



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:42 PM GMT

PDB ID : 1QB2  
Title : CRYSTAL STRUCTURE OF THE CONSERVED SUBDOMAIN OF HUMAN PROTEIN SRP54M AT 2.1A 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

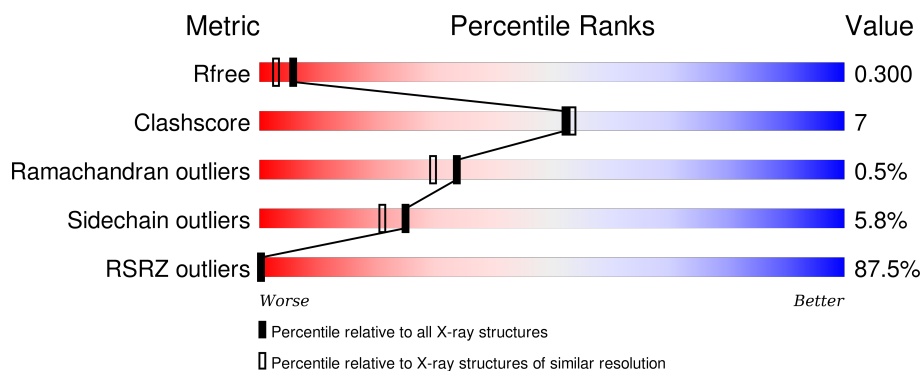
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>84%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>••</div> </div> </div>
1	B	109	<div> <div>89%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>•</div> </div> </div>

## 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			

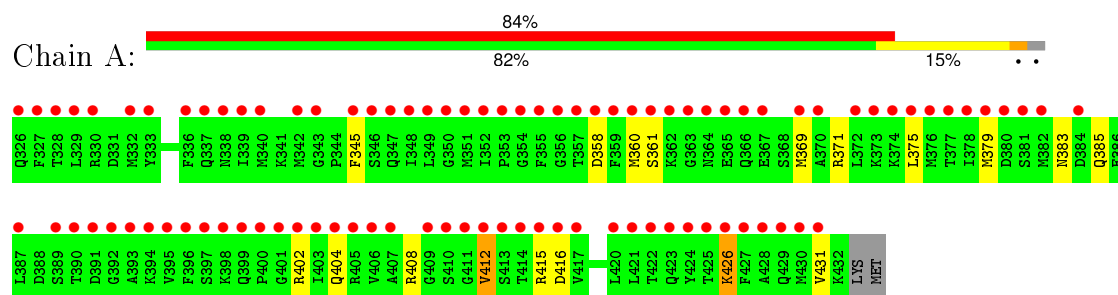
- Molecule 2 is water.

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

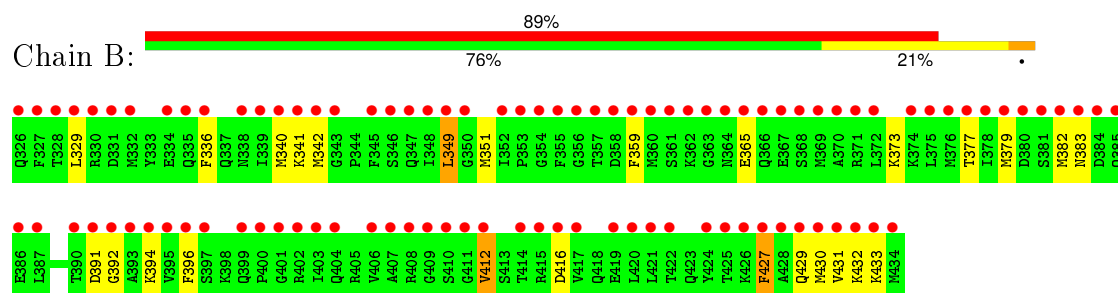
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	28.91Å 61.34Å 129.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 19.49 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 97.8 (19.49-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.10 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.245 , 0.318 0.237 , 0.300	Depositor DCC
$R_{free}$ test set	444 reflections (3.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 24798 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1790	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	0.42	0/851	0.55	0/1135
1	B	0.37	0/877	0.53	0/1165
All	All	0.39	0/1728	0.54	0/2300

There are no bond length outliers.

