



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:40 PM UTC

PDB ID : 1A8Y / pdb_00001a8y
Title : CRYSTAL STRUCTURE OF CALSEQUESTRIN FROM RABBIT SKELETAL MUSCLE SARCOPLASMIC RETICULUM AT 2.4 Å RESOLUTION
Authors : Wang, S.; Trumble, W.R.; Liao, H.; Wesson, C.R.; Dunker, A.K.; Kang, C.
Deposited on : 1998-03-31
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

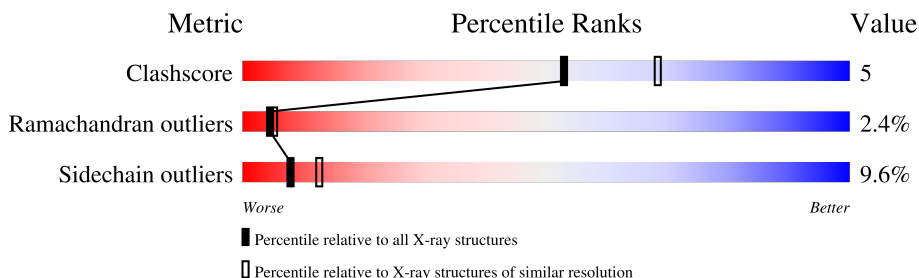
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	367	 61% 25% 6% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2800 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 CALSEQUESTIN.

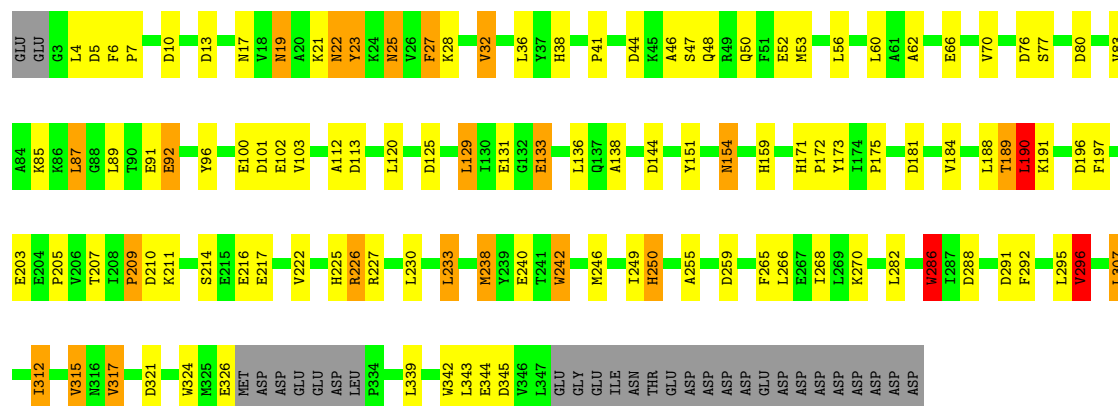
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2760	1775	413	567	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		

Note EDS was not executed.

Chain A: 61% 25% 6% 8%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	59.74Å 145.56Å 111.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	78.3 (10.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.188 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2800	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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	1.00	7/2824 (0.2%)	1.87	78/3832 (2.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	VAL	CA-CB	7.62	1.64	1.54
1	A	159	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	225	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	38	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	250	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	171	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	205	PRO	CA-CB	-5.50	1.47	1.54

