



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 3W3X / pdb_00003w3x
Title : Crystal structure of Kap121p bound to Pho4p
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

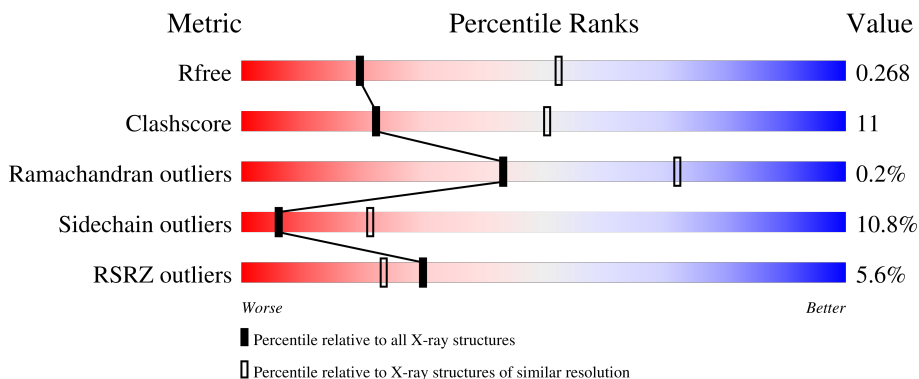
1 Overall quality at a glance

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	5% 73% 18% • 5%
2	B	27	19% 7% 11% 63%

2 Entry composition

There are 2 unique types of molecules 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
1	A	1021	Total	C	N	O	S	0	0	0
			7773	4994	1246	1498	35			

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

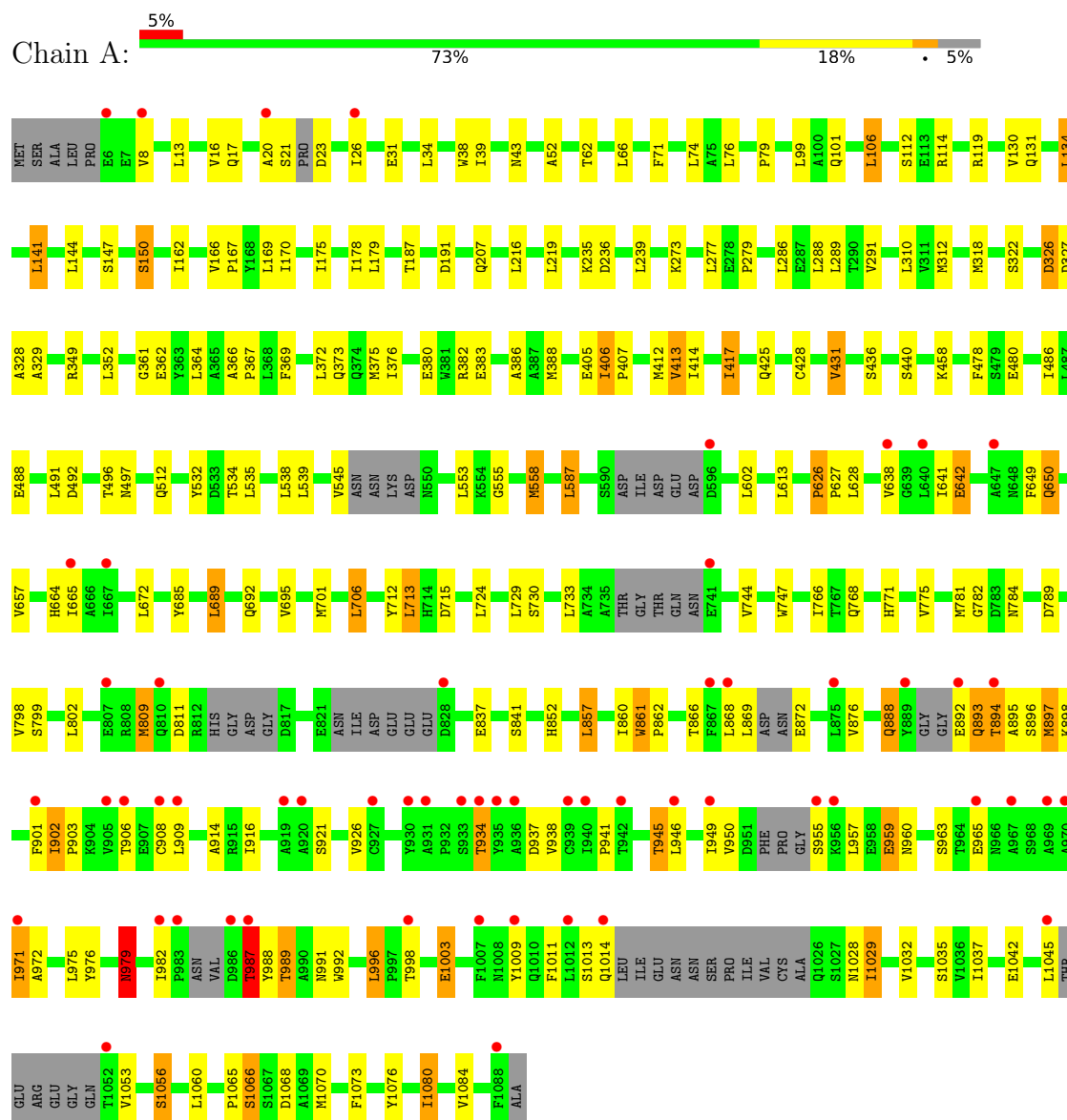
- Molecule 2 is a protein called Phosphate system positive regulatory protein PHO4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			76	45	16	15			

