



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 03:13 AM UTC

PDB ID : 1KJU / pdb_00001kju
Title : Ca²⁺-ATPase in the E2 State
Authors : Xu, C.; Rice, W.J.; He, W.; Stokes, D.L.
Deposited on : 2001-12-05
Resolution : 6.00 Å(reported)
Based on initial model : 1EUL

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

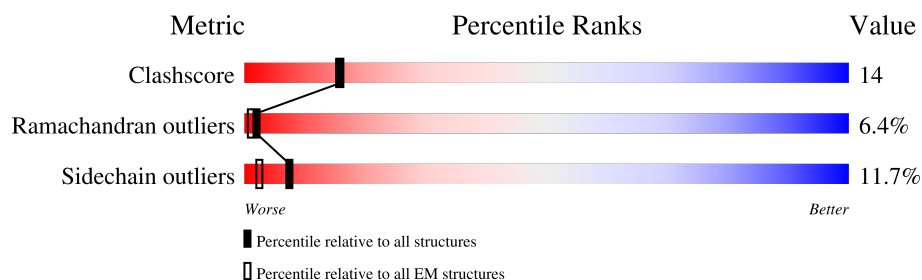
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	994	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7671 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	994	Total	C	N	O	S	0	0
			7671	4876	1287	1451	57		

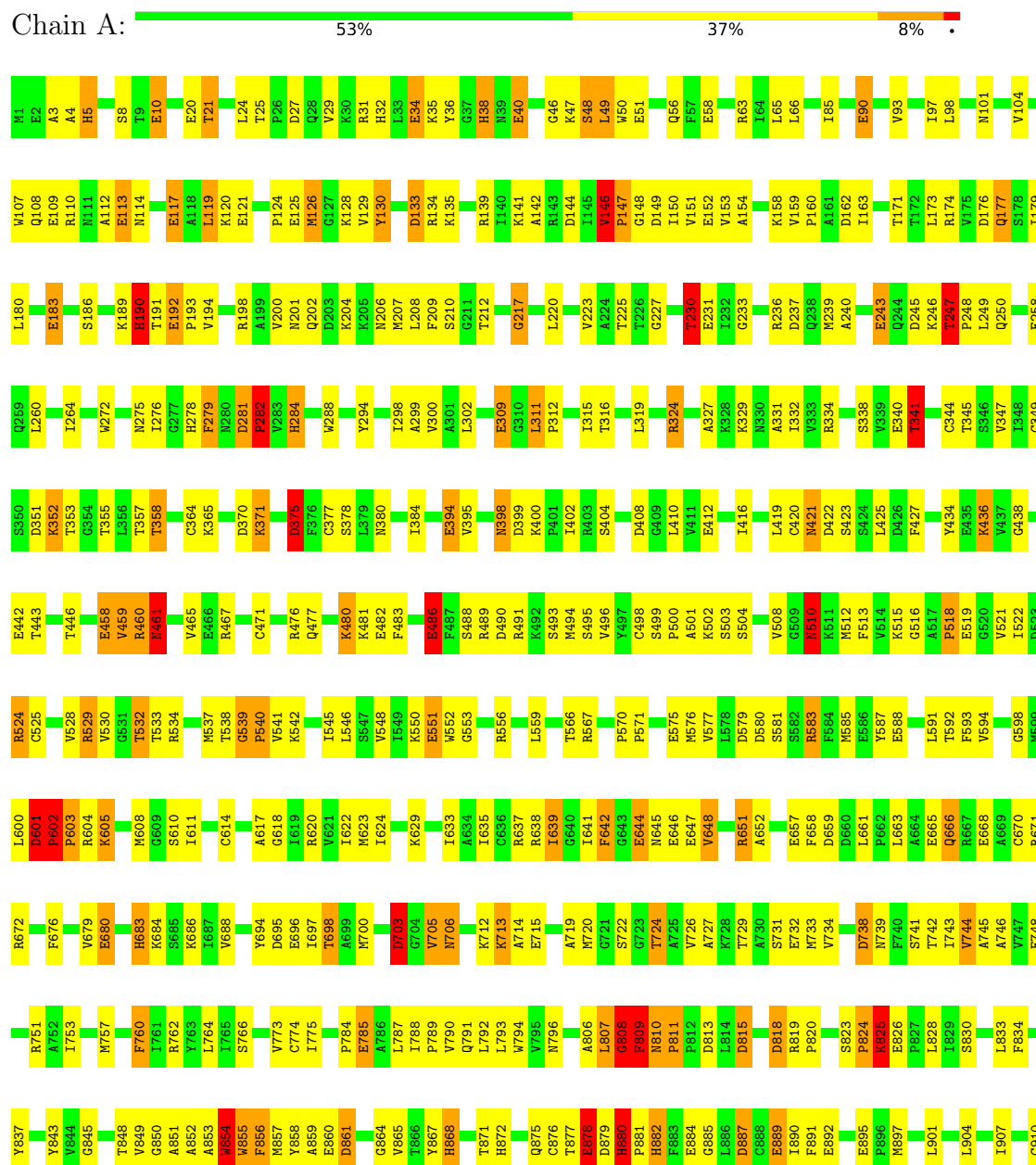
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

