



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:18 PM UTC

PDB ID : 2F55 / pdb\_00002f55  
Title : Two hepatitis c virus ns3 helicase domains complexed with the same strand of dna  
Authors : Lu, J.Z.; Jordan, J.B.; Sakon, J.  
Deposited on : 2005-11-25  
Resolution : 3.30 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](mailto: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>.

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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)  
Xtrriage (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

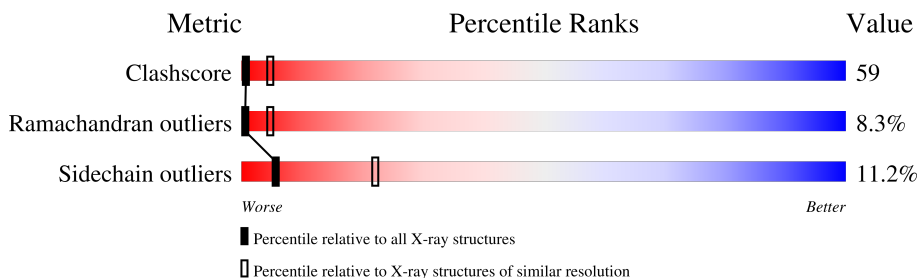
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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  $\geq 3$ , 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	D	13	23% 38% 38%
2	E	3	67% 33%
3	A	435	35% 51% 12% ..
3	B	435	24% 58% 17% ..
3	C	435	33% 52% 12% ..





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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	3	Total O 3 3	0	0
5	A	20	Total O 20 20	0	0
5	B	14	Total O 14 14	0	0
5	C	25	Total O 25 25	0	0



T612
H613
P614
I615
T616
K617
Y618
M620
A621
C622
M623
S624

• Molecule 3: polyprotein



P190	P191	A192	Y193	P194	Q195	Q196	H201	L202	H203	G209	K210	S211	S212	K213	Y214	P215	A216	A217	Y218	A219	Q221	G222	Y223	K224	Y225	L226	Y227	L228	N229	P230	S231	Y232	A233	A234	L236	G237	F238	G239	A240	Y241	N242	S243	K244	A245	H246	G247	D249	P250	N251	L252	R253	T254	G255							
Y256	R257	T261	G262	G263	S264	L265	T266	Y267	S268	H269	K270	G271	K272	F273	L274	A275	D276	G277	G278	C279	S280	G281	Y284	D285	L286	L287	L288	C289	D290	E291	C292	H293	T295	D296	S297	T298	T299	I300	L301	G302	I303	G304	T305	S306	K307	L307	I308	Q309	A310	L311	T312	A313	K314	A315	R316	L317	V318			
T322	A323	T324	P325	G326	G327	V328	H333	P334	I335	L336	E337	E338	L339	G340	L341	S342	N343	N344	G345	G346	I347	P348	F349	Y350	L286	G351	L288	A352	A353	L354	P355	L356	K360	G361	G362	H363	H364	L365	L366	F367	C368	H369	I303	G370	K371	T305	K372	K373	C374	S375	G376	L377	E311	A378	A379	K380	L381	L382	G383	L384
L386	N387	A388	V389	A390	Y391	Y392	R393	G394	L395	D396	P401	P402	L403	G404	D405	V406	V407	V408	V409	A410	T411	D412	L286	G351	L288	A352	A353	L354	P355	L356	K360	G361	G362	H363	H364	L365	L366	F367	C368	H369	I303	G370	K371	T305	K372	K373	C374	S375	G376	L377	E311	A378	A379	K380	L381	L382	G383	L384		
L448	L449	T450	V451	P452	D453	D454	S457	R458	S459	A460	R461	R462	G463	R464	T465	L466	G466	R467	G468	R469	S470	G471	L472	Y473	R474	F475	V476	R481	L482	S483	G484	R485	F486	D487	S488	V489	C492	L491	G492	D493	C494	Y495	D496	A497	L498	G499	V501	Y502	E503	L504	T505	L506	A507	E508	L509	S510	V511	R512		
L513	R514	A515	Y516	L517	N518	T519	P520	P523	V524	C525	O526	D527	H528	L529	E530	F531	R532	A533	E534	S535	S536	G537	F538	Y539	T540	H541	L542	A543	D544	A545	H546	F547	S548	K551	Q552	A553	G554	D555	E493	C494	Y495	D496	A497	L498	G499	V501	Y502	E503	L504	T505	L506	A507	E508	L509	S510	V511	R512			
P575	P576	S577	H578	D579	O580	N581	H582	K583	L584	L585	L586	L587	L588	T591	L592	H593	G594	P595	S596	P597	L598	L599	Y600	R601	L602	G603	H604	L605	V606	L607	L608	L609	L610	L611	T612	H613	L614	L615	L616	K617	Y618	L619	M620	S624																

