



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 1F9F / pdb_00001f9f
Title : CRYSTAL STRUCTURE OF THE HPV-18 E2 DNA-BINDING DOMAIN
Authors : Kim, S.S.; Tam, J.; Wang, A.F.; Hegde, R.
Deposited on : 2000-07-10
Resolution : 1.90 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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

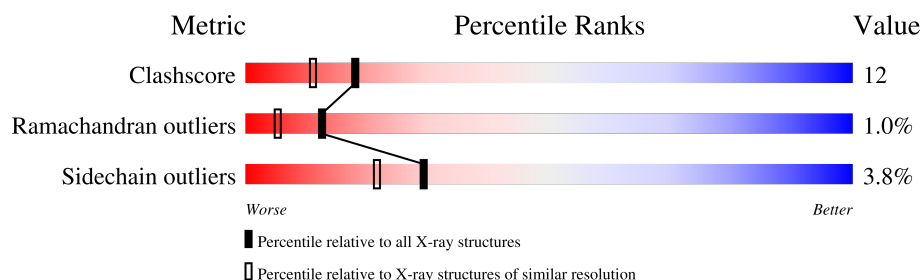
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 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	83	 57% 29% 6% 8%
1	B	83	 60% 25% 6% 7%
1	C	83	 65% 19% 7% 8%
1	D	83	 77% 19% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2560 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.

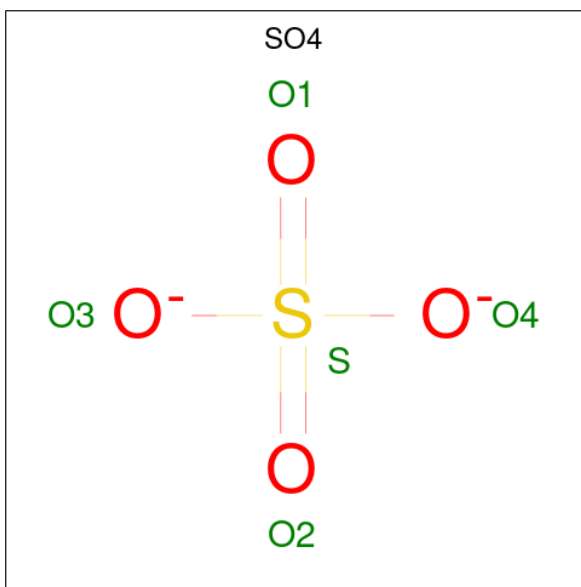
- Molecule 1 is a protein called Regulatory protein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	S	0	0	0
			605	380	112	109	4			
1	B	77	Total	C	N	O	S	0	0	0
			592	375	106	108	3			
1	C	76	Total	C	N	O	S	0	0	0
			597	377	108	108	4			
1	D	82	Total	C	N	O	S	0	0	0
			657	413	121	119	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	GLY	-	expression tag	UNP P06790
A	284	SER	-	expression tag	UNP P06790
A	285	HIS	-	expression tag	UNP P06790
A	286	MET	-	expression tag	UNP P06790
B	283	GLY	-	expression tag	UNP P06790
B	284	SER	-	expression tag	UNP P06790
B	285	HIS	-	expression tag	UNP P06790
B	286	MET	-	expression tag	UNP P06790
C	283	GLY	-	expression tag	UNP P06790
C	284	SER	-	expression tag	UNP P06790
C	285	HIS	-	expression tag	UNP P06790
C	286	MET	-	expression tag	UNP P06790
D	283	GLY	-	expression tag	UNP P06790
D	284	SER	-	expression tag	UNP P06790
D	285	HIS	-	expression tag	UNP P06790
D	286	MET	-	expression tag	UNP P06790

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	12	Total	O	0	0
			12	12		
3	C	23	Total	O	0	0
			23	23		
3	D	43	Total	O	0	0
			43	43		

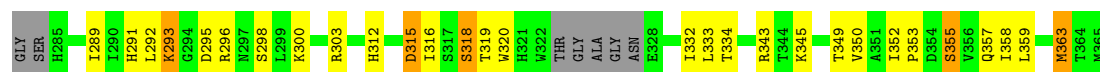
3 Residue-property plots [i](#)

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 E2

Chain A: 



• Molecule 1: Regulatory protein E2

Chain B: 



• Molecule 1: Regulatory protein E2

Chain C: 



