Full wwPDB X-ray Structure Validation Report (i)

May 27, 2020 – 12:11 am BST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

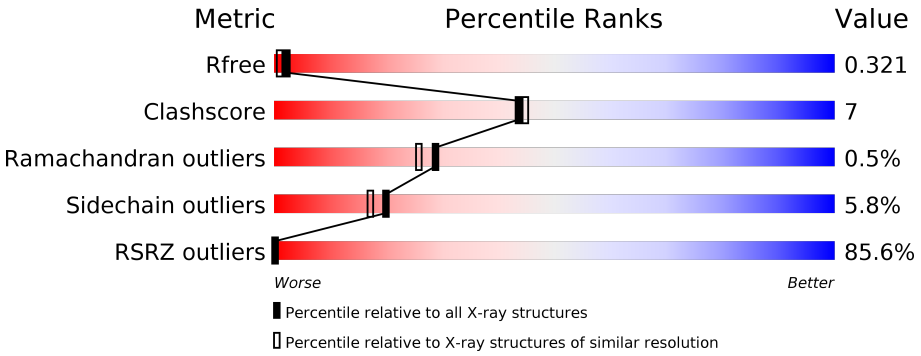
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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 <=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	83% 82% 15%
1	B	109	87% 76% 21%

2 Entry composition (i)

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.

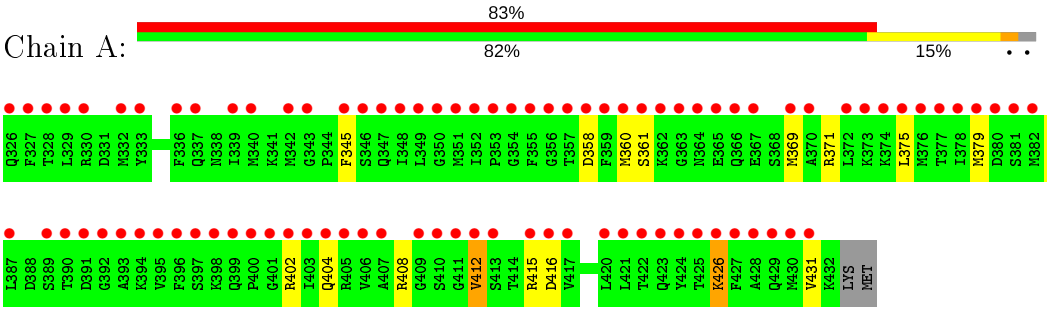
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	53	Total	O	0	0
			53	53		
2	B	31	Total	O	0	0
			31	31		

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 (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.

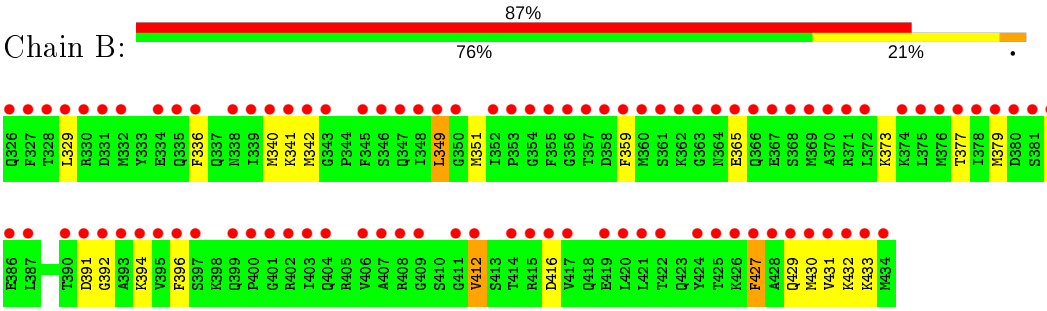
• Molecule 1: HUMAN SIGNAL RECOGNITION PARTICLE 54 KD PROTEIN

Chain A:



• Molecule 1: HUMAN SIGNAL RECOGNITION PARTICLE 54 KD PROTEIN

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	0.10 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.245 , 0.318 0.270 , 0.321	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)	0.34 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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%)	15 11
1	B	107/109 (98%)	102 (95%)	5 (5%)	0	100 100
All	All	212/218 (97%)	205 (97%)	6 (3%)	1 (0%)	29 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	VAL

5.3.2 Protein sidechains (i)

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%)	22	20
1	B	96/96 (100%)	90 (94%)	6 (6%)	18	15
All	All	189/192 (98%)	178 (94%)	11 (6%)	20	17

