



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:28 PM UTC

PDB ID : 1G8Y / pdb_00001g8y
Title : CRYSTAL STRUCTURE OF THE HEXAMERIC REPLICATIVE HELI-
CASE REPA OF PLASMID RSF1010
Authors : Niedenzu, T.; Roeleke, D.; Bains, G.; Scherzinger, E.; Saenger, W.
Deposited on : 2000-11-21
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

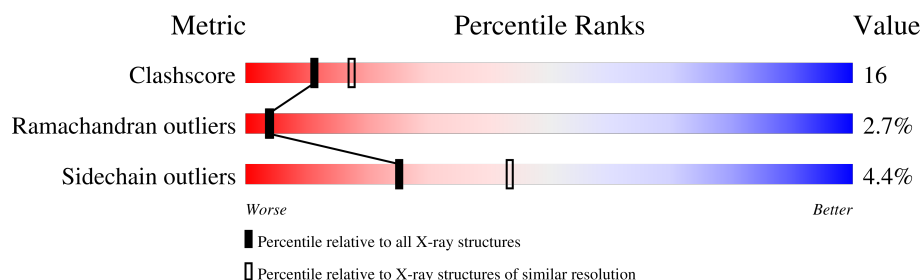
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 of 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	279	62% 23% • 13%
1	B	279	57% 24% 5% 13%
1	C	279	59% 23% • 13%
1	D	279	61% 23% • 13%
1	E	279	58% 24% • 13%
1	F	279	63% 20% •• 13%
1	G	279	59% 22% 5% 13%
1	H	279	63% 21% • 13%

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Mol	Chain	Length	Quality of chain
1	I	279	59%23%••13%
1	J	279	59%23%•13%
1	K	279	62%19%5%13%
1	L	279	63%19%•13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22536 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 REGULATORY PROTEIN REPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	B	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	C	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	D	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	E	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	F	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	G	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	H	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	I	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	J	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	K	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	L	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total	O	0	0
			41	41		
2	B	40	Total	O	0	0
			40	40		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	40	Total 40	O 40	0	0
2	D	39	Total 39	O 39	0	0
2	E	41	Total 41	O 41	0	0
2	F	39	Total 39	O 39	0	0
2	G	41	Total 41	O 41	0	0
2	H	38	Total 38	O 38	0	0
2	I	41	Total 41	O 41	0	0
2	J	41	Total 41	O 41	0	0
2	K	38	Total 38	O 38	0	0
2	L	41	Total 41	O 41	0	0

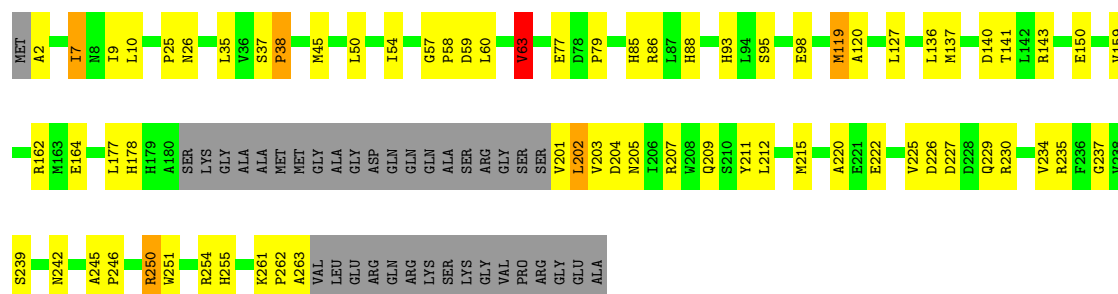
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

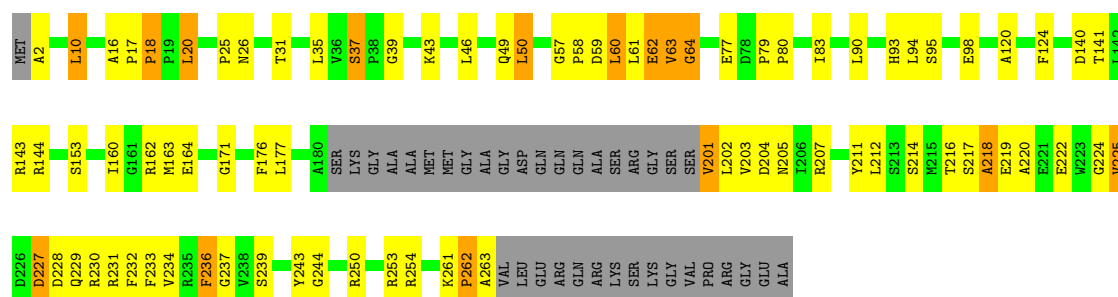
• Molecule 1: REGULATORY PROTEIN REPA

Chain A: 