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ASN	N-CA-C	12.02	125.69	111.02
1	A	19	ASN	CA-CB-CG	8.16	120.77	112.60
1	A	23	TYR	N-CA-C	8.14	121.18	111.33
1	A	196	ASP	CA-CB-CG	7.79	120.39	112.60
1	A	144	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	291	ASP	CA-CB-CG	7.62	120.22	112.60
1	A	321	ASP	CA-CB-CG	7.50	120.10	112.60
1	A	52	GLU	CA-C-N	7.25	129.86	120.44
1	A	52	GLU	C-N-CA	7.25	129.86	120.44
1	A	345	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	173	TYR	N-CA-C	7.03	119.97	111.82
1	A	238	MET	N-CA-C	7.01	125.73	110.80
1	A	209	PRO	N-CA-C	7.00	126.89	112.47
1	A	125	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	282	LEU	N-CA-C	6.86	120.32	110.10
1	A	21	LYS	CA-C-N	6.76	130.19	120.79
1	A	21	LYS	C-N-CA	6.76	130.19	120.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	HIS	CA-CB-CG	-6.76	107.04	113.80
1	A	210	ASP	O-C-N	6.63	130.04	122.55
1	A	189	THR	CA-CB-OG1	-6.55	99.78	109.60
1	A	292	PHE	CA-C-N	6.50	126.26	119.05
1	A	292	PHE	C-N-CA	6.50	126.26	119.05
1	A	113	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	181	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	286	TRP	CA-CB-CG	6.27	125.52	113.60
1	A	259	ASP	CA-CB-CG	6.24	118.83	112.60
1	A	103	VAL	N-CA-C	6.12	116.97	108.89
1	A	286	TRP	CB-CG-CD1	-6.09	117.76	126.90
1	A	102	GLU	CA-C-N	6.05	130.02	121.66
1	A	102	GLU	C-N-CA	6.05	130.02	121.66
1	A	22	ASN	CB-CA-C	-5.95	101.45	110.92
1	A	210	ASP	CA-C-O	5.93	128.83	122.13
1	A	13	ASP	O-C-N	5.88	129.93	123.22
1	A	190	LEU	N-CA-C	5.85	123.25	110.80
1	A	205	PRO	N-CA-C	5.83	123.17	111.69
1	A	85	LYS	N-CA-C	5.80	118.07	111.11
1	A	27	PHE	CA-CB-CG	-5.79	108.01	113.80
1	A	77	SER	N-CA-C	5.79	118.53	111.82
1	A	17	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	203	GLU	CA-C-N	5.75	129.60	121.61
1	A	203	GLU	C-N-CA	5.75	129.60	121.61
1	A	288	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	226	ARG	N-CA-C	5.64	117.51	111.36
1	A	154	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	317	VAL	CA-CB-CG2	-5.63	100.83	110.40
1	A	326	GLU	CB-CG-CD	5.59	122.10	112.60
1	A	76	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	10	ASP	N-CA-C	5.53	119.88	113.18
1	A	53	MET	N-CA-C	5.50	116.95	111.07
1	A	133	GLU	N-CA-C	5.45	122.40	110.80
1	A	62	ALA	N-CA-C	5.44	116.89	111.07
1	A	80	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	216	GLU	CB-CG-CD	5.35	121.70	112.60
1	A	129	LEU	N-CA-C	5.34	118.80	110.32
1	A	171	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	85	LYS	CB-CA-C	-5.32	102.31	110.81
1	A	44	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	210	ASP	N-CA-C	5.31	117.85	108.24
1	A	296	VAL	CA-C-O	-5.29	112.86	119.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	TRP	CG-CD2-CE3	5.29	139.19	133.90
1	A	225	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	A	240	GLU	N-CA-C	-5.26	105.46	111.14
1	A	175	PRO	N-CA-C	5.26	118.75	110.50
1	A	210	ASP	CA-C-N	5.24	128.33	120.83
1	A	210	ASP	C-N-CA	5.24	128.33	120.83
1	A	113	ASP	N-CA-CB	-5.23	102.27	109.91
1	A	92	GLU	N-CA-C	5.17	121.81	110.80
1	A	240	GLU	CA-CB-CG	5.08	124.27	114.10
1	A	112	ALA	CA-C-N	5.08	127.35	120.65
1	A	112	ALA	C-N-CA	5.08	127.35	120.65
1	A	242	TRP	CG-CD2-CE3	5.06	138.96	133.90
1	A	317	VAL	CA-CB-CG1	5.05	118.99	110.40
1	A	197	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	250	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	286	TRP	CE2-CD2-CG	-5.03	101.17	107.20
1	A	66	GLU	N-CA-C	5.02	117.14	111.11
1	A	38	HIS	N-CA-C	5.01	116.86	108.99
1	A	342	TRP	CE2-CD2-CG	-5.01	101.19	107.20

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	2760	0	2611	27	0
2	A	40	0	0	2	0
All	All	2800	0	2611	27	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 5.

