Full wwPDB EM Validation Report

Feb 3, 2024 – 09:20 AM EST

PDB ID	:	1KJU
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 (i) 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 (i)) were used in the production of this report:

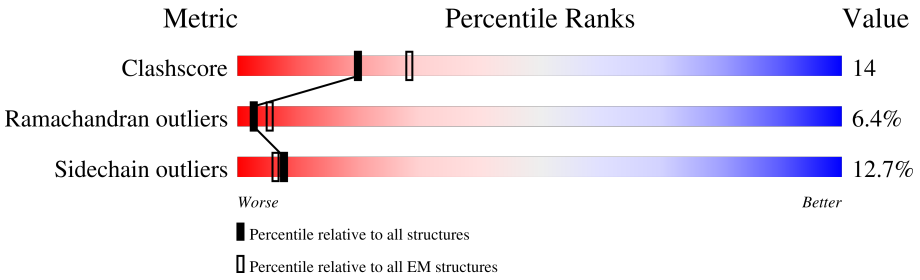
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	994	56% 35% 7% ·

2 Entry composition (i)

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
			Total	C	N	O	S		
1	A	994	7671	4876	1287	1451	57	0	0

There is a discrepancy between the modelled and reference sequences:

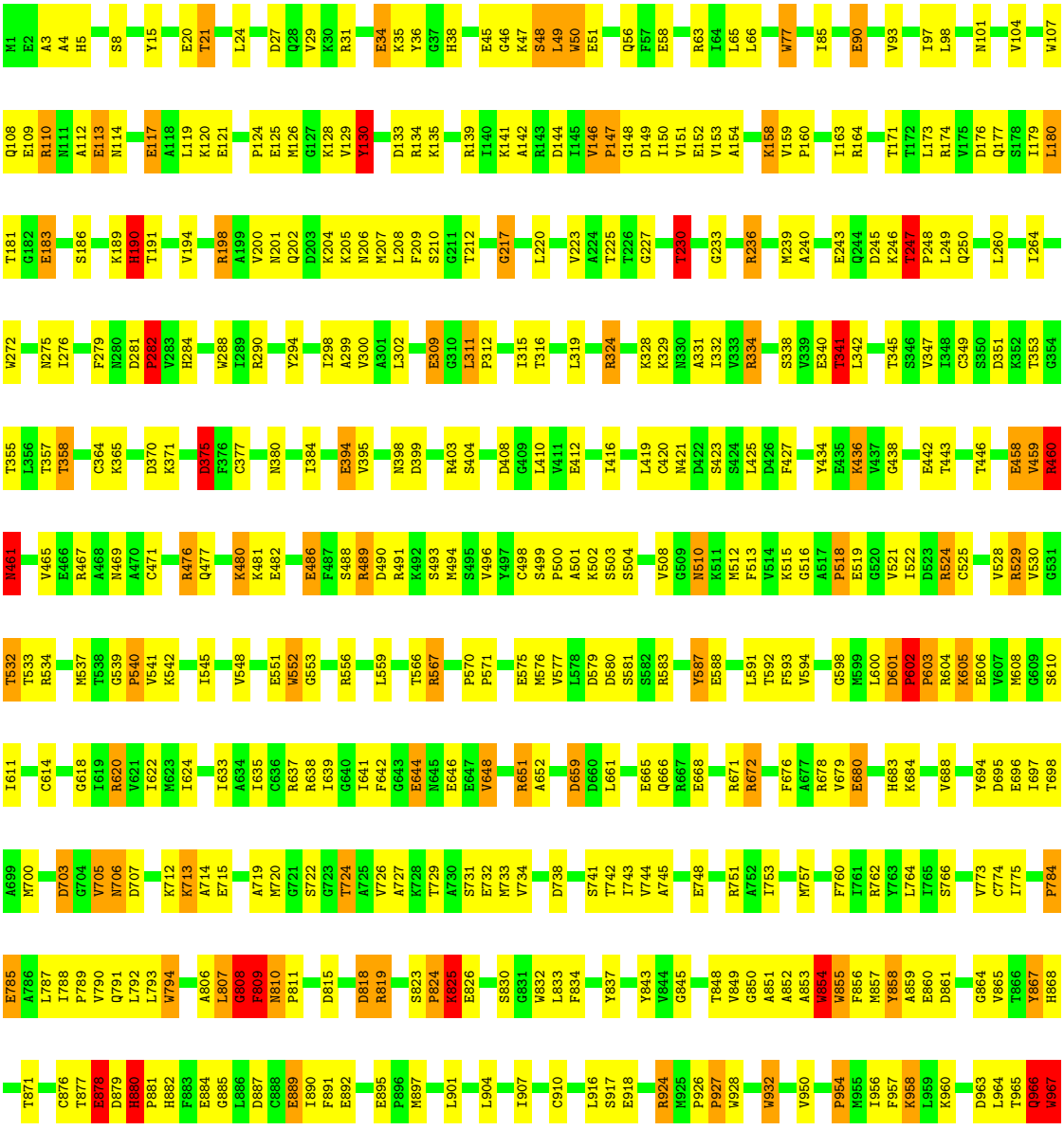
Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

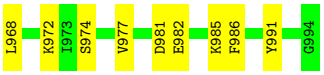
3 Residue-property plots (i)

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. 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

Chain A:




L968
K972
I973
S974
V977
D981
E982
K985
F986
Y991
G994

4 Data and refinement statistics (i)

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 (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	0.64	0/7812	1.33	74/10592 (0.7%)

