



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2021 – 09:39 PM EDT

PDB ID : 1NKK
Title : COMPLEX STRUCTURE OF HCMV PROTEASE AND A PEP-
TIDOMIMETIC INHIBITOR
Authors : Khayat, R.; Batra, R.; Qian, C.; Halmos, T.; Bailey, M.; Tong, L.
Deposited on : 2003-01-03
Resolution : 2.60 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)
Xtrriage (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) : 2.23.2

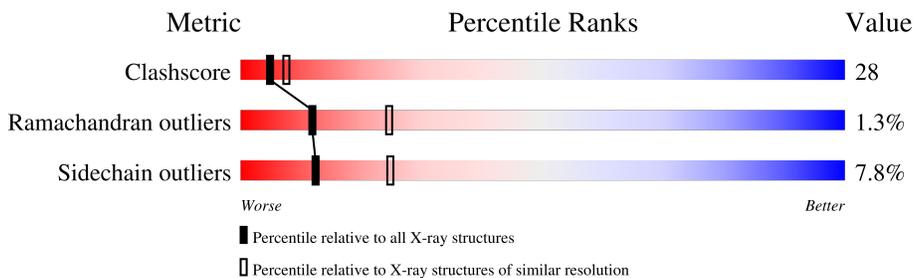
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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	256	
1	B	256	
1	C	256	
1	D	256	
2	E	6	
2	F	6	
2	G	6	
2	H	6	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7431 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 Capsid protein P40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	Total 1749	C 1097	N 324	O 324	S 4	0	0	0
1	B	226	Total 1770	C 1108	N 328	O 328	S 6	0	0	0
1	C	226	Total 1776	C 1112	N 328	O 330	S 6	0	0	0
1	D	220	Total 1731	C 1087	N 319	O 321	S 4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ARG	GLU	engineered mutation	UNP P16753
A	143	GLN	ALA	engineered mutation	UNP P16753
B	331	ARG	GLU	engineered mutation	UNP P16753
B	443	GLN	ALA	engineered mutation	UNP P16753
C	1031	ARG	GLU	engineered mutation	UNP P16753
C	1143	GLN	ALA	engineered mutation	UNP P16753
D	1331	ARG	GLU	engineered mutation	UNP P16753
D	1443	GLN	ALA	engineered mutation	UNP P16753

- Molecule 2 is a protein called Peptidomimetic inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	F	N	O			
2	E	6	Total 39	C 23	F 3	N 5	O 8	0	0	0
2	F	6	Total 39	C 23	F 3	N 5	O 8	0	0	0
2	G	6	Total 39	C 23	F 3	N 5	O 8	0	0	0
2	H	6	Total 39	C 23	F 3	N 5	O 8	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	68	Total O 68 68	0	0
3	B	61	Total O 61 61	0	0
3	C	64	Total O 64 64	0	0
3	D	49	Total O 49 49	0	0
3	E	2	Total O 2 2	0	0
3	F	3	Total O 3 3	0	0
3	G	1	Total O 1 1	0	0
3	H	1	Total O 1 1	0	0

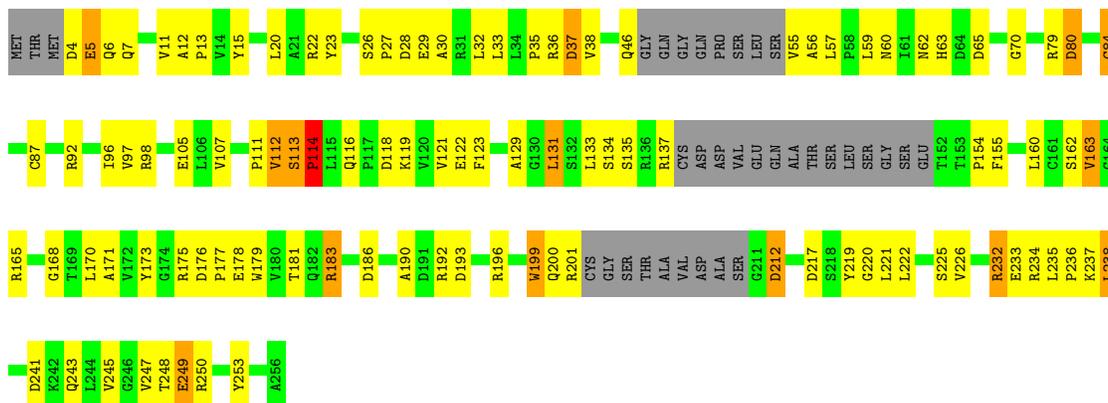
3 Residue-property plots [i](#)

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.