• Molecule 1: Regulatory protein E2

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.50 Å 46.80 Å 161.06 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.52 – 1.90	Depositor
% Data completeness (in resolution range)	94.3 (30.52-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2560	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.46	3/619 (0.5%)	1.48	8/836 (1.0%)
1	B	1.42	6/604 (1.0%)	1.44	7/819 (0.9%)
1	C	1.64	5/609 (0.8%)	1.53	5/824 (0.6%)
1	D	1.72	5/672 (0.7%)	1.45	2/909 (0.2%)
All	All	1.57	19/2504 (0.8%)	1.48	22/3388 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	363	MET	SD-CE	-7.38	1.61	1.79
1	C	304	TYR	CA-CB	7.34	1.64	1.53
1	D	360	VAL	CA-CB	7.05	1.63	1.54
1	C	312	HIS	N-CA	-6.95	1.37	1.46
1	A	350	VAL	CA-CB	6.91	1.62	1.54
1	A	363	MET	SD-CE	-6.45	1.63	1.79
1	D	346	PHE	N-CA	6.39	1.53	1.46
1	B	289	ILE	CA-CB	6.24	1.62	1.54
1	B	350	VAL	CA-CB	6.12	1.62	1.54
1	B	316	ILE	CA-CB	5.81	1.62	1.54
1	D	363	MET	N-CA	5.73	1.52	1.46
1	C	311	ASP	CA-C	-5.40	1.45	1.52
1	D	352	ILE	CA-C	5.39	1.58	1.52
1	C	365	MET	CG-SD	5.35	1.94	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	363	MET	CG-SD	5.26	1.94	1.80
1	B	294	GLY	CA-C	-5.19	1.45	1.51
1	D	346	PHE	CA-C	5.17	1.59	1.52
1	B	352	ILE	C-O	-5.09	1.19	1.23
1	A	343	ARG	CZ-NH2	5.03	1.40	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	312	HIS	N-CA-C	-10.73	96.35	111.81
1	D	318	SER	N-CA-C	-9.04	99.29	110.41
1	D	310	SER	N-CA-C	-8.78	101.87	112.58
1	B	318	SER	N-CA-C	-7.93	100.30	110.53
1	B	352	ILE	CB-CA-C	-6.99	103.35	110.13
1	B	307	ARG	CA-C-N	6.88	133.57	123.12
1	B	307	ARG	C-N-CA	6.88	133.57	123.12
1	A	318	SER	N-CA-C	-6.73	100.83	110.59
1	B	304	TYR	N-CA-C	-6.38	104.25	111.14
1	A	355	SER	CA-C-N	-6.27	115.42	123.19
1	A	355	SER	C-N-CA	-6.27	115.42	123.19
1	C	318	SER	N-CA-C	-6.25	102.11	110.55
1	C	311	ASP	CA-C-O	6.22	129.41	120.51
1	A	353	PRO	N-CA-C	5.99	120.49	111.14
1	B	312	HIS	N-CA-C	5.97	120.30	113.19
1	A	312	HIS	N-CA-C	5.87	119.73	112.58
1	A	292	LEU	N-CA-C	-5.70	99.22	108.52
1	C	313	TYR	N-CA-C	5.59	117.89	109.23
1	A	291	HIS	N-CA-C	-5.38	100.94	109.59
1	A	349	THR	CB-CA-C	-5.23	101.40	109.29
1	C	317	SER	N-CA-C	5.14	117.44	110.35
1	B	310	SER	N-CA-C	-5.03	107.20	113.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	362	TYR	Sidechain

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	605	0	582	20	0
1	B	592	0	559	15	0
1	C	597	0	583	15	0
1	D	657	0	648	11	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	21	0	0	2	0
3	B	12	0	0	0	0
3	C	23	0	0	2	0
3	D	43	0	0	0	0
All	All	2560	0	2372	59	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 12.