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



SER	K141	N142	K143	N147	K148	S149	N150	SER	PRO	TYR	LEU	ASN	LYS	ARG	ARG	GLY	LYS	PRO	GLY	PRO	ASP	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.09Å 126.31Å 128.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.50 – 2.90 29.50 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.50-2.90) 98.5 (29.50-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.224 , 0.268 0.224 , 0.268	Depositor DCC
R_{free} test set	1426 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7849	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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	0.74	0/7908	1.04	12/10781 (0.1%)
2	B	0.82	0/75	1.48	1/98 (1.0%)
All	All	0.74	0/7983	1.04	13/10879 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	979	ASN	N-CA-C	10.08	123.31	111.02
1	A	987	THR	N-CA-C	-7.17	102.51	111.11
2	B	143	LYS	N-CA-C	-6.39	99.86	109.96
1	A	982	ILE	N-CA-C	6.08	115.23	108.05
1	A	406	ILE	N-CA-CB	-6.07	102.71	111.21
1	A	491	LEU	N-CA-C	5.77	117.24	111.07
1	A	782	GLY	N-CA-C	5.58	119.55	111.24
1	A	279	PRO	N-CA-C	5.53	117.44	110.70
1	A	497	ASN	N-CA-C	5.37	116.81	111.07
1	A	1029	ILE	N-CA-C	5.26	115.88	110.36
1	A	626	PRO	N-CA-C	5.25	117.10	110.70
1	A	431	VAL	CB-CA-C	-5.21	105.03	112.22
1	A	364	LEU	N-CA-C	5.09	119.76	113.50

There are no chirality outliers.

There are no planarity outliers.

