



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:47 PM GMT

PDB ID : 1R5N
Title : Crystal Structure Analysis of sup35 complexed with GDP
Authors : Kong, C.; Song, H.
Deposited on : 2003-10-10
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

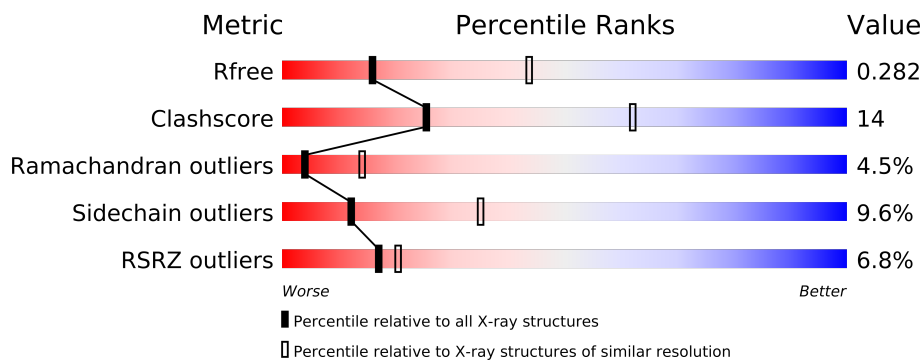
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. 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	467	

2 Entry composition i

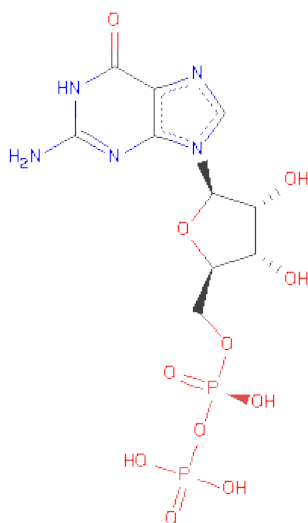
There are 3 unique types of molecules in this entry. The entry contains 3316 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Eukaryotic peptide chain release factor GTP-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	3213	2019	556	619	19	0	0	0

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	28	10	5	11	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	75	Total 75 O 75	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.76 Å 82.76 Å 169.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 46.61 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 100.0 (46.61-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.256 , 0.284 0.258 , 0.282	Depositor DCC
R_{free} test set	674 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 16860 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3316	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP

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	0.46	0/3264	0.76	9/4400 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	647	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	538	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	232	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	387	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	540	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	518	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	322	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	515	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	636	ASP	CB-CG-OD2	5.05	122.84	118.30

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	3213	0	3228	88	0
2	A	28	0	12	1	0
3	A	75	0	0	10	0
All	All	3316	0	3240	88	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 14.