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 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 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^{th} 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%)	0	0	23, 41, 75, 88	0
1	B	109/109 (100%)	3.39	95 (87%)	0	0	25, 43, 77, 85	0
All	All	216/218 (99%)	3.41	185 (85%)	0	0	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	327	PHE	7.4
1	A	346	SER	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	B	360	MET	6.0
1	A	404	GLN	6.0
1	A	326	GLN	5.9
1	A	345	PHE	5.7
1	A	394	LYS	5.5
1	B	332	MET	5.5
1	B	379	MET	5.5
1	A	328	THR	5.4
1	A	427	PHE	5.4
1	B	364	ASN	5.4
1	A	353	PRO	5.4
1	A	403	ILE	5.4
1	B	341	LYS	5.2
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	4.5
1	B	361	SER	4.5
1	A	332	MET	4.5
1	A	369	MET	4.5
1	A	382	MET	4.5
1	A	351	MET	4.5
1	B	431	VAL	4.5
1	B	339	ILE	4.4
1	A	366	GLN	4.4
1	A	420	LEU	4.4
1	A	411	GLY	4.4
1	B	419	GLU	4.4
1	A	342	MET	4.4
1	B	353	PRO	4.3
1	B	359	PHE	4.3
1	B	369	MET	4.3
1	A	329	LEU	4.2
1	B	365	GLU	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	A	407	ALA	4.0
1	B	427	PHE	4.0
1	A	370	ALA	4.0
1	A	362	LYS	4.0
1	B	425	THR	3.9
1	A	372	LEU	3.9
1	A	395	VAL	3.9
1	A	412	VAL	3.9
1	B	415	ARG	3.9
1	A	429	GLN	3.9
1	A	367	GLU	3.9
1	A	340	MET	3.9
1	A	363	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	424	TYR	3.9
1	A	426	LYS	3.9
1	B	362	LYS	3.9
1	A	364	ASN	3.8
1	B	376	MET	3.8
1	B	408	ARG	3.8
1	A	399	GLN	3.8
1	B	363	GLY	3.8
1	B	338	ASN	3.7
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	356	GLY	3.7
1	B	411	GLY	3.7
1	B	328	THR	3.7
1	B	417	VAL	3.6
1	A	336	PHE	3.6
1	A	339	ILE	3.6
1	B	329	LEU	3.6
1	A	389	SER	3.6
1	A	349	LEU	3.6
1	A	384	ASP	3.6
1	B	358	ASP	3.6
1	B	336	PHE	3.6
1	A	377	THR	3.6
1	B	400	PRO	3.6
1	A	398	LYS	3.5
1	B	394	LYS	3.5
1	A	348	ILE	3.5
1	B	386	GLU	3.5
1	A	376	MET	3.5
1	A	430	MET	3.5
1	A	390	THR	3.5
1	A	361	SER	3.5
1	A	355	PHE	3.5
1	A	330	ARG	3.4
1	B	366	GLN	3.4
1	A	374	LYS	3.4
1	A	428	ALA	3.4
1	B	334	GLU	3.4
1	B	391	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	415	ARG	3.3
1	B	357	THR	3.3
1	A	378	ILE	3.2
1	A	413	SER	3.2
1	A	391	ASP	3.2
1	A	392	GLY	3.2
1	A	410	SER	3.2
1	B	397	SER	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	373	LYS	2.9
1	B	393	ALA	2.9
1	A	337	GLN	2.8
1	A	343	GLY	2.8
1	A	396	PHE	2.8
1	A	354	GLY	2.8
1	B	396	PHE	2.8
1	A	417	VAL	2.8
1	A	405	ARG	2.8
1	B	387	LEU	2.8
1	B	381	SER	2.8
1	B	352	ILE	2.7
1	A	357	THR	2.7
1	B	350	GLY	2.7
1	B	385	GLN	2.7
1	B	404	GLN	2.7
1	A	375	LEU	2.7
1	B	345	PHE	2.6
1	B	372	LEU	2.6
1	B	346	SER	2.6
1	B	331	ASP	2.6
1	B	371	ARG	2.6
1	B	327	PHE	2.6
1	A	422	THR	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	375	LEU	2.6
1	B	356	GLY	2.5
1	B	392	GLY	2.5
1	B	335	GLN	2.5
1	A	400	PRO	2.5
1	B	383	ASN	2.5
1	B	420	LEU	2.5
1	A	393	ALA	2.5
1	B	428	ALA	2.5
1	A	409	GLY	2.4
1	B	407	ALA	2.4
1	B	354	GLY	2.4
1	B	355	PHE	2.4
1	B	367	GLU	2.4
1	B	349	LEU	2.4
1	B	422	THR	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	399	GLN	2.2
1	B	374	LYS	2.2
1	A	350	GLY	2.2
1	A	425	THR	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	2.1
1	A	352	ILE	2.0
1	B	416	ASP	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

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.