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	7773	0	7641	163	0
2	B	76	0	82	4	0
All	All	7849	0	7723	165	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 (165) 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:558:MET:SD	1:A:602:LEU:HD23	1.72	1.29
1:A:1011:PHE:CE1	1:A:1014:GLN:OE1	1.86	1.28
1:A:1011:PHE:CD1	1:A:1014:GLN:OE1	1.94	1.20
1:A:406:ILE:HG23	1:A:407:PRO:HD3	1.21	1.13
1:A:892:GLU:CB	1:A:934:THR:HG21	1.82	1.09
1:A:1009:TYR:HB3	1:A:1053:VAL:HG21	1.40	1.02
1:A:558:MET:SD	1:A:602:LEU:CD2	2.49	1.00
1:A:902:ILE:N	1:A:903:PRO:HD2	1.81	0.95
1:A:638:VAL:HG23	1:A:665:ILE:CG2	1.96	0.94
1:A:1011:PHE:HE1	1:A:1014:GLN:OE1	1.43	0.92
1:A:1011:PHE:HD1	1:A:1014:GLN:OE1	1.58	0.87
1:A:892:GLU:CB	1:A:934:THR:CG2	2.52	0.87
1:A:987:THR:HG23	1:A:991:ASN:HD21	1.40	0.86
1:A:406:ILE:CG2	1:A:407:PRO:HD3	2.04	0.85
1:A:558:MET:HE1	1:A:587:LEU:HD23	1.60	0.84
1:A:1011:PHE:O	1:A:1014:GLN:HG2	1.80	0.82
1:A:988:TYR:HA	1:A:991:ASN:HD22	1.49	0.78
1:A:894:THR:O	1:A:897:MET:HG3	1.83	0.78
2:B:147:ASN:C	2:B:148:LYS:HG2	2.09	0.77
1:A:1013:SER:HG	1:A:1056:SER:HG	1.29	0.77
1:A:965:GLU:HG2	1:A:998:THR:HG23	1.67	0.77
1:A:641:ILE:HG23	1:A:664:HIS:HB3	1.66	0.76
1:A:1011:PHE:HD1	1:A:1014:GLN:CD	1.93	0.76
1:A:534:THR:O	1:A:538:LEU:HD13	1.85	0.75
1:A:406:ILE:HG23	1:A:407:PRO:CD	2.11	0.75
1:A:987:THR:HG23	1:A:991:ASN:ND2	2.01	0.75
1:A:638:VAL:HG23	1:A:665:ILE:HG22	1.69	0.74
1:A:414:ILE:O	1:A:417:ILE:HG22	1.85	0.74
1:A:638:VAL:CG2	1:A:665:ILE:CG2	2.67	0.72
1:A:1011:PHE:CD1	1:A:1014:GLN:CD	2.68	0.72
1:A:1013:SER:OG	1:A:1056:SER:OG	2.00	0.72
1:A:480:GLU:OE2	2:B:143:LYS:NZ	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PHE:O	1:A:373:GLN:HG2	1.89	0.71
1:A:650:GLN:HG2	1:A:657:VAL:HG22	1.73	0.71
1:A:937:ASP:O	1:A:941:PRO:HG2	1.91	0.71
1:A:898:LYS:HG3	1:A:902:ILE:HD11	1.72	0.71
1:A:987:THR:HG22	1:A:988:TYR:N	2.06	0.70
1:A:626:PRO:HB2	1:A:627:PRO:HD3	1.73	0.70
1:A:902:ILE:N	1:A:903:PRO:CD	2.56	0.68
1:A:1066:SER:O	1:A:1070:MET:HG2	1.97	0.65
1:A:492:ASP:O	1:A:496:THR:HG23	1.97	0.64
1:A:638:VAL:CG2	1:A:665:ILE:HG23	2.29	0.63
1:A:558:MET:CE	1:A:587:LEU:HD23	2.28	0.62
1:A:987:THR:CG2	1:A:988:TYR:N	2.62	0.62
1:A:131:GLN:HB3	1:A:134:LEU:HB2	1.81	0.62
1:A:987:THR:CG2	1:A:991:ASN:HD21	2.11	0.62
1:A:893:GLN:HG2	1:A:893:GLN:O	2.00	0.62
1:A:901:PHE:C	1:A:903:PRO:HD2	2.25	0.62
1:A:375:MET:HE2	1:A:383:GLU:O	2.00	0.61
1:A:20:ALA:O	1:A:21:SER:HB2	1.99	0.61
1:A:641:ILE:HG22	1:A:664:HIS:O	2.01	0.60
1:A:908:CYS:HB3	1:A:916:ILE:HG22	1.82	0.60
1:A:975:LEU:HD22	1:A:989:THR:HG22	1.82	0.60