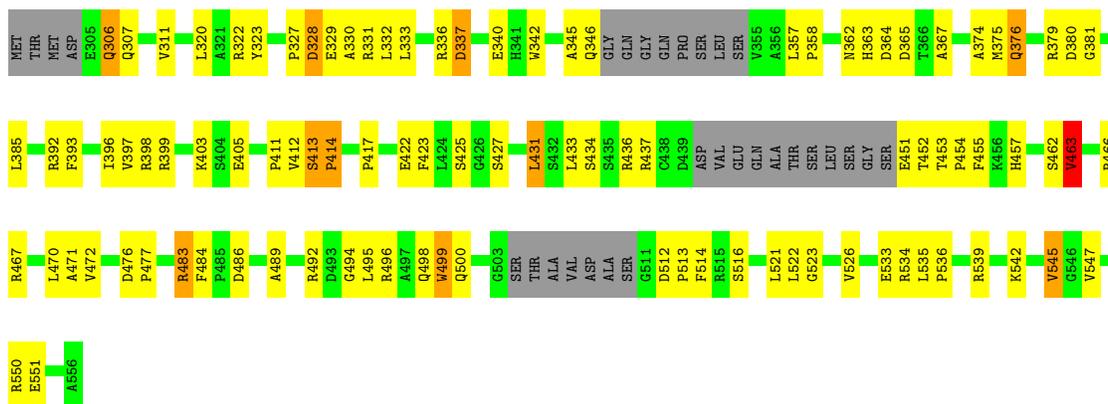
- Molecule 1: Capsid protein P40

Chain A: 



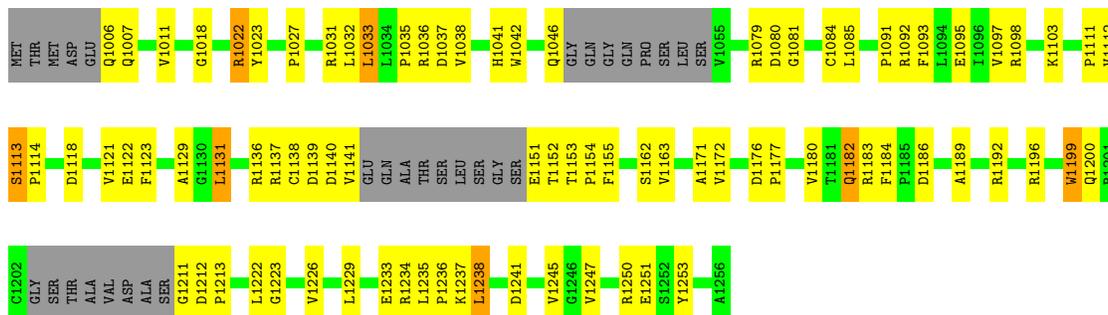
- Molecule 1: Capsid protein P40

Chain B: 



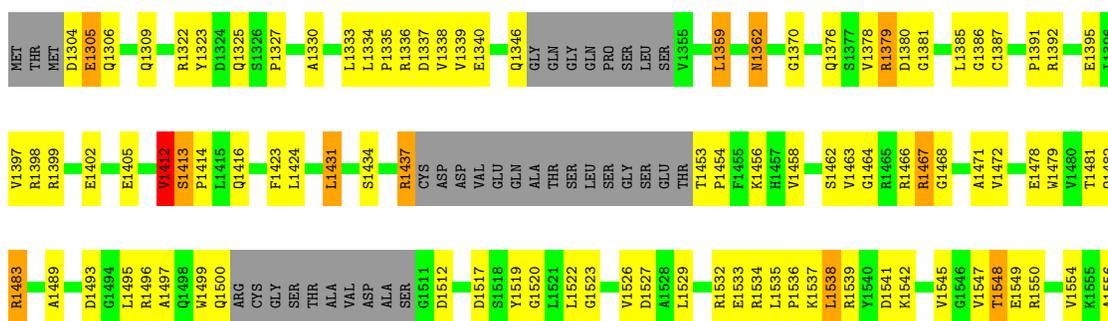
- Molecule 1: Capsid protein P40

Chain C: 



- Molecule 1: Capsid protein P40

Chain D: 48% 33% 14%



- Molecule 2: Peptidomimetic inhibitor

Chain E: 33% 33% 33%



- Molecule 2: Peptidomimetic inhibitor

Chain F: 50% 50%



- Molecule 2: Peptidomimetic inhibitor

Chain G: 67% 17% 17%



- Molecule 2: Peptidomimetic inhibitor

Chain H: 67% 33%

ACE1560
T1561
D1562
H1563
A1564
CF11565

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 2	Depositor
Cell constants a, b, c, α , β , γ	105.17Å 215.25Å 52.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.60	Depositor
% Data completeness (in resolution range)	82.6 (19.98-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7431	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: DMK, DMH, ACE, CFT

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	0.39	0/1784	0.62	0/2417
1	B	0.41	0/1805	0.63	0/2445
1	C	0.38	0/1811	0.62	0/2454
1	D	0.38	0/1766	0.61	0/2393
2	E	2.53	1/11 (9.1%)	1.68	1/13 (7.7%)
2	F	2.78	1/11 (9.1%)	1.62	1/13 (7.7%)
2	G	2.56	1/11 (9.1%)	1.52	1/13 (7.7%)
2	H	2.61	1/11 (9.1%)	1.75	1/13 (7.7%)
All	All	0.44	4/7210 (0.1%)	0.63	4/9761 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	564	ALA	C-O	8.90	1.40	1.23
2	H	1564	ALA	C-O	8.57	1.39	1.23
2	E	264	ALA	C-O	8.17	1.38	1.23
2	G	1264	ALA	C-O	8.17	1.38	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	264	ALA	CA-C-O	-5.77	107.97	120.10
2	H	1564	ALA	CA-C-O	-5.71	108.10	120.10
2	F	564	ALA	CA-C-O	-5.40	108.76	120.10
2	G	1264	ALA	CA-C-O	-5.19	109.20	120.10

