Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:40 am BST

PDB ID	:	1R5B
Title	:	Crystal structure analysis of sup35
Authors	:	Kong, C.; Song, H.
Deposited on	:	2003-10-10
Resolution	:	2.35 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 following versions of software and data (see references ①) were used in the production of this report:

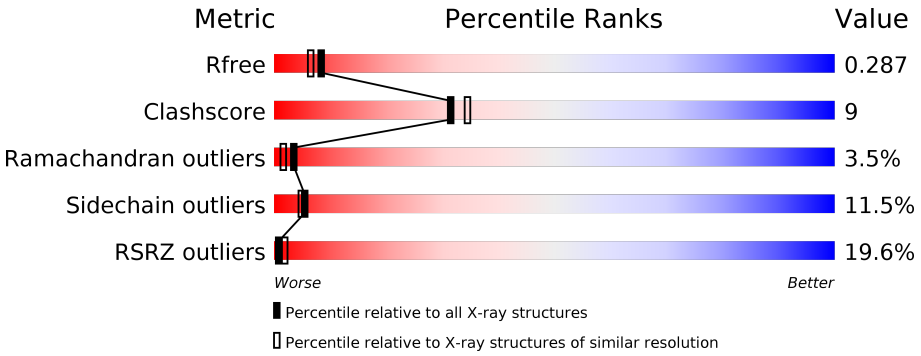
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	467	17% 65% 17% 5% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3381 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 Eukaryotic peptide chain release factor GTP-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3222	2024	557	622	19			

- Molecule 2 is water.

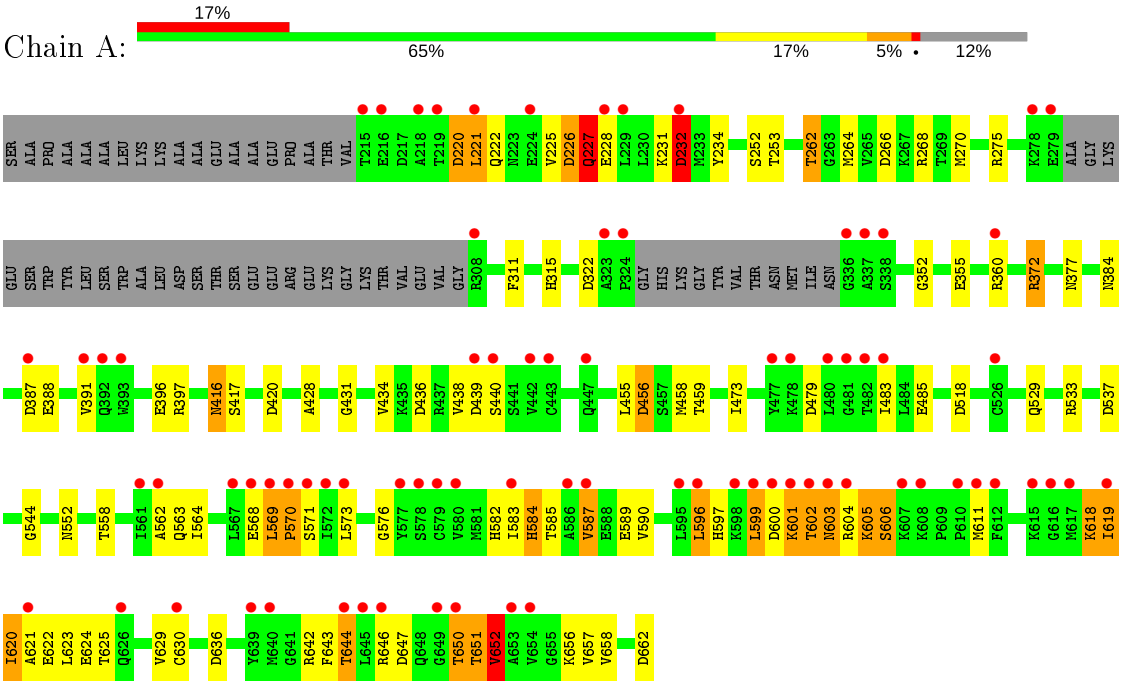
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	159	Total	O	0	0
			159	159		

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: Eukaryotic peptide chain release factor GTP-binding subunit

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	83.80Å 83.80Å 165.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 40.62 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.35) 99.2 (40.62-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.255 , 0.284 0.258 , 0.287	Depositor DCC
R_{free} test set	1284 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3381	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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	0.54	1/3273 (0.0%)	0.81	15/4412 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	ARG	NE-CZ	7.43	1.42	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	232	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	436	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	220	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	266	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	636	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	275	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	322	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	439	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	456	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	537	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	226	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	387	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	600	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	662	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	479	ASP	CB-CG-OD2	5.04	122.83	118.30

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	3222	0	3234	58	0
2	A	159	0	0	6	0
All	All	3381	0	3234	58	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 9.

