



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:33 PM UTC

PDB ID : 1QB2 / pdb_00001qb2
Title : CRYSTAL STRUCTURE OF THE CONSERVED SUBDOMAIN OF HUMAN PROTEIN SRP54M AT 2.1Å RESOLUTION: EVIDENCE FOR THE MECHANISM OF SIGNAL PEPTIDE BINDING
Authors : Clemons Jr., W.M.; Gowda, K.; Black, S.D.; Zwieb, C.; Ramakrishnan, V.
Deposited on : 1999-04-29
Resolution : 2.10 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

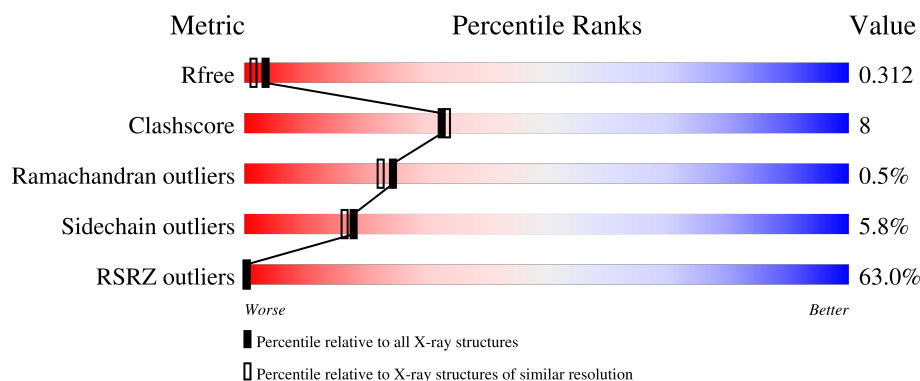
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	109	62% 79% 17% • •
1	B	109	62% 74% 23% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1790 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 HUMAN SIGNAL RECOGNITION PARTICLE 54 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	0	1
			840	523	146	161	10			
1	B	109	Total	C	N	O	S	0	0	0
			866	540	150	165	11			

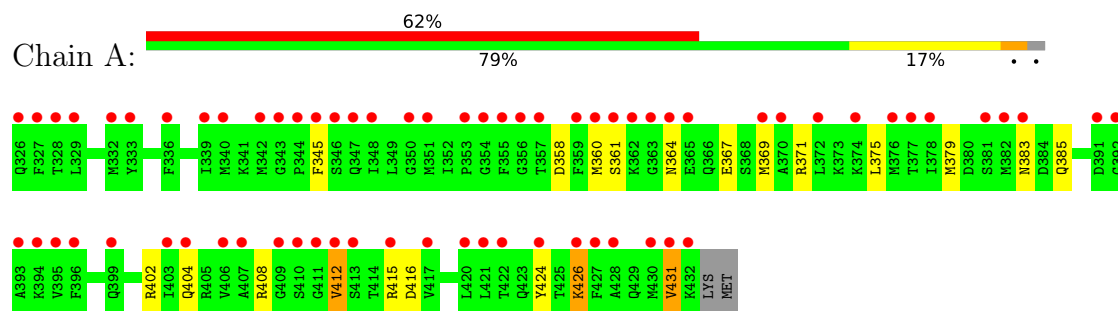
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	53	Total	O	0	0
			53	53		
2	B	31	Total	O	0	0
			31	31		

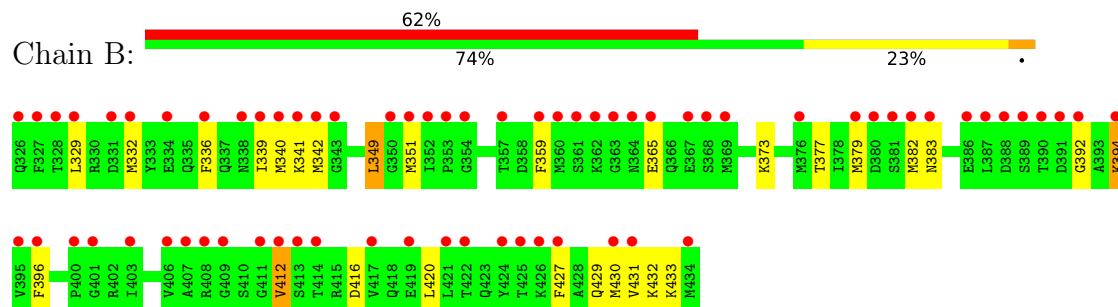
3 Residue-property plots [i](#)

