



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:58 pm BST

PDB ID : 1CU1
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

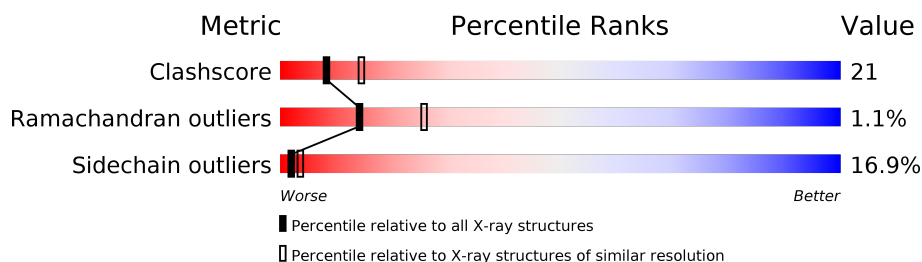
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 on 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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is PHOSPHATE ION (three-letter code: 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.

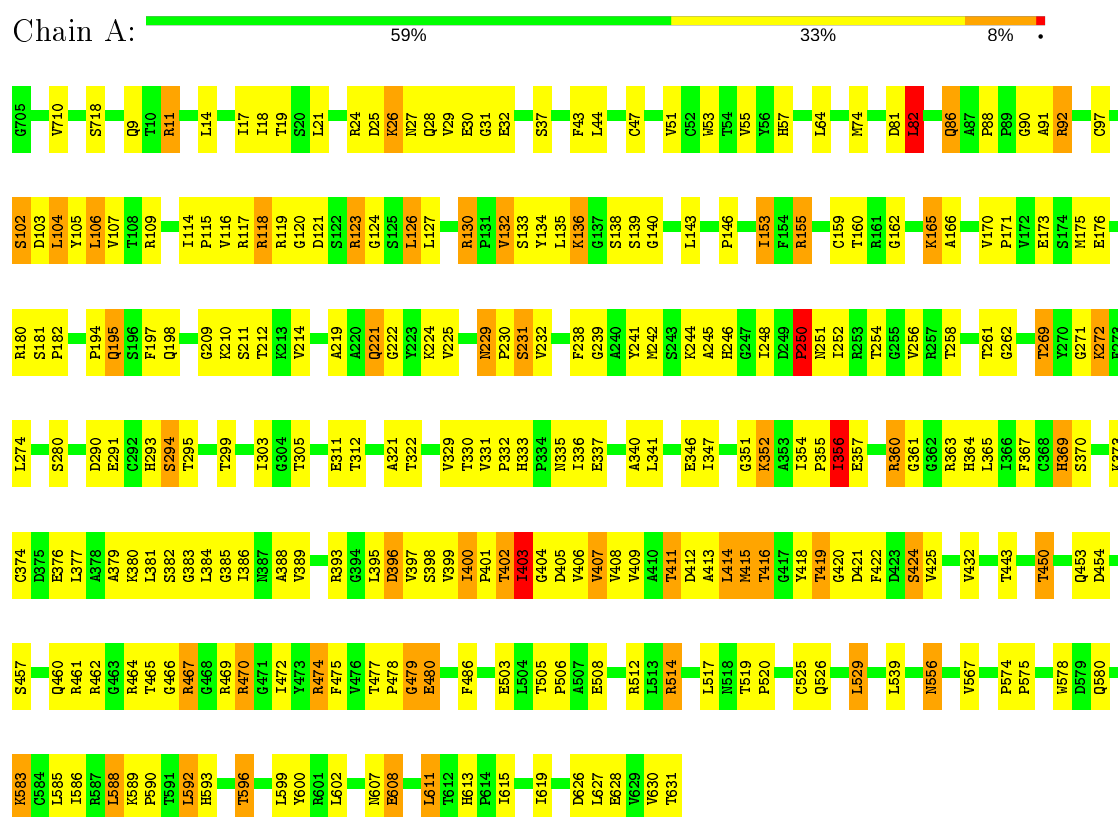
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	150	Total	O	0	0
			150	150		
4	B	118	Total	O	0	0
			118	118		

3 Residue-property plots

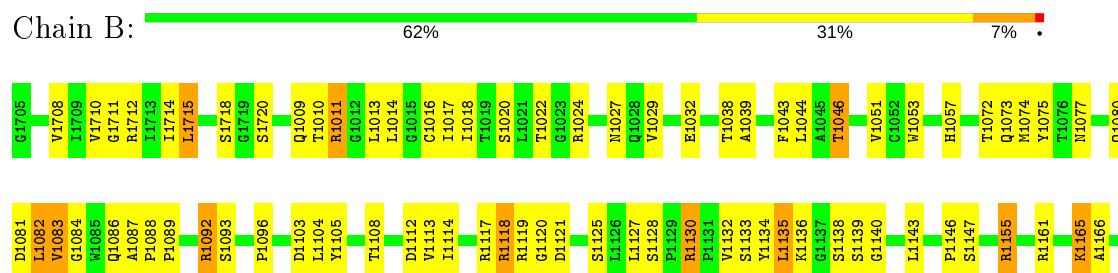
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