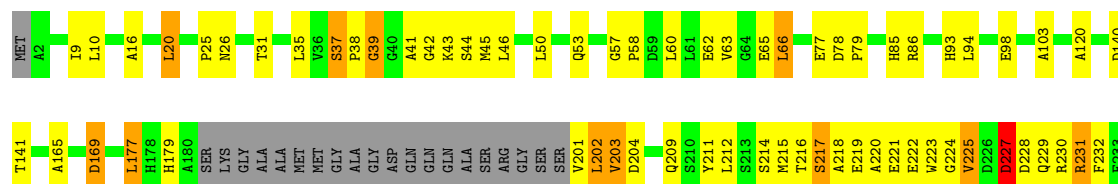
• Molecule 1: REGULATORY PROTEIN REPA

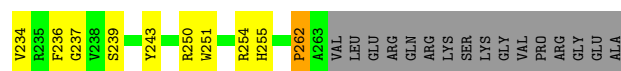
Chain B: 



• Molecule 1: REGULATORY PROTEIN REPA

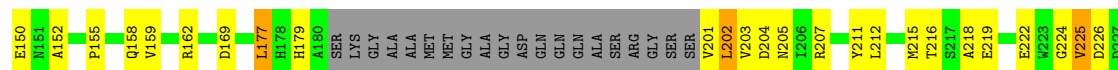
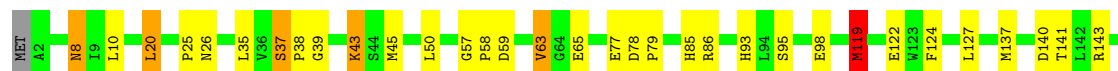
Chain C: 





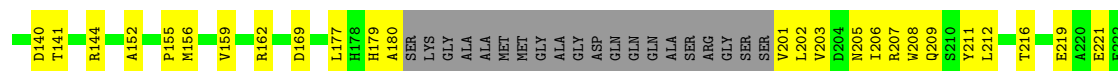
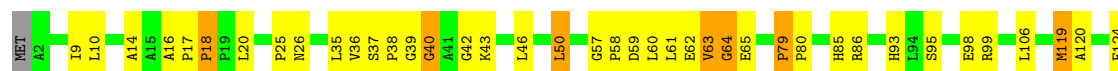
• Molecule 1: REGULATORY PROTEIN REPA

Chain D: 61% 23% 13%



• Molecule 1: REGULATORY PROTEIN REPA

Chain E: 58% 24% 13%



• Molecule 1: REGULATORY PROTEIN REPA

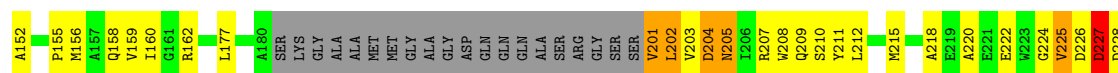
Chain F: 63% 20% 13%



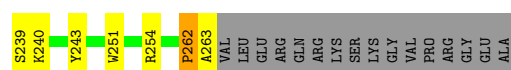
• Molecule 1: REGULATORY PROTEIN REPA

Chain G: 59% 22% 5% 13%

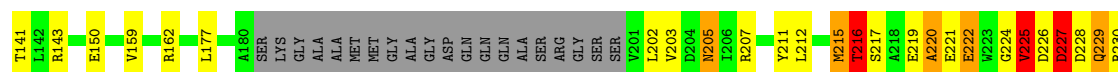




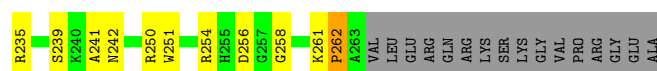
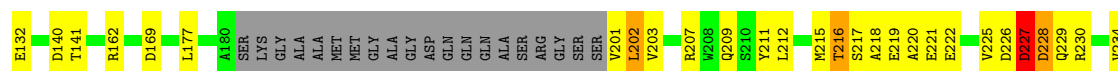
• Molecule 1: REGULATORY PROTEIN REPA



• Molecule 1: REGULATORY PROTEIN REPA



• Molecule 1: REGULATORY PROTEIN REPA



• Molecule 1: REGULATORY PROTEIN REPA



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.43Å 179.16Å 116.29Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	92.0 (30.00-2.40)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22536	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.62	1/1884 (0.1%)	1.00	6/2564 (0.2%)
1	B	0.58	0/1884	1.04	10/2564 (0.4%)
1	C	0.62	0/1884	1.02	11/2564 (0.4%)
1	D	0.63	1/1884 (0.1%)	0.97	4/2564 (0.2%)
1	E	0.60	2/1884 (0.1%)	1.02	13/2564 (0.5%)
1	F	0.60	0/1884	1.04	9/2564 (0.4%)
1	G	0.68	1/1884 (0.1%)	1.05	8/2564 (0.3%)
1	H	0.67	1/1884 (0.1%)	1.04	11/2564 (0.4%)
1	I	0.60	1/1884 (0.1%)	1.01	13/2564 (0.5%)
1	J	0.67	0/1884	1.07	10/2564 (0.4%)
1	K	0.64	0/1884	1.01	10/2564 (0.4%)
1	L	0.62	1/1884 (0.1%)	0.99	5/2564 (0.2%)
All	All	0.63	8/22608 (0.0%)	1.02	110/30768 (0.4%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	119	MET	SD-CE	-8.51	1.58	1.79
1	E	119	MET	SD-CE	-8.41	1.58	1.79
1	D	119	MET	SD-CE	-7.34	1.61	1.79
1	A	119	MET	SD-CE	-7.01	1.62	1.79
1	L	119	MET	SD-CE	-6.71	1.62	1.79

