wwPDB EM Validation Summary Report (i)

Nov 22, 2022 – 01:02 AM EST

PDB ID	:	3J5M
EMDB ID	:	EMD-5779
Title	:	Cryo-EM structure of the BG505 SOSIP.664 HIV-1 Env trimer with 3 PGV04 Fabs
Authors	:	Lyumkis, D.; Julien, J.-P.; Wilson, I.A.; Ward, A.B.
Deposited on	:	2013-10-26
Resolution	:	5.80 Å(reported)
Based on initial models	:	3SE9, 2B4C, 1ENV, 3U2S

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

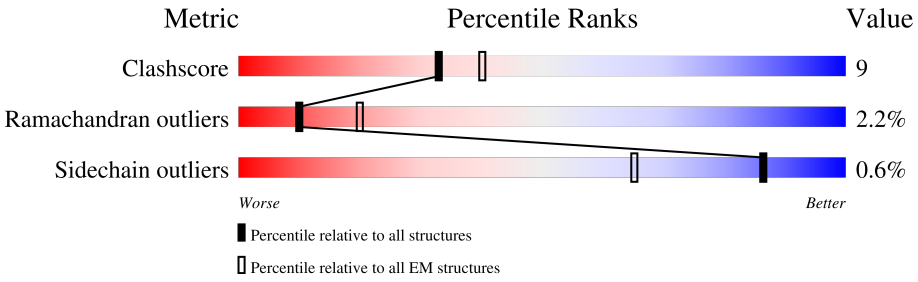
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	475	70% 14% · 13%
1	E	475	69% 15% · 13%
1	I	475	70% 13% · 13%
2	B	64	98% ·
2	F	64	98% ·
2	J	64	98% ·
3	C	208	95% ·
3	G	208	96% ·
3	K	208	96% ·

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Mol	Chain	Length	Quality of chain
4	D	228	
4	H	228	
4	L	228	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20394 atoms, of which 15 are hydrogens and 0 are deuteriums.

In the tables below, 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 BG505 SOSIP gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	415	Total 3140	C 1964	N 554	O 595	S 27	0	0
1	E	415	Total 3140	C 1964	N 554	O 595	S 27	0	0
1	I	415	Total 3140	C 1964	N 554	O 595	S 27	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
A	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6
E	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
E	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6
I	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
I	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP gp41.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	63	Total 315	C 189	N 63	O 63	0	0
2	F	63	Total 315	C 189	N 63	O 63	0	0
2	J	63	Total 315	C 189	N 63	O 63	0	0

- Molecule 3 is a protein called PGV04 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	208	Total 1621	C 1018	N 275	O 321	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	208	Total	C	N	O	S	0	0
			1621	1018	275	321	7		
3	K	208	Total	C	N	O	S	0	0
			1621	1018	275	321	7		

- Molecule 4 is a protein called PGV04 heavy chain.

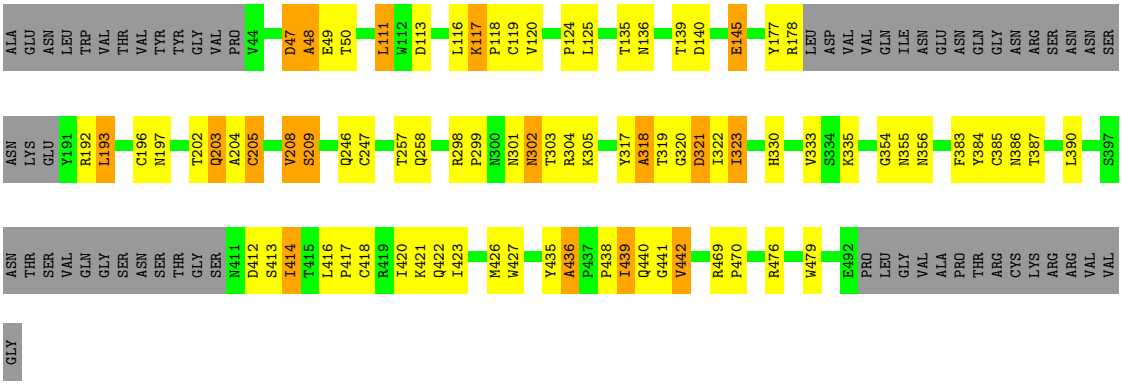
Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	225	Total	C	H	N	O	S	0	0
			1722	1090	5	298	324	5		
4	H	225	Total	C	H	N	O	S	0	0
			1722	1090	5	298	324	5		
4	L	225	Total	C	H	N	O	S	0	0
			1722	1090	5	298	324	5		

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.