There are no bond angle outliers.

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	840	0	837	9	0
1	B	866	0	872	15	0
2	A	53	0	0	1	0
2	B	31	0	0	1	0
All	All	1790	0	1709	23	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 7.

All (23) 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:351:MET:HG2	2:B:88:HOH:O	1.84	0.75

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:379:MET:HE1	1:B:329:LEU:O	2.05	0.57
1:B:379:MET:HA	1:B:382:MET:HG3	1.87	0.56
1:B:391:ASP:HB3	1:B:394:LYS:HZ2	1.70	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:B:394:LYS:NZ	1:B:394:LYS:HB3	2.27	0.50
1:B:373:LYS:O	1:B:377:THR:HG23	2.13	0.48
1:A:426:LYS:HB2	1:A:426:LYS:NZ	2.31	0.45
1:A:360:MET:HE1	1:A:369:MET:HG3	1.98	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%)	19	13
1	B	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
All	All	212/218 (97%)	205 (97%)	6 (3%)	1 (0%)	34	30

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%)	27	24
1	B	96/96 (100%)	90 (94%)	6 (6%)	22	18
All	All	189/192 (98%)	178 (94%)	11 (6%)	25	21

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	412	VAL
1	B	427	PHE

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

Mol	Chain	Res	Type
1	A	364	ASN
1	A	383	ASN
1	A	385	GLN
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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	107/109 (98%)	3.59	92 (85%)  	23, 41, 75, 88	0
1	B	109/109 (100%)	3.54	97 (88%)  	25, 43, 77, 85	0
All	All	216/218 (99%)	3.57	189 (87%)  	23, 43, 77, 88	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	GLN	11.8
1	B	390	THR	10.3
1	B	412	VAL	8.0
1	A	327	PHE	7.7
1	A	346	SER	7.7
1	A	358	ASP	7.4
1	A	347	GLN	7.0
1	B	433	LYS	6.8
1	B	402	ARG	6.3
1	A	360	MET	6.2
1	A	404	GLN	6.2
1	B	360	MET	6.1
1	A	326	GLN	6.1
1	A	345	PHE	6.0
1	A	394	LYS	5.7
1	A	403	ILE	5.7
1	A	328	THR	5.7
1	A	427	PHE	5.7
1	B	332	MET	5.6
1	B	379	MET	5.6
1	A	353	PRO	5.6
1	B	364	ASN	5.6
1	B	341	LYS	5.3
1	A	406	VAL	5.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	409	GLY	5.2
1	B	434	MET	5.2
1	A	359	PHE	5.1
1	B	406	VAL	5.0
1	B	342	MET	4.9
1	B	403	ILE	4.9
1	B	430	MET	4.9
1	B	431	VAL	4.8
1	B	361	SER	4.8
1	B	339	ILE	4.7
1	A	332	MET	4.7
1	A	411	GLY	4.7
1	A	369	MET	4.7
1	A	382	MET	4.6
1	A	420	LEU	4.6
1	A	351	MET	4.6
1	A	366	GLN	4.6
1	B	359	PHE	4.5
1	B	419	GLU	4.5
1	A	342	MET	4.5
1	B	353	PRO	4.5
1	B	369	MET	4.4
1	A	329	LEU	4.4
1	B	365	GLU	4.3
1	B	382	MET	4.3
1	B	432	LYS	4.3
1	B	427	PHE	4.2
1	A	407	ALA	4.2
1	A	365	GLU	4.2
