



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:55 PM UTC

PDB ID : 6AHO / pdb_00006aho
Title : Crystal structure of Kap114p
Authors : Liao, C.C.; Shankar, S.; Ahmed, G.R.; Hsia, K.C.
Deposited on : 2018-08-20
Resolution : 2.50 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

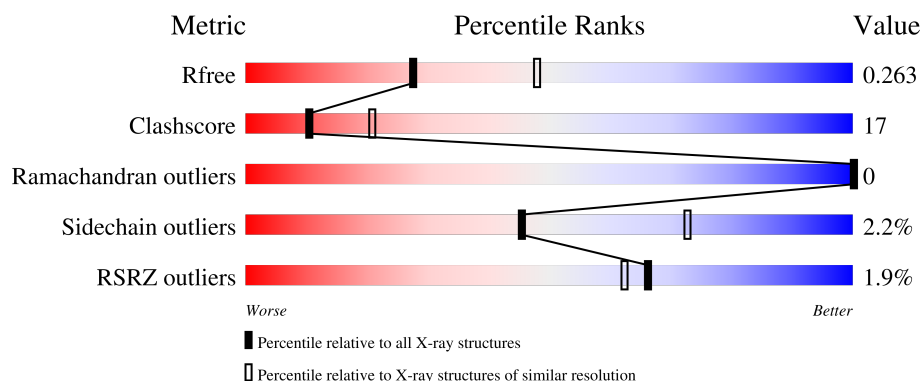
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1009	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7294 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-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	916	Total	C	N	O	S	0	0	0
			7294	4681	1175	1406	32			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P53067
A	-3	PRO	-	expression tag	UNP P53067
A	-2	LEU	-	expression tag	UNP P53067
A	-1	GLY	-	expression tag	UNP P53067
A	0	SER	-	expression tag	UNP P53067

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.62Å 116.62Å 189.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.97-2.50) 98.5 (19.97-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.50Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.211 , 0.263 0.212 , 0.263	Depositor DCC
R_{free} test set	1993 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7294	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.45	1/7407 (0.0%)	0.72	8/10036 (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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	ILE	CG1-CD1	-5.62	1.29	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ASP	CA-C-N	-10.56	108.11	119.83
1	A	122	ASP	C-N-CA	-10.56	108.11	119.83
1	A	25	LEU	CA-CB-CG	-9.14	84.30	116.30
1	A	123	PHE	N-CA-CB	7.13	117.17	110.39
1	A	6	LEU	CB-CG-CD2	-5.75	93.44	110.70
1	A	23	THR	N-CA-CB	5.09	117.91	110.47
1	A	120	ALA	CA-C-N	-5.03	113.55	120.74
1	A	120	ALA	C-N-CA	-5.03	113.55	120.74

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	440	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	545	GLU	Peptide
1	A	897	GLN	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	7294	0	7413	249	0
All	All	7294	0	7413	249	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 17.

All (249) 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:62:ARG:HH21	1:A:117:GLN:NE2	1.14	1.43
1:A:62:ARG:NH2	1:A:117:GLN:NE2	1.79	1.30
1:A:19:GLU:OE1	1:A:22:GLU:HG2	1.47	1.13
1:A:288:VAL:HG13	1:A:307:VAL:HG23	1.35	1.06
