



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:54 PM BST

PDB ID : 3JBA  
EMDB ID: : EMD-6424  
Title : The U4 antibody epitope on human papillomavirus 16 identified by cryo-EM  
Authors : Guan, J.; Bywaters, S.M.; Brendle, S.A.; Lee, H.; Ashley, R.E.; Christensen, N.D.; Hafenstein, S.  
Deposited on : 2015-08-11  
Resolution : 12.00 Å(reported)  
Based on PDB ID : 3J6R

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

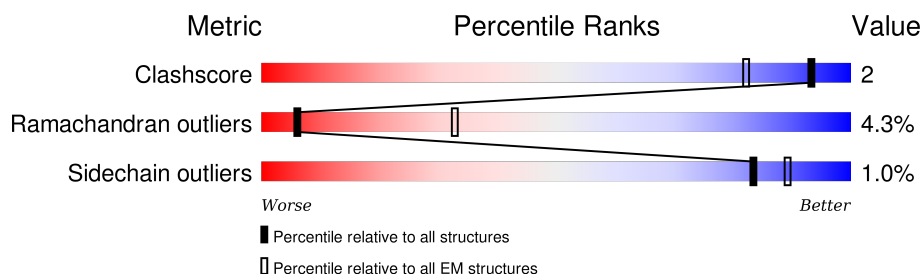
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	L	115	91% 9%
2	H	115	90% 9% .
3	A	478	92% 7% .
3	B	478	90% 8% .
3	C	478	89% 10% .
3	D	478	90% 8% .
3	E	478	91% 8%
3	F	478	91% 8% .

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 20721 atoms, of which 7468 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 H16.U4 antibody light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	115	Total	C	H	N	O	0	0
			1772	567	879	144	178		

- Molecule 2 is a protein called H16.U4 antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	115	Total	C	H	N	O	0	0
			1735	560	841	151	178		

- Molecule 3 is a protein called Major capsid protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	A	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	E	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	D	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	C	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		
3	F	478	Total	C	H	N	O	0	0
			2869	956	958	478	477		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	GLN	ASN	CONFLICT	UNP C9E771
B	181	GLN	ASN	CONFLICT	UNP C9E771
B	472	LEU	ALA	CONFLICT	UNP C9E771
A	177	GLN	ASN	CONFLICT	UNP C9E771
A	181	GLN	ASN	CONFLICT	UNP C9E771

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Chain	Residue	Modelled	Actual	Comment	Reference
A	472	LEU	ALA	CONFLICT	UNP C9E771
E	177	GLN	ASN	CONFLICT	UNP C9E771
E	181	GLN	ASN	CONFLICT	UNP C9E771
E	472	LEU	ALA	CONFLICT	UNP C9E771
D	177	GLN	ASN	CONFLICT	UNP C9E771
D	181	GLN	ASN	CONFLICT	UNP C9E771
D	472	LEU	ALA	CONFLICT	UNP C9E771
C	177	GLN	ASN	CONFLICT	UNP C9E771
C	181	GLN	ASN	CONFLICT	UNP C9E771
C	472	LEU	ALA	CONFLICT	UNP C9E771
F	177	GLN	ASN	CONFLICT	UNP C9E771
F	181	GLN	ASN	CONFLICT	UNP C9E771
F	472	LEU	ALA	CONFLICT	UNP C9E771

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: H16.U4 antibody light chain

Chain L:  91% 9%



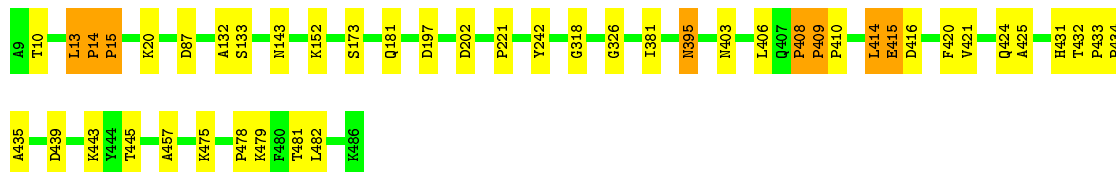
- Molecule 2: H16.U4 antibody heavy chain

Chain H:  90% 9% .