1:A:388:MET:SD	1:A:413:VAL:HG22	2.42	0.59
1:A:898:LYS:O	1:A:902:ILE:CG1	2.51	0.59
1:A:715:ASP:HB2	1:A:766:ILE:HD11	1.84	0.58
1:A:1003:GLU:H	1:A:1003:GLU:CD	2.12	0.58
1:A:170:ILE:HG23	1:A:178:ILE:HG12	1.87	0.57
1:A:972:ALA:HB2	1:A:992:TRP:NE1	2.19	0.56
1:A:712:TYR:CD1	1:A:713:LEU:HD13	2.39	0.56
1:A:638:VAL:HG23	1:A:665:ILE:HG23	1.85	0.56
1:A:1009:TYR:O	1:A:1053:VAL:HG22	2.06	0.55
1:A:971:ILE:HD11	1:A:992:TRP:HB2	1.89	0.55
1:A:902:ILE:HG21	1:A:938:VAL:HG11	1.89	0.54
1:A:747:TRP:CG	1:A:781:MET:HG3	2.43	0.54
1:A:898:LYS:NZ	1:A:937:ASP:OD1	2.41	0.54
1:A:898:LYS:O	1:A:902:ILE:HG12	2.08	0.54
1:A:893:GLN:O	1:A:893:GLN:CG	2.56	0.54
1:A:112:SER:O	1:A:119:ARG:NH2	2.42	0.53
1:A:1080:ILE:O	1:A:1080:ILE:HD12	2.08	0.53
1:A:20:ALA:O	1:A:21:SER:CB	2.57	0.53
1:A:1037:ILE:HD12	1:A:1084:VAL:HG22	1.90	0.53
1:A:809:MET:C	1:A:811:ASP:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ALA:O	1:A:329:ALA:C	2.51	0.52
1:A:650:GLN:CG	1:A:657:VAL:HG22	2.36	0.52
1:A:191:ASP:OD2	1:A:235:LYS:HG2	2.08	0.52
1:A:898:LYS:HG3	1:A:902:ILE:CD1	2.40	0.52
1:A:366:ALA:HB3	1:A:367:PRO:CD	2.40	0.52
1:A:945:THR:O	1:A:949:ILE:HG13	2.09	0.52
1:A:16:VAL:HG23	1:A:66:LEU:HD12	1.91	0.52
1:A:512:GLN:OE1	2:B:142:ASN:ND2	2.43	0.52
1:A:861:TRP:NE1	1:A:897:MET:HE2	2.25	0.52
1:A:76:LEU:O	1:A:79:PRO:HB3	2.10	0.51
1:A:861:TRP:HE1	1:A:897:MET:CE	2.22	0.51
1:A:144:LEU:HD21	1:A:162:ILE:HD12	1.92	0.51
1:A:861:TRP:N	1:A:862:PRO:HD2	2.24	0.51
1:A:372:LEU:O	1:A:376:ILE:HG12	2.12	0.50
1:A:413:VAL:HG13	1:A:428:CYS:SG	2.52	0.50
1:A:898:LYS:O	1:A:902:ILE:HG13	2.11	0.50
1:A:39:ILE:HG22	1:A:39:ILE:O	2.10	0.50
1:A:906:THR:HA	1:A:909:LEU:HD12	1.93	0.50
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.92	0.50
1:A:369:PHE:CD1	1:A:412:MET:HE1	2.47	0.50
1:A:641:ILE:HG22	1:A:664:HIS:C	2.36	0.50
1:A:641:ILE:HG12	1:A:642:GLU:N	2.27	0.50
1:A:934:THR:O	1:A:934:THR:OG1	2.30	0.50
1:A:946:LEU:CD1	1:A:971:ILE:HG22	2.42	0.49
1:A:417:ILE:O	1:A:425:GLN:HG2	2.12	0.49
1:A:861:TRP:NE1	1:A:897:MET:CE	2.75	0.49
1:A:914:ALA:O	1:A:963:SER:OG	2.22	0.49
1:A:66:LEU:C	1:A:66:LEU:HD13	2.38	0.49
1:A:1073:PHE:HA	1:A:1076:TYR:CD2	2.48	0.48
1:A:130:VAL:HG11	1:A:169:LEU:HD21	1.96	0.48
1:A:167:PRO:HG3	1:A:207:GLN:CB	2.44	0.47
1:A:641:ILE:CG2	1:A:664:HIS:HB3	2.42	0.47
1:A:366:ALA:HB3	1:A:367:PRO:HD3	1.97	0.47
1:A:976:TYR:HE1	1:A:1014:GLN:HE22	1.62	0.46
1:A:1009:TYR:O	1:A:1053:VAL:CG2	2.63	0.46
1:A:322:SER:O	1:A:382:ARG:NH2	2.46	0.46
1:A:417:ILE:HG13	1:A:458:LYS:HD3	1.97	0.46
1:A:1009:TYR:CB	1:A:1053:VAL:HG21	2.30	0.45
1:A:641:ILE:HG12	1:A:642:GLU:H	1.80	0.45