1:A:988:TYR:HA	1:A:991:LEU:HD13	1.43	0.98
1:A:62:ARG:NH2	1:A:117:GLN:HE21	1.56	0.96
1:A:19:GLU:OE1	1:A:22:GLU:CG	2.23	0.86
1:A:288:VAL:HG13	1:A:307:VAL:CG2	2.06	0.85
1:A:62:ARG:NH2	1:A:117:GLN:HE22	1.58	0.81
1:A:443:GLU:N	1:A:443:GLU:OE2	2.13	0.81
1:A:409:LEU:HD23	1:A:455:ILE:HD11	1.63	0.80
1:A:153:ILE:HG23	1:A:157:VAL:HG22	1.63	0.80
1:A:557:SER:HG	1:A:601:CYS:HG	1.12	0.80
1:A:153:ILE:HG23	1:A:157:VAL:CG2	2.11	0.79
1:A:987:ILE:O	1:A:991:LEU:CD1	2.31	0.78
1:A:7:ILE:HG21	1:A:56:PHE:CE2	2.19	0.77
1:A:61:LEU:CD1	1:A:65:ILE:HD11	2.15	0.77
1:A:6:LEU:HD21	1:A:25:LEU:HD22	1.67	0.77
1:A:62:ARG:CZ	1:A:117:GLN:NE2	2.48	0.76
1:A:21:ALA:HA	1:A:24:GLN:HB3	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:ILE:HD11	1:A:825:ARG:HB3	1.68	0.76
1:A:798:PHE:CE2	1:A:800:ILE:HD11	2.20	0.75
1:A:719:GLU:OE1	1:A:755:ARG:NH2	2.17	0.75
1:A:807:THR:HG22	1:A:811:ARG:HD2	1.69	0.74
1:A:155:ASP:OD1	1:A:155:ASP:N	2.21	0.72
1:A:69:TRP:NE1	1:A:122:ASP:OD2	2.22	0.72
1:A:881:THR:HG22	1:A:987:ILE:HG12	1.72	0.71
1:A:62:ARG:HH21	1:A:117:GLN:HE22	0.72	0.71
1:A:988:TYR:CA	1:A:991:LEU:HD13	2.18	0.71
1:A:964:SER:HB3	1:A:967:GLN:HG3	1.73	0.70
1:A:20:VAL:O	1:A:24:GLN:HB2	1.92	0.70
1:A:829:ASN:O	1:A:833:LEU:HD12	1.92	0.70
1:A:512:CYS:HB3	1:A:558:GLN:OE1	1.91	0.69
1:A:444:ASN:HA	1:A:447:VAL:HG22	1.72	0.69
1:A:985:HIS:O	1:A:989:GLU:HG2	1.94	0.68
1:A:3:ILE:HA	1:A:6:LEU:HD13	1.76	0.67
1:A:794:PHE:HD2	1:A:795:LEU:HD12	1.60	0.67
1:A:424:ASP:OD1	1:A:425:GLU:N	2.28	0.67
1:A:59:LEU:HA	1:A:62:ARG:HB3	1.76	0.66
1:A:62:ARG:CZ	1:A:117:GLN:HE21	2.08	0.66
1:A:467:LEU:HD13	1:A:481:THR:HG22	1.77	0.66
1:A:784:THR:HG22	1:A:791:THR:HG21	1.77	0.66
1:A:24:GLN:O	1:A:27:GLN:HB2	1.95	0.66
1:A:2:ASP:OD1	1:A:6:LEU:HD12	1.96	0.66
1:A:6:LEU:HD23	1:A:7:ILE:HD12	1.78	0.65
1:A:962:LYS:HD2	1:A:962:LYS:N	2.11	0.65
1:A:29:CYS:SG	1:A:68:TYR:CZ	2.89	0.65
1:A:83:GLU:OE2	1:A:86:VAL:HG23	1.97	0.65
1:A:6:LEU:HD21	1:A:25:LEU:CD2	2.26	0.65
1:A:765:ILE:HD11	1:A:800:ILE:HG21	1.79	0.65
1:A:987:ILE:O	1:A:991:LEU:HD13	1.96	0.65
1:A:988:TYR:CE1	1:A:996:ARG:HG3	2.32	0.65
1:A:37:PHE:HB3	1:A:90:ILE:HD11	1.77	0.65
1:A:243:VAL:HA	1:A:246:GLN:HB2	1.79	0.64
1:A:5:GLU:HA	1:A:8:ILE:HB	1.78	0.64
1:A:11:GLN:O	1:A:18:ARG:NH1	2.31	0.64
1:A:34:SER:OG	1:A:83:GLU:N	2.30	0.63
1:A:42:ASN:O	1:A:46:GLN:HG2	1.98	0.63
