	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:375:MET:HE2	1:A:383:GLU:O	1.88	0.73
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:901:PHE:C	1:A:903:PRO:HD2	2.18	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:B:615:ILE:HG22	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:715:ASP:HB2	1:A:766:ILE:HD11	1.82	0.62
1:A:375:MET:HE1	1:A:386:ALA:HB3	1.81	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
1:A:328:ALA:O	1:A:329:ALA:C	2.43	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:O	1:A:1080:ILE:HD12	2.05	0.56
1:A:20:ALA:O	1:A:21:SER:CB	2.54	0.56
1:A:893:GLN:CG	1:A:893:GLN:O	2.53	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:1003:GLU:H	1:A:1003:GLU:CD	2.13	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:369:PHE:CD1	1:A:412:MET:HE1	2.41	0.55
1:A:191:ASP:OD2	1:A:235:LYS:HG2	2.07	0.55
1:A:857:LEU:O	1:A:857:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:809:MET:C	1:A:811:ASP:H	2.16	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:933:SER:C	1:A:935:TYR:H	2.18	0.51
1:A:747:TRP:CG	1:A:781:MET:HG3	2.46	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:641:ILE:HG22	1:A:664:HIS:C	2.37	0.49
1:A:908:CYS:HB3	1:A:916:ILE:HG22	1.94	0.49
1:A:264:ILE:O	1:A:264:ILE:HG13	2.11	0.49
1:A:375:MET:HE3	1:A:383:GLU:HG2	1.94	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:O	1:A:893:GLN:HG2	2.13	0.48
1:A:939:CYS:HB3	1:A:974:ILE:HG12	1.95	0.48
1:A:170:ILE:HG23	1:A:178:ILE:HG12	1.96	0.48
1:A:897:MET:O	1:A:898:LYS:C	2.57	0.48
1:A:898:LYS:NZ	1:A:937:ASP:OD1	2.43	0.48
1:A:66:LEU:C	1:A:66:LEU:HD13	2.38	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:436:SER:HB3	1:A:478:PHE:HA	1.97	0.47
1:A:413:VAL:HG13	1:A:428:CYS:SG	2.55	0.46
1:A:1076:TYR:CG	1:A:1080:ILE:HD11	2.51	0.46
1:A:326:ASP:OD1	1:A:382:ARG:NH1	2.47	0.46
1:A:375:MET:CE	1:A:386:ALA:HB3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:692:GLN:HG2	1.55	0.46
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.96	0.46
1:A:695:VAL:O	1:A:695:VAL:CG2	2.62	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:369:PHE:CE1	1:A:412:MET:HE1	2.52	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:310:LEU:C	1:A:310:LEU:HD13	2.42	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:959:GLU:CD	1:A:959:GLU:H	2.22	0.44
1:A:934:THR:O	1:A:934:THR:OG1	2.29	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
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:213:TRP:C	1:A:215:LYS:H	2.27	0.43
1:A:38:TRP:CE3	1:A:43:ASN:HB3	2.54	0.43
1:A:317:MET:HB2	1:A:348:ALA:HB2	2.01	0.43
1:A:608:ARG:NH2	3:A:1178:HOH:O	2.52	0.42
1:A:1080:ILE:HD12	1:A:1080:ILE:C	2.44	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:747:TRP:CD1	1:A:781:MET:HG3	2.54	0.42
1:A:1073:PHE:HA	1:A:1076:TYR:CD2	2.54	0.42
1:A:957:LEU:O	1:A:958:GLU:C	2.62	0.42
1:A:946:LEU:HD13	1:A:971:ILE:HG22	2.02	0.42
1:A:532:TYR:CD2	1:A:532:TYR:C	2.98	0.41
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:66:LEU:HD13	1:A:66:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLN:CB	1:A:134:LEU:HD22	2.51	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:ND2	1:A:979:ASN:H	2.19	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:1011:PHE:HA	1:A:1014:GLN:HG3	2.03	0.41
1:A:326:ASP:CG	1:A:382:ARG:NH1	2.79	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:385:PHE:O	1:A:386:ALA:C	2.64	0.40
1:A:581:ILE:O	1:A:585:VAL:HG23	2.21	0.40
1:A:933:SER:C	1:A:935:TYR:N	2.80	0.40
1:A:78:ALA:N	1:A:79:PRO:HA	2.35	0.40
1:A:931:ALA:O	1:A:932:PRO:C	2.65	0.40
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.91	0.40
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.69	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 [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	1002/1078 (93%)	953 (95%)	45 (4%)	4 (0%)	30	34
2	B	10/69 (14%)	8 (80%)	2 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1012/1147 (88%)	961 (95%)	47 (5%)	4 (0%)	30	34