• Molecule 3: polyprotein



P190	P191	P194	Q198	V199	A200	H203	T206	G209	K210	S211	T212	K213	Y214	P215	A216	A219	Q221	G222	Y223	K224	Y225	L226	V227	S231	V232	A233	T235	L236	G237	F238	G239	M242	A245	I248	D249	P250	N251	L252	R253	V256	T257	P258	L259	T261	G262									
I265	T266	Y267	Y270	G271	K272	L273	L274	D276	S280	G281	A282	A283	D285	L286	L287	I288	C289	D290	E291	C292	H293	S294	T295	D296	T299	L300	L301	T305	V306	L307	A315	R316	L317	V318	L319	L320	A321	T322	P325	P326	V329	T330	V331	P332	E337	E338	L339	G340						
L341	S342	N343	G345	E346	L347	F348	F349	K352	A353	L354	P355	R363	H364	L365	I366	F367	K371	K372	S294	K373	C374	D375	E376	L377	A378	A379	K380	L381	L382	G383	L384	G385	L386	N387	A388	V389	A390	Y391	Y392	R393	G394	L395	D396	V397	V399	I400	P401	P402	G404					
D405	V406	V407	V408	A409	T411	D412	A413	L414	MET	THR	GLY	F416	D421	V425	I426	D427	C428	N429	V432	T433	G434	T435	T436	F438	A439	L440	D441	T444	T445	L446	E447	T448	T449	Q453	D454	S457	R458	S459	Q460	R461	S464	R465	G466	F467	G468	R469	S470	G471	I472	Y473				
R474	F475	V476	T477	P478	G479	E480	R481	P482	G483	S484	S485	V486	G487	A488	G489	V490	L491	C492	D496	A497	G498	C499	H501	Y502	P506	A507	E508	T509	S510	V511	R512	L513	L514	R515	Y516	L517	G525	Q526	D527	H528	L529	E530	F531	W532	E533	S534	V535	F536	T537	G538	I542	D543	A544	H545



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	108.20Å 109.80Å 183.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30	Depositor
% Data completeness (in resolution range)	83.2 (50.00-3.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.247 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	D	1.19	4/272 (1.5%)	0.98	1/412 (0.2%)
2	E	1.20	1/62 (1.6%)	0.99	0/92
3	A	0.71	5/3331 (0.2%)	1.11	20/4548 (0.4%)
3	B	0.76	6/3331 (0.2%)	1.12	20/4548 (0.4%)
3	C	0.64	6/3331 (0.2%)	1.08	24/4548 (0.5%)
All	All	0.73	22/10327 (0.2%)	1.10	65/14148 (0.5%)

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	469	ARG	NE-CZ	8.88	1.42	1.33
3	B	469	ARG	NE-CZ	8.83	1.42	1.33
3	A	469	ARG	NE-CZ	8.81	1.42	1.33
3	B	469	ARG	CZ-NH2	7.11	1.42	1.33
3	C	469	ARG	CZ-NH2	7.07	1.42	1.33

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	PRO	CA-N-CD	-13.11	93.64	112.00
3	B	402	PRO	CA-N-CD	-13.09	93.67	112.00
3	A	402	PRO	CA-N-CD	-11.59	95.78	112.00
3	B	566	THR	N-CA-C	-11.45	97.70	112.93
3	B	298	THR	N-CA-C	9.30	121.03	111.07

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	D	247	0	131	18	0
2	E	57	0	31	6	0
3	A	3251	0	3216	347	0
3	B	3251	0	3215	455	0
3	C	3251	0	3215	378	0
4	A	5	0	0	0	0
4	C	5	0	0	1	0
5	A	20	0	0	2	0
5	B	14	0	0	0	0
5	C	25	0	0	3	0
5	D	3	0	0	0	0
All	All	10129	0	9808	1178	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 59.

The worst 5 of 1178 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:469:ARG:HB2	3:A:469:ARG:NH1	1.31	1.43
3:C:513:LEU:O	3:C:517:LEU:CD2	1.65	1.42
3:A:360:LYS:NZ	3:A:386:LEU:HD21	1.06	1.36
3:A:360:LYS:NZ	3:A:386:LEU:CD2	1.88	1.35
3:A:339:ILE:CG2	3:A:474:ARG:HG2	1.54	1.35

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	
3	A	428/435 (98%)	318 (74%)	86 (20%)	24 (6%)	1	9
3	B	428/435 (98%)	282 (66%)	104 (24%)	42 (10%)	0	3
3	C	428/435 (98%)	296 (69%)	92 (22%)	40 (9%)	0	3
All	All	1284/1305 (98%)	896 (70%)	282 (22%)	106 (8%)	0	5

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	246	HIS
3	A	349	PHE
3	A	413	ALA
3	A	583	LYS
3	B	245	ALA

### 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	
3	A	352/354 (99%)	314 (89%)	38 (11%)	6	23
3	B	352/354 (99%)	307 (87%)	45 (13%)	4	18
3	C	352/354 (99%)	317 (90%)	35 (10%)	7	27
All	All	1056/1062 (99%)	938 (89%)	118 (11%)	6	22

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	380	LYS
3	C	572	GLN
3	B	524	VAL
3	C	557	PHE
3	C	402	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	460	GLN
3	C	526	GLN
3	C	564	GLN
3	B	387	ASN
3	B	344	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](#)

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	$\# Z  > 2$
4	SO4	A	101	-	4,4,4	0.35	0	6,6,6	0.19	0
4	SO4	C	102	-	4,4,4	0.31	0	6,6,6	0.23	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	102	SO4	1	0

## 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

### 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.