



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:33 PM GMT

PDB ID : 1KU1
Title : Crystal Structure of the Sec7 Domain of Yeast GEA2
Authors : Renault, L.; Christova, P.; Guibert, B.; Pasqualato, S.; Cherfils, J.
Deposited on : 2002-01-20
Resolution : 1.93 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

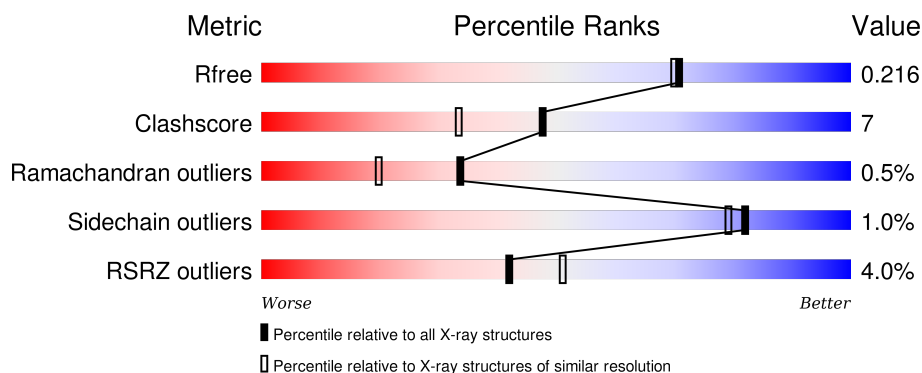
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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	230	<div> <div>4%</div> <div>80%</div> <div>10%</div> <div>8%</div> </div>
1	B	230	<div> <div>3%</div> <div>76%</div> <div>16%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3629 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 ARF guanine-nucleotide exchange factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1706	1080	286	328	12			
1	B	211	Total	C	N	O	S	0	0	0
			1706	1080	286	328	12			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	CLONING ARTIFACT	UNP P39993
A	-20	GLY	-	CLONING ARTIFACT	UNP P39993
A	-19	SER	-	CLONING ARTIFACT	UNP P39993
A	-18	SER	-	CLONING ARTIFACT	UNP P39993
A	-17	HIS	-	CLONING ARTIFACT	UNP P39993
A	-16	HIS	-	CLONING ARTIFACT	UNP P39993
A	-15	HIS	-	CLONING ARTIFACT	UNP P39993
A	-14	HIS	-	CLONING ARTIFACT	UNP P39993
A	-13	HIS	-	CLONING ARTIFACT	UNP P39993
A	-12	HIS	-	CLONING ARTIFACT	UNP P39993
A	-11	SER	-	CLONING ARTIFACT	UNP P39993
A	-10	SER	-	CLONING ARTIFACT	UNP P39993
A	-9	GLY	-	CLONING ARTIFACT	UNP P39993
A	-8	LEU	-	CLONING ARTIFACT	UNP P39993
A	-7	VAL	-	CLONING ARTIFACT	UNP P39993
A	-6	PRO	-	CLONING ARTIFACT	UNP P39993
A	-5	ARG	-	CLONING ARTIFACT	UNP P39993
A	-4	GLY	-	CLONING ARTIFACT	UNP P39993
A	-3	SER	-	CLONING ARTIFACT	UNP P39993
A	-2	HIS	-	CLONING ARTIFACT	UNP P39993
A	-1	MET	-	CLONING ARTIFACT	UNP P39993
A	747	VAL	ILE	CLONING ARTIFACT	UNP P39993
B	-21	MET	-	CLONING ARTIFACT	UNP P39993
B	-20	GLY	-	CLONING ARTIFACT	UNP P39993
B	-19	SER	-	CLONING ARTIFACT	UNP P39993

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	CLONING ARTIFACT	UNP P39993
B	-17	HIS	-	CLONING ARTIFACT	UNP P39993
B	-16	HIS	-	CLONING ARTIFACT	UNP P39993
B	-15	HIS	-	CLONING ARTIFACT	UNP P39993
B	-14	HIS	-	CLONING ARTIFACT	UNP P39993
B	-13	HIS	-	CLONING ARTIFACT	UNP P39993
B	-12	HIS	-	CLONING ARTIFACT	UNP P39993
B	-11	SER	-	CLONING ARTIFACT	UNP P39993
B	-10	SER	-	CLONING ARTIFACT	UNP P39993
B	-9	GLY	-	CLONING ARTIFACT	UNP P39993
B	-8	LEU	-	CLONING ARTIFACT	UNP P39993
B	-7	VAL	-	CLONING ARTIFACT	UNP P39993
B	-6	PRO	-	CLONING ARTIFACT	UNP P39993
B	-5	ARG	-	CLONING ARTIFACT	UNP P39993
B	-4	GLY	-	CLONING ARTIFACT	UNP P39993
B	-3	SER	-	CLONING ARTIFACT	UNP P39993
B	-2	HIS	-	CLONING ARTIFACT	UNP P39993
B	-1	MET	-	CLONING ARTIFACT	UNP P39993
B	747	VAL	ILE	CLONING ARTIFACT	UNP P39993

