



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:45 PM UTC

PDB ID : 1CU1 / pdb_00001cu1
Title : CRYSTAL STRUCTURE OF AN ENZYME COMPLEX FROM HEPATITIS C VIRUS
Authors : Yao, N.; Weber, P.C.
Deposited on : 1999-08-20
Resolution : 2.50 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
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

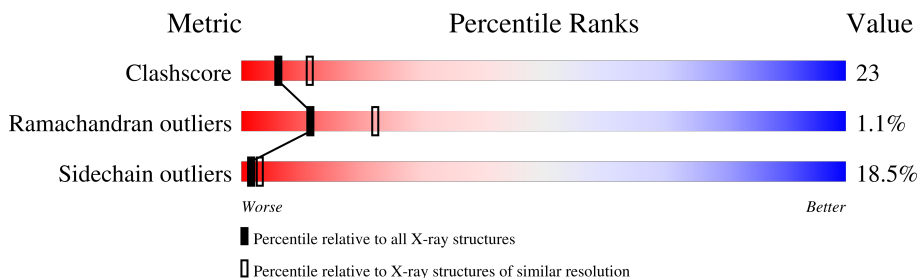
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	645	
1	B	645	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9894 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 PROTEIN (PROTEASE/HELICASE NS3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	645	Total	C	N	O	S	0	0	0
			4807	3026	834	917	30			
1	B	645	Total	C	N	O	S	0	0	0
			4807	3026	834	917	30			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

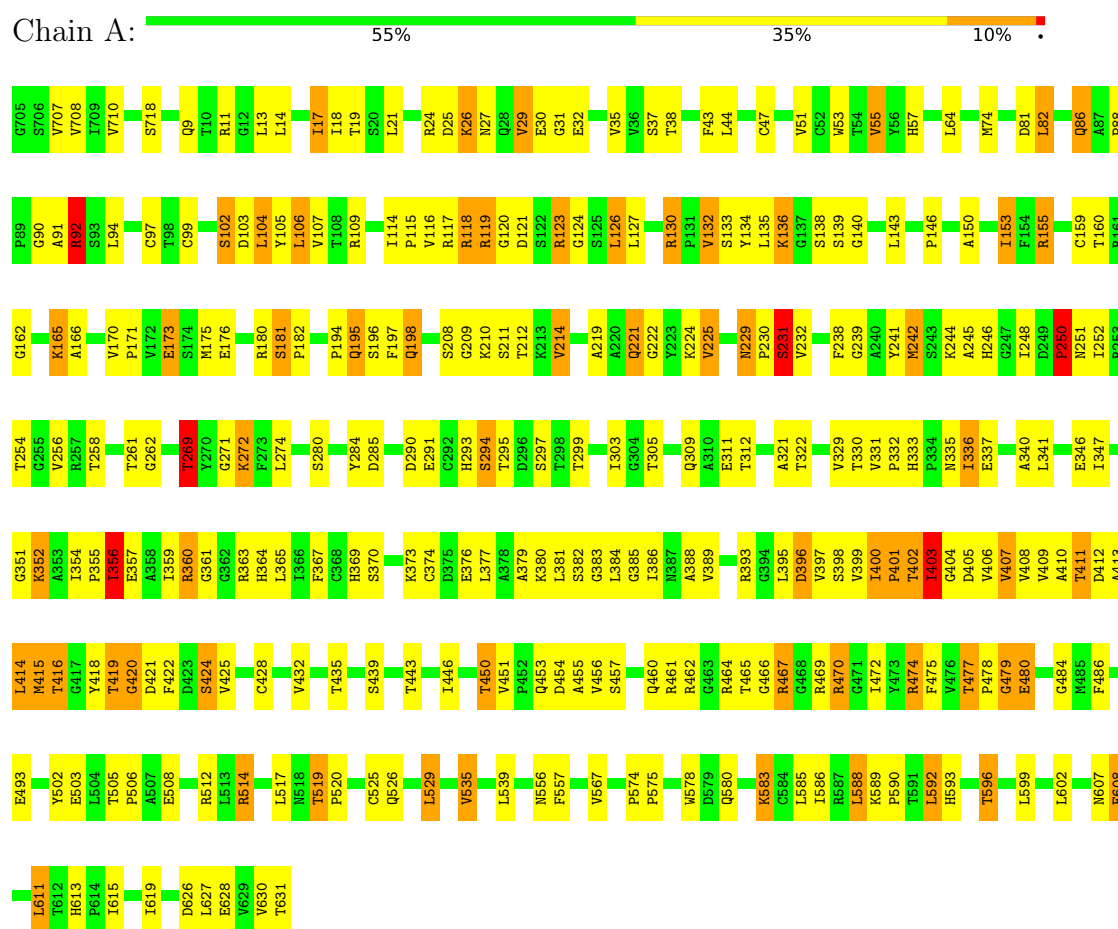
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	150	Total	O	0	0
			150	150		
4	B	118	Total	O	0	0
			118	118		