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: HUMAN SIGNAL RECOGNITION PARTICLE 54 KD PROTEIN



• Molecule 1: HUMAN SIGNAL RECOGNITION PARTICLE 54 KD PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	28.91Å 61.34Å 129.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 93.6 (50.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.10 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.245 , 0.318 0.262 , 0.312	Depositor DCC
R_{free} test set	2474 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1790	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% 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	0.51	1/851 (0.1%)	0.93	0/1135
1	B	0.42	0/877	0.91	0/1165
All	All	0.47	1/1728 (0.1%)	0.92	0/2300

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	VAL	C-N	-5.64	1.25	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	840	0	837	13	0
1	B	866	0	872	17	0
2	A	53	0	0	1	0
2	B	31	0	0	1	0
All	All	1790	0	1709	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 8.

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:B:394:LYS:HZ3	1:B:394:LYS:HB3	1.45	0.80
1:A:379:MET:HE1	1:B:329:LEU:O	1.87	0.75
1:B:351:MET:HG2	2:B:88:HOH:O	1.84	0.75
1:B:349:LEU:HD22	1:B:359:PHE:HE2	1.59	0.68
1:A:345:PHE:HB2	2:A:20:HOH:O	2.02	0.59
1:A:360:MET:HE1	1:A:369:MET:HG3	1.85	0.57
1:B:379:MET:HA	1:B:382:MET:HG3	1.87	0.56
1:B:429:GLN:O	1:B:432:LYS:HG2	2.06	0.55
1:B:336:PHE:O	1:B:340:MET:HG2	2.07	0.55
1:A:404:GLN:O	1:A:408:ARG:HG3	2.09	0.53
1:B:349:LEU:HD22	1:B:359:PHE:CE2	2.40	0.52
1:A:375:LEU:O	1:A:379:MET:HG3	2.10	0.52
1:B:392:GLY:O	1:B:396:PHE:HD1	1.95	0.50
1:A:424:TYR:HA	1:B:332:MET:HE1	1.95	0.49
1:B:373:LYS:O	1:B:377:THR:HG23	2.13	0.48
1:A:360:MET:HE1	1:A:369:MET:CG	2.45	0.46
1:A:360:MET:HE3	1:B:339:ILE:HG22	1.97	0.46
1:A:364:ASN:HA	1:A:367:GLU:CD	2.42	0.45
1:A:426:LYS:HB2	1:A:426:LYS:NZ	2.31	0.45
1:B:420:LEU:C	1:B:420:LEU:HD23	2.42	0.45
1:A:385:GLN:NE2	1:A:402:ARG:HH22	2.15	0.44
1:B:427:PHE:O	1:B:431:VAL:HG23	2.17	0.44
1:A:358:ASP:HB3	1:A:361:SER:OG	2.17	0.44
1:B:430:MET:HA	1:B:433:LYS:HB3	2.00	0.42
1:B:412:VAL:HG22	1:B:416:ASP:OD2	2.20	0.41
1:B:341:LYS:HD3	1:B:341:LYS:HA	1.85	0.41
1:A:412:VAL:HG22	1:A:416:ASP:OD1	2.22	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	105/109 (96%)	103 (98%)	1 (1%)	1 (1%)	12	9
1	B	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
All	All	212/218 (97%)	205 (97%)	6 (3%)	1 (0%)	24	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	VAL

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	93/96 (97%)	88 (95%)	5 (5%)	20	18
1	B	96/96 (100%)	90 (94%)	6 (6%)	16	14
All	All	189/192 (98%)	178 (94%)	11 (6%)	18	16

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	ARG
1	A	383	ASN
1	A	412	VAL
1	A	415	ARG
1	A	426	LYS
1	B	342	MET
1	B	349	LEU
1	B	365	GLU
1	B	383	ASN
1	B	394	LYS
1	B	412	VAL

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	335	GLN
1	A	337	GLN
1	A	383	ASN
1	A	385	GLN
1	A	429	GLN
1	B	364	ASN
1	B	383	ASN
1	B	385	GLN
1	B	429	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.

