Full wwPDB Geometry-Only Validation Report

Jun 12, 2024 – 04:01 PM EDT

PDB ID	:	1ERF
Title	:	CONFORMATIONAL MAPPING OF THE N-TERMINAL FUSION PEPTIDE OF HIV-1 GP41 USING 13C-ENHANCED FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR)
Authors	:	Gordon, L.M.; Mobley, P.W.; Pilpa, R.; Sherman, M.A.; Waring, A.J.
Deposited on	:	2000-04-06
Resolution	:	Not provided

This is a Full wwPDB Geometry-Only 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:

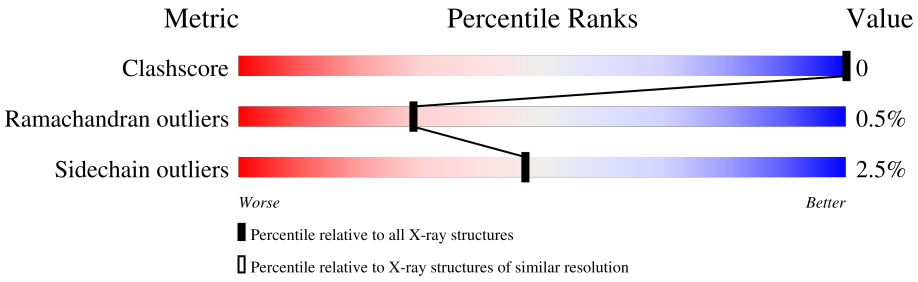
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
INFRARED SPECTROSCOPY

The reported resolution of this entry is unknown.

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	-
Ramachandran outliers	138981	-
Sidechain outliers	138945	-

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1-A	24	96% .
1	10-A	24	92% 8%
1	11-A	24	96% .
1	12-A	24	96% .
1	13-A	24	96% .
1	14-A	24	96% .
1	15-A	24	96% .
1	16-A	24	92% 8%

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Mol	Chain	Length	Quality of chain
1	17-A	24	96%
1	2-A	24	96%
1	3-A	24	96%
1	4-A	24	96%
1	5-A	24	96%
1	6-A	24	96%
1	7-A	24	92% 8%
1	8-A	24	96%
1	9-A	24	92% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5168 atoms, of which 2635 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 TRANSMEMBRANE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	2-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	3-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	4-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	5-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	6-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	7-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	8-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	9-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	10-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	11-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	12-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	13-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	14-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	15-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			
1	16-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	24	Total	C	H	N	O	S	0	0	1
			304	95	155	27	26	1			

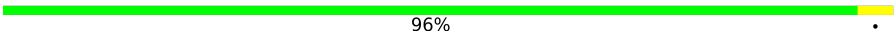
3 Residue-property plots (i)

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.

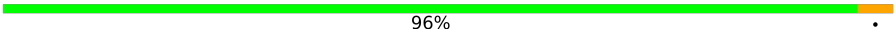
- Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 1-A:



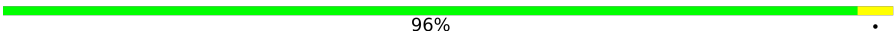
- Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 2-A:



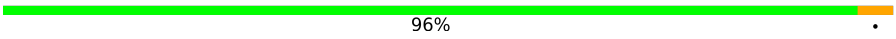
- Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 3-A:



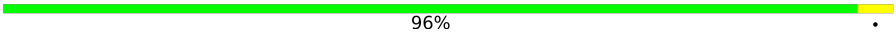
- Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 4-A:



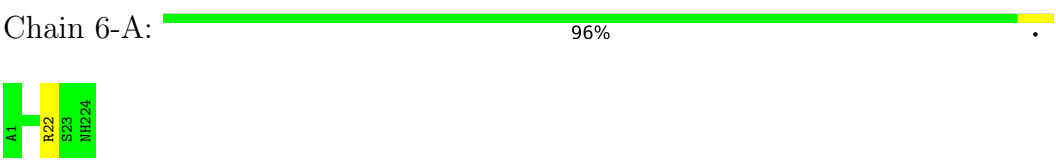
- Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 5-A:



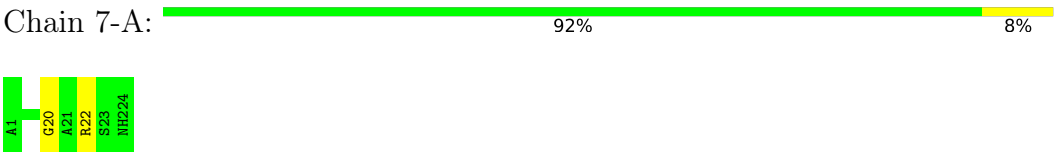
- Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 6-A:



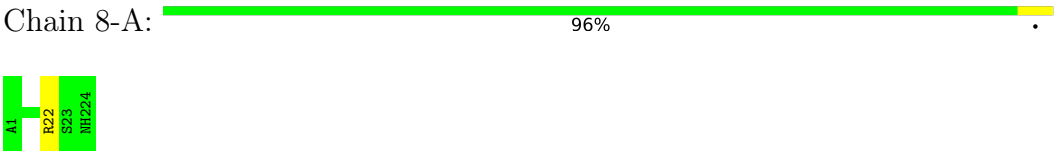
• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 7-A:



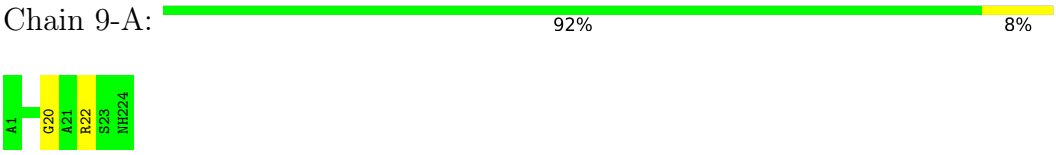
• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 8-A:



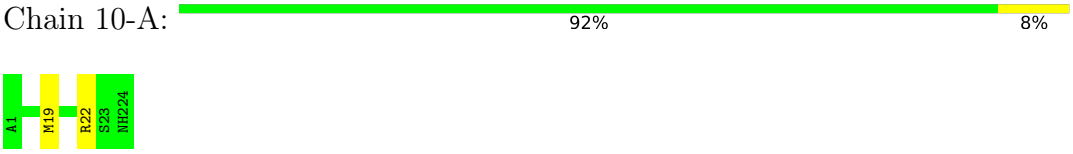
• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 9-A:



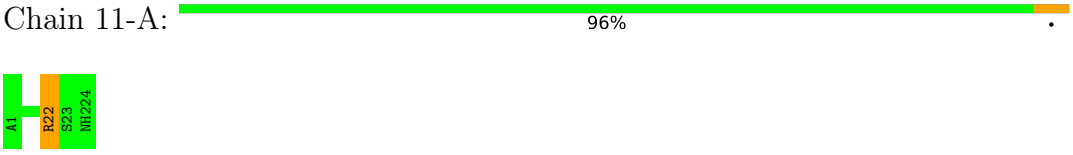
• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 10-A:



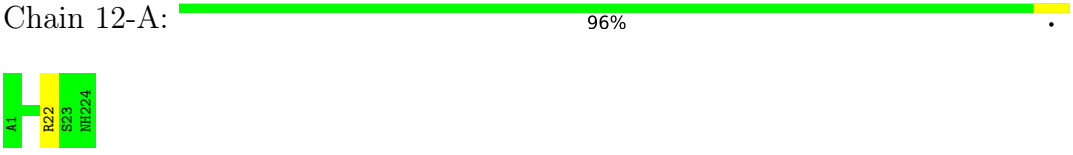
• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 11-A:



• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 12-A:



• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 13-A:

• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

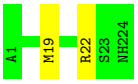
Chain 14-A:

• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 15-A:

• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 16-A:



• Molecule 1: TRANSMEMBRANE GLYCOPROTEIN

Chain 17-A:

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	1-A	1.33	0/149	1.48	2/198 (1.0%)
1	2-A	1.34	0/149	1.46	2/198 (1.0%)
1	3-A	1.34	0/149	1.58	2/198 (1.0%)
1	4-A	1.32	0/149	1.52	2/198 (1.0%)
1	5-A	1.31	0/149	1.44	2/198 (1.0%)
1	6-A	1.30	0/149	1.41	2/198 (1.0%)
1	7-A	1.31	0/149	1.49	2/198 (1.0%)
1	8-A	1.31	0/149	1.43	2/198 (1.0%)
1	9-A	1.33	0/149	1.39	2/198 (1.0%)
1	10-A	1.33	0/149	1.48	2/198 (1.0%)
1	11-A	1.36	0/149	1.51	2/198 (1.0%)
1	12-A	1.35	0/149	1.54	2/198 (1.0%)
1	13-A	1.31	0/149	1.45	2/198 (1.0%)
1	14-A	1.33	0/149	1.47	2/198 (1.0%)
1	15-A	1.32	0/149	1.45	2/198 (1.0%)
1	16-A	1.35	0/149	1.47	2/198 (1.0%)
1	17-A	1.32	0/149	1.46	2/198 (1.0%)
All	All	1.33	0/2533	1.47	34/3366 (1.0%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	22	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	7-A	22	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	6-A	22	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	16-A	22	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	12-A	22	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	15-A	22	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	4-A	22	ARG	NE-CZ-NH1	8.21	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	14-A	22	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	5-A	22	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	13-A	22	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	8-A	22	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	2-A	22	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	13-A	22	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	10-A	22	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	17-A	22	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	2-A	22	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	3-A	22	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	17-A	22	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	3-A	22	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	11-A	22	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	10-A	22	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	9-A	22	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	5-A	22	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	1-A	22	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	11-A	22	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	6-A	22	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	15-A	22	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	7-A	22	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	12-A	22	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	16-A	22	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	14-A	22	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	9-A	22	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	4-A	22	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	8-A	22	ARG	NE-CZ-NH2	-5.44	117.58	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1-A	149	155	155	0	0
1	2-A	149	155	155	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-A	149	155	155	0	0
1	4-A	149	155	155	0	0
1	5-A	149	155	155	0	0
1	6-A	149	155	155	0	0
1	7-A	149	155	155	0	0
1	8-A	149	155	155	0	0
1	9-A	149	155	155	0	0
1	10-A	149	155	155	0	0
1	11-A	149	155	155	0	0
1	12-A	149	155	155	0	0
1	13-A	149	155	155	0	0
1	14-A	149	155	155	0	0
1	15-A	149	155	155	0	0
1	16-A	149	155	155	0	0
1	17-A	149	155	155	0	0
All	All	2533	2635	2635	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	1-A	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
1	2-A	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
1	3-A	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
1	4-A	22/24 (92%)	16 (73%)	6 (27%)	0	100	100
1	5-A	22/24 (92%)	21 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	6-A	22/24 (92%)	20 (91%)	2 (9%)	0	100 100
1	7-A	22/24 (92%)	20 (91%)	1 (4%)	1 (4%)	2 2
1	8-A	22/24 (92%)	18 (82%)	4 (18%)	0	100 100
1	9-A	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	2 2
1	10-A	22/24 (92%)	21 (96%)	1 (4%)	0	100 100
1	11-A	22/24 (92%)	22 (100%)	0	0	100 100
1	12-A	22/24 (92%)	21 (96%)	1 (4%)	0	100 100
1	13-A	22/24 (92%)	19 (86%)	3 (14%)	0	100 100
1	14-A	22/24 (92%)	19 (86%)	3 (14%)	0	100 100
1	15-A	22/24 (92%)	20 (91%)	2 (9%)	0	100 100
1	16-A	22/24 (92%)	21 (96%)	1 (4%)	0	100 100
1	17-A	22/24 (92%)	19 (86%)	3 (14%)	0	100 100
All	All	374/408 (92%)	339 (91%)	33 (9%)	2 (0%)	29 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	9-A	20	GLY
1	7-A	20	GLY

4.3.2 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	1-A	12/12 (100%)	12 (100%)	0	100 100
1	2-A	12/12 (100%)	11 (92%)	1 (8%)	11 11
1	3-A	12/12 (100%)	12 (100%)	0	100 100
1	4-A	12/12 (100%)	11 (92%)	1 (8%)	11 11
1	5-A	12/12 (100%)	12 (100%)	0	100 100
1	6-A	12/12 (100%)	12 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	7-A	12/12 (100%)	12 (100%)	0	100 100
1	8-A	12/12 (100%)	12 (100%)	0	100 100
1	9-A	12/12 (100%)	12 (100%)	0	100 100
1	10-A	12/12 (100%)	11 (92%)	1 (8%)	11 11
1	11-A	12/12 (100%)	11 (92%)	1 (8%)	11 11
1	12-A	12/12 (100%)	12 (100%)	0	100 100
1	13-A	12/12 (100%)	12 (100%)	0	100 100
1	14-A	12/12 (100%)	12 (100%)	0	100 100
1	15-A	12/12 (100%)	12 (100%)	0	100 100
1	16-A	12/12 (100%)	11 (92%)	1 (8%)	11 11
1	17-A	12/12 (100%)	12 (100%)	0	100 100
All	All	204/204 (100%)	199 (98%)	5 (2%)	47 47

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2-A	22	ARG
1	4-A	22	ARG
1	10-A	19	MET
1	11-A	22	ARG
1	16-A	19	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.