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. 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. 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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1a





4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 6.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-6.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

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	0.69	13/7812 (0.2%)	1.58	103/10592 (1.0%)

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	21

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	HIS	CD2-NE2	-7.17	1.29	1.37
1	A	5	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	683	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	278	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	882	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	38	HIS	CD2-NE2	-6.73	1.30	1.37
1	A	880	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	944	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	190	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	32	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	868	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	872	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	882	HIS	CG-ND1	-5.32	1.32	1.38

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	PRO	N-CA-C	10.86	123.94	110.70
1	A	604	ARG	O-C-N	-9.13	113.09	123.40
1	A	670	CYS	N-CA-C	9.07	123.36	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	ASP	CA-CB-CG	8.98	121.58	112.60
1	A	861	ASP	CA-CB-CG	8.15	120.75	112.60
1	A	282	PRO	N-CA-C	8.15	129.25	112.47
1	A	34	GLU	CA-CB-CG	7.73	129.57	114.10
1	A	880	HIS	CB-CG-CD2	-7.61	121.31	131.20
1	A	746	ALA	N-CA-C	-7.60	102.83	112.93
1	A	114	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	A	944	HIS	CB-CG-CD2	-7.16	121.89	131.20
1	A	278	HIS	CB-CG-CD2	-7.05	122.03	131.20
1	A	279	PHE	CA-CB-CG	7.03	120.83	113.80
1	A	642	PHE	N-CA-C	-6.92	97.62	108.90
1	A	683	HIS	CB-CG-CD2	-6.86	122.29	131.20
1	A	878	GLU	CA-CB-CG	6.69	127.49	114.10
1	A	605	LYS	O-C-N	-6.66	112.35	123.00
1	A	808	GLY	O-C-N	-6.57	114.16	122.70
1	A	785	GLU	N-CA-C	6.46	124.56	110.80
1	A	856	PHE	CA-CB-CG	6.45	120.25	113.80
1	A	642	PHE	CA-CB-CG	6.43	120.23	113.80
1	A	808	GLY	CA-C-N	6.42	133.26	121.70
1	A	808	GLY	C-N-CA	6.42	133.26	121.70
1	A	739	ASN	N-CA-C	6.41	119.66	110.24
1	A	617	ALA	N-CA-C	6.38	120.64	112.34
1	A	243	GLU	N-CA-C	6.35	119.57	110.24
1	A	601	ASP	CA-C-N	6.33	126.90	120.38
1	A	601	ASP	C-N-CA	6.33	126.90	120.38
1	A	119	LEU	N-CA-C	6.25	117.78	110.97
1	A	5	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	A	327	ALA	N-CA-C	6.21	119.99	111.54
1	A	344	CYS	N-CA-C	-6.20	103.09	110.41
1	A	281	ASP	CA-C-N	6.16	127.54	119.84
1	A	281	ASP	C-N-CA	6.16	127.54	119.84
1	A	872	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	A	658	PHE	CA-CB-CG	6.07	119.86	113.80
1	A	190	HIS	CB-CG-CD2	-6.06	123.33	131.20
1	A	134	ARG	N-CA-C	-6.05	98.42	108.34
1	A	489	ARG	CA-CB-CG	6.04	126.19	114.10
1	A	951	ASP	N-CA-C	6.04	123.17	109.81
1	A	34	GLU	N-CA-CB	-6.02	100.31	110.49
1	A	981	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	38	HIS	CB-CG-CD2	-5.93	123.48	131.20
1	A	486	GLU	N-CA-C	5.90	117.51	110.19
1	A	398	ASN	N-CA-C	5.87	118.36	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	828	LEU	N-CA-C	-5.86	103.61	112.04
1	A	162	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	868	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	A	944	HIS	CB-CG-ND1	5.76	131.34	122.70
1	A	604	ARG	CA-C-N	5.72	132.00	121.70
1	A	604	ARG	C-N-CA	5.72	132.00	121.70
1	A	278	HIS	CB-CG-ND1	5.72	131.28	122.70
1	A	483	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	133	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	926	PRO	N-CA-C	5.62	117.56	110.70
1	A	811	PRO	CA-C-N	5.58	124.78	118.97
1	A	811	PRO	C-N-CA	5.58	124.78	118.97
1	A	114	ASN	CB-CG-ND2	5.58	124.77	116.40
1	A	796	ASN	CA-CB-CG	5.49	118.09	112.60
1	A	760	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	400	LYS	CA-C-N	5.45	125.38	119.76
1	A	400	LYS	C-N-CA	5.45	125.38	119.76
1	A	645	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	813	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	809	PHE	N-CA-CB	5.43	119.73	110.50
1	A	738	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	230	THR	CA-CB-CG2	5.39	119.67	110.50
1	A	149	ASP	CA-CB-CG	5.33	117.94	112.60
1	A	378	SER	N-CA-C	-5.33	101.47	109.15
1	A	854	TRP	CE2-CD2-CG	-5.33	100.80	107.20
1	A	284	HIS	CB-CG-CD2	-5.31	124.29	131.20
1	A	666	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	177	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	A	605	LYS	N-CA-CB	5.27	119.46	110.50
1	A	887	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	237	ASP	CA-CB-CG	-5.27	107.33	112.60
1	A	966	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	875	GLN	N-CA-CB	-5.23	102.23	110.49
1	A	25	THR	CA-C-N	5.22	124.67	119.24
1	A	25	THR	C-N-CA	5.22	124.67	119.24
1	A	539	GLY	CA-C-N	5.21	125.52	119.47
1	A	539	GLY	C-N-CA	5.21	125.52	119.47
1	A	146	VAL	CA-C-N	5.21	126.35	119.84
1	A	146	VAL	C-N-CA	5.21	126.35	119.84
1	A	107	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	510	ASN	CB-CG-ND2	5.16	124.14	116.40
1	A	820	PRO	N-CA-C	5.16	116.99	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	GLU	CA-CB-CG	5.15	124.40	114.10
1	A	990	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	510	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	880	HIS	CA-C-O	-5.11	113.16	120.16
1	A	272	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	A	193	PRO	N-CA-C	5.10	119.25	111.34
1	A	583	ARG	CA-CB-CG	5.10	124.30	114.10
1	A	854	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	A	281	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	663	LEU	N-CA-C	5.05	118.90	112.34
1	A	421	ASN	N-CA-C	-5.03	100.08	110.80
1	A	815	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	10	GLU	N-CA-C	-5.02	105.72	111.14
1	A	855	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	A	107	TRP	CG-CD2-CE3	5.01	138.91	133.90
1	A	288	TRP	CE2-CD2-CG	-5.00	101.20	107.20