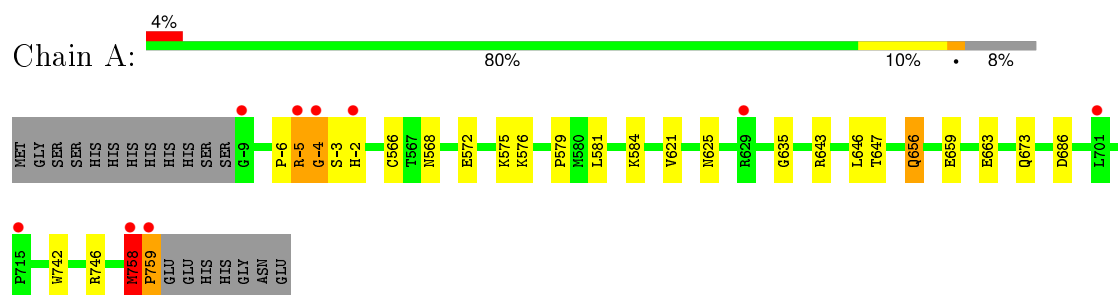
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	110	Total O 110 110	0	0
2	B	107	Total O 107 107	0	0

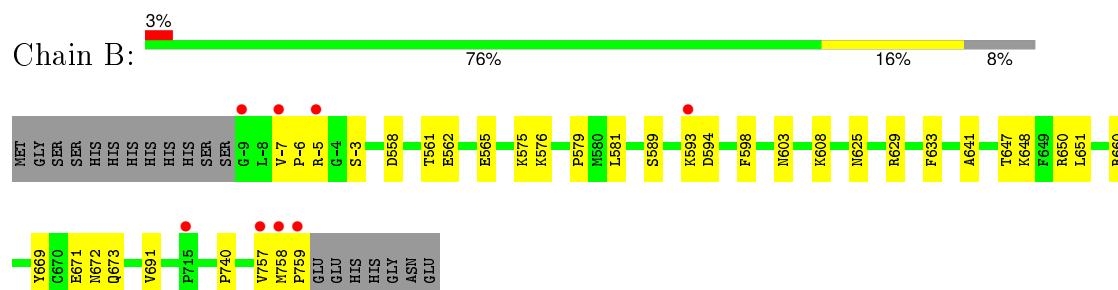
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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: ARF guanine-nucleotide exchange factor 2



- Molecule 1: ARF guanine-nucleotide exchange factor 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.05Å 75.88Å 76.20Å 90.00° 105.37° 90.00°	Depositor
Resolution (Å)	24.04 – 1.93 24.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.04-1.93) 96.9 (24.04-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.228 0.214 , 0.216	Depositor DCC
R_{free} test set	3541 reflections (7.04%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 52653 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3629	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.33 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7814e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/1742	0.68	3/2349 (0.1%)
1	B	0.33	0/1742	0.54	0/2349
All	All	0.34	0/3484	0.61	3/4698 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	-4	GLY	N-CA-C	-10.76	86.21	113.10
1	A	758	MET	N-CA-C	8.23	133.23	111.00
1	A	-3	SER	N-CA-C	-6.36	93.84	111.00