1:A:114:ARG:HA	1:A:114:ARG:HD2	1.90	0.45
1:A:369:PHE:CE1	1:A:412:MET:HE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:MET:O	1:A:898:LYS:C	2.59	0.45
1:A:768:GLN:HG3	1:A:837:GLU:HG3	1.98	0.45
1:A:558:MET:HE2	1:A:558:MET:HB3	1.82	0.45
2:B:147:ASN:O	2:B:148:LYS:HG2	2.16	0.45
1:A:13:LEU:HG	1:A:17:GLN:OE1	2.17	0.44
1:A:327:ASP:O	1:A:328:ALA:HB3	2.17	0.44
1:A:996:LEU:N	1:A:996:LEU:HD23	2.32	0.44
1:A:1028:ASN:O	1:A:1032:VAL:HG23	2.17	0.44
1:A:857:LEU:O	1:A:857:LEU:HD12	2.17	0.44
1:A:959:GLU:CD	1:A:959:GLU:H	2.23	0.44
1:A:175:ILE:HA	1:A:178:ILE:HG22	2.00	0.44
1:A:318:MET:HE2	1:A:349:ARG:HA	2.00	0.44
1:A:436:SER:HB3	1:A:478:PHE:HA	2.00	0.44
1:A:987:THR:HG22	1:A:988:TYR:H	1.77	0.44
1:A:361:GLY:O	1:A:362:GLU:C	2.61	0.43
1:A:988:TYR:O	1:A:991:ASN:HB2	2.18	0.43
1:A:558:MET:HE1	1:A:602:LEU:HD21	2.00	0.43
1:A:417:ILE:CG1	1:A:458:LYS:HD3	2.48	0.43
1:A:273:LYS:NZ	1:A:312:MET:SD	2.89	0.43
1:A:1009:TYR:OH	1:A:1035:SER:O	2.23	0.43
1:A:326:ASP:OD1	1:A:382:ARG:NH1	2.52	0.43
1:A:685:TYR:O	1:A:689:LEU:HB2	2.19	0.43
1:A:701:MET:HG3	1:A:706:LEU:HD22	2.00	0.43
1:A:147:SER:O	1:A:150:SER:HB3	2.19	0.43
1:A:406:ILE:CG2	1:A:407:PRO:CD	2.84	0.43
1:A:310:LEU:C	1:A:310:LEU:HD13	2.44	0.43
1:A:1076:TYR:CG	1:A:1080:ILE:HD11	2.54	0.43
1:A:52:ALA:HB1	1:A:106:LEU:HD13	2.01	0.42
1:A:695:VAL:O	1:A:695:VAL:HG22	2.17	0.42
1:A:375:MET:HE1	1:A:386:ALA:HB3	2.00	0.42
1:A:775:VAL:HG22	1:A:841:SER:HA	2.01	0.42
1:A:1073:PHE:HA	1:A:1076:TYR:HD2	1.84	0.42
1:A:979:ASN:ND2	1:A:979:ASN:H	2.16	0.42
1:A:771:HIS:O	1:A:775:VAL:HG23	2.20	0.42
1:A:532:TYR:CD2	1:A:532:TYR:C	2.98	0.42
1:A:959:GLU:N	1:A:959:GLU:OE1	2.52	0.42
1:A:555:GLY:O	1:A:558:MET:HG2	2.20	0.42
1:A:902:ILE:CG2	1:A:938:VAL:HG11	2.49	0.42
1:A:13:LEU:O	1:A:17:GLN:HG3	2.19	0.41
1:A:436:SER:O	1:A:440:SER:HB3	2.20	0.41
1:A:1065:PRO:HG2	1:A:1068:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TRP:CE3	1:A:43:ASN:HB3	2.55	0.41
1:A:798:VAL:O	1:A:802:LEU:HG	2.20	0.41
1:A:628:LEU:HD23	1:A:628:LEU:HA	1.89	0.41
1:A:799:SER:HB2	1:A:860:ILE:CG2	2.51	0.40
1:A:888:GLN:HE21	1:A:888:GLN:HB2	1.68	0.40
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.81	0.40
1:A:872:GLU:O	1:A:876:VAL:HG23	2.22	0.40
1:A:747:TRP:CD1	1:A:781:MET:HG3	2.57	0.40
1:A:895:ALA:C	1:A:897:MET:N	2.80	0.40
1:A:71:PHE:CD2	1:A:71:PHE:C	2.99	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	995/1078 (92%)	951 (96%)	42 (4%)	2 (0%)	43	72
2	B	8/27 (30%)	6 (75%)	2 (25%)	0	100	100
All	All	1003/1105 (91%)	957 (95%)	44 (4%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	852	HIS
1	A	8	VAL