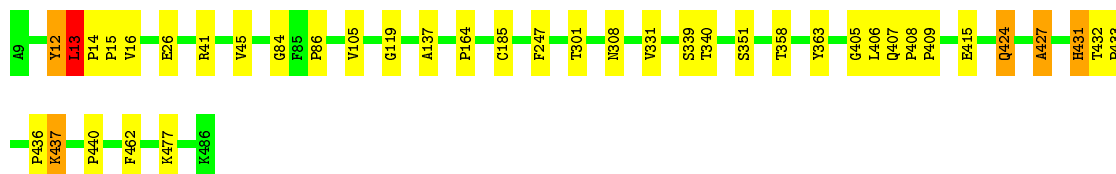
- Molecule 3: Major capsid protein L1

Chain B:  90% 8% .



- Molecule 3: Major capsid protein L1

Chain A:  92% 7% .



- Molecule 3: Major capsid protein L1

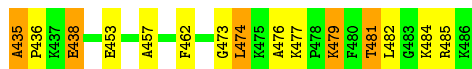
Chain E:  91% 8%





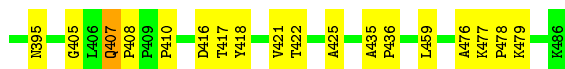
- Molecule 3: Major capsid protein L1

Chain D: 90% 8%



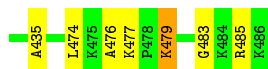
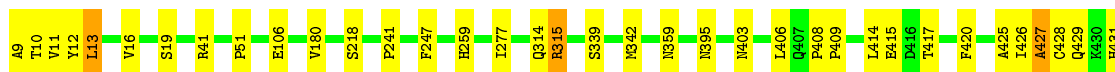
- Molecule 3: Major capsid protein L1

Chain C: 89% 10%



- Molecule 3: Major capsid protein L1

Chain F: 91% 8%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	5806	Depositor
Resolution determination method	FSC 0.5	Depositor
CTF correction method	each particle	Depositor
Microscope	JEOL 2100	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	5430	Depositor
Magnification	50000	Depositor
Image detector	GATAN ULTRASCAN 4000 (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  > 2$	RMSZ	# $ Z  > 2$
1	L	0.69	1/913 (0.1%)	0.68	0/1236
2	H	1.07	1/916 (0.1%)	1.04	5/1236 (0.4%)
3	A	1.50	3/1910 (0.2%)	1.73	10/2386 (0.4%)
3	B	1.52	1/1910 (0.1%)	1.76	10/2386 (0.4%)
3	C	1.55	11/1910 (0.6%)	1.72	11/2386 (0.5%)
3	D	1.58	7/1910 (0.4%)	1.75	13/2386 (0.5%)
3	E	1.58	5/1910 (0.3%)	1.72	17/2386 (0.7%)
3	F	1.51	4/1910 (0.2%)	1.73	17/2386 (0.7%)
All	All	1.47	33/13289 (0.2%)	1.64	83/16788 (0.5%)

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
3	A	0	12
3	B	0	10
3	C	0	13
3	D	0	15
3	E	0	9
3	F	0	11
All	All	0	70

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	94	ARG	C-N	23.30	1.75	1.33
3	E	206	GLY	N-CA	-6.92	1.35	1.46
3	C	290	ASN	N-CA	-6.25	1.33	1.46
3	A	164	PRO	N-CA	-6.25	1.36	1.47
3	E	165	ILE	C-N	6.13	1.44	1.33
3	E	482	LEU	C-N	6.10	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	119	GLY	CA-C	-6.03	1.42	1.51
3	E	197	ASP	N-CA	-5.92	1.34	1.46
3	A	119	GLY	N-CA	-5.85	1.37	1.46
3	C	85	PHE	CA-C	-5.82	1.37	1.52
3	C	38	GLY	CA-C	-5.65	1.42	1.51
3	A	84	GLY	N-CA	-5.64	1.37	1.46
3	C	268	GLY	N-CA	-5.61	1.37	1.46
3	E	83	PHE	C-N	5.58	1.43	1.33
3	D	110	GLY	N-CA	-5.54	1.37	1.46
3	D	67	GLY	N-CA	-5.42	1.38	1.46
3	F	51	PRO	CA-C	-5.33	1.42	1.52
1	L	30(B)	SER	C-N	-5.32	1.21	1.34
3	D	159	ILE	C-N	5.29	1.42	1.33
3	D	435	ALA	N-CA	-5.29	1.35	1.46
3	C	116	GLY	CA-C	-5.29	1.43	1.51
3	C	280	SER	C-N	5.25	1.42	1.33
3	D	214	GLN	N-CA	-5.17	1.36	1.46
3	D	408	PRO	C-N	5.14	1.44	1.34
3	F	359	ASN	N-CA	-5.14	1.36	1.46
3	C	12	TYR	N-CA	-5.11	1.36	1.46
3	C	53	LYS	C-N	5.11	1.45	1.34
3	C	149	MET	CA-C	-5.10	1.39	1.52
3	D	182	PRO	N-CA	-5.09	1.38	1.47
3	C	38	GLY	N-CA	-5.09	1.38	1.46
3	B	197	ASP	C-N	5.06	1.42	1.33
3	F	277	ILE	C-N	5.06	1.45	1.34
3	F	13	LEU	N-CA	5.04	1.56	1.46