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	1706	0	1669	24	0
1	B	1706	0	1669	26	0
2	A	110	0	0	0	0
2	B	107	0	0	2	0
All	All	3629	0	3338	50	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 (50) 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:-4:GLY:H	1:A:-2:HIS:H	1.17	0.89
1:A:656:GLN:H	1:A:656:GLN:NE2	1.73	0.87
1:A:656:GLN:H	1:A:656:GLN:HE21	1.39	0.69
1:A:659:GLU:O	1:A:663:GLU:HG3	1.96	0.66
1:A:-4:GLY:H	1:A:-2:HIS:N	1.93	0.65
1:B:651:LEU:H	1:B:758:MET:HE1	1.62	0.64
1:A:643:ARG:O	1:A:647:THR:HG23	1.98	0.62
1:A:646:LEU:O	1:A:759:PRO:HG2	1.99	0.61
1:B:593:LYS:NZ	1:B:593:LYS:HB3	2.16	0.61
1:B:-7:VAL:HG22	1:B:-3:SER:OG	2.02	0.59
1:A:758:MET:HB3	1:A:759:PRO:CD	2.34	0.57
1:A:-6:PRO:O	1:A:-5:ARG:HB3	2.04	0.57
1:B:648:LYS:O	1:B:759:PRO:HG2	2.05	0.57
1:A:635:GLY:H	1:A:673:GLN:HE22	1.55	0.55
1:B:650:ARG:HH11	1:B:650:ARG:HG3	1.73	0.54
1:A:566:CYS:SG	1:A:584:LYS:HG3	2.47	0.53
1:B:625:ASN:O	1:B:629:ARG:HG3	2.09	0.53
1:B:651:LEU:H	1:B:758:MET:CE	2.22	0.52
1:B:651:LEU:HG	1:B:758:MET:HE1	1.91	0.51
1:A:742:TRP:O	1:A:746:ARG:HD3	2.11	0.50
1:B:647:THR:HA	1:B:757:VAL:O	2.12	0.49
1:B:603:ASN:ND2	1:B:608:LYS:HE3	2.28	0.49
1:B:558:ASP:O	1:B:562:GLU:HG3	2.13	0.48
1:B:648:LYS:O	1:B:759:PRO:CG	2.63	0.47
1:A:-4:GLY:HA2	1:A:-2:HIS:CD2	2.50	0.47
1:A:-6:PRO:O	1:A:-5:ARG:O	2.32	0.47
1:B:581:LEU:HD13	1:B:598:PHE:CE2	2.49	0.47
1:A:758:MET:CB	1:A:759:PRO:CD	2.93	0.47
1:A:568:ASN:O	1:A:572:GLU:HG2	2.15	0.47
1:A:-4:GLY:N	1:A:-2:HIS:H	1.98	0.46
1:A:621:VAL:HG22	1:A:625:ASN:ND2	2.31	0.46
1:B:669:TYR:O	1:B:673:GLN:HG2	2.16	0.46
1:B:593:LYS:HZ2	1:B:593:LYS:HB3	1.80	0.46
1:B:-5:ARG:NH1	2:B:217:HOH:O	2.47	0.45
1:B:650:ARG:CG	1:B:650:ARG:HH11	2.29	0.45
1:B:576:LYS:O	1:B:579:PRO:HG2	2.17	0.44
1:A:576:LYS:O	1:A:579:PRO:HG2	2.18	0.44
1:B:589:SER:OG	1:B:594:ASP:OD2	2.29	0.43
1:B:660:ARG:HD2	2:B:169:HOH:O	2.19	0.43
1:B:575:LYS:HB3	1:B:575:LYS:NZ	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:PHE:CD1	1:B:641:ALA:HB1	2.53	0.43
1:A:575:LYS:HB3	1:A:575:LYS:NZ	2.34	0.42
1:A:656:GLN:N	1:A:656:GLN:NE2	2.55	0.42
1:B:-7:VAL:HG22	1:B:-6:PRO:HD2	2.00	0.42
1:B:648:LYS:O	1:B:759:PRO:CD	2.68	0.42
1:A:686:ASP:HA	1:A:742:TRP:CZ3	2.55	0.41
1:A:575:LYS:HZ3	1:A:575:LYS:HB3	1.86	0.41
1:B:691:VAL:HG22	1:B:740:PRO:HG2	2.03	0.41
1:B:561:THR:O	1:B:565:GLU:HG3	2.21	0.40
1:A:566:CYS:HB3	1:A:581:LEU:CD2	2.51	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	209/230 (91%)	200 (96%)	7 (3%)	2 (1%)	19	7
1	B	209/230 (91%)	206 (99%)	3 (1%)	0	100	100
All	All	418/460 (91%)	406 (97%)	10 (2%)	2 (0%)	34	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	MET
1	A	-5	ARG

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	194/211 (92%)	192 (99%)	2 (1%)	82	79
1	B	194/211 (92%)	192 (99%)	2 (1%)	82	79
All	All	388/422 (92%)	384 (99%)	4 (1%)	82	79

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	656	GLN
1	A	759	PRO
1	B	671	GLU
1	B	672	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	604	ASN
1	A	625	ASN
1	A	656	GLN
1	A	673	GLN
1	A	720	HIS
1	B	-2	HIS
1	B	601	ASN
1	B	602	ASN
1	B	603	ASN

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, 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	211/230 (91%)	0.08	9 (4%)	39 48	18, 29, 57, 98	0
1	B	211/230 (91%)	0.21	8 (3%)	44 54	18, 34, 62, 95	0
All	All	422/460 (91%)	0.15	17 (4%)	42 51	18, 31, 60, 98	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	759	PRO	7.6
1	A	758	MET	5.7
1	A	-5	ARG	5.1
1	B	-5	ARG	4.3
1	B	-9	GLY	3.4
1	A	629	ARG	2.9
1	A	-9	GLY	2.8
1	B	715	PRO	2.8
1	B	758	MET	2.7
1	A	701	LEU	2.5
1	A	715	PRO	2.5
1	B	-7	VAL	2.2
1	B	757	VAL	2.2
1	B	593	LYS	2.2
1	A	-2	HIS	2.1
1	A	-4	GLY	2.1
1	B	759	PRO	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.