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	833/937 (89%)	745 (89%)	88 (11%)	6	22
2	B	9/24 (38%)	6 (67%)	3 (33%)	0	0
All	All	842/961 (88%)	751 (89%)	91 (11%)	6	21

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	26	ILE
1	A	31	GLU
1	A	34	LEU
1	A	62	THR
1	A	74	LEU
1	A	101	GLN
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	216	LEU
1	A	219	LEU
1	A	236	ASP
1	A	239	LEU
1	A	277	LEU
1	A	286	LEU
1	A	288	LEU
1	A	289	LEU
1	A	291	VAL
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	486	ILE
1	A	488	GLU
1	A	535	LEU

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Mol	Chain	Res	Type
1	A	539	LEU
1	A	545	VAL
1	A	553	LEU
1	A	558	MET
1	A	587	LEU
1	A	613	LEU
1	A	642	GLU
1	A	649	PHE
1	A	650	GLN
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
1	A	744	VAL
1	A	784	ASN
1	A	789	ASP
1	A	809	MET
1	A	857	LEU
1	A	861	TRP
1	A	866	THR
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	921	SER
1	A	926	VAL
1	A	934	THR
1	A	945	THR
1	A	950	VAL
1	A	955	SER
1	A	957	LEU
1	A	959	GLU
1	A	960	ASN

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Mol	Chain	Res	Type
1	A	971	ILE
1	A	979	ASN
1	A	987	THR
1	A	989	THR
1	A	996	LEU
1	A	1003	GLU
1	A	1029	ILE
1	A	1042	GLU
1	A	1045	LEU
1	A	1056	SER
1	A	1060	LEU
1	A	1066	SER
1	A	1080	ILE
2	B	142	ASN
2	B	148	LYS
2	B	149	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	303	ASN
1	A	468	GLN
1	A	510	GLN
1	A	541	ASN
1	A	692	GLN
1	A	801	ASN
1	A	856	ASN
1	A	888	GLN
1	A	893	GLN
1	A	899	ASN
1	A	918	GLN
1	A	979	ASN
1	A	991	ASN
1	A	1014	GLN
2	B	150	ASN

5.3.3 RNA ⓘ

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 [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	1021/1078 (94%)	0.07	58 (5%) 29 23	30, 68, 147, 212	0
2	B	10/27 (37%)	-0.27	0 100 100	38, 49, 72, 85	0
All	All	1031/1105 (93%)	0.06	58 (5%) 30 23	30, 68, 147, 212	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	946	LEU	5.2
1	A	905	VAL	5.2
1	A	983	PRO	4.5
1	A	1045	LEU	4.0
1	A	596	ASP	3.8
1	A	971	ILE	3.6
1	A	828	ASP	3.5
1	A	894	THR	3.4
1	A	908	CYS	3.2
1	A	969	ALA	3.1
1	A	982	ILE	3.1
1	A	939	CYS	3.1
1	A	8	VAL	3.0
1	A	867	PHE	3.0
1	A	901	PHE	2.9
1	A	741	GLU	2.9
1	A	6	GLU	2.8
1	A	1009	TYR	2.8
1	A	933	SER	2.7
1	A	940	ILE	2.7
1	A	1007	PHE	2.7
1	A	967	ALA	2.6
1	A	1012	LEU	2.6
1	A	647	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	931	ALA	2.5
1	A	1014	GLN	2.5
1	A	667	ILE	2.5
1	A	955	SER	2.5
1	A	892	GLU	2.4
1	A	810	GLN	2.4
1	A	942	THR	2.4
1	A	998	THR	2.3
1	A	987	THR	2.3
1	A	935	TYR	2.3
1	A	919	ALA	2.3
1	A	875	LEU	2.2
1	A	889	TYR	2.2
1	A	909	LEU	2.2
1	A	956	LYS	2.2
1	A	868	LEU	2.2
1	A	665	ILE	2.2
1	A	906	THR	2.2
1	A	927	CYS	2.2
1	A	20	ALA	2.2
1	A	807	GLU	2.2
1	A	934	THR	2.1
1	A	930	TYR	2.1
1	A	949	ILE	2.1
1	A	986	ASP	2.1
1	A	640	LEU	2.1
1	A	920	ALA	2.1
1	A	936	ALA	2.1
1	A	970	ALA	2.1
1	A	26	ILE	2.1
1	A	1088	PHE	2.0
1	A	638	VAL	2.0
1	A	1052	THR	2.0
1	A	965	GLU	2.0

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

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.