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	LEU	Peptide
1	A	130	TYR	Sidechain
1	A	133	ASP	Peptide
1	A	174	ARG	Sidechain
1	A	247	THR	Peptide
1	A	294	TYR	Sidechain
1	A	324	ARG	Sidechain
1	A	36	TYR	Sidechain
1	A	461	ASN	Peptide
1	A	482	GLU	Peptide
1	A	524	ARG	Sidechain
1	A	534	ARG	Sidechain
1	A	583	ARG	Sidechain
1	A	587	TYR	Sidechain
1	A	601	ASP	Peptide
1	A	63	ARG	Sidechain
1	A	694	TYR	Sidechain
1	A	697	ILE	Peptide
1	A	745	ALA	Peptide
1	A	858	TYR	Sidechain
1	A	880	HIS	Sidechain

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	7671	0	7766	223	0
All	All	7671	0	7766	223	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 14.

All (223) 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:332:ILE:HB	1:A:734:VAL:HB	1.63	0.80
1:A:248:PRO:HD3	1:A:715:GLU:HB3	1.63	0.79
1:A:370:ASP:HB2	1:A:380:ASN:HB2	1.63	0.79
1:A:889:GLU:HB3	1:A:892:GLU:HB2	1.63	0.79
1:A:176:ASP:HA	1:A:186:SER:HA	1.63	0.78
1:A:201:ASN:HB2	1:A:680:GLU:HG3	1.68	0.74
1:A:65:LEU:HB2	1:A:300:VAL:HG11	1.69	0.72
1:A:412:GLU:HB3	1:A:566:THR:HG21	1.71	0.72
1:A:703:ASP:HB3	1:A:720:MET:HB2	1.71	0.72
1:A:171:THR:HB	1:A:488:SER:HB3	1.72	0.71
1:A:676:PHE:HB3	1:A:679:VAL:HG21	1.72	0.70
1:A:358:THR:HG22	1:A:738:ASP:HB3	1.74	0.68
1:A:787:LEU:HD13	1:A:792:LEU:HA	1.74	0.68
1:A:512:MET:HB2	1:A:571:PRO:HG3	1.74	0.67
1:A:878:GLU:HA	1:A:889:GLU:HG2	1.76	0.67
1:A:423:SER:HB2	1:A:442:GLU:HB2	1.77	0.67
1:A:719:ALA:HB2	1:A:731:SER:HB2	1.76	0.67
1:A:762:ARG:HD3	1:A:833:LEU:HD11	1.77	0.67
1:A:49:LEU:HB3	1:A:112:ALA:HB1	1.78	0.66
1:A:302:LEU:HB2	1:A:775:ILE:HG21	1.78	0.65
1:A:249:LEU:HB2	1:A:341:THR:HA	1.79	0.65
1:A:642:PHE:HZ	1:A:652:ALA:HB2	1.61	0.64
1:A:861:ASP:HB2	1:A:966:GLN:HE21	1.62	0.64
1:A:855:TRP:HE1	1:A:967:TRP:HA	1.62	0.63
1:A:773:VAL:HG21	1:A:845:GLY:HA2	1.80	0.63
1:A:633:ILE:HG23	1:A:648:VAL:HG21	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LYS:HB2	1:A:742:THR:HA	1.82	0.62
1:A:202:GLN:HG2	1:A:680:GLU:HB3	1.82	0.62
1:A:364:CYS:SG	1:A:600:LEU:HB3	2.40	0.61
1:A:329:LYS:HD2	1:A:742:THR:HA	1.81	0.61
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.82	0.61
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.41	0.60
1:A:120:LYS:HE3	1:A:236:ARG:HB3	1.83	0.60
1:A:635:ILE:HG23	1:A:638:ARG:NH2	2.16	0.60
1:A:528:VAL:HG23	1:A:537:MET:HA	1.82	0.60
1:A:246:LYS:HE2	1:A:246:LYS:HA	1.82	0.60
1:A:880:HIS:HA	1:A:885:GLY:O	2.02	0.60
1:A:298:ILE:HG22	1:A:775:ILE:HG23	1.83	0.60
1:A:661:LEU:HB3	1:A:665:GLU:HB2	1.84	0.60
1:A:659:ASP:CG	1:A:686:LYS:HZ2	2.10	0.60
1:A:200:VAL:HG21	1:A:683:HIS:CE1	2.37	0.59
1:A:377:CYS:HB3	1:A:541:VAL:HG22	1.84	0.59
1:A:638:ARG:HD2	1:A:639:ILE:HG23	1.84	0.59