All (59) 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)
3:A:62:HOH:O	1:D:301:CYS:HB2	1.26	1.28
1:A:357:GLN:NE2	1:A:359:LEU:HD21	1.62	1.11
1:B:310:SER:HA	1:B:313:TYR:CE2	1.93	1.03
1:D:352:ILE:HG12	1:D:358:ILE:HD11	1.41	0.97
1:D:340:GLU:OE2	1:D:362:TYR:OH	1.91	0.89
1:C:332:ILE:HG22	3:C:99:HOH:O	1.73	0.86
1:A:303:ARG:NH2	1:A:319:THR:H	1.75	0.84
1:C:309:HIS:O	1:C:310:SER:O	1.99	0.80
1:A:303:ARG:HH21	1:A:318:SER:HA	1.55	0.72
1:A:296:ARG:O	1:A:300:LYS:HG3	1.91	0.70
1:A:357:GLN:HE21	1:A:359:LEU:HD21	1.60	0.66
1:A:295:ASP:HB3	1:A:298:SER:OG	1.97	0.65
1:D:352:ILE:CG1	1:D:358:ILE:HD11	2.23	0.64
1:B:300:LYS:HE3	1:B:300:LYS:C	2.23	0.64
1:B:303:ARG:HB2	1:B:333:LEU:HD21	1.80	0.63
1:A:316:ILE:HD11	1:A:333:LEU:HD22	1.81	0.62
1:B:310:SER:HA	1:B:313:TYR:CZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HH21	1:A:318:SER:CA	2.16	0.58
1:A:303:ARG:NH2	1:A:319:THR:N	2.49	0.57
1:A:293:LYS:HG2	1:A:332:ILE:HG12	1.88	0.56
1:A:334:THR:HG21	1:A:363:MET:HE1	1.88	0.56
1:B:364:THR:O	1:B:365:MET:HB3	2.06	0.56
1:D:295:ASP:OD2	1:D:297:ASN:HB2	2.06	0.55
1:B:306:LEU:O	1:B:308:LYS:N	2.41	0.54
1:A:315:ASP:OD1	3:A:80:HOH:O	2.19	0.53
1:A:352:ILE:HD12	1:A:358:ILE:HD13	1.91	0.53
1:B:288:PRO:HG3	1:B:340:GLU:OE1	2.10	0.52
1:C:332:ILE:CG2	3:C:99:HOH:O	2.47	0.51
1:B:306:LEU:C	1:B:308:LYS:N	2.65	0.51
1:C:314:ARG:HH21	1:C:338:HIS:CB	2.24	0.50
1:A:357:GLN:NE2	1:A:359:LEU:CD2	2.55	0.50
1:D:310:SER:HA	1:D:313:TYR:CE2	2.46	0.50
1:A:334:THR:HG21	1:A:363:MET:CE	2.42	0.49
1:C:309:HIS:O	1:C:310:SER:C	2.56	0.48
1:B:306:LEU:C	1:B:308:LYS:H	2.21	0.48
1:C:359:LEU:N	1:C:359:LEU:HD22	2.29	0.48
1:B:300:LYS:HE3	1:B:300:LYS:O	2.15	0.47
1:C:314:ARG:HH21	1:C:338:HIS:HB2	1.79	0.46
1:D:299:LEU:HD23	1:D:299:LEU:HA	1.82	0.46
1:C:289:ILE:HG22	1:C:336:THR:HG22	1.98	0.45
1:A:303:ARG:HH22	1:A:319:THR:H	1.59	0.45
1:C:284:SER:HA	1:C:365:MET:OXT	2.17	0.44
1:C:311:ASP:C	1:C:313:TYR:H	2.26	0.44
1:D:284:SER:OG	1:D:285:HIS:N	2.51	0.44
1:A:352:ILE:HD12	1:A:358:ILE:CD1	2.48	0.44
1:A:293:LYS:HB2	1:A:357:GLN:HG3	2.00	0.43
1:C:289:ILE:HG21	1:C:363:MET:HE2	2.00	0.43
1:B:309:HIS:C	1:B:311:ASP:H	2.26	0.42
1:A:289:ILE:HG21	1:A:363:MET:HE3	2.02	0.42
1:C:293:LYS:HG2	1:C:332:ILE:HG12	2.02	0.42
1:C:323:THR:HG21	1:D:307:ARG:NE	2.34	0.41
1:B:304:TYR:O	1:B:305:ARG:C	2.64	0.41
1:D:284:SER:OG	1:D:365:MET:O	2.34	0.41
1:B:284:SER:HA	1:B:365:MET:OXT	2.21	0.41
1:D:310:SER:HA	1:D:313:TYR:CZ	2.56	0.41
1:A:320:TRP:HB3	1:B:320:TRP:HB3	2.02	0.40
1:C:322:TRP:HA	1:C:322:TRP:CE3	2.56	0.40
1:B:306:LEU:O	1:B:307:ARG:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ASP:C	1:C:313:TYR:N	2.78	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	72/83 (87%)	70 (97%)	2 (3%)	0	100	100
1	B	73/83 (88%)	66 (90%)	5 (7%)	2 (3%)	4	1
1	C	72/83 (87%)	69 (96%)	2 (3%)	1 (1%)	9	3
1	D	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
All	All	297/332 (90%)	284 (96%)	10 (3%)	3 (1%)	12	5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	309	HIS
1	C	310	SER
1	B	307	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	66/75 (88%)	62 (94%)	4 (6%)	17	9
1	B	61/75 (81%)	58 (95%)	3 (5%)	22	14
1	C	65/75 (87%)	63 (97%)	2 (3%)	35	29
1	D	72/75 (96%)	71 (99%)	1 (1%)	59	59
All	All	264/300 (88%)	254 (96%)	10 (4%)	29	21

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	LYS
1	A	315	ASP
1	A	345	LYS
1	A	355	SER
1	B	300	LYS
1	B	340	GLU
1	B	348	ASN
1	C	353	PRO
1	C	359	LEU
1	D	352	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	GLN
1	B	348	ASN
1	C	338	HIS
1	D	338	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are 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	SO4	D	901	-	4,4,4	0.29	0	6,6,6	0.69	0
2	SO4	C	902	-	4,4,4	0.44	0	6,6,6	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.