1:A:707:MET:HB3	1:A:745:PHE:HZ	1.64	0.63
1:A:795:LEU:HD23	1:A:809:VAL:HG21	1.81	0.62
1:A:159:SER:H	1:A:162:MET:HE3	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG21	1:A:56:PHE:HE2	1.63	0.61
1:A:963:GLU:HB3	1:A:967:GLN:HB2	1.83	0.61
1:A:65:ILE:HG23	1:A:69:TRP:CE3	2.36	0.61
1:A:765:ILE:CD1	1:A:800:ILE:HG21	2.32	0.60
1:A:622:LEU:O	1:A:626:ILE:HD12	2.02	0.60
1:A:7:ILE:CD1	1:A:25:LEU:HD13	2.31	0.59
1:A:182:THR:HG22	1:A:184:THR:H	1.68	0.59
1:A:780:LEU:O	1:A:784:THR:HG23	2.03	0.59
1:A:69:TRP:CZ2	1:A:87:LYS:HB2	2.38	0.58
1:A:61:LEU:HD13	1:A:65:ILE:HD11	1.86	0.58
1:A:84:ILE:HG13	1:A:87:LYS:HE3	1.85	0.58
1:A:84:ILE:O	1:A:87:LYS:HG2	2.03	0.58
1:A:131:LEU:O	1:A:135:TYR:HD1	1.86	0.58
1:A:87:LYS:HG3	1:A:88:ASP:N	2.17	0.58
1:A:477:ILE:O	1:A:481:THR:HG23	2.04	0.58
1:A:56:PHE:CZ	1:A:60:SER:HB3	2.39	0.58
1:A:91:ARG:HD3	1:A:127:TRP:CE2	2.38	0.58
1:A:103:GLU:HG3	1:A:104:ASN:H	1.69	0.58
1:A:436:GLN:O	1:A:440:LYS:HB2	2.04	0.58
1:A:204:MET:HE1	1:A:222:CYS:HB2	1.84	0.57
1:A:446:LEU:HB3	1:A:491:LEU:HD11	1.86	0.57
1:A:516:GLU:HG2	1:A:518:ASP:OD1	2.05	0.57
1:A:644:SER:O	1:A:648:GLU:HG3	2.05	0.57
1:A:897:GLN:HB3	1:A:898:PRO:HD3	1.86	0.57
1:A:61:LEU:HD12	1:A:65:ILE:HD11	1.87	0.56
1:A:987:ILE:O	1:A:991:LEU:HD12	2.03	0.56
1:A:433:GLN:O	1:A:437:ILE:HG13	2.06	0.56
1:A:188:ILE:HD12	1:A:188:ILE:H	1.70	0.56
1:A:62:ARG:HA	1:A:65:ILE:HD12	1.87	0.55
1:A:91:ARG:HD3	1:A:127:TRP:CD2	2.41	0.55
1:A:341:LEU:HB3	1:A:372:VAL:HG11	1.89	0.55
1:A:153:ILE:HG23	1:A:157:VAL:HG21	1.87	0.55
1:A:187:LEU:CD2	1:A:245:SER:HB3	2.36	0.55
1:A:703:ASP:OD1	1:A:704:THR:N	2.40	0.55
1:A:698:LEU:O	1:A:702:THR:HG23	2.07	0.55
1:A:849:VAL:HG21	1:A:882:LYS:HG2	1.89	0.55
1:A:21:ALA:HB1	1:A:25:LEU:HD12	1.88	0.54
1:A:980:ASP:CG	1:A:985:HIS:HD1	2.15	0.54
1:A:7:ILE:HG13	1:A:10:ALA:HB3	1.89	0.54
1:A:60:SER:O	1:A:64:LEU:HD23	2.07	0.54
1:A:895:SER:O	1:A:897:GLN:HG3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLN:HB3	1:A:48:GLU:CG	2.38	0.54
1:A:61:LEU:HD13	1:A:65:ILE:CG1	2.38	0.54
1:A:204:MET:CE	1:A:219:VAL:HA	2.37	0.54
1:A:663:LEU:HB2	1:A:702:THR:HG22	1.90	0.54
1:A:548:THR:O	1:A:552:LEU:HG	2.07	0.53
1:A:452:PRO:O	1:A:455:ILE:HG22	2.07	0.53
1:A:73:PHE:O	1:A:73:PHE:CD1	2.61	0.53
1:A:105:THR:HA	1:A:108:LYS:HE3	1.89	0.53
1:A:83:GLU:OE2	1:A:86:VAL:N	2.39	0.53
1:A:7:ILE:HD11	1:A:25:LEU:HD13	1.89	0.53