1:A:349:CYS:HB2	1:A:700:MET:SD	2.41	0.59
1:A:559:LEU:HD13	1:A:598:GLY:HA3	1.84	0.59
1:A:163:ILE:HB	1:A:208:LEU:HB2	1.85	0.58
1:A:459:VAL:HG11	1:A:471:CYS:SG	2.43	0.58
1:A:525:CYS:HB3	1:A:593:PHE:HB2	1.84	0.58
1:A:542:LYS:HA	1:A:545:ILE:HG12	1.85	0.58
1:A:774:CYS:SG	1:A:787:LEU:HB2	2.43	0.58
1:A:408:ASP:HB2	1:A:532:THR:HG23	1.84	0.58
1:A:204:LYS:HB3	1:A:207:MET:HB2	1.85	0.58
1:A:364:CYS:SG	1:A:559:LEU:HD22	2.44	0.58
1:A:480:LYS:HB2	1:A:501:ALA:HB2	1.86	0.57
1:A:176:ASP:HB3	1:A:212:THR:HB	1.86	0.57
1:A:29:VAL:HG13	1:A:146:VAL:HG21	1.86	0.56
1:A:351:ASP:HA	1:A:624:ILE:HB	1.88	0.56
1:A:794:TRP:HB3	1:A:901:LEU:HD11	1.87	0.55
1:A:125:GLU:HG3	1:A:139:ARG:NH1	2.20	0.55
1:A:239:MET:SD	1:A:713:LYS:HB2	2.46	0.55
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.89	0.55
1:A:357:THR:HG21	1:A:601:ASP:HB2	1.87	0.55
1:A:375:ASP:HB3	1:A:540:PRO:HD2	1.89	0.55
1:A:623:MET:HE3	1:A:641:ILE:HD12	1.88	0.54
1:A:981:ASP:CG	1:A:985:LYS:HZ1	2.16	0.54
1:A:525:CYS:HA	1:A:591:LEU:HB2	1.89	0.54
1:A:741:SER:HA	1:A:744:VAL:HG23	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HB2	1:A:158:LYS:HG3	1.89	0.54
1:A:353:THR:HA	1:A:357:THR:O	2.09	0.53
1:A:491:ARG:HA	1:A:585:MET:HE3	1.89	0.53
1:A:855:TRP:NE1	1:A:967:TRP:HA	2.22	0.53
1:A:719:ALA:HB3	1:A:734:VAL:HA	1.91	0.53
1:A:806:ALA:HA	1:A:932:TRP:HB2	1.90	0.53
1:A:230:THR:HG22	1:A:233:GLY:H	1.75	0.52
1:A:31:ARG:O	1:A:35:LYS:HG2	2.10	0.51
1:A:422:ASP:CG	1:A:481:LYS:HZ2	2.18	0.51
1:A:611:ILE:HA	1:A:614:CYS:HB2	1.91	0.51
1:A:93:VAL:HG21	1:A:956:ILE:HG21	1.92	0.51
1:A:245:ASP:HB3	1:A:713:LYS:HA	1.92	0.51
1:A:247:THR:HG22	1:A:250:GLN:HE21	1.76	0.51
1:A:815:ASP:O	1:A:819:ARG:HB2	2.10	0.51
1:A:481:LYS:HA	1:A:498:CYS:SG	2.49	0.51
1:A:420:CYS:SG	1:A:494:MET:HG3	2.50	0.51
1:A:499:SER:HB3	1:A:510:ASN:HA	1.93	0.51
1:A:190:HIS:HE1	1:A:194:VAL:HG22	1.76	0.50
1:A:807:LEU:HG	1:A:916:LEU:HA	1.92	0.50
1:A:611:ILE:HG21	1:A:641:ILE:HA	1.93	0.50
1:A:347:VAL:HG23	1:A:696:GLU:HB3	1.93	0.50
1:A:404:SER:HB3	1:A:410:LEU:HD13	1.94	0.50
1:A:614:CYS:O	1:A:620:ARG:HA	2.11	0.49
1:A:349:CYS:SG	1:A:622:ILE:HD12	2.52	0.49
1:A:352:LYS:HG3	1:A:623:MET:HE2	1.95	0.49
1:A:38:HIS:CE1	1:A:144:ASP:HA	2.47	0.49
1:A:810:ASN:HB3	1:A:811:PRO:HD2	1.94	0.49
1:A:548:VAL:HA	1:A:551:GLU:HB3	1.95	0.48
1:A:50:TRP:HZ3	1:A:312:PRO:HG2	1.78	0.48
1:A:808:GLY:HA3	1:A:809:PHE:CB	2.43	0.48
1:A:808:GLY:HA3	1:A:809:PHE:HB2	1.94	0.48
1:A:180:LEU:HD12	1:A:706:ASN:HD21	1.77	0.48
1:A:299:ALA:O	1:A:302:LEU:HB3	2.12	0.48
1:A:340:GLU:HG3	1:A:753:ILE:HG23	1.95	0.48
1:A:97:ILE:HG12	1:A:793:LEU:HD13	1.95	0.48
1:A:852:ALA:HA	1:A:855:TRP:HE3	1.79	0.48
1:A:427:PHE:HB2	1:A:434:TYR:CE2	2.49	0.48