All (27) 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:255:ALA:O	1:A:286:TRP:HZ3	1.77	0.67
1:A:87:LEU:HB3	1:A:89:LEU:HD13	1.80	0.64
1:A:296:VAL:HB	1:A:307:LEU:HD23	1.80	0.63
1:A:41:PRO:HB2	1:A:48:GLN:HG2	1.81	0.63
1:A:214:SER:OG	1:A:217:GLU:HG3	2.01	0.60
1:A:46:ALA:O	1:A:50:GLN:HG3	2.03	0.58
1:A:227:ARG:HH12	1:A:246:MET:HB3	1.71	0.56
1:A:242:TRP:O	1:A:250:HIS:HE1	1.90	0.55
1:A:19:ASN:H	1:A:22:ASN:HB2	1.72	0.54
1:A:154:ASN:HB2	2:A:519:HOH:O	2.12	0.49
1:A:266:LEU:O	1:A:270:LYS:HG3	2.14	0.48
1:A:25:ASN:HA	1:A:28:LYS:HG2	1.98	0.46
1:A:151:TYR:HB2	1:A:190:LEU:HD23	1.98	0.45
1:A:136:LEU:HD12	1:A:184:VAL:HG22	1.98	0.45
1:A:91:GLU:HG2	1:A:96:TYR:OH	2.18	0.44
1:A:191:LYS:HD2	1:A:211:LYS:NZ	2.33	0.43
1:A:246:MET:O	1:A:249:ILE:HG22	2.19	0.42
1:A:32:VAL:O	1:A:70:VAL:HA	2.20	0.42
1:A:83:VAL:O	1:A:87:LEU:HB2	2.20	0.42
1:A:265:PHE:HA	1:A:268:ILE:HD12	2.02	0.42
1:A:6:PHE:HB3	2:A:501:HOH:O	2.20	0.41
1:A:222:VAL:O	1:A:226:ARG:HG3	2.20	0.41
1:A:23:TYR:O	1:A:27:PHE:HD2	2.03	0.41
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.79	0.41
1:A:6:PHE:HA	1:A:7:PRO:HD3	1.90	0.40
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.89	0.40
1:A:265:PHE:HZ	1:A:312:ILE:HB	1.87	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	334/367 (91%)	313 (94%)	13 (4%)	8 (2%)	4 5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	GLU
1	A	133	GLU
1	A	189	THR
1	A	190	LEU
1	A	100	GLU
1	A	238	MET
1	A	138	ALA
1	A	209	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	303/331 (92%)	274 (90%)	29 (10%)	8 12

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	ASP
1	A	25	ASN
1	A	32	VAL
1	A	36	LEU
1	A	47	SER
1	A	56	LEU
1	A	60	LEU
1	A	87	LEU
1	A	101	ASP
1	A	120	LEU
1	A	129	LEU
1	A	131	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	172	PRO
1	A	188	LEU
1	A	207	THR
1	A	230	LEU
1	A	233	LEU
1	A	286	TRP
1	A	295	LEU
1	A	296	VAL
1	A	307	LEU
1	A	312	ILE
1	A	315	VAL
1	A	317	VAL
1	A	324	TRP
1	A	339	LEU
1	A	343	LEU
1	A	344	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	159	HIS
1	A	171	HIS
1	A	193	ASN
1	A	220	ASN
1	A	311	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 oligosaccharides 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.