3 Residue-property plots

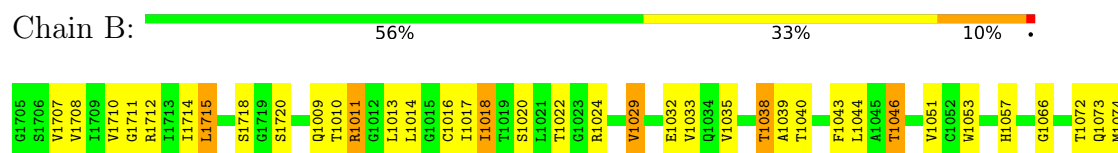
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PROTEIN (PROTEASE/HELICASE NS3)



• Molecule 1: PROTEIN (PROTEASE/HELICASE NS3)



M1620	Q1549	EL447	Y1350	N1229	P1146	Y1075
L1627	D1555	T1450	G1351	P1230	S1147	T1076
V1630	M1556	V1451	K1352	S1231		M1077
T1631	F1557	P1452	I1353	S1243	A1150	
	P1558		P1355			G1080
	A1562	V1456	I1356	D1249	I1153	D1081
	Y1563	Q1460	E1357	P1250	F1154	L1082
	Q1564	A1358	A1358	N1251	P1155	V1083
		I1359	I1359	I1252	G1159	G1084
	A1565	R1467			T1160	V1085
	T1566	H1364		T1258	R1161	Q1086
	V1567	L1365			A1087	A1087
	C1568	R1470		T1266		P1088
	A1569	I1471	S1370	Y1267	A1166	P1089
	R1570	Y1472	K1371	S1268		
	A1571	R1474	K1372	T1269	V1170	R1092
	Q1572	F1475	K1373		P1171	S1093
	A1573	V1476	L1381	K1272	E1172	L1094
	P1575	G1479	I1386	F1273	V1173	T1095
	P1576	E1480		L1274	S1175	P1096
	S1577	R1481	V1389	C1279	M1175	
	W1578	P1482	A1390	S1280	E1176	D1103
	D1579	S1483			R1177	L1104
	Q1580	Y1391	Y1392	Y1284	T1178	Y1105
	M1581	D1487				
	V1582	L1491	L1395	I1287	S1181	T1108
	K1583	G1492	D1396		P1182	R1109
	C1584	E1493	P1397	S1294	V1183	H1110
	L1585		D1296	T1295	F1184	A1111
	T1586		S1398		T1185	D1112
	R1587	E1503			D1186	V1113
	L1588	L1504	I1403	T1305	P1115	T1114
	K1589	T1505			N1187	P1115
	P1590		V1407		S1188	V1116
	T1591	E1508		Q1309	R1117	R1117
	L1592		A1410		P1190	A1118
	H1593	R1514	T1411	T1312	P1191	R1119
	G1594	A1515	D1412	A1313	A1192	G1120
	P1595	Y1516	A1413	G1314	V1193	D1121
	T1596	L1517	L1414	A1315	Q1195	
	P1597	W1518	M1415	R1316	S1196	
	L1598	T1519	T1416	V1329	P1197	S1125
	L1599	P1520	G1417	T1330	Q1198	L1126
	V1600	G1521	Y1418	V1331	T1199	L1127
	R1601		T1419	P1332	H1201	S1128
	L1602	Q1526			I1203	P1129
		L1529	V1425	N1335	A1204	P1131
	M1607		C1428	E1338	K1210	V1132
	E1608	F1536	N1429		S1211	S1133
	V1609			A1340	T1212	Y1134
	T1610	L1539	Q1434	L1341	K1136	K1136
	L1611		T1435		T1217	G1137
	T1612	I1542		T1344		S1138
	H1613	D1543	S1439	G1345		S1139
	P1614	A1544	L1440	L1446	K1224	G1140
		H1545	D1441	I1347	V1225	L1143
					L1227	L1144
						T1145