1:A:125:GLU:CD	1:A:141:LYS:HZ1	2.21	0.47
1:A:51:GLU:HG2	1:A:56:GLN:HG3	1.96	0.47
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.74	0.47
1:A:425:LEU:H	1:A:446:THR:HG21	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ILE:HD13	1:A:684:LYS:HE2	1.97	0.47
1:A:633:ILE:HG12	1:A:648:VAL:HG11	1.96	0.47
1:A:246:LYS:O	1:A:250:GLN:HB3	2.13	0.47
1:A:104:VAL:HG12	1:A:108:GLN:NE2	2.29	0.47
1:A:398:ASN:N	1:A:399:ASP:HA	2.30	0.47
1:A:624:ILE:HD11	1:A:700:MET:SD	2.55	0.47
1:A:427:PHE:HB3	1:A:465:VAL:HA	1.97	0.47
1:A:614:CYS:SG	1:A:743:ILE:HG22	2.54	0.47
1:A:416:ILE:HD11	1:A:566:THR:HG23	1.96	0.46
1:A:101:ASN:HD22	1:A:309:GLU:HG3	1.79	0.46
1:A:703:ASP:HA	1:A:727:ALA:HB2	1.96	0.46
1:A:916:LEU:HD13	1:A:924:ARG:HD3	1.96	0.46
1:A:957:PHE:O	1:A:958:LYS:HD2	2.15	0.46
1:A:880:HIS:HB2	1:A:881:PRO:HD3	1.97	0.46
1:A:324:ARG:HG2	1:A:324:ARG:HH11	1.80	0.46
1:A:179:ILE:HG23	1:A:210:SER:O	2.16	0.46
1:A:281:ASP:HB2	1:A:882:HIS:CE1	2.51	0.46
1:A:331:ALA:HA	1:A:733:MET:SD	2.56	0.46
1:A:371:LYS:HA	1:A:530:VAL:HG13	1.97	0.46
1:A:602:PRO:HA	1:A:603:PRO:HD3	1.72	0.46
1:A:784:PRO:HB2	1:A:853:ALA:HB2	1.96	0.46
1:A:130:TYR:HB2	1:A:150:ILE:HB	1.97	0.46
1:A:365:LYS:HD2	1:A:559:LEU:HD21	1.97	0.46
1:A:398:ASN:HA	1:A:399:ASP:CG	2.42	0.45
1:A:705:VAL:HG13	1:A:724:THR:HG21	1.98	0.45
1:A:688:VAL:HG11	1:A:714:ALA:HA	1.99	0.45
1:A:204:LYS:HE3	1:A:209:PHE:CZ	2.51	0.45
1:A:458:GLU:OE1	1:A:461:ASN:HB3	2.16	0.45
1:A:260:LEU:O	1:A:264:ILE:HG12	2.17	0.45
1:A:774:CYS:SG	1:A:775:ILE:N	2.89	0.45
1:A:904:LEU:HA	1:A:907:ILE:HG13	1.99	0.45
1:A:762:ARG:NH2	1:A:918:GLU:HA	2.31	0.45
1:A:854:TRP:HA	1:A:868:HIS:CE1	2.52	0.45
1:A:567:ARG:HD3	1:A:571:PRO:HD3	1.99	0.45
1:A:48:SER:HA	1:A:113:GLU:HB3	1.99	0.44
1:A:384:ILE:HD12	1:A:395:VAL:HG22	1.99	0.44
1:A:90:GLU:HG2	1:A:790:VAL:HG13	1.99	0.44
1:A:338:SER:HB3	1:A:732:GLU:HB3	1.99	0.44
1:A:865:VAL:HG11	1:A:890:ILE:HD11	1.98	0.44
1:A:546:LEU:O	1:A:550:LYS:NZ	2.50	0.44
1:A:648:VAL:HG13	1:A:651:ARG:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HD2	1:A:659:ASP:HB3	1.99	0.44
1:A:416:ILE:HG12	1:A:513:PHE:HB3	1.98	0.44
1:A:460:ARG:H	1:A:460:ARG:HG3	1.65	0.44
1:A:834:PHE:HA	1:A:837:TYR:HD2	1.82	0.44
1:A:66:LEU:HB2	1:A:98:LEU:HG	1.98	0.44
1:A:891:PHE:O	1:A:897:MET:HG3	2.18	0.44
1:A:849:VAL:O	1:A:854:TRP:HB2	2.18	0.44
1:A:148:GLY:H	1:A:223:VAL:HB	1.82	0.44
1:A:815:ASP:HB2	1:A:818:ASP:HB2	2.00	0.44
1:A:153:VAL:HG11	1:A:159:VAL:HG22	2.00	0.43
1:A:315:ILE:HB	1:A:760:PHE:CZ	2.53	0.43
1:A:751:ARG:NH2	1:A:819:ARG:O	2.51	0.43
1:A:364:CYS:SG	1:A:600:LEU:CB	3.06	0.43
1:A:150:ILE:HG22	1:A:220:LEU:HD11	2.01	0.43
1:A:249:LEU:HD22	1:A:757:MET:SD	2.59	0.43
