



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 10:28 PM EDT

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 : unknown
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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

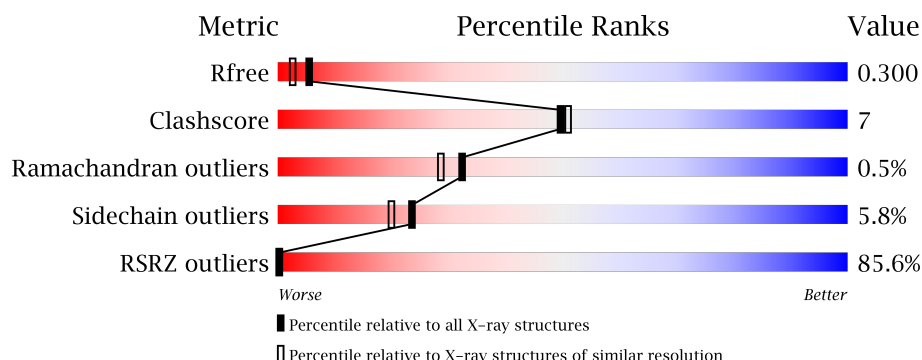
1 Overall quality at a glance

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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 ≥ 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>83%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>••</div> </div> </div>
1	B	109	<div> <div>87%</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			

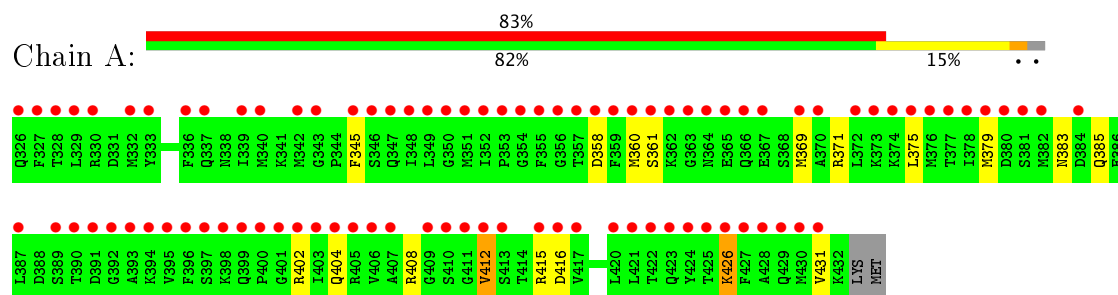
- Molecule 2 is water.

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

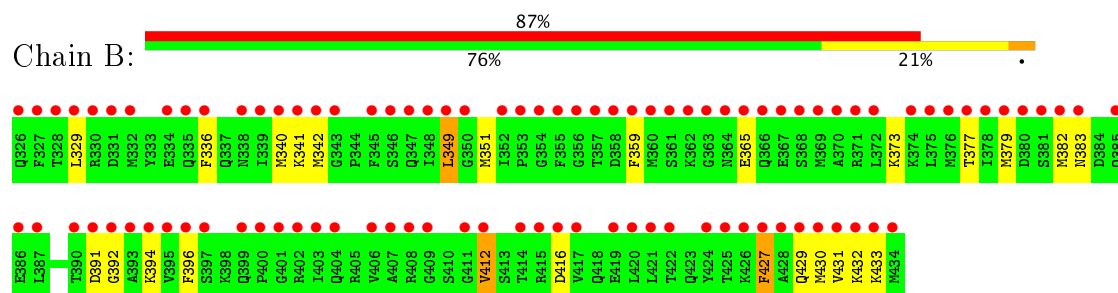
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	18.8	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.3	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

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

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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%)	18	12
1	B	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
All	All	212/218 (97%)	205 (97%)	6 (3%)	1 (0%)	32	28

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%)	26	23
1	B	96/96 (100%)	90 (94%)	6 (6%)	21	17
All	All	189/192 (98%)	178 (94%)	11 (6%)	23	20