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	91.36Å 110.51Å 141.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.200 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9894	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: ZN, PO4

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	0.85	2/4916 (0.0%)	1.26	46/6714 (0.7%)
1	B	0.84	4/4916 (0.1%)	1.20	41/6714 (0.6%)
All	All	0.85	6/9832 (0.1%)	1.23	87/13428 (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	A	0	2
1	B	0	2
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ALA	C-N	15.31	1.56	1.33
1	B	1183	VAL	C-N	-8.14	1.15	1.33
1	B	1081	ASP	C-N	-7.57	1.21	1.33
1	B	1084	GLY	C-N	6.90	1.43	1.33
1	B	1094	LEU	C-N	-5.81	1.24	1.33

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	ASN	N-CA-C	15.31	128.05	111.36
1	B	1183	VAL	CA-C-N	14.09	143.66	120.70
1	B	1183	VAL	C-N-CA	14.09	143.66	120.70
1	A	250	PRO	O-C-N	-13.78	104.04	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ALA	CA-C-N	-12.22	103.23	122.29

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Sidechain
1	A	250	PRO	Mainchain
1	B	1084	GLY	Mainchain
1	B	1183	VAL	Peptide

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	A	4807	0	4781	234	0
1	B	4807	0	4780	203	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	150	0	0	9	1
4	B	118	0	0	7	1
All	All	9894	0	9561	433	1

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 23.

The worst 5 of 433 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:400:ILE:HD12	1:A:400:ILE:H	1.18	1.07
1:A:212:THR:HG22	1:A:242:MET:HE1	1.33	1.06
1:A:596:THR:HG22	1:A:607:ASN:HD22	1.19	1.06
1:A:269:THR:HG22	1:A:272:LYS:H	1.21	1.02
1:A:360:ARG:HD2	1:A:361:GLY:H	1.27	0.99

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:783:HOH:O	4:B:1838:HOH:O[4_567]	2.11	0.09

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	643/645 (100%)	609 (95%)	28 (4%)	6 (1%)	14	27
1	B	643/645 (100%)	609 (95%)	26 (4%)	8 (1%)	10	20
All	All	1286/1290 (100%)	1218 (95%)	54 (4%)	14 (1%)	11	22

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	THR
1	B	1571	ALA
1	A	356	ILE
1	A	397	VAL
1	A	479	GLY

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	526/526 (100%)	435 (83%)	91 (17%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	526/526 (100%)	422 (80%)	104 (20%)	1	2
All	All	1052/1052 (100%)	857 (82%)	195 (18%)	1	3

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1155	ARG
1	B	1346	GLU
1	B	1181	SER
1	B	1228	LEU
1	B	1395	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1545	HIS
1	B	1556	ASN
1	B	1613	HIS
1	A	541	HIS
1	A	526	GLN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	PO4	A	800	-	4,4,4	1.61	0	6,6,6	0.54	0
3	PO4	B	1800	-	4,4,4	1.68	0	6,6,6	0.80	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
3	A	800	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1183:VAL	C	1184:PHE	N	1.15

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.