1:A:250:LYS:HE2	1:A:284:ASP:CG	2.34	0.53
1:A:173:MET:HE2	1:A:222:CYS:HB3	1.91	0.53
1:A:360:VAL:HG11	1:A:548:THR:HB	1.90	0.53
1:A:153:ILE:CG2	1:A:157:VAL:HG22	2.37	0.52
1:A:801:ASP:O	1:A:802:ASN:ND2	2.41	0.52
1:A:37:PHE:HB3	1:A:90:ILE:CD1	2.40	0.52
1:A:62:ARG:NE	1:A:117:GLN:NE2	2.57	0.52
1:A:5:GLU:O	1:A:8:ILE:HG22	2.10	0.52
1:A:385:ASN:ND2	1:A:424:ASP:OD1	2.42	0.52
1:A:557:SER:OG	1:A:601:CYS:SG	2.38	0.52
1:A:707:MET:HE2	1:A:714:ILE:HD11	1.92	0.52
1:A:2:ASP:HB3	1:A:3:ILE:HD12	1.92	0.51
1:A:2:ASP:O	1:A:6:LEU:HB2	2.10	0.51
1:A:571:LYS:O	1:A:575:GLN:HG3	2.10	0.51
1:A:572:GLU:OE2	1:A:572:GLU:N	2.35	0.51
1:A:464:PRO:HG3	1:A:511:TYR:CE2	2.45	0.51
1:A:187:LEU:HD21	1:A:245:SER:HB3	1.92	0.51
1:A:46:GLN:HB3	1:A:48:GLU:HG3	1.92	0.51
1:A:441:THR:O	1:A:445:ILE:HD13	2.11	0.51
1:A:104:ASN:HB3	1:A:107:ILE:HG12	1.93	0.51
1:A:7:ILE:O	1:A:7:ILE:CG2	2.59	0.51
1:A:811:ARG:NH1	1:A:848:VAL:O	2.43	0.51
1:A:21:ALA:HB1	1:A:25:LEU:CD1	2.40	0.50
1:A:446:LEU:HD11	1:A:463:ILE:HD11	1.92	0.50
1:A:807:THR:O	1:A:811:ARG:HG3	2.10	0.50
1:A:311:SER:HA	1:A:314:ILE:HD12	1.92	0.50
1:A:485:LEU:O	1:A:489:LEU:HD22	2.12	0.50
1:A:65:ILE:HG21	1:A:118:ILE:CD1	2.42	0.50
1:A:529:THR:O	1:A:533:VAL:HG13	2.12	0.49
1:A:811:ARG:O	1:A:815:GLU:HG3	2.12	0.49
1:A:987:ILE:HG22	1:A:991:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:OE2	1:A:74:GLU:N	2.46	0.49
1:A:614:TYR:CE2	1:A:667:ILE:HD11	2.47	0.49
1:A:569:SER:O	1:A:570:ARG:HG2	2.13	0.48
1:A:973:PHE:CD1	1:A:999:LEU:HD21	2.48	0.48
1:A:29:CYS:SG	1:A:30:ASP:N	2.86	0.48
1:A:823:GLU:HG2	1:A:827:LYS:HE3	1.95	0.48
1:A:271:SER:O	1:A:275:LYS:HG3	2.13	0.48
1:A:335:ILE:O	1:A:339:THR:OG1	2.27	0.48
1:A:351:ILE:CG2	1:A:358:THR:HG21	2.43	0.48
1:A:673:GLU:HG3	1:A:674:PRO:HD3	1.95	0.48
1:A:386:PRO:O	1:A:390:LEU:HG	2.13	0.48
1:A:21:ALA:HA	1:A:24:GLN:CB	2.39	0.48
1:A:395:VAL:O	1:A:399:ILE:HG13	2.14	0.48
1:A:440:LYS:HA	1:A:443:GLU:CD	2.39	0.48
1:A:445:ILE:HG21	1:A:459:ALA:CB	2.43	0.48
1:A:123:PHE:O	1:A:124:PRO:C	2.56	0.48
1:A:7:ILE:O	1:A:7:ILE:HG22	2.14	0.47
1:A:91:ARG:HB3	1:A:127:TRP:CZ2	2.49	0.47
1:A:10:ALA:HB2	1:A:21:ALA:HB3	1.95	0.47
1:A:62:ARG:HE	1:A:117:GLN:NE2	2.11	0.47
1:A:61:LEU:HD12	1:A:114:CYS:SG	2.54	0.47
1:A:400:GLU:OE1	1:A:441:THR:HG21	2.14	0.47
1:A:805:ALA:O	1:A:809:VAL:HG23	2.15	0.47
1:A:707:MET:HB3	1:A:745:PHE:CZ	2.47	0.47
1:A:34:SER:O	1:A:86:VAL:HG11	2.14	0.47