All (58) 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:A:597:HIS:HB2	1:A:620:ILE:HG23	1.65	0.77
1:A:388:GLU:O	1:A:391:VAL:O	2.05	0.74
1:A:590:VAL:HG21	1:A:623:LEU:HD23	1.70	0.74
1:A:262:THR:HG21	1:A:311:PHE:HB2	1.71	0.72
1:A:384:ASN:HD21	1:A:428:ALA:H	1.34	0.71
1:A:584:HIS:HE1	1:A:630:CYS:O	1.78	0.66
1:A:431:GLY:O	1:A:434:VAL:HG12	1.96	0.65
1:A:599:LEU:HD11	1:A:620:ILE:HG22	1.80	0.64
1:A:222:GLN:O	1:A:225:VAL:HG22	2.00	0.61
1:A:651:THR:O	1:A:652:VAL:HG13	2.02	0.58
1:A:620:ILE:O	1:A:620:ILE:HG13	2.05	0.56
1:A:355:GLU:OE1	2:A:57:HOH:O	2.18	0.56
1:A:416:ASN:HD22	1:A:416:ASN:C	2.10	0.55
1:A:596:LEU:HD22	1:A:597:HIS:CE1	2.42	0.55
1:A:352:GLY:C	2:A:57:HOH:O	2.45	0.55
1:A:619:ILE:HD11	1:A:621:ALA:HB3	1.88	0.54
1:A:544:GLY:HA2	1:A:585:THR:HG23	1.90	0.53
1:A:562:ALA:HB1	1:A:643:PHE:HZ	1.73	0.53
1:A:552:ASN:HB3	2:A:99:HOH:O	2.10	0.52
1:A:372:ARG:HH11	1:A:377:ASN:HD22	1.58	0.52
1:A:221:LEU:HD23	1:A:644:THR:HG23	1.92	0.51
1:A:558:THR:O	1:A:624:GLU:HA	2.10	0.51
1:A:619:ILE:CD1	1:A:621:ALA:HB3	2.40	0.51
1:A:582:HIS:O	1:A:643:PHE:HB2	2.10	0.51
1:A:563:GLN:HA	1:A:619:ILE:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:HIS:CB	1:A:620:ILE:HG23	2.40	0.50
1:A:596:LEU:HB3	1:A:597:HIS:ND1	2.26	0.50
1:A:605:LYS:O	1:A:606:SER:CB	2.60	0.50
1:A:234:TYR:CE2	1:A:642:ARG:HG3	2.47	0.49
1:A:221:LEU:HD12	1:A:584:HIS:HA	1.95	0.49
1:A:262:THR:HG23	1:A:264:MET:CE	2.43	0.48
1:A:473:ILE:O	1:A:585:THR:HG21	2.14	0.48
1:A:582:HIS:ND1	1:A:587:VAL:HG22	2.29	0.48
1:A:658:VAL:HB	2:A:117:HOH:O	2.13	0.48
1:A:596:LEU:H	1:A:621:ALA:HB2	1.79	0.47
1:A:221:LEU:HD13	1:A:222:GLN:HG2	1.96	0.47
1:A:231:LYS:O	1:A:232:ASP:CB	2.62	0.47
1:A:352:GLY:N	2:A:57:HOH:O	2.50	0.46
1:A:416:ASN:ND2	1:A:416:ASN:C	2.69	0.45
1:A:315:HIS:HD2	1:A:456:ASP:OD2	1.97	0.45
1:A:569:LEU:N	1:A:570:PRO:CD	2.79	0.45
1:A:622:GLU:O	1:A:623:LEU:HD12	2.17	0.45
1:A:602:THR:O	1:A:604:ARG:N	2.50	0.45
1:A:483:ILE:HD13	1:A:533:ARG:HA	2.00	0.44
1:A:226:ASP:O	1:A:227:GLN:HB2	2.18	0.43
1:A:231:LYS:O	1:A:232:ASP:HB3	2.19	0.43
1:A:564:ILE:O	1:A:618:LYS:HA	2.19	0.43
1:A:603:ASN:ND2	2:A:138:HOH:O	2.53	0.42
1:A:225:VAL:HG21	1:A:642:ARG:HH21	1.85	0.42
1:A:596:LEU:HD22	1:A:597:HIS:HE1	1.82	0.42
1:A:582:HIS:O	1:A:643:PHE:CB	2.67	0.42
1:A:589:GLU:O	1:A:625:THR:HG22	2.20	0.42
1:A:650:THR:O	1:A:651:THR:HG22	2.19	0.42
1:A:416:ASN:O	1:A:420:ASP:HB2	2.19	0.41
1:A:564:ILE:N	1:A:619:ILE:HG22	2.34	0.41
1:A:563:GLN:HE21	1:A:563:GLN:HB3	1.74	0.41
1:A:582:HIS:CE1	1:A:587:VAL:HG22	2.56	0.41
1:A:597:HIS:O	1:A:619:ILE:HA	2.21	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	403/467 (86%)	359 (89%)	30 (7%)	14 (4%)	3 1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	PRO
1	A	603	ASN
1	A	606	SER
1	A	220	ASP
1	A	227	GLN
1	A	518	ASP
1	A	605	LYS
1	A	652	VAL
1	A	576	GLY
1	A	228	GLU
1	A	232	ASP
1	A	601	LYS
1	A	573	LEU
1	A	587	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	356/398 (89%)	315 (88%)	41 (12%)	5 5