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, 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%)	3.44	90 (84%)  	23, 41, 75, 88	0
1	B	109/109 (100%)	3.39	95 (87%)  	25, 43, 77, 85	0
All	All	216/218 (99%)	3.41	185 (85%)  	23, 43, 77, 88	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	GLN	11.5
1	B	390	THR	9.9
1	B	412	VAL	7.5
1	A	346	SER	7.4
1	A	327	PHE	7.4
1	A	358	ASP	7.1
1	A	347	GLN	6.8
1	B	433	LYS	6.6
1	B	402	ARG	6.1
1	A	360	MET	6.0
1	A	404	GLN	6.0
1	B	360	MET	6.0
1	A	326	GLN	5.9
1	A	345	PHE	5.7
1	A	394	LYS	5.6
1	B	332	MET	5.5
1	B	379	MET	5.5
1	A	328	THR	5.5
1	B	364	ASN	5.4
1	A	427	PHE	5.4
1	A	353	PRO	5.4
1	A	403	ILE	5.4
1	B	341	LYS	5.1
1	B	434	MET	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	409	GLY	5.0
1	A	406	VAL	4.9
1	A	359	PHE	4.8
1	B	342	MET	4.8
1	B	430	MET	4.7
1	B	406	VAL	4.7
1	B	403	ILE	4.6
1	B	361	SER	4.6
1	A	332	MET	4.5
1	A	369	MET	4.5
1	B	431	VAL	4.5
1	A	382	MET	4.5
1	A	351	MET	4.5
1	A	411	GLY	4.4
1	B	339	ILE	4.4
1	A	366	GLN	4.4
1	A	420	LEU	4.4
1	B	419	GLU	4.4
1	A	342	MET	4.4
1	B	353	PRO	4.3
1	B	369	MET	4.3
1	B	359	PHE	4.3
1	B	365	GLU	4.2
1	A	329	LEU	4.2
1	B	382	MET	4.2
1	B	432	LYS	4.1
1	A	365	GLU	4.1
1	A	333	TYR	4.0
1	B	424	TYR	4.0
1	B	427	PHE	4.0
1	A	407	ALA	4.0
1	B	415	ARG	4.0
1	B	425	THR	4.0
1	A	362	LYS	4.0
1	A	370	ALA	4.0
1	A	429	GLN	3.9
1	A	372	LEU	3.9
1	A	412	VAL	3.9
1	A	364	ASN	3.9
1	A	340	MET	3.9
1	A	395	VAL	3.9
1	A	367	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	424	TYR	3.9
1	A	426	LYS	3.9
1	A	363	GLY	3.8
1	B	362	LYS	3.8
1	B	376	MET	3.8
1	B	363	GLY	3.8
1	B	408	ARG	3.8
1	A	399	GLN	3.8
1	B	338	ASN	3.8
1	B	421	LEU	3.7
1	A	379	MET	3.7
1	B	395	VAL	3.7
1	B	370	ALA	3.7
1	A	336	PHE	3.7
1	B	328	THR	3.7
1	A	339	ILE	3.6
1	B	411	GLY	3.6
1	B	329	LEU	3.6
1	A	356	GLY	3.6
1	A	349	LEU	3.6
1	A	384	ASP	3.6
1	B	417	VAL	3.6
1	A	389	SER	3.6
1	B	358	ASP	3.6
1	B	400	PRO	3.6
1	A	398	LYS	3.5
1	B	336	PHE	3.5
1	A	377	THR	3.5
1	A	430	MET	3.5
1	B	386	GLU	3.5
1	A	376	MET	3.5
1	A	361	SER	3.5
1	A	390	THR	3.5
1	B	394	LYS	3.5
1	A	355	PHE	3.5
1	A	348	ILE	3.5
1	A	330	ARG	3.5
1	A	374	LYS	3.4
1	A	428	ALA	3.4
1	B	366	GLN	3.4
1	B	334	GLU	3.4
1	B	391	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	357	THR	3.3
1	A	415	ARG	3.3
1	A	413	SER	3.2
1	B	397	SER	3.2
1	A	378	ILE	3.2
1	A	392	GLY	3.2
1	A	410	SER	3.2
1	A	391	ASP	3.2
1	B	340	MET	3.1
1	B	348	ILE	3.1
1	B	429	GLN	3.1
1	B	414	THR	3.0
1	A	380	ASP	3.0
1	B	368	SER	3.0
1	A	387	LEU	3.0
1	A	421	LEU	3.0
1	B	378	ILE	2.9
1	B	426	LYS	2.9
1	A	343	GLY	2.9
1	A	337	GLN	2.9
1	B	393	ALA	2.9
1	A	373	LYS	2.8
1	A	396	PHE	2.8
1	A	354	GLY	2.8
1	A	417	VAL	2.8
1	B	396	PHE	2.8
1	B	381	SER	2.8
1	A	405	ARG	2.8
1	A	357	THR	2.7
1	B	352	ILE	2.7
1	B	387	LEU	2.7
1	B	350	GLY	2.7
1	B	385	GLN	2.7
1	A	375	LEU	2.7
1	B	372	LEU	2.7
1	B	346	SER	2.6
1	B	404	GLN	2.6
1	B	345	PHE	2.6
1	B	371	ARG	2.6
1	B	331	ASP	2.6
1	A	422	THR	2.6
1	B	327	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	343	GLY	2.6
1	B	380	ASP	2.6
1	A	416	ASP	2.5
1	B	356	GLY	2.5
1	B	375	LEU	2.5
1	B	392	GLY	2.5
1	B	335	GLN	2.5
1	A	400	PRO	2.5
1	A	393	ALA	2.5
1	B	420	LEU	2.5
1	B	428	ALA	2.5
1	B	383	ASN	2.5
1	B	354	GLY	2.4
1	B	367	GLU	2.4
1	A	409	GLY	2.4
1	B	407	ALA	2.4
1	B	422	THR	2.4
1	B	349	LEU	2.3
1	B	355	PHE	2.3
1	B	330	ARG	2.3
1	B	347	GLN	2.3
1	A	381	SER	2.3
1	A	401	GLY	2.3
1	B	374	LYS	2.2
1	A	425	THR	2.2
1	B	399	GLN	2.2
1	A	350	GLY	2.2
1	B	377	THR	2.2
1	A	431	VAL	2.1
1	B	401	GLY	2.1
1	A	423	GLN	2.1
1	A	402	ARG	2.1
1	A	397	SER	2.0
1	A	352	ILE	2.0
1	B	416	ASP	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 [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.