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

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	334	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	967	TRP	CD1-CG-CD2	8.76	113.31	106.30
1	A	854	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	A	855	TRP	CD1-CG-CD2	8.55	113.14	106.30
1	A	567	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	A	272	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	A	288	TRP	CD1-CG-CD2	8.39	113.02	106.30
1	A	794	TRP	CD1-CG-CD2	8.38	113.00	106.30
1	A	928	TRP	CD1-CG-CD2	8.32	112.95	106.30
1	A	107	TRP	CD1-CG-CD2	8.19	112.86	106.30
1	A	854	TRP	CE2-CD2-CG	-8.12	100.80	107.30
1	A	77	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	A	832	TRP	CD1-CG-CD2	7.98	112.68	106.30
1	A	932	TRP	CD1-CG-CD2	7.97	112.67	106.30
1	A	107	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	A	272	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	552	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	A	855	TRP	CE2-CD2-CG	-7.65	101.18	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	A	832	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	A	967	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	A	794	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	552	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	928	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	A	50	TRP	CD1-CG-CD2	7.42	112.23	106.30
1	A	50	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	A	34	GLU	CA-CB-CG	7.35	129.57	113.40
1	A	77	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	605	LYS	CA-C-N	6.86	132.30	117.20
1	A	932	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	282	PRO	N-CA-C	6.60	129.25	112.10
1	A	605	LYS	O-C-N	-6.47	112.35	122.70
1	A	878	GLU	CA-CB-CG	6.40	127.49	113.40
1	A	334	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	460	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	290	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	604	ARG	CA-C-N	6.04	130.49	117.20
1	A	604	ARG	O-C-N	-6.01	113.09	122.70
1	A	489	ARG	CA-CB-CG	5.81	126.19	113.40
1	A	130	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	A	34	GLU	N-CA-CB	-5.72	100.31	110.60
1	A	107	TRP	CB-CG-CD1	-5.68	119.62	127.00
1	A	854	TRP	CB-CG-CD1	-5.67	119.62	127.00
1	A	290	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	854	TRP	CG-CD2-CE3	5.63	138.97	133.90
1	A	107	TRP	CG-CD2-CE3	5.57	138.91	133.90
1	A	967	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	476	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	272	TRP	CB-CG-CD1	-5.50	119.86	127.00
1	A	808	GLY	CA-C-N	5.47	129.24	117.20
1	A	180	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	981	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	77	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	A	832	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	A	808	GLY	O-C-N	-5.34	114.16	122.70
1	A	587	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	A	50	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	A	855	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	A	236	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	342	LEU	CA-CB-CG	5.24	127.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	THR	CA-CB-CG2	5.19	119.67	112.40
1	A	272	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	A	794	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	A	928	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	A	467	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	110	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	288	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	809	PHE	N-CA-CB	5.08	119.73	110.60
1	A	552	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	A	164	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	785	GLU	N-CA-C	5.02	124.56	111.00
1	A	403	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	50	TRP	CB-CG-CD1	-5.01	120.49	127.00
1	A	15	TYR	CB-CG-CD1	-5.00	118.00	121.00

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 (i)

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	213	0
All	All	7671	0	7766	213	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 (213) 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

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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: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: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
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:855:TRP:NE1	1:A:967:TRP:HA	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:774:CYS:SG	1:A:775:ILE:N	2.89	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: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: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:648:VAL:HG13	1:A:651:ARG:HB2	2.00	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:982:GLU:CD	1:A:985:LYS:HZ3	2.22	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: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:125:GLU:CD	1:A:141:LYS:HZ1	2.23	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: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: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
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:328:LYS:HZ2	1:A:328:LYS:HG3	1.77	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:181:THR:O	1:A:684:LYS:NZ	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:398:ASN:HA	1:A:399:ASP:CG	2.42	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: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: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 (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 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 16

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
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

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Mol	Chain	Res	Type
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%)	733 (87%)	107 (13%)	4 19

All (107) 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	45	GLU
1	A	47	LYS
1	A	77	TRP

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Mol	Chain	Res	Type
1	A	90	GLU
1	A	110	ARG
1	A	113	GLU
1	A	114	ASN
1	A	121	GLU
1	A	134	ARG
1	A	146	VAL
1	A	147	PRO
1	A	149	ASP
1	A	158	LYS
1	A	183	GLU
1	A	190	HIS
1	A	191	THR
1	A	198	ARG
1	A	205	LYS
1	A	225	THR
1	A	230	THR
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	375	ASP
1	A	394	GLU
1	A	436	LYS
1	A	458	GLU
1	A	460	ARG
1	A	461	ASN
1	A	469	ASN
1	A	480	LYS
1	A	486	GLU
1	A	489	ARG
1	A	490	ASP
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

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Mol	Chain	Res	Type
1	A	532	THR
1	A	533	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	606	GLU
1	A	610	SER
1	A	620	ARG
1	A	644	GLU
1	A	646	GLU
1	A	651	ARG
1	A	659	ASP
1	A	668	GLU
1	A	671	ARG
1	A	672	ARG
1	A	678	ARG
1	A	680	GLU
1	A	703	ASP
1	A	705	VAL
1	A	706	ASN
1	A	707	ASP
1	A	712	LYS
1	A	713	LYS
1	A	724	THR
1	A	766	SER
1	A	784	PRO
1	A	788	ILE
1	A	789	PRO
1	A	807	LEU
1	A	818	ASP
1	A	819	ARG
1	A	825	LYS
1	A	826	GLU
1	A	830	SER
1	A	854	TRP
1	A	856	PHE
1	A	858	TYR

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Mol	Chain	Res	Type
1	A	860	GLU
1	A	867	TYR
1	A	871	THR
1	A	876	CYS
1	A	887	ASP
1	A	889	GLU
1	A	895	GLU
1	A	924	ARG
1	A	954	PRO
1	A	958	LYS
1	A	960	LYS
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	359	ASN
1	A	966	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.