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	A	227	GLN
1	A	252	SER
1	A	253	THR
1	A	262	THR
1	A	270	MET
1	A	360	ARG
1	A	372	ARG
1	A	396	GLU
1	A	397	ARG
1	A	416	ASN
1	A	417	SER
1	A	438	VAL
1	A	440	SER
1	A	455	LEU
1	A	458	MET
1	A	459	THR
1	A	485	GLU
1	A	529	GLN
1	A	568	GLU
1	A	569	LEU
1	A	571	SER
1	A	583	ILE
1	A	584	HIS
1	A	596	LEU
1	A	599	LEU
1	A	601	LYS
1	A	602	THR
1	A	611	MET
1	A	618	LYS
1	A	619	ILE
1	A	620	ILE
1	A	629	VAL
1	A	644	THR
1	A	646	ARG
1	A	647	ASP
1	A	650	THR
1	A	651	THR
1	A	652	VAL
1	A	656	LYS
1	A	657	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	315	HIS
1	A	367	HIS
1	A	377	ASN
1	A	378	HIS
1	A	384	ASN
1	A	416	ASN
1	A	460	HIS
1	A	506	GLN
1	A	542	GLN
1	A	563	GLN
1	A	584	HIS
1	A	648	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	409/467 (87%)	1.09	80 (19%) 1 2	25, 36, 42, 52	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	ALA	9.5
1	A	568	GLU	9.5
1	A	567	LEU	6.8
1	A	573	LEU	6.3
1	A	596	LEU	6.3
1	A	650	THR	6.3
1	A	570	PRO	6.1
1	A	621	ALA	5.9
1	A	601	LYS	5.6
1	A	600	ASP	5.6
1	A	338	SER	5.3
1	A	215	THR	5.3
1	A	229	LEU	5.1
1	A	218	ALA	5.1
1	A	616	GLY	5.1
1	A	477	TYR	4.9
1	A	583	ILE	4.9
1	A	569	LEU	4.5
1	A	649	GLY	4.5
1	A	360	ARG	4.3
1	A	572	ILE	4.3
1	A	579	CYS	4.2
1	A	216	GLU	4.2
1	A	595	LEU	4.1
1	A	480	LEU	4.0
1	A	324	PRO	3.8
1	A	639	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	645	LEU	3.6
1	A	644	THR	3.6
1	A	571	SER	3.5
1	A	447	GLN	3.4
1	A	603	ASN	3.4
1	A	604	ARG	3.4
1	A	221	LEU	3.2
1	A	611	MET	3.2
1	A	440	SER	3.0
1	A	478	LYS	2.9
1	A	608	LYS	2.9
1	A	598	LYS	2.9
1	A	580	VAL	2.8
1	A	481	GLY	2.8
1	A	653	ALA	2.7
1	A	387	ASP	2.7
1	A	607	LYS	2.7
1	A	561	ILE	2.6
1	A	562	ALA	2.6
1	A	442	VAL	2.6
1	A	654	VAL	2.6
1	A	640	MET	2.6
1	A	336	GLY	2.5
1	A	577	TYR	2.5
1	A	615	LYS	2.5
1	A	279	GLU	2.4
1	A	619	ILE	2.4
1	A	610	PRO	2.4
1	A	483	ILE	2.4
1	A	391	VAL	2.4
1	A	443	CYS	2.4
1	A	323	ALA	2.3
1	A	482	THR	2.3
1	A	602	THR	2.3
1	A	578	SER	2.3
1	A	586	ALA	2.3
1	A	224	GLU	2.2
1	A	278	LYS	2.2
1	A	232	ASP	2.2
1	A	587	VAL	2.2
1	A	626	GLN	2.2
1	A	612	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	393	TRP	2.2
1	A	219	THR	2.2
1	A	599	LEU	2.2
1	A	308	ARG	2.1
1	A	526	CYS	2.1
1	A	228	GLU	2.1
1	A	392	GLN	2.1
1	A	617	MET	2.1
1	A	439	ASP	2.0
1	A	630	CYS	2.0
1	A	646	ARG	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.