1:A:316:THR:HA	1:A:319:LEU:HD23	2.00	0.43
1:A:774:CYS:HA	1:A:848:THR:HG21	1.99	0.43
1:A:117:GLU:O	1:A:334:ARG:NH2	2.52	0.43
1:A:128:LYS:NZ	1:A:152:GLU:O	2.51	0.43
1:A:570:PRO:HA	1:A:571:PRO:HD2	1.84	0.43
1:A:688:VAL:HG11	1:A:713:LYS:O	2.18	0.43
1:A:486:GLU:O	1:A:491:ARG:NH2	2.51	0.43
1:A:659:ASP:HA	1:A:666:GLN:NE2	2.34	0.43
1:A:791:GLN:HG2	1:A:901:LEU:HD22	2.00	0.43
1:A:173:LEU:HA	1:A:217:GLY:HA3	2.00	0.43
1:A:179:ILE:HG13	1:A:724:THR:OG1	2.19	0.43
1:A:192:GLU:CD	1:A:192:GLU:H	2.26	0.43
1:A:319:LEU:HD13	1:A:340:GLU:H	1.83	0.42
1:A:419:LEU:HD13	1:A:498:CYS:SG	2.59	0.42
1:A:986:PHE:HB3	1:A:991:TYR:O	2.19	0.42
1:A:419:LEU:HD23	1:A:476:ARG:HG2	2.01	0.42
1:A:436:LYS:NZ	1:A:438:GLY:O	2.51	0.42
1:A:496:VAL:HG12	1:A:513:PHE:HB2	2.01	0.42
1:A:637:ARG:NH1	1:A:644:GLU:O	2.51	0.42
1:A:40:GLU:H	1:A:40:GLU:CD	2.27	0.42
1:A:358:THR:HA	1:A:738:ASP:CG	2.45	0.42
1:A:762:ARG:NH2	1:A:917:SER:O	2.53	0.42
1:A:311:LEU:HD13	1:A:764:LEU:HG	2.01	0.42
1:A:647:GLU:CD	1:A:651:ARG:HH22	2.27	0.42
1:A:966:GLN:HE21	1:A:966:GLN:HA	1.84	0.42
1:A:521:VAL:HG12	1:A:525:CYS:SG	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:VAL:HG13	1:A:683:HIS:HB2	2.02	0.42
1:A:477:GLN:O	1:A:502:LYS:NZ	2.52	0.41
1:A:493:SER:HA	1:A:516:GLY:HA3	2.02	0.41
1:A:843:TYR:CD1	1:A:977:VAL:HG11	2.56	0.41
1:A:177:GLN:HG2	1:A:180:LEU:HD23	2.02	0.41
1:A:347:VAL:HG12	1:A:349:CYS:SG	2.60	0.41
1:A:50:TRP:HD1	1:A:109:GLU:HG2	1.85	0.41
1:A:552:TRP:HB3	1:A:559:LEU:HG	2.03	0.41
1:A:21:THR:O	1:A:135:LYS:NZ	2.53	0.41
1:A:240:ALA:HA	1:A:243:GLU:HG3	2.02	0.41
1:A:861:ASP:HB2	1:A:966:GLN:NE2	2.34	0.41
1:A:637:ARG:NH1	1:A:642:PHE:HB2	2.35	0.41
1:A:859:ALA:HB1	1:A:968:LEU:HB2	2.03	0.41
1:A:867:TYR:CE2	1:A:884:GLU:HG3	2.55	0.41
1:A:950:VAL:O	1:A:954:PRO:HD2	2.21	0.41
1:A:227:GLY:O	1:A:230:THR:HB	2.21	0.41
1:A:420:CYS:SG	1:A:515:LYS:HB3	2.60	0.41
1:A:700:MET:HB3	1:A:714:ALA:HB1	2.01	0.41
1:A:3:ALA:O	1:A:5:HIS:N	2.53	0.41
1:A:524:ARG:HH21	1:A:588:GLU:HB2	1.86	0.41
1:A:529:ARG:HB3	1:A:594:VAL:HA	2.02	0.41
1:A:556:ARG:HG3	1:A:637:ARG:HB3	2.01	0.41
1:A:688:VAL:HG22	1:A:698:THR:HG21	2.03	0.41
1:A:436:LYS:HA	1:A:443:THR:HG21	2.02	0.41
1:A:629:LYS:HZ3	1:A:657:GLU:CD	2.29	0.41
1:A:695:ASP:HB2	1:A:825:LYS:NZ	2.36	0.41
1:A:248:PRO:HG2	1:A:341:THR:O	2.20	0.40
1:A:726:VAL:HA	1:A:729:THR:OG1	2.20	0.40
1:A:823:SER:HA	1:A:824:PRO:HD3	1.85	0.40
1:A:10:GLU:CD	1:A:10:GLU:H	2.30	0.40
1:A:633:ILE:HA	1:A:642:PHE:CE1	2.56	0.40
1:A:751:ARG:HH11	1:A:751:ARG:HD3	1.79	0.40
1:A:910:CYS:SG	1:A:974:SER:HB3	2.61	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 PDB entries followed by that with respect to all EM entries.