L1598	L1599	M1600	R1601	L1602	M1607	E1608	V1609	T1610	L1611	T1612	H1613	P1614	I1615	M1620	L1627	V1630	T1631	L1517	M1518	T1519	P1520	G1521	Q1526	L1529	F1536	L1539	I1542	D1543	A1544	H1545	Q1549	D1555	M1556	F1557	P1558	A1562	Y1563	T1566	V1567	R1570	A1571	Q1572	A1573	P1574	P1575	F1576	S1577	W1578	D1579	Q1580	M1581	W1582	K1583	C1584	L1585	I1586	R1587	L1588	K1589	P1590	T1591	L1592	H1593	G1594	P1595	T1596	P1597	G1279	S1280	S1294	T1295	D1296	T1305	Q1309	R1316	V1329	T1330	V1331	P1332	E1338	V1339	A1340	L1341	T1344	L1347	Y1350	H1203	G1351	K1352	A1353	L1354	P1355	E1356	E1357	A1358	L1359	R1363	H1364	L1365	S1370	K1371	K1372	K1373	L1381	I1252	T1258	T1266	Y1267	S1268	T1269	K1272	F1273	L1274	I1403	T1411	D1412	A1413	L1414	M1415	T1416	G1417	Y1418	T1419	V1425	C1428	N1429	Q1434	T1435	D1441	E1447	T1450	V1451	P1452	V1456	Q1460	R1467	R1470	G1471	I1472	T1473	R1474	G1479	E1480	E1481	P1482	S1483	D1487	E1493	E1503	L1504	T1505	E1508	R1514	A1515	Y1516	V1170	P1171	V1172	E1173	S1174	M1175	E1176	T1177	T1178	S1181	P1182	V1183	F1184	T1185	D1186	S1187	S1188	P1194	Q1195	S1196	F1197	Q1198	H1201	L1202	H1203	A1204	K1210	K1213	K1224	V1225	L1226	V1227	L1228	N1229	P1230	S1231	S1243	D1249	I1252	T1258	T1266	Y1267	S1268	T1269	K1272	F1273	L1274
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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	91.36 Å 110.51 Å 141.20 Å 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	0.67	1/4916 (0.0%)	0.83	7/6714 (0.1%)
1	B	0.67	2/4916 (0.0%)	0.83	7/6714 (0.1%)
All	All	0.67	3/9832 (0.0%)	0.83	14/13428 (0.1%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ALA	C-N	9.91	1.56	1.34
1	B	1183	VAL	C-N	-8.09	1.15	1.34
1	B	1081	ASP	C-N	-5.32	1.21	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	PRO	O-C-N	-11.66	104.04	122.70
1	B	1183	VAL	C-N-CA	8.79	143.66	121.70
1	A	245	ALA	C-N-CA	-7.39	103.23	121.70
1	B	1092	ARG	NE-CZ-NH2	6.53	123.57	120.30
1	A	556	ASN	N-CA-C	6.31	128.05	111.00

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

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	222	0
1	B	4807	0	4779	185	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	9560	404	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 21.

The worst 5 of 404 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:H	1:A:400:ILE:HD12	1.18	1.07
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
1:B:1411:THR:HG23	1:B:1413:ALA:H	1.26	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%)	17	31
1	B	643/645 (100%)	609 (95%)	26 (4%)	8 (1%)	13	24
All	All	1286/1290 (100%)	1218 (95%)	54 (4%)	14 (1%)	14	26

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%)	440 (84%)	86 (16%)	2	4
1	B	526/526 (100%)	434 (82%)	92 (18%)	2	3
All	All	1052/1052 (100%)	874 (83%)	178 (17%)	2	3

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	596	THR
1	B	1104	LEU
1	B	1586	ILE
1	A	602	LEU
1	B	1009	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1027	ASN
1	B	1149	HIS
1	B	1572	GLN
1	B	1034	GLN
1	B	1086	GLN

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 ⓘ

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	B	1800	-	4,4,4	1.63	0	6,6,6	0.76	0
3	PO4	A	800	-	4,4,4	1.56	0	6,6,6	0.51	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 ⓘ

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.