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	1749	0	1731	108	0
1	B	1770	0	1746	107	0
1	C	1776	0	1754	85	0
1	D	1731	0	1711	101	0
2	E	39	0	33	4	0
2	F	39	0	33	1	0
2	G	39	0	33	1	0
2	H	39	0	33	0	0
3	A	68	0	0	6	0
3	B	61	0	0	9	0
3	C	64	0	0	2	0
3	D	49	0	0	5	0
3	E	2	0	0	1	0
3	F	3	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	7431	0	7074	393	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 28.

The worst 5 of 393 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:C:1182:GLN:HA	1:C:1182:GLN:HE21	1.16	1.09
1:D:1413:SER:HB3	1:D:1414:PRO:HD3	1.37	1.07
1:C:1042:TRP:HE1	1:C:1140:ASP:HB3	1.11	1.06
1:B:462:SER:HB2	1:B:534:ARG:HE	1.17	1.03
1:B:331:ARG:HD3	1:B:437:ARG:HH21	1.22	1.03

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	214/256 (84%)	199 (93%)	11 (5%)	4 (2%)	8	15
1	B	218/256 (85%)	198 (91%)	18 (8%)	2 (1%)	17	35
1	C	218/256 (85%)	198 (91%)	17 (8%)	3 (1%)	11	22
1	D	212/256 (83%)	190 (90%)	20 (9%)	2 (1%)	17	35
2	E	1/6 (17%)	1 (100%)	0	0	100	100
2	F	1/6 (17%)	1 (100%)	0	0	100	100
2	G	1/6 (17%)	1 (100%)	0	0	100	100
2	H	1/6 (17%)	1 (100%)	0	0	100	100
All	All	866/1048 (83%)	789 (91%)	66 (8%)	11 (1%)	12	24

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	B	413	SER
1	C	1113	SER
1	D	1413	SER
1	A	212	ASP

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	188/215 (87%)	170 (90%)	18 (10%)	8	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	190/215 (88%)	175 (92%)	15 (8%)	12	24
1	C	192/215 (89%)	183 (95%)	9 (5%)	26	50
1	D	186/215 (86%)	169 (91%)	17 (9%)	9	18
2	E	1/1 (100%)	1 (100%)	0	100	100
2	F	1/1 (100%)	1 (100%)	0	100	100
2	G	1/1 (100%)	1 (100%)	0	100	100
2	H	1/1 (100%)	1 (100%)	0	100	100
All	All	760/864 (88%)	701 (92%)	59 (8%)	12	25

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	463	VAL
1	D	1483	ARG
1	C	1084	CYS
1	D	1467	ARG
1	D	1392	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1362	ASN
1	D	1543	GLN
1	D	1500	GLN
1	B	482	GLN
1	D	1306	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](#)

8 non-standard protein/DNA/RNA residues 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	DMK	G	1262	2	5,9,10	1.46	1 (20%)	6,13,15	0.88	0
2	DMH	G	1263	2	8,9,10	0.71	0	8,11,13	0.60	0
2	DMH	E	263	2	8,9,10	0.61	0	8,11,13	0.79	0
2	DMH	H	1563	2	8,9,10	0.71	0	8,11,13	0.64	0
2	DMK	E	262	2	5,9,10	1.66	1 (20%)	6,13,15	0.84	0
2	DMK	F	562	2	5,9,10	1.15	1 (20%)	6,13,15	1.15	0
2	DMK	H	1562	2	5,9,10	1.56	1 (20%)	6,13,15	0.97	1 (16%)
2	DMH	F	563	2	8,9,10	0.75	0	8,11,13	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DMK	G	1262	2	-	2/4/14/16	-
2	DMH	G	1263	2	-	0/9/10/12	-
2	DMH	E	263	2	-	0/9/10/12	-
2	DMH	H	1563	2	-	1/9/10/12	-
2	DMK	E	262	2	-	0/4/14/16	-
2	DMK	F	562	2	-	4/4/14/16	-
2	DMK	H	1562	2	-	2/4/14/16	-
2	DMH	F	563	2	-	0/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	262	DMK	CB-CG1	3.20	1.56	1.50
2	H	1562	DMK	CB-CG1	2.91	1.55	1.50
2	G	1262	DMK	CB-CG1	2.83	1.55	1.50
2	F	562	DMK	CB-CG1	2.15	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1562	DMK	CG3-CB-CG2	2.03	109.91	107.43

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	562	DMK	N-CA-CB-CG2
2	F	562	DMK	C-CA-CB-CG2
2	G	1262	DMK	C-CA-CB-CG2
2	H	1562	DMK	C-CA-CB-CG2
2	H	1563	DMH	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1262	DMK	1	0
2	E	262	DMK	1	0
2	F	563	DMH	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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.