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	94	ARG	CA-C-N	-22.36	71.48	116.20
2	H	102	TYR	O-C-N	-8.84	108.56	122.70
3	B	420	PHE	C-N-CA	8.65	143.34	121.70
3	B	15	PRO	C-N-CA	8.15	142.07	121.70
3	F	427	ALA	O-C-N	-8.11	109.73	122.70
3	F	485	ARG	C-N-CA	8.08	141.90	121.70
2	H	94	ARG	C-N-CA	-7.90	105.71	122.30
3	C	354	THR	O-C-N	7.33	134.43	122.70
3	A	339	SER	C-N-CA	7.11	139.48	121.70
3	F	431	HIS	C-N-CA	7.06	139.34	121.70
3	E	479	LYS	C-N-CA	6.94	139.05	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	482	LEU	O-C-N	-6.92	111.44	123.20
3	D	256	PHE	O-C-N	-6.76	111.89	122.70
3	B	431	HIS	C-N-CA	6.74	138.55	121.70
3	F	431	HIS	O-C-N	-6.72	111.95	122.70
3	E	434	PRO	O-C-N	-6.43	112.42	122.70
3	A	45	VAL	N-CA-C	-6.29	94.03	111.00
3	F	426	ILE	CA-C-N	6.25	130.94	117.20
3	D	92	ASN	N-CA-C	-6.22	94.19	111.00
3	C	172	GLY	C-N-CA	6.22	137.25	121.70
3	F	483	GLY	C-N-CA	6.21	137.23	121.70
3	D	474	LEU	C-N-CA	6.21	137.22	121.70
3	D	438	GLU	N-CA-C	-6.19	94.28	111.00
3	D	428	CYS	C-N-CA	6.17	137.12	121.70
3	E	341	ASN	N-CA-C	-6.08	94.59	111.00
3	B	415	GLU	C-N-CA	6.03	136.79	121.70
3	D	265	GLY	N-CA-C	-5.96	98.21	113.10
3	C	410	PRO	C-N-CA	5.90	134.69	122.30
3	A	406	LEU	C-N-CA	5.90	136.45	121.70
2	H	102	TYR	CA-C-N	5.89	130.16	117.20
3	A	424	GLN	N-CA-C	-5.84	95.23	111.00
3	C	10	THR	C-N-CA	5.81	136.23	121.70
3	B	425	ALA	C-N-CA	5.70	135.94	121.70
2	H	102	TYR	C-N-CA	5.66	135.86	121.70
3	B	395	ASN	C-N-CA	5.65	135.83	121.70
3	D	462	PHE	N-CA-C	-5.64	95.76	111.00
3	F	474	LEU	N-CA-C	-5.62	95.82	111.00
3	A	12	TYR	C-N-CA	5.62	135.74	121.70
3	F	9	ALA	CA-C-N	5.61	129.55	117.20
3	B	10	THR	C-N-CA	5.60	135.71	121.70
3	F	429	GLN	C-N-CA	5.46	135.35	121.70
3	D	422	THR	CA-C-N	5.45	129.20	117.20
3	E	475	LYS	N-CA-C	5.43	125.67	111.00
3	D	479	LYS	O-C-N	-5.42	114.03	122.70
3	C	359	ASN	O-C-N	5.41	131.35	122.70
3	A	431	HIS	O-C-N	-5.38	114.09	122.70
3	C	341	ASN	N-CA-C	-5.36	96.53	111.00
3	E	474	LEU	C-N-CA	5.36	135.09	121.70
3	B	432	THR	N-CA-C	-5.35	96.55	111.00
3	E	442	LYS	O-C-N	5.31	131.20	122.70
3	A	301	THR	N-CA-C	-5.30	96.68	111.00
3	D	414	LEU	C-N-CA	5.30	134.94	121.70
3	F	359	ASN	O-C-N	-5.29	114.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	422	THR	C-N-CA	5.28	134.90	121.70
3	E	434	PRO	C-N-CA	5.25	134.81	121.70
3	E	482	LEU	CA-C-N	5.24	126.69	116.20
3	D	107	VAL	O-C-N	5.24	132.11	123.20
3	D	139	ALA	N-CA-C	-5.23	96.89	111.00
3	C	296	SER	C-N-CA	5.22	133.25	122.30
3	E	461	GLN	C-N-CA	5.21	134.72	121.70
3	D	481	THR	C-N-CA	5.16	134.59	121.70
3	A	363	TYR	N-CA-C	-5.15	97.09	111.00
3	C	311	TYR	N-CA-C	-5.15	97.10	111.00
3	F	426	ILE	O-C-N	-5.14	114.47	122.70
3	E	420	PHE	C-N-CA	5.14	134.54	121.70
3	F	427	ALA	C-N-CA	5.12	134.51	121.70
3	F	106	GLU	N-CA-C	-5.12	97.18	111.00
3	C	371	ASP	N-CA-C	-5.09	97.26	111.00
3	B	406	LEU	N-CA-C	-5.08	97.27	111.00
3	F	315	ARG	N-CA-C	-5.08	97.27	111.00
3	E	45	VAL	N-CA-C	-5.06	97.33	111.00
3	B	381	ILE	N-CA-C	-5.04	97.38	111.00
3	F	342	MET	N-CA-C	-5.04	97.38	111.00
3	E	479	LYS	CA-C-N	5.04	128.28	117.20
3	A	331	VAL	N-CA-C	-5.03	97.41	111.00
3	E	323	ILE	N-CA-C	-5.03	97.42	111.00
3	E	431	HIS	N-CA-C	-5.03	97.43	111.00
3	C	10	THR	O-C-N	-5.02	114.67	122.70
3	A	427	ALA	O-C-N	-5.02	114.67	122.70
3	F	359	ASN	C-N-CA	5.02	134.25	121.70
3	E	428	CYS	CA-C-N	5.01	128.23	117.20
3	F	429	GLN	N-CA-C	-5.01	97.47	111.00
3	E	419	ARG	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	105	VAL	Peptide
3	A	13	LEU	Peptide
3	A	16	VAL	Peptide
3	A	405	GLY	Peptide
3	A	407	GLN	Peptide
3	A	408	PRO	Peptide
3	A	409	PRO	Peptide

