



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:58 PM GMT

PDB ID : 1QB2  
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 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/ValidationPDFNotes.html>

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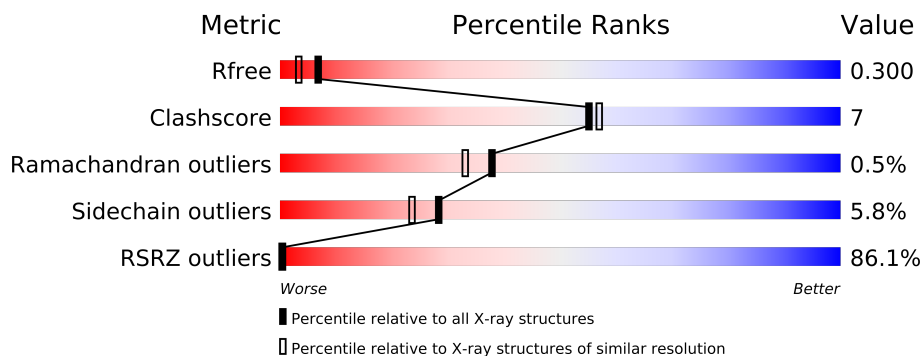
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	109	
1	B	109	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1790 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

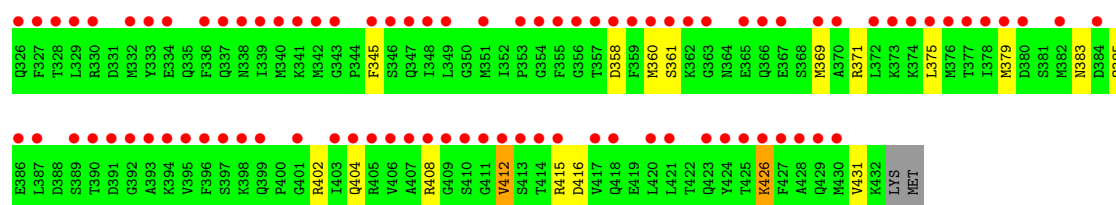
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	53	Total	O	0	0
			53	53		
2	B	31	Total	O	0	0
			31	31		

### 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 ( $RSRZ > 2$ ). 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.

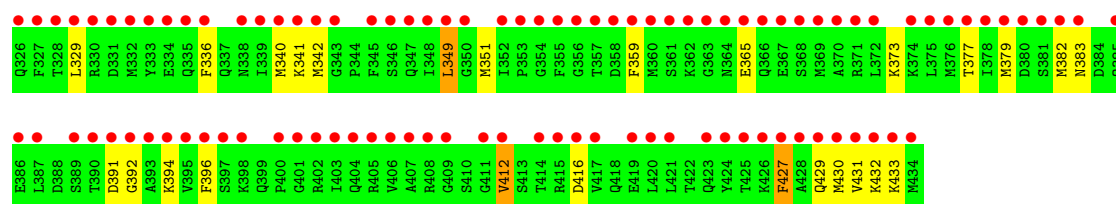
#### • Molecule 1: HUMAN SIGNAL RECOGNITION PARTICLE 54 KD PROTEIN

Chain A: 



#### • Molecule 1: HUMAN SIGNAL RECOGNITION PARTICLE 54 KD PROTEIN

Chain B: 



## 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> )	0.36 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (23) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:351:MET:HG2	2:B:88:HOH:O	1.84	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(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

### 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 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%)	22	14
1	B	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
All	All	212/218 (97%)	205 (97%)	6 (3%)	1 (0%)	38	33

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%)	31	27
1	B	96/96 (100%)	90 (94%)	6 (6%)	25	21
All	All	189/192 (98%)	178 (94%)	11 (6%)	28	23

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 ⓘ

There are no RNA chains 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 carbohydrates 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 ⓘ