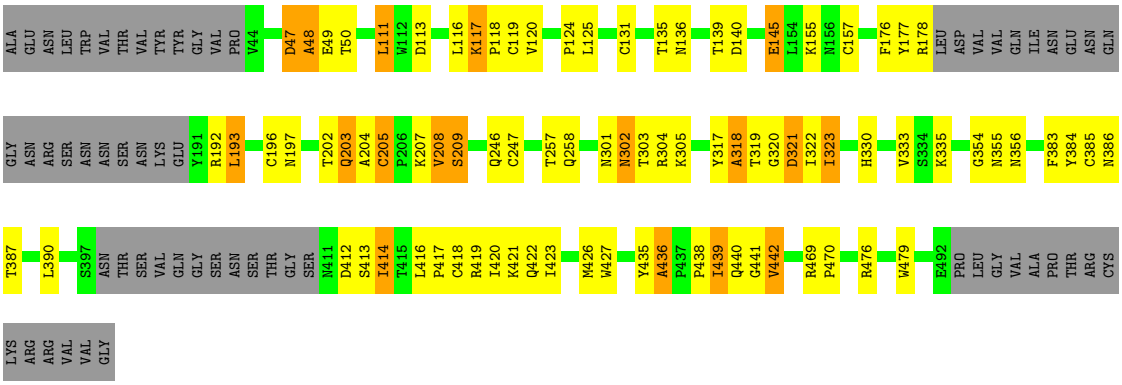
- Molecule 1: BG505 SOSIP gp120

Chain A:



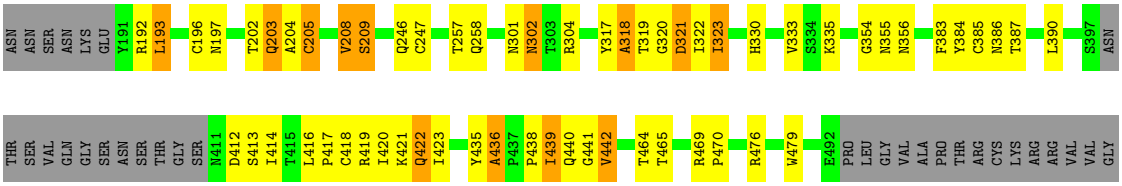
- Molecule 1: BG505 SOSIP gp120

Chain E:



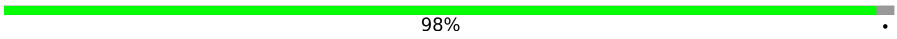
- Molecule 1: BG505 SOSIP gp120

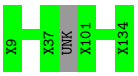
Chain I:



• Molecule 2: BG505 SOSIP gp41

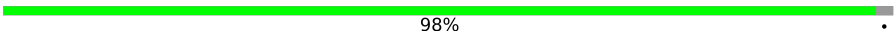
Chain B:

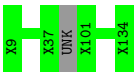




• Molecule 2: BG505 SOSIP gp41

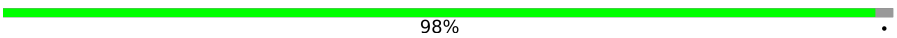
Chain F:

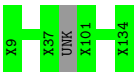




• Molecule 2: BG505 SOSIP gp41

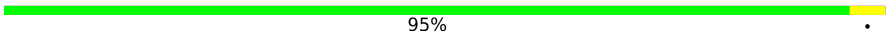
Chain J:





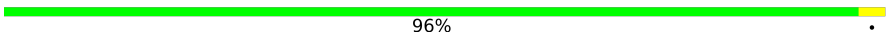
• Molecule 3: PGV04 light chain

Chain C:



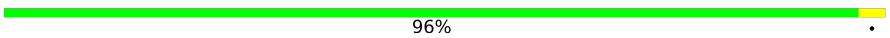
• Molecule 3: PGV04 light chain

Chain G:



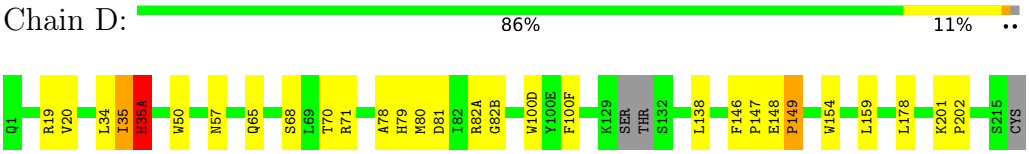
• Molecule 3: PGV04 light chain

Chain K:



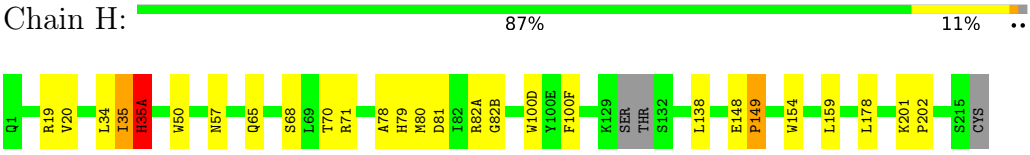
• Molecule 4: PGV04 heavy chain

Chain D:



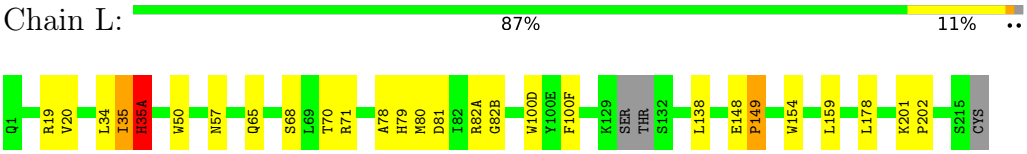
• Molecule 4: PGV04 heavy chain

Chain H:



• Molecule 4: PGV04 heavy chain

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	49572	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Frealign	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.59	0/3206	0.57	1/4358 (0.0%)
1	E	0.60	0/3206	0.57	1/4358 (0.0%)
1	I	0.60	1/3206 (0.0%)	0.57	1/4358 (0.0%)
3	C	0.67	0/1658	0.56	1/2244 (0.0%)
3	G	0.67	0/1658	0.56	1/2244 (0.0%)
3	K	0.67	0/1658	0.56	1/2244 (0.0%)
4	D	0.58	2/1761 (0.1%)	0.57	2/2396 (0.1%)
4	H	0.58	2/1761 (0.1%)	0.57	2/2396 (0.1%)
4	L	0.58	2/1761 (0.1%)	0.57	2/2396 (0.1%)
All	All	0.61	7/19875 (0.0%)	0.57	12/26994 (0.0%)

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	E	0	2
1	I	0	2
3	C	0	1
3	G	0	1
3	K	0	1
4	D	0	1
4	H	0	1
4	L	0	1
All	All	0	12

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	82(B)	GLY	C-N	5.29	1.46	1.34
4	D	82(B)	GLY	C-N	5.27	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	82(B)	GLY	C-N	5.27	1.46	1.34
4	D	149	PRO	N-CD	5.11	1.55	1.47
1	I	422	GLN	C-N	5.09	1.45	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	145	GLU	O-C-N	-12.75	102.31	122.70
1	A	145	GLU	O-C-N	-12.73	102.32	122.70
1	I	145	GLU	O-C-N	-12.73	102.33	122.70
3	G	91	LEU	O-C-N	-8.36	109.33	122.70
3	C	91	LEU	O-C-N	-8.34	109.36	122.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLU	Mainchain
1	A	47	ASP	Peptide
3	C	91	LEU	Mainchain
4	D	35(A)	HIS	Mainchain
1	E	47	ASP	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	3140	0	2943	90	0
1	E	3140	0	2943	93	0
1	I	3140	0	2943	90	0
2	B	315	0	67	0	0
2	F	315	0	67	0	0
2	J	315	0	67	0	0
3	C	1621	0	1579	6	0
3	G	1621	0	1579	5	0
3	K	1621	0	1579	5	0
4	D	1717	5	1690	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1717	5	1690	25	0
4	L	1717	5	1690	23	0
All	All	20379	15	18837	361	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 9.

The worst 5 of 361 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:384:TYR:CE1	1:A:421:LYS:HG2	1.30	1.66
1:E:384:TYR:CE1	1:E:421:LYS:HG2	1.30	1.63
1:I:384:TYR:CE1	1:I:421:LYS:HG2	1.30	1.60
1:E:384:TYR:CE1	1:E:421:LYS:CG	1.89	1.55
1:I:384:TYR:CE1	1:I:421:LYS:CG	1.89	1.54

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 PDB entries followed by that with respect to all EM entries.

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	409/475 (86%)	359 (88%)	33 (8%)	17 (4%)	3 22
1	E	409/475 (86%)	359 (88%)	33 (8%)	17 (4%)	3 22
1	I	409/475 (86%)	359 (88%)	33 (8%)	17 (4%)	3 22
3	C	206/208 (99%)	198 (96%)	7 (3%)	1 (0%)	29 69
3	G	206/208 (99%)	198 (96%)	7 (3%)	1 (0%)	29 69
3	K	206/208 (99%)	198 (96%)	7 (3%)	1 (0%)	29 69
4	D	221/228 (97%)	212 (96%)	9 (4%)	0	100 100
4	H	221/228 (97%)	212 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	L	221/228 (97%)	212 (96%)	9 (4%)	0	100 100
All	All	2508/2733 (92%)	2307 (92%)	147 (6%)	54 (2%)	10 35

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	LEU
1	A	302	ASN
1	A	318	ALA
1	A	321	ASP
1	A	323	ILE

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 PDB entries followed by that with respect to all EM entries.

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	333/422 (79%)	330 (99%)	3 (1%)	78 87
1	E	333/422 (79%)	330 (99%)	3 (1%)	78 87
1	I	333/422 (79%)	330 (99%)	3 (1%)	78 87
3	C	182/182 (100%)	181 (100%)	1 (0%)	88 93
3	G	182/182 (100%)	181 (100%)	1 (0%)	88 93
3	K	182/182 (100%)	181 (100%)	1 (0%)	88 93
4	D	190/193 (98%)	190 (100%)	0	100 100
4	H	190/193 (98%)	190 (100%)	0	100 100
4	L	190/193 (98%)	190 (100%)	0	100 100
All	All	2115/2391 (88%)	2103 (99%)	12 (1%)	86 92

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	91	LEU
1	I	111	LEU

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Mol	Chain	Res	Type
3	K	91	LEU
1	I	412	ASP
3	C	91	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	171	GLN
1	I	67	ASN
4	L	171	GLN
4	D	171	GLN
1	A	67	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 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-5779. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.