1:A:61:LEU:HD13	1:A:65:ILE:CD1	2.44	0.47
1:A:204:MET:HE3	1:A:219:VAL:HA	1.96	0.47
1:A:988:TYR:HA	1:A:991:LEU:CD1	2.29	0.47
1:A:351:ILE:HG22	1:A:358:THR:HG21	1.97	0.46
1:A:822:GLY:O	1:A:826:ILE:HG13	2.15	0.46
1:A:87:LYS:O	1:A:91:ARG:HG3	2.16	0.46
1:A:34:SER:HA	1:A:82:VAL:HG23	1.97	0.46
1:A:546:GLU:HG3	1:A:591:ASN:HD22	1.80	0.46
1:A:83:GLU:CD	1:A:85:ASP:H	2.23	0.46
1:A:17:THR:O	1:A:20:VAL:HG22	2.15	0.46
1:A:398:ASP:HB3	1:A:412:LEU:HD11	1.98	0.46
1:A:153:ILE:CG2	1:A:157:VAL:CG2	2.90	0.45
1:A:390:LEU:O	1:A:394:VAL:HG23	2.15	0.45
1:A:7:ILE:HD12	1:A:25:LEU:HD13	1.97	0.45
1:A:103:GLU:O	1:A:108:LYS:HE2	2.17	0.45
1:A:471:ILE:HG13	1:A:477:ILE:HG12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:VAL:O	1:A:796:SER:HB3	2.16	0.45
1:A:961:VAL:HG11	1:A:968:LEU:HD11	1.99	0.45
1:A:49:ALA:HB3	1:A:54:ARG:HG3	1.98	0.45
1:A:62:ARG:HD3	1:A:113:TYR:HB3	1.98	0.45
1:A:7:ILE:HG23	1:A:10:ALA:HB3	1.99	0.45
1:A:679:LEU:O	1:A:720:ARG:NH1	2.50	0.45
1:A:722:LEU:O	1:A:763:ARG:HD3	2.16	0.44
1:A:7:ILE:O	1:A:8:ILE:C	2.60	0.44
1:A:173:MET:HE3	1:A:177:PHE:CZ	2.53	0.44
1:A:33:ALA:HB3	1:A:81:ASN:O	2.17	0.44
1:A:61:LEU:HD13	1:A:65:ILE:HG13	1.99	0.44
1:A:553:MET:CG	1:A:597:GLN:HB2	2.48	0.44
1:A:788:PRO:O	1:A:792:VAL:HG23	2.17	0.44
1:A:451:ILE:HG13	1:A:455:ILE:HG23	2.00	0.44
1:A:19:GLU:O	1:A:20:VAL:C	2.61	0.44
1:A:65:ILE:HG21	1:A:118:ILE:HD13	2.00	0.44
1:A:385:ASN:N	1:A:386:PRO:HD2	2.33	0.44
1:A:537:ILE:HD11	1:A:555:VAL:HG12	1.99	0.43
1:A:3:ILE:HG13	1:A:6:LEU:HD13	1.99	0.43
1:A:157:VAL:O	1:A:162:MET:HE1	2.18	0.43
1:A:409:LEU:CD2	1:A:455:ILE:HD11	2.40	0.43
1:A:715:MET:O	1:A:719:GLU:HG3	2.17	0.43
1:A:873:ARG:HG2	1:A:873:ARG:HH11	1.83	0.43
1:A:15:LYS:HG3	1:A:18:ARG:HG3	2.00	0.43
1:A:546:GLU:HG3	1:A:591:ASN:ND2	2.33	0.43
1:A:363:GLU:OE1	1:A:461:LEU:HD13	2.19	0.43
1:A:758:GLU:O	1:A:762:VAL:HG13	2.19	0.43
1:A:498:GLU:OE2	1:A:543:ASP:HB2	2.18	0.43
1:A:71:PRO:HA	1:A:72:GLY:HA3	1.83	0.43
1:A:251:SER:HB3	1:A:310:CYS:HA	2.01	0.43
1:A:442:LEU:O	1:A:446:LEU:HD12	2.18	0.43
1:A:87:LYS:HD2	1:A:91:ARG:NH2	2.34	0.43
1:A:525:VAL:O	1:A:528:GLU:HG2	2.19	0.43
1:A:227:LEU:HA	1:A:227:LEU:HD23	1.80	0.42
1:A:728:ASP:O	1:A:732:MET:HG3	2.19	0.42
1:A:986:CYS:O	1:A:990:THR:HG23	2.19	0.42
1:A:439:ILE:O	1:A:443:GLU:OE2	2.37	0.42
1:A:59:LEU:HA	1:A:62:ARG:CB	2.48	0.42
1:A:71:PRO:HG3	1:A:75:SER:OG	2.19	0.42