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%)	3.30	88 (82%) 0 0	23, 41, 75, 88	0
1	B	109/109 (100%)	3.49	98 (89%) 0 0	25, 43, 77, 85	0
All	All	216/218 (99%)	3.40	186 (86%) 0 0	23, 43, 77, 88	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	GLN	18.4
1	B	412	VAL	8.7
1	A	327	PHE	8.3
1	A	346	SER	7.7
1	B	390	THR	6.9
1	B	402	ARG	6.7
1	A	347	GLN	6.6
1	B	432	LYS	6.1
1	B	433	LYS	6.1
1	A	360	MET	5.7
1	A	345	PHE	5.5
1	B	332	MET	5.5
1	A	404	GLN	5.4
1	B	360	MET	5.3
1	A	394	LYS	5.3
1	B	359	PHE	5.3
1	A	336	PHE	5.2
1	A	359	PHE	5.2
1	B	364	ASN	5.1
1	B	365	GLU	4.9
1	B	434	MET	4.9
1	B	408	ARG	4.9
1	B	339	ILE	4.9
1	A	358	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	412	VAL	4.8
1	B	361	SER	4.8
1	A	326	GLN	4.7
1	A	366	GLN	4.7
1	B	338	ASN	4.7
1	B	370	ALA	4.6
1	B	362	LYS	4.5
1	A	411	GLY	4.5
1	A	342	MET	4.5
1	B	379	MET	4.5
1	A	427	PHE	4.5
1	A	328	THR	4.4
1	A	384	ASP	4.4
1	B	417	VAL	4.4
1	B	341	LYS	4.4
1	A	378	ILE	4.4
1	B	395	VAL	4.4
1	B	431	VAL	4.3
1	B	406	VAL	4.3
1	A	365	GLU	4.3
1	A	413	SER	4.3
1	A	348	ILE	4.3
1	A	382	MET	4.2
1	A	406	VAL	4.2
1	A	355	PHE	4.2
1	B	430	MET	4.2
1	A	370	ALA	4.2
1	B	425	THR	4.2
1	B	382	MET	4.2
1	A	362	LYS	4.2
1	A	332	MET	4.1
1	B	385	GLN	4.1
1	A	387	LEU	4.0
1	B	378	ILE	4.0
1	B	363	GLY	4.0
1	A	377	THR	4.0
1	A	392	GLY	3.9
1	A	349	LEU	3.9
1	A	399	GLN	3.9
1	B	345	PHE	3.9
1	A	426	LYS	3.8
1	A	429	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	369	MET	3.8
1	B	366	GLN	3.8
1	A	407	ALA	3.8
1	B	357	THR	3.8
1	B	427	PHE	3.8
1	A	430	MET	3.8
1	A	339	ILE	3.8
1	A	403	ILE	3.7
1	A	363	GLY	3.7
1	B	342	MET	3.7
1	A	398	LYS	3.7
1	B	407	ALA	3.6
1	B	358	ASP	3.6
1	A	329	LEU	3.6
1	B	396	PHE	3.6
1	B	400	PRO	3.6
1	A	369	MET	3.6
1	B	424	TYR	3.5
1	A	333	TYR	3.5
1	B	392	GLY	3.5
1	B	331	ASP	3.5
1	B	397	SER	3.5
1	B	329	LEU	3.5
1	A	424	TYR	3.5
1	B	419	GLU	3.5
1	A	375	LEU	3.4
1	B	352	ILE	3.4
1	A	379	MET	3.4
1	B	336	PHE	3.4
1	A	340	MET	3.4
1	A	351	MET	3.4
1	B	328	THR	3.4
1	A	420	LEU	3.3
1	B	405	ARG	3.3
1	B	387	LEU	3.3
1	A	374	LYS	3.3
1	A	405	ARG	3.3
1	B	415	ARG	3.3
1	A	356	GLY	3.3
1	B	416	ASP	3.3
1	A	376	MET	3.3
1	B	429	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	421	LEU	3.2
1	B	421	LEU	3.2
1	B	355	PHE	3.2
1	B	393	ALA	3.2
1	B	376	MET	3.2
1	A	389	SER	3.2
1	A	380	ASP	3.1
1	B	403	ILE	3.1
1	A	390	THR	3.1
1	B	394	LYS	3.1
1	A	409	GLY	3.1
1	B	411	GLY	3.1
1	A	410	SER	3.1
1	B	380	ASP	3.0
1	A	354	GLY	3.0
1	A	353	PRO	3.0
1	B	343	GLY	3.0
1	A	423	GLN	3.0
1	A	397	SER	3.0
1	B	371	ARG	2.9
1	A	373	LYS	2.9
1	B	335	GLN	2.8
1	B	347	GLN	2.8
1	B	340	MET	2.8
1	B	383	ASN	2.8
1	B	420	LEU	2.8
1	B	401	GLY	2.8
1	A	395	VAL	2.7
1	B	327	PHE	2.7
1	A	372	LEU	2.7
1	B	330	ARG	2.7
1	B	333	TYR	2.7
1	B	409	GLY	2.7
1	A	391	ASP	2.7
1	A	396	PHE	2.7
1	A	337	GLN	2.7
1	B	377	THR	2.7
1	B	353	PRO	2.6
1	A	330	ARG	2.6
1	B	426	LYS	2.6
1	B	349	LEU	2.6
1	B	423	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	381	SER	2.5
1	A	357	THR	2.5
1	A	417	VAL	2.5
1	A	343	GLY	2.5
1	B	414	THR	2.5
1	A	334	GLU	2.5
1	B	334	GLU	2.5
1	B	367	GLU	2.5
1	B	372	LEU	2.4
1	B	368	SER	2.4
1	A	425	THR	2.4
1	B	346	SER	2.4
1	B	374	LYS	2.4
1	A	428	ALA	2.4
1	B	354	GLY	2.4
1	A	341	LYS	2.4
1	B	404	GLN	2.4
1	B	389	SER	2.3
1	A	414	THR	2.3
1	B	391	ASP	2.3
1	A	386	GLU	2.3
1	A	401	GLY	2.3
1	A	393	ALA	2.2
1	B	428	ALA	2.2
1	A	408	ARG	2.2
1	B	350	GLY	2.2
1	B	356	GLY	2.2
1	A	361	SER	2.2
1	B	375	LEU	2.2
1	A	415	ARG	2.1
1	B	348	ILE	2.1
1	A	338	ASN	2.1
1	B	386	GLU	2.0
1	B	398	LYS	2.0
1	A	418	GLN	2.0
1	A	367	GLU	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.