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%)	749 (89%)	96 (11%)	5	5
2	B	10/59 (17%)	9 (90%)	1 (10%)	7	7
All	All	855/996 (86%)	758 (89%)	97 (11%)	5	5

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	31	GLU
1	A	62	THR
1	A	66	LEU
1	A	74	LEU
1	A	101	GLN
1	A	106	LEU
1	A	113	GLU
1	A	134	LEU
1	A	141	LEU
1	A	150	SER
1	A	166	VAL
1	A	179	LEU
1	A	187	THR

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Mol	Chain	Res	Type
1	A	206	LYS
1	A	216	LEU
1	A	219	LEU
1	A	235	LYS
1	A	236	ASP
1	A	239	LEU
1	A	264	ILE
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	413	VAL
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	624	VAL
1	A	642	GLU
1	A	649	PHE
1	A	650	GLN
1	A	667	ILE
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
1	A	730	SER
1	A	733	LEU

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Mol	Chain	Res	Type
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	866	THR
1	A	868	LEU
1	A	869	LEU
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	929	GLN
1	A	934	THR
1	A	945	THR
1	A	950	VAL
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	994	LYS
1	A	996	LEU
1	A	1003	GLU
1	A	1014	GLN
1	A	1029	ILE
1	A	1042	GLU
1	A	1045	LEU
1	A	1056	SER
1	A	1066	SER
1	A	1080	ILE
2	B	613	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	303	ASN
1	A	430	ASN
1	A	434	GLN
1	A	510	GLN
1	A	541	ASN
1	A	801	ASN
1	A	856	ASN
1	A	888	GLN
1	A	893	GLN
1	A	918	GLN
1	A	966	ASN
1	A	979	ASN
1	A	981	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 oligosaccharides 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 ⓘ

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%)	0.25	74 (7%) 21 18	23, 48, 93, 131	0
2	B	12/69 (17%)	0.18	1 (8%) 17 15	27, 42, 66, 82	0
All	All	1040/1147 (90%)	0.25	75 (7%) 21 18	23, 47, 93, 131	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	828	ASP	5.7
1	A	983	PRO	5.6
1	A	596	ASP	5.3
1	A	982	ILE	5.2
1	A	1052	THR	5.0
1	A	1073	PHE	4.4
1	A	1025	ALA	4.2
1	A	986	ASP	3.8
1	A	1023	VAL	3.7
1	A	812	ARG	3.7
1	A	1045	LEU	3.6
1	A	661	GLN	3.5
1	A	895	ALA	3.4
1	A	4	LEU	3.3
1	A	894	THR	3.3
1	A	638	VAL	3.3
1	A	1014	GLN	3.3
1	A	869	LEU	3.2
1	A	892	GLU	3.2
1	A	905	VAL	3.2
1	A	990	ALA	3.1
1	A	545	VAL	3.1
1	A	639	GLY	3.1
1	A	1061	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	666	ALA	3.0
1	A	980	SER	2.9
1	A	641	ILE	2.9
2	B	617	THR	2.9
1	A	989	THR	2.8
1	A	978	TYR	2.8
1	A	954	GLY	2.8
1	A	26	ILE	2.7
1	A	857	LEU	2.7
1	A	652	TYR	2.7
1	A	889	TYR	2.7
1	A	861	TRP	2.7
1	A	987	THR	2.6
1	A	1065	PRO	2.6
1	A	654	ASP	2.5
1	A	887	ILE	2.5
1	A	971	ILE	2.5
1	A	23	ASP	2.4
1	A	860	ILE	2.4
1	A	951	ASP	2.4
1	A	741	GLU	2.4
1	A	1063	PHE	2.4
1	A	640	LEU	2.4
1	A	979	ASN	2.3
1	A	1030	SER	2.3
1	A	1057	VAL	2.3
1	A	658	VAL	2.3
1	A	168	TYR	2.3
1	A	943	LEU	2.3
1	A	649	PHE	2.2
1	A	1088	PHE	2.2
1	A	977	ALA	2.2
1	A	1066	SER	2.2
1	A	874	ILE	2.2
1	A	854	LEU	2.2
1	A	1026	GLN	2.2
1	A	20	ALA	2.2
1	A	647	ALA	2.2
1	A	406	ILE	2.2
1	A	1064	LEU	2.2
1	A	21	SER	2.2
1	A	1012	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1011	PHE	2.1
1	A	810	GLN	2.1
1	A	133	ASP	2.1
1	A	933	SER	2.1
1	A	786	LEU	2.1
1	A	660	VAL	2.1
1	A	947	VAL	2.1
1	A	25	GLN	2.0
1	A	550	ASN	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 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.