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	104	ASP	N-CA-C	-12.75	94.73	110.41
1	F	57	GLY	CA-C-N	11.03	130.99	119.85
1	F	57	GLY	C-N-CA	11.03	130.99	119.85
1	B	57	GLY	CA-C-N	9.58	130.17	119.92
1	B	57	GLY	C-N-CA	9.58	130.17	119.92

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	1838	0	1819	60	0
1	B	1838	0	1819	73	0
1	C	1838	0	1819	65	0
1	D	1838	0	1819	66	0
1	E	1838	0	1819	64	0
1	F	1838	0	1819	49	0
1	G	1838	0	1819	61	0
1	H	1838	0	1819	53	0
1	I	1838	0	1819	78	0
1	J	1838	0	1819	63	0
1	K	1838	0	1819	56	0
1	L	1838	0	1819	60	0
2	A	41	0	0	2	0
2	B	40	0	0	0	0
2	C	40	0	0	1	0
2	D	39	0	0	0	0
2	E	41	0	0	1	0
2	F	39	0	0	0	0
2	G	41	0	0	0	0
2	H	38	0	0	0	0
2	I	41	0	0	0	0
2	J	41	0	0	1	0
2	K	38	0	0	1	0
2	L	41	0	0	2	0
All	All	22536	0	21828	709	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 16.

The worst 5 of 709 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:F:203:VAL:HG23	1:F:209:GLN:HE22	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:HG3	1:A:250:ARG:HH11	1.19	1.05
1:B:250:ARG:HG3	1:B:250:ARG:HH11	1.31	0.95
1:H:203:VAL:HG23	1:H:209:GLN:HE22	1.33	0.94
1:B:62:GLU:HB2	1:B:262:PRO:HG3	1.56	0.88

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	238/279 (85%)	215 (90%)	19 (8%)	4 (2%)	7	10
1	B	238/279 (85%)	214 (90%)	15 (6%)	9 (4%)	2	2
1	C	238/279 (85%)	215 (90%)	13 (6%)	10 (4%)	2	2
1	D	238/279 (85%)	221 (93%)	14 (6%)	3 (1%)	9	14
1	E	238/279 (85%)	220 (92%)	13 (6%)	5 (2%)	5	7
1	F	238/279 (85%)	220 (92%)	12 (5%)	6 (2%)	4	5
1	G	238/279 (85%)	222 (93%)	12 (5%)	4 (2%)	7	10
1	H	238/279 (85%)	219 (92%)	15 (6%)	4 (2%)	7	10
1	I	238/279 (85%)	212 (89%)	16 (7%)	10 (4%)	2	2
1	J	238/279 (85%)	222 (93%)	10 (4%)	6 (2%)	4	5
1	K	238/279 (85%)	216 (91%)	14 (6%)	8 (3%)	3	2
1	L	238/279 (85%)	215 (90%)	15 (6%)	8 (3%)	3	2
All	All	2856/3348 (85%)	2611 (91%)	168 (6%)	77 (3%)	4	4

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	PRO

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Mol	Chain	Res	Type
1	B	217	SER
1	B	218	ALA
1	B	225	VAL
1	C	225	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	186/212 (88%)	180 (97%)	6 (3%)	34	56
1	B	186/212 (88%)	179 (96%)	7 (4%)	29	49
1	C	186/212 (88%)	176 (95%)	10 (5%)	20	35
1	D	186/212 (88%)	177 (95%)	9 (5%)	23	40
1	E	186/212 (88%)	179 (96%)	7 (4%)	29	49
1	F	186/212 (88%)	178 (96%)	8 (4%)	26	44
1	G	186/212 (88%)	173 (93%)	13 (7%)	14	24
1	H	186/212 (88%)	180 (97%)	6 (3%)	34	56
1	I	186/212 (88%)	179 (96%)	7 (4%)	29	49
1	J	186/212 (88%)	177 (95%)	9 (5%)	23	40
1	K	186/212 (88%)	178 (96%)	8 (4%)	26	44
1	L	186/212 (88%)	177 (95%)	9 (5%)	23	40
All	All	2232/2544 (88%)	2133 (96%)	99 (4%)	25	43

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	231	ARG
1	I	227	ASP
1	G	261	LYS
1	H	219	GLU
1	J	43	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	109	GLN
1	J	242	ASN
1	H	209	GLN
1	I	205	ASN
1	K	242	ASN

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.