1	A	333	TYR	4.2
1	A	370	ALA	4.2
1	A	412	VAL	4.2
1	B	424	TYR	4.2
1	A	395	VAL	4.1
1	B	425	THR	4.1
1	A	372	LEU	4.1
1	B	415	ARG	4.1
1	A	362	LYS	4.1
1	A	429	GLN	4.1
1	A	364	ASN	4.0
1	A	363	GLY	4.0
1	A	340	MET	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	424	TYR	4.0
1	B	363	GLY	4.0
1	A	426	LYS	4.0
1	A	367	GLU	4.0
1	B	362	LYS	4.0
1	B	395	VAL	4.0
1	B	376	MET	3.9
1	B	421	LEU	3.9
1	B	408	ARG	3.9
1	A	399	GLN	3.9
1	B	338	ASN	3.9
1	A	339	ILE	3.9
1	B	370	ALA	3.9
1	A	336	PHE	3.9
1	B	417	VAL	3.9
1	B	328	THR	3.8
1	B	411	GLY	3.8
1	B	329	LEU	3.8
1	A	379	MET	3.8
1	A	349	LEU	3.8
1	A	356	GLY	3.8
1	A	384	ASP	3.8
1	B	336	PHE	3.8
1	A	389	SER	3.7
1	B	358	ASP	3.7
1	B	400	PRO	3.7
1	A	377	THR	3.7
1	A	348	ILE	3.7
1	A	398	LYS	3.7
1	A	355	PHE	3.7
1	A	390	THR	3.7
1	A	361	SER	3.6
1	A	428	ALA	3.6
1	A	430	MET	3.6
1	B	386	GLU	3.6
1	A	376	MET	3.6
1	B	394	LYS	3.6
1	A	330	ARG	3.6
1	A	374	LYS	3.5
1	B	366	GLN	3.5
1	B	334	GLU	3.5
1	B	391	ASP	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	378	ILE	3.4
1	B	357	THR	3.4
1	A	413	SER	3.4
1	B	397	SER	3.4
1	A	415	ARG	3.4
1	A	392	GLY	3.4
1	A	410	SER	3.3
1	B	348	ILE	3.3
1	A	391	ASP	3.3
1	B	340	MET	3.2
1	B	429	GLN	3.2
1	B	414	THR	3.2
1	A	380	ASP	3.1
1	A	387	LEU	3.1
1	A	421	LEU	3.1
1	B	368	SER	3.1
1	B	378	ILE	3.1
1	B	393	ALA	3.0
1	A	343	GLY	3.0
1	B	426	LYS	3.0
1	A	417	VAL	3.0
1	A	396	PHE	3.0
1	A	337	GLN	3.0
1	A	354	GLY	3.0
1	B	396	PHE	3.0
1	B	352	ILE	2.9
1	A	373	LYS	2.9
1	B	381	SER	2.9
1	B	387	LEU	2.9
1	A	357	THR	2.9
1	B	350	GLY	2.9
1	A	405	ARG	2.9
1	A	375	LEU	2.8
1	B	372	LEU	2.8
1	B	385	GLN	2.8
1	B	345	PHE	2.8
1	B	346	SER	2.8
1	B	327	PHE	2.7
1	B	331	ASP	2.7
1	B	404	GLN	2.7
1	B	343	GLY	2.7
1	A	422	THR	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	371	ARG	2.7
1	B	380	ASP	2.7
1	B	375	LEU	2.7
1	B	356	GLY	2.7
1	A	416	ASP	2.7
1	B	392	GLY	2.7
1	A	393	ALA	2.6
1	B	428	ALA	2.6
1	B	420	LEU	2.6
1	A	400	PRO	2.6
1	B	335	GLN	2.6
1	B	354	GLY	2.6
1	B	407	ALA	2.6
1	A	409	GLY	2.6
1	B	383	ASN	2.6
1	B	367	GLU	2.5
1	B	355	PHE	2.5
1	B	349	LEU	2.5
1	B	422	THR	2.5
1	B	330	ARG	2.4
1	B	347	GLN	2.4
1	A	401	GLY	2.4
1	A	381	SER	2.4
1	A	425	THR	2.3
1	A	431	VAL	2.3
1	A	350	GLY	2.3
1	B	374	LYS	2.3
1	B	377	THR	2.3
1	B	399	GLN	2.3
1	B	401	GLY	2.3
1	A	423	GLN	2.2
1	A	352	ILE	2.2
1	A	402	ARG	2.2
1	A	397	SER	2.2
1	B	416	ASP	2.1
1	A	338	ASN	2.1
1	B	384	ASP	2.1
1	A	414	THR	2.0
1	B	410	SER	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 carbohydrates 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.