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	992/994 (100%)	756 (76%)	173 (17%)	63 (6%)	1	12

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ALA
1	A	126	MET
1	A	282	PRO
1	A	394	GLU
1	A	504	SER
1	A	602	PRO
1	A	605	LYS
1	A	722	SER
1	A	809	PHE
1	A	810	ASN
1	A	825	LYS
1	A	877	THR
1	A	880	HIS
1	A	24	LEU
1	A	34	GLU
1	A	58	GLU
1	A	85	ILE
1	A	117	GLU
1	A	147	PRO
1	A	154	ALA
1	A	160	PRO
1	A	190	HIS
1	A	206	ASN
1	A	284	HIS
1	A	341	THR
1	A	355	THR
1	A	459	VAL
1	A	518	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	576	MET
1	A	648	VAL
1	A	808	GLY
1	A	878	GLU
1	A	879	ASP
1	A	183	GLU
1	A	189	LYS
1	A	358	THR
1	A	375	ASP
1	A	785	GLU
1	A	851	ALA
1	A	857	MET
1	A	927	PRO
1	A	21	THR
1	A	48	SER
1	A	49	LEU
1	A	142	ALA
1	A	461	ASN
1	A	553	GLY
1	A	966	GLN
1	A	247	THR
1	A	311	LEU
1	A	421	ASN
1	A	508	VAL
1	A	603	PRO
1	A	608	MET
1	A	672	ARG
1	A	824	PRO
1	A	748	GLU
1	A	539	GLY
1	A	618	GLY
1	A	217	GLY
1	A	864	GLY
1	A	46	GLY
1	A	850	GLY