1:A:444:ASN:HA	1:A:447:VAL:CG2	2.47	0.42
1:A:452:PRO:HD2	1:A:455:ILE:HG21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:SER:OG	1:A:843:ARG:HD2	2.19	0.42
1:A:973:PHE:CG	1:A:999:LEU:HD21	2.55	0.42
1:A:278:LYS:O	1:A:282:ILE:HG13	2.19	0.42
1:A:3:ILE:HD11	1:A:28:TRP:HH2	1.85	0.42
1:A:103:GLU:HG3	1:A:104:ASN:N	2.33	0.42
1:A:169:GLY:O	1:A:173:MET:HG2	2.20	0.41
1:A:384:PRO:HG2	1:A:387:GLN:OE1	2.20	0.41
1:A:386:PRO:HG2	1:A:387:GLN:OE1	2.20	0.41
1:A:33:ALA:O	1:A:36:VAL:HG12	2.21	0.41
1:A:435:LEU:O	1:A:439:ILE:HG12	2.20	0.41
1:A:823:GLU:CG	1:A:827:LYS:HE3	2.49	0.41
1:A:666:GLU:N	1:A:666:GLU:OE1	2.51	0.41
1:A:677:LYS:O	1:A:678:VAL:C	2.62	0.41
1:A:116:VAL:O	1:A:119:SER:OG	2.39	0.41
1:A:744:ARG:HG3	1:A:744:ARG:HH11	1.85	0.41
1:A:757:LEU:HG	1:A:783:LEU:HD13	2.03	0.41
1:A:33:ALA:HA	1:A:36:VAL:HG12	2.03	0.41
1:A:872:ASP:OD1	1:A:872:ASP:N	2.51	0.41
1:A:3:ILE:HD12	1:A:3:ILE:H	1.86	0.41
1:A:622:LEU:HD13	1:A:671:LEU:HD13	2.03	0.41
1:A:357:ASN:HA	1:A:548:THR:HG21	2.03	0.41
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.86	0.40
1:A:589:PRO:HB3	1:A:642:LEU:HD13	2.04	0.40
1:A:331:MET:SD	1:A:391:ILE:HD12	2.62	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	900/1009 (89%)	851 (95%)	49 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	846/931 (91%)	827 (98%)	19 (2%)	45 73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	CYS
1	A	125	ASP
1	A	155	ASP
1	A	369	SER
1	A	443	GLU
1	A	458	ARG
1	A	482	SER
1	A	519	SER
1	A	529	THR
1	A	533	VAL
1	A	542	SER
1	A	548	THR
1	A	569	SER
1	A	734	VAL
1	A	767	THR
1	A	786	ASN
1	A	959	MET
1	A	979	LYS
1	A	994	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	129	GLN
1	A	274	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	283	GLN
1	A	308	HIS
1	A	325	GLN
1	A	385	ASN
1	A	668	ASN
1	A	786	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 [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	916/1009 (90%)	-0.08	17 (1%) 66 62	54, 78, 129, 159	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ILE	3.6
1	A	121	VAL	2.9
1	A	871	PRO	2.9
1	A	67	MET	2.8
1	A	902	GLN	2.8
1	A	157	VAL	2.7
1	A	567	PRO	2.7
1	A	26	LEU	2.6
1	A	10	ALA	2.5
1	A	82	VAL	2.5
1	A	855	PRO	2.4
1	A	16	HIS	2.3
1	A	73	PHE	2.3
1	A	302	PRO	2.3
1	A	17	THR	2.2
1	A	241	VAL	2.1
1	A	903	LEU	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.