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Mol	Chain	Res	Type	Group
3	A	415	GLU	Peptide
3	A	433	PRO	Peptide
3	A	436	PRO	Peptide
3	A	437	LYS	Peptide
3	A	477	LYS	Peptide
3	B	13	LEU	Peptide
3	B	14	PRO	Peptide
3	B	181	GLN	Peptide
3	B	408	PRO	Peptide
3	B	409	PRO	Peptide
3	B	414	LEU	Peptide
3	B	424	GLN	Peptide
3	B	433	PRO	Peptide
3	B	443	LYS	Peptide
3	B	481	THR	Peptide
3	C	12	TYR	Peptide
3	C	13	LEU	Peptide
3	C	14	PRO	Peptide
3	C	16	VAL	Peptide
3	C	181	GLN	Peptide
3	C	405	GLY	Peptide
3	C	407	GLN	Peptide
3	C	416	ASP	Peptide
3	C	418	TYR	Peptide
3	C	421	VAL	Peptide
3	C	435	ALA	Peptide
3	C	476	ALA	Peptide
3	C	477	LYS	Peptide
3	D	13	LEU	Peptide
3	D	17	PRO	Peptide
3	D	407	GLN	Peptide
3	D	408	PRO	Peptide
3	D	409	PRO	Peptide
3	D	422	THR	Peptide
3	D	424	GLN	Peptide
3	D	432	THR	Peptide
3	D	433	PRO	Peptide
3	D	435	ALA	Peptide
3	D	438	GLU	Peptide
3	D	473	GLY	Peptide
3	D	477	LYS	Peptide
3	D	481	THR	Peptide