All (88) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:598:LYS:HA	1:A:619:ILE:HG22	1.63	0.80
1:A:228:GLU:O	1:A:231:LYS:NZ	2.16	0.74
1:A:433:ASN:HB2	1:A:438:VAL:HG13	1.69	0.72
1:A:455:LEU:HA	1:A:458:MET:HE2	1.74	0.68
1:A:494:LYS:O	1:A:513:ILE:HD11	1.94	0.68
1:A:384:ASN:HD21	1:A:428:ALA:H	1.42	0.67
1:A:246:HIS:ND1	1:A:247:VAL:HG23	2.09	0.67
1:A:372:ARG:NH1	1:A:377:ASN:HD22	1.94	0.66
1:A:593:ALA:O	1:A:594:LYS:HB2	1.98	0.63
1:A:544:GLY:HA3	1:A:586:ALA:HA	1.81	0.61
1:A:392:GLN:N	3:A:24:HOH:O	2.27	0.60
1:A:393:TRP:CZ3	1:A:438:VAL:HG11	2.36	0.60
1:A:384:ASN:ND2	1:A:385:LYS:H	2.00	0.59
1:A:544:GLY:CA	1:A:586:ALA:HA	2.32	0.59
1:A:372:ARG:HH11	1:A:377:ASN:HD22	1.51	0.59
1:A:420:ASP:HB3	3:A:35:HOH:O	2.02	0.58
1:A:435:LYS:HA	1:A:452:LEU:HD12	1.84	0.58
1:A:581:MET:HE2	1:A:643:PHE:CG	2.39	0.58
1:A:510:VAL:HA	1:A:534:VAL:HG12	1.86	0.58
1:A:262:THR:HG21	1:A:311:PHE:HB2	1.85	0.58
1:A:644:THR:HG22	1:A:654:VAL:HG12	1.88	0.55
1:A:393:TRP:CH2	1:A:438:VAL:HG11	2.41	0.55
1:A:372:ARG:HH11	1:A:377:ASN:ND2	2.05	0.54
1:A:246:HIS:NE2	1:A:363:GLN:HG2	2.23	0.54
1:A:593:ALA:O	1:A:594:LYS:CB	2.55	0.54
1:A:602:THR:O	1:A:603:ASN:C	2.46	0.53
1:A:224:GLU:O	3:A:59:HOH:O	2.18	0.53
1:A:266:ASP:OD2	1:A:269:THR:N	2.34	0.53
1:A:246:HIS:CE1	1:A:363:GLN:HG2	2.44	0.52
1:A:240:ASN:HB3	1:A:321:LEU:HD11	1.90	0.52
1:A:460:HIS:HE1	1:A:462:GLU:OE2	1.94	0.51
1:A:597:HIS:HB2	1:A:620:ILE:HG12	1.93	0.51
1:A:342:ILE:HD13	1:A:458:MET:HE1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:267:LYS:O	1:A:271:GLU:HG3	2.11	0.50
1:A:363:GLN:HG3	1:A:367:HIS:CE1	2.47	0.50
1:A:633:ARG:HG3	3:A:41:HOH:O	2.12	0.50
1:A:584:HIS:O	1:A:585:THR:HB	2.11	0.50
1:A:582:HIS:O	1:A:643:PHE:HA	2.12	0.49
1:A:227:GLN:HE21	1:A:229:LEU:HB3	1.78	0.49
1:A:590:VAL:HG21	1:A:623:LEU:HD23	1.93	0.49
1:A:571:SER:O	1:A:572:ILE:HB	2.12	0.49
1:A:246:HIS:HE2	1:A:363:GLN:H	1.59	0.48
1:A:346:VAL:HA	1:A:382:VAL:HG12	1.95	0.48
1:A:416:ASN:ND2	1:A:419:THR:OG1	2.46	0.48
1:A:224:GLU:HG2	1:A:644:THR:CG2	2.44	0.48
1:A:566:ILE:HG22	1:A:615:LYS:HA	1.94	0.48
1:A:460:HIS:CE1	1:A:462:GLU:OE2	2.67	0.47
1:A:651:THR:O	1:A:652:VAL:HG13	2.14	0.47
1:A:372:ARG:NH1	1:A:377:ASN:ND2	2.62	0.47
1:A:315:HIS:HD2	1:A:456:ASP:OD2	1.98	0.47
1:A:339:GLN:NE2	1:A:374:GLN:O	2.48	0.46
1:A:590:VAL:CG2	1:A:623:LEU:HD23	2.45	0.46
1:A:581:MET:HE2	1:A:643:PHE:CD1	2.51	0.46
1:A:572:ILE:HG23	1:A:573:LEU:N	2.31	0.46
1:A:240:ASN:ND2	3:A:70:HOH:O	2.49	0.45
1:A:658:VAL:HB	3:A:32:HOH:O	2.17	0.45
1:A:471:MET:HE2	1:A:547:LEU:HD12	1.99	0.45
1:A:576:GLY:O	1:A:577:TYR:O	2.35	0.45
1:A:584:HIS:HE1	1:A:630:CYS:O	2.00	0.45
1:A:575:THR:HG23	1:A:593:ALA:HA	2.00	0.44
1:A:566:ILE:N	1:A:566:ILE:HD12	2.31	0.44
1:A:598:LYS:H	1:A:606:SER:HB2	1.83	0.44
1:A:572:ILE:HG23	1:A:573:LEU:HD13	1.99	0.44
1:A:388:GLU:O	1:A:391:VAL:O	2.36	0.44
1:A:598:LYS:HG3	1:A:617:MET:HE3	2.00	0.44
1:A:258:ILE:O	1:A:262:THR:HB	2.17	0.44
1:A:589:GLU:O	1:A:625:THR:HG22	2.18	0.44
1:A:582:HIS:HA	3:A:42:HOH:O	2.18	0.43
1:A:471:MET:CE	1:A:547:LEU:HD12	2.48	0.43
1:A:584:HIS:HD2	1:A:585:THR:HG22	1.83	0.43
1:A:566:ILE:HG21	3:A:33:HOH:O	2.18	0.43
1:A:462:GLU:OE2	3:A:28:HOH:O	2.21	0.43
1:A:495:LYS:NZ	1:A:520:GLU:HG2	2.34	0.43
1:A:237:GLU:HB3	1:A:316:ARG:HG2	2.00	0.43
1:A:563:GLN:HG2	1:A:620:ILE:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:354:PHE:CZ	1:A:401:CYS:HA	2.55	0.42
1:A:502:MET:HB3	1:A:503:PRO:HA	2.01	0.42
1:A:221:LEU:CD1	1:A:644:THR:HG23	2.50	0.42
1:A:262:THR:CG2	1:A:264:MET:HG2	2.49	0.42
1:A:248:ASP:HB3	2:A:663:GDP:H5"	2.02	0.42
1:A:581:MET:HE2	1:A:643:PHE:CD2	2.55	0.41
1:A:220:ASP:OD1	1:A:220:ASP:O	2.38	0.41
1:A:359:GLU:O	1:A:360:ARG:C	2.59	0.41
1:A:564:ILE:HG22	1:A:565:ALA:N	2.35	0.41
1:A:432:GLN:HB3	1:A:438:VAL:HG12	2.02	0.41
1:A:455:LEU:HD12	1:A:458:MET:CE	2.51	0.41
1:A:237:GLU:OE2	1:A:464:LYS:NZ	2.42	0.40
1:A:610:PRO:HA	3:A:68:HOH:O	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	402/467 (86%)	339 (84%)	45 (11%)	18 (4%)	4 14