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	107/109 (98%)	2.35	68 (63%)  	23, 41, 75, 87	0
1	B	109/109 (100%)	2.29	68 (62%)  	25, 43, 77, 85	0
All	All	216/218 (99%)	2.32	136 (62%)  	23, 43, 77, 87	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	412	VAL	4.8
1	B	425	THR	4.7
1	A	427	PHE	4.6
1	A	356	GLY	4.4
1	B	360	MET	4.2
1	A	431	VAL	4.2
1	A	355	PHE	4.2
1	A	346	SER	4.0
1	A	351	MET	3.9
1	B	409	GLY	3.8
1	B	342	MET	3.7
1	A	345	PHE	3.7
1	A	406	VAL	3.6
1	A	430	MET	3.5
1	A	369	MET	3.5
1	A	354	GLY	3.4
1	B	379	MET	3.4
1	A	370	ALA	3.3
1	B	391	ASP	3.3
1	A	404	GLN	3.3
1	A	327	PHE	3.3
1	A	359	PHE	3.3
1	B	353	PRO	3.2
1	A	342	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	351	MET	3.2
1	A	347	GLN	3.2
1	B	326	GLN	3.2
1	B	390	THR	3.2
1	A	350	GLY	3.2
1	A	411	GLY	3.2
1	B	339	ILE	3.1
1	B	408	ARG	3.1
1	B	431	VAL	3.1
1	B	434	MET	3.1
1	B	422	THR	3.1
1	A	340	MET	3.1
1	A	377	THR	3.0
1	A	374	LYS	3.0
1	A	329	LEU	3.0
1	A	403	ILE	3.0
1	B	421	LEU	3.0
1	A	360	MET	2.9
1	B	430	MET	2.9
1	B	332	MET	2.9
1	A	365	GLU	2.9
1	B	417	VAL	2.9
1	A	328	THR	2.9
1	A	407	ALA	2.9
1	A	391	ASP	2.8
1	B	343	GLY	2.9
1	B	380	ASP	2.8
1	B	361	SER	2.8
1	B	357	THR	2.8
1	B	367	GLU	2.8
1	B	340	MET	2.8
1	A	336	PHE	2.8
1	A	424	TYR	2.8
1	A	399	GLN	2.7
1	B	427	PHE	2.7
1	A	428	ALA	2.7
1	B	352	ILE	2.7
1	A	420	LEU	2.7
1	B	387	LEU	2.7
1	B	395	VAL	2.7
1	B	362	LYS	2.7
1	A	392	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	326	GLN	2.6
1	B	329	LEU	2.6
1	B	382	MET	2.6
1	A	339	ILE	2.6
1	B	386	GLU	2.6
1	A	393	ALA	2.6
1	A	396	PHE	2.6
1	B	350	GLY	2.6
1	B	376	MET	2.6
1	A	432	LYS	2.6
1	A	344	PRO	2.6
1	A	421	LEU	2.6
1	B	411	GLY	2.5
1	B	424	TYR	2.5
1	A	362	LYS	2.5
1	B	407	ALA	2.5
1	B	336	PHE	2.5
1	A	412	VAL	2.5
1	A	357	THR	2.5
1	B	328	THR	2.5
1	A	382	MET	2.5
1	B	406	VAL	2.4
1	B	365	GLU	2.4
1	B	368	SER	2.4
1	A	378	ILE	2.4
1	A	343	GLY	2.4
1	B	354	GLY	2.4
1	B	419	GLU	2.4
1	B	369	MET	2.4
1	B	394	LYS	2.4
1	A	333	TYR	2.4
1	A	409	GLY	2.4
1	B	363	GLY	2.4
1	B	327	PHE	2.4
1	B	403	ILE	2.4
1	A	417	VAL	2.3
1	B	413	SER	2.3
1	B	359	PHE	2.3
1	B	396	PHE	2.3
1	A	410	SER	2.3
1	B	381	SER	2.3
1	A	363	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	388	ASP	2.3
1	A	361	SER	2.3
1	B	334	GLU	2.3
1	B	400	PRO	2.3
1	B	414	THR	2.3
1	A	383	ASN	2.3
1	A	394	LYS	2.3
1	B	401	GLY	2.3
1	A	353	PRO	2.2
1	A	395	VAL	2.2
1	A	364	ASN	2.2
1	A	422	THR	2.2
1	A	413	SER	2.2
1	A	426	LYS	2.2
1	B	341	LYS	2.2
1	B	389	SER	2.2
1	B	426	LYS	2.2
1	B	338	ASN	2.2
1	A	415	ARG	2.1
1	B	364	ASN	2.1
1	A	372	LEU	2.1
1	B	392	GLY	2.1
1	A	332	MET	2.1
1	B	383	ASN	2.1
1	B	331	ASP	2.1
1	A	381	SER	2.1
1	A	348	ILE	2.0
1	A	376	MET	2.0

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.