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Mol	Chain	Res	Type	Group
3	D	9	ALA	Peptide
3	E	10	THR	Peptide
3	E	13	LEU	Peptide
3	E	14	PRO	Peptide
3	E	406	LEU	Peptide
3	E	407	GLN	Peptide
3	E	408	PRO	Peptide
3	E	433	PRO	Peptide
3	E	477	LYS	Peptide
3	E	481	THR	Peptide
3	F	10	THR	Peptide
3	F	12	TYR	Peptide
3	F	13	LEU	Peptide
3	F	16	VAL	Peptide
3	F	19	SER	Peptide
3	F	408	PRO	Peptide
3	F	409	PRO	Peptide
3	F	414	LEU	Peptide
3	F	435	ALA	Peptide
3	F	476	ALA	Peptide
3	F	479	LYS	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	L	893	879	878	8	0
2	H	894	841	836	20	0
3	A	1911	958	512	2	0
3	B	1911	958	512	1	0
3	C	1911	958	512	0	0
3	D	1911	958	512	0	0
3	E	1911	958	512	0	0
3	F	1911	958	512	1	0
All	All	13253	7468	4786	30	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 2.

All (30) 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)
2:H:94:ARG:C	2:H:95:GLY:N	1.75	1.39
2:H:94:ARG:CA	2:H:95:GLY:N	1.92	1.30
2:H:94:ARG:HA	2:H:95:GLY:N	1.70	1.04
2:H:103:TRP:CE3	2:H:103:TRP:O	2.17	0.96
2:H:103:TRP:O	2:H:103:TRP:HE3	1.57	0.86
2:H:103:TRP:N	2:H:103:TRP:CE3	2.47	0.83
2:H:103:TRP:N	2:H:103:TRP:HE3	1.83	0.74
2:H:94:ARG:C	2:H:95:GLY:CA	2.56	0.73
2:H:94:ARG:HG3	2:H:94:ARG:O	1.90	0.69
1:L:50:TRP:CD2	1:L:50:TRP:O	2.47	0.68
1:L:44:PRO:O	2:H:103:TRP:NE1	2.28	0.66
1:L:50:TRP:CE3	1:L:50:TRP:O	2.50	0.64
2:H:94:ARG:CB	2:H:95:GLY:N	2.62	0.61
2:H:94:ARG:CG	2:H:94:ARG:O	2.50	0.59
1:L:50:TRP:CG	1:L:50:TRP:O	2.61	0.54
2:H:35:SER:N	2:H:93:ALA:O	2.42	0.53
2:H:103:TRP:CE3	2:H:103:TRP:C	2.84	0.49
3:F:427:ALA:H	3:F:428:CYS:CA	2.27	0.48
2:H:42:GLU:O	2:H:43:LYS:HB2	2.14	0.47
2:H:103:TRP:CE3	2:H:103:TRP:CA	2.99	0.45
3:A:12:TYR:H	3:A:13:LEU:CA	2.31	0.43
1:L:19:VAL:HG22	1:L:75:ILE:HB	2.00	0.43
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.53	0.43
2:H:109:LEU:HD23	2:H:109:LEU:C	2.40	0.42
2:H:12:VAL:O	2:H:111:VAL:HA	2.20	0.41
1:L:43:SER:HB3	2:H:103:TRP:NE1	2.36	0.41
1:L:32:TYR:CD2	1:L:32:TYR:N	2.88	0.41
3:A:431:HIS:H	3:A:432:THR:CA	2.34	0.41
2:H:94:ARG:O	2:H:101:ASP:N	2.53	0.40
3:B:242:TYR:O	3:B:318:GLY:HA3	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	L	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	H	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
3	A	476/478 (100%)	403 (85%)	55 (12%)	18 (4%)	4	37
3	B	476/478 (100%)	395 (83%)	50 (10%)	31 (6%)	1	25
3	C	476/478 (100%)	402 (84%)	52 (11%)	22 (5%)	3	33
3	D	476/478 (100%)	404 (85%)	47 (10%)	25 (5%)	2	29
3	E	476/478 (100%)	417 (88%)	43 (9%)	16 (3%)	5	40
3	F	476/478 (100%)	405 (85%)	52 (11%)	19 (4%)	4	35
All	All	3082/3098 (100%)	2646 (86%)	305 (10%)	131 (4%)	6	34