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	573	LEU
1	A	577	TYR
1	A	585	THR
1	A	594	LYS
1	A	601	LYS
1	A	605	LYS
1	A	227	GLN
1	A	572	ILE
1	A	584	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	603	ASN
1	A	652	VAL
1	A	247	VAL
1	A	568	GLU
1	A	595	LEU
1	A	587	VAL
1	A	518	ASP
1	A	389	PRO

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	355/398 (89%)	321 (90%)	34 (10%)	12	35

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	THR
1	A	221	LEU
1	A	231	LYS
1	A	232	ASP
1	A	262	THR
1	A	391	VAL
1	A	397	ARG
1	A	435	LYS
1	A	438	VAL
1	A	455	LEU
1	A	459	THR
1	A	462	GLU
1	A	466	ASN
1	A	482	THR
1	A	485	GLU
1	A	515	ASP
1	A	519	GLU
1	A	524	SER
1	A	549	SER
1	A	568	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	569	LEU
1	A	572	ILE
1	A	575	THR
1	A	596	LEU
1	A	600	ASP
1	A	602	THR
1	A	605	LYS
1	A	619	ILE
1	A	625	THR
1	A	629	VAL
1	A	645	LEU
1	A	652	VAL
1	A	657	VAL
1	A	659	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	227	GLN
1	A	240	ASN
1	A	315	HIS
1	A	377	ASN
1	A	378	HIS
1	A	384	ASN
1	A	416	ASN
1	A	460	HIS
1	A	466	ASN
1	A	506	GLN
1	A	542	GLN
1	A	563	GLN
1	A	584	HIS

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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GDP	A	663	-	30,30,30	1.04	1 (3%)	44,47,47	2.07	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	663	-	-	0/16/32/32	0/1/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	663	GDP	C2-N3	4.06	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	663	GDP	C6-C5-N7	-8.24	133.03	134.14
2	A	663	GDP	O4'-C1'-N9	5.49	113.55	108.44
2	A	663	GDP	PA-O3A-PB	-4.26	119.20	131.68
2	A	663	GDP	C2-N3-C4	3.52	120.04	115.09
2	A	663	GDP	C5-C4-N3	-3.19	121.32	125.94
2	A	663	GDP	N3-C4-N9	3.00	131.31	126.91
2	A	663	GDP	N7-C8-N9	-2.10	108.42	114.36
2	A	663	GDP	O2A-PA-O3A	2.00	114.64	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	408/467 (87%)	0.22	28 (6%) 17 20	28, 60, 99, 111	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	LEU	9.2
1	A	217	ASP	4.4
1	A	572	ILE	4.1
1	A	569	LEU	4.1
1	A	568	GLU	4.0
1	A	337	ALA	3.9
1	A	580	VAL	3.5
1	A	215	THR	3.2
1	A	600	ASP	2.7
1	A	651	THR	2.6
1	A	223	ASN	2.6
1	A	571	SER	2.6
1	A	648	GLN	2.6
1	A	360	ARG	2.4
1	A	586	ALA	2.4
1	A	567	LEU	2.4
1	A	229	LEU	2.3
1	A	227	GLN	2.2
1	A	219	THR	2.2
1	A	226	ASP	2.2
1	A	535	ARG	2.2
1	A	481	GLY	2.2
1	A	216	GLU	2.2
1	A	225	VAL	2.2
1	A	649	GLY	2.1
1	A	607	LYS	2.1
1	A	621	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	480	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GDP	A	663	28/28	0.15	-0.49	63,65,66,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.