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 PDB entries followed by that with respect to all EM entries.

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	840/840 (100%)	742 (88%)	98 (12%)	5 18

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	20	GLU
1	A	27	ASP
1	A	40	GLU
1	A	47	LYS
1	A	90	GLU
1	A	110	ARG
1	A	113	GLU
1	A	121	GLU
1	A	126	MET
1	A	146	VAL
1	A	147	PRO
1	A	183	GLU
1	A	191	THR
1	A	192	GLU
1	A	225	THR
1	A	230	THR
1	A	231	GLU
1	A	258	GLU
1	A	275	ASN
1	A	276	ILE
1	A	279	PHE
1	A	282	PRO
1	A	309	GLU
1	A	341	THR
1	A	345	THR
1	A	352	LYS
1	A	371	LYS
1	A	375	ASP
1	A	394	GLU
1	A	402	ILE
1	A	436	LYS
1	A	458	GLU
1	A	460	ARG
1	A	461	ASN
1	A	467	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	480	LYS
1	A	486	GLU
1	A	490	ASP
1	A	495	SER
1	A	500	PRO
1	A	503	SER
1	A	510	ASN
1	A	518	PRO
1	A	519	GLU
1	A	522	ILE
1	A	529	ARG
1	A	532	THR
1	A	533	THR
1	A	538	THR
1	A	540	PRO
1	A	575	GLU
1	A	577	VAL
1	A	579	ASP
1	A	580	ASP
1	A	581	SER
1	A	592	THR
1	A	602	PRO
1	A	610	SER
1	A	639	ILE
1	A	644	GLU
1	A	646	GLU
1	A	651	ARG
1	A	668	GLU
1	A	671	ARG
1	A	680	GLU
1	A	698	THR
1	A	703	ASP
1	A	705	VAL
1	A	706	ASN
1	A	712	LYS
1	A	713	LYS
1	A	724	THR
1	A	744	VAL
1	A	766	SER
1	A	788	ILE
1	A	789	PRO
1	A	807	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	818	ASP
1	A	825	LYS
1	A	826	GLU
1	A	830	SER
1	A	854	TRP
1	A	856	PHE
1	A	860	GLU
1	A	871	THR
1	A	876	CYS
1	A	887	ASP
1	A	889	GLU
1	A	895	GLU
1	A	916	LEU
1	A	954	PRO
1	A	963	ASP
1	A	964	LEU
1	A	965	THR
1	A	966	GLN
1	A	967	TRP
1	A	972	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	ASN
1	A	966	GLN

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.