All (131) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	15	PRO
3	B	87	ASP
3	B	133	SER
3	B	395	ASN
3	B	408	PRO
3	B	409	PRO
3	B	414	LEU
3	B	415	GLU
3	B	439	ASP
3	A	41	ARG
3	A	86	PRO
3	A	340	THR
3	A	427	ALA
3	E	11	VAL
3	E	289	SER
3	E	475	LYS
3	E	480	PHE
3	D	152	LYS
3	D	290	ASN
3	D	476	ALA
3	C	89	SER
3	C	202	ASP
3	C	355	TYR
3	C	395	ASN

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Mol	Chain	Res	Type
3	C	408	PRO
3	C	417	THR
3	C	425	ALA
3	C	478	PRO
3	F	339	SER
3	B	143	ASN
3	B	152	LYS
3	B	410	PRO
3	B	421	VAL
3	A	14	PRO
3	A	15	PRO
3	A	26	GLU
3	A	424	GLN
3	E	425	ALA
3	D	41	ARG
3	D	408	PRO
3	D	409	PRO
3	D	457	ALA
3	D	474	LEU
3	D	482	LEU
3	C	14	PRO
3	C	26	GLU
3	C	41	ARG
3	F	315	ARG
3	F	406	LEU
3	F	415	GLU
3	B	13	LEU
3	B	14	PRO
3	B	132	ALA
3	B	202	ASP
3	B	221	PRO
3	B	326	GLY
3	B	457	ALA
3	A	351	SER
3	A	358	THR
3	E	48	PRO
3	E	110	GLY
3	E	202	ASP
3	E	308	ASN
3	E	423	SER
3	E	479	LYS
3	D	78	PRO

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Mol	Chain	Res	Type
3	D	89	SER
3	D	395	ASN
3	D	427	ALA
3	D	433	PRO
3	D	436	PRO
3	D	453	GLU
3	D	479	LYS
3	C	133	SER
3	C	182	PRO
3	C	459	LEU
3	C	479	LYS
3	F	314	GLN
3	F	395	ASN
3	F	425	ALA
3	F	477	LYS
3	B	435	ALA
3	B	475	LYS
3	B	478	PRO
3	B	479	LYS
3	B	482	LEU
3	A	13	LEU
3	A	185	CYS
3	A	247	PHE
3	A	308	ASN
3	A	437	LYS
3	A	440	PRO
3	A	462	PHE
3	E	314	GLN
3	E	439	ASP
3	D	90	PHE
3	D	139	ALA
3	D	259	HIS
3	D	410	PRO
3	D	434	PRO
3	C	16	VAL
3	C	161	CYS
3	C	173	SER
3	C	436	PRO
3	F	11	VAL
3	F	241	PRO
3	F	247	PHE
3	F	259	HIS

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Mol	Chain	Res	Type
3	F	479	LYS
3	B	20	LYS
3	B	173	SER
3	B	403	ASN
3	B	416	ASP
3	B	445	THR
3	E	409	PRO
3	D	484	LYS
3	D	485	ARG
3	C	90	PHE
3	F	41	ARG
3	F	218	SER
3	F	403	ASN
3	F	420	PHE
3	A	137	ALA
3	E	41	ARG
3	E	259	HIS
3	D	403	ASN
3	F	417	THR
3	B	434	PRO
3	F	180	VAL
3	C	407	GLN
3	C	164	PRO

### 5.3.2 Protein sidechains ⓘ

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	L	100/100 (100%)	99 (99%)	1 (1%)	82	92
2	H	95/95 (100%)	94 (99%)	1 (1%)	80	91
All	All	195/195 (100%)	193 (99%)	2 (1%)	83	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	30(F)	LYS
2	H	103	TRP

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

### 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 carbohydrates 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.