



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:53 PM BST

PDB ID : 3J8V
EMDB ID: : EMD-6121
Title : Cryo-EM reconstruction of quasi-HPV16 complex with H16.14J Fab
Authors : Guan, J.; Hafenstein, S.
Deposited on : 2014-11-19
Resolution : 13.90 Å(reported)
Based on PDB ID : 3OAE

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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

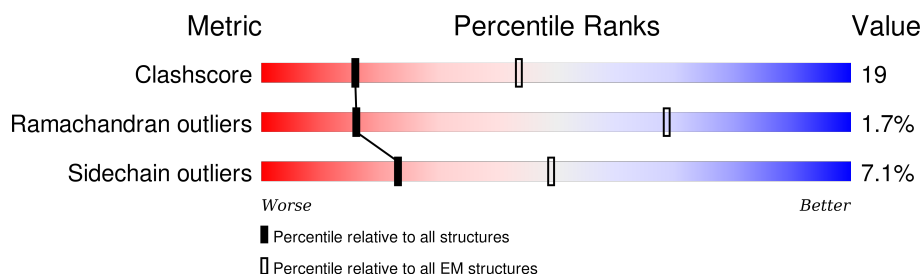
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.90 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 ≥ 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	A	455	55% 31% 6% 7%
1	B	455	56% 30% 6% 7%
1	C	455	56% 31% 6% 7%
1	D	455	55% 32% 5% 7%
1	E	455	55% 31% 6% 7%
2	J	109	92% 7% .
2	K	109	92% 7% .
2	L	109	92% 7% .
2	M	109	92% 7% .

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Mol	Chain	Length	Quality of chain
3	F	119	 90%9% •
3	G	119	 90%9% •
3	H	119	 88%11% •
3	I	119	 90%9% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30346 atoms, of which 6752 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 L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
1	B	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
1	C	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
1	D	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
1	E	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
A	177	GLN	ASN	CONFLICT	UNP Q4VRM0
A	181	GLN	ASN	CONFLICT	UNP Q4VRM0
A	472	LEU	ALA	CONFLICT	UNP Q4VRM0
B	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
B	177	GLN	ASN	CONFLICT	UNP Q4VRM0
B	181	GLN	ASN	CONFLICT	UNP Q4VRM0
B	472	LEU	ALA	CONFLICT	UNP Q4VRM0
C	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
C	177	GLN	ASN	CONFLICT	UNP Q4VRM0
C	181	GLN	ASN	CONFLICT	UNP Q4VRM0
C	472	LEU	ALA	CONFLICT	UNP Q4VRM0
D	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
D	177	GLN	ASN	CONFLICT	UNP Q4VRM0
D	181	GLN	ASN	CONFLICT	UNP Q4VRM0
D	472	LEU	ALA	CONFLICT	UNP Q4VRM0
E	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
E	177	GLN	ASN	CONFLICT	UNP Q4VRM0
E	181	GLN	ASN	CONFLICT	UNP Q4VRM0
E	472	LEU	ALA	CONFLICT	UNP Q4VRM0

- Molecule 2 is a protein called H16.14J light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	L	109	Total	C	H	N	O	S	0	0
			1651	523	820	142	163	3		
2	J	109	Total	C	H	N	O	S	0	0
			1651	523	820	142	163	3		
2	K	109	Total	C	H	N	O	S	0	0
			1651	523	820	142	163	3		
2	M	109	Total	C	H	N	O	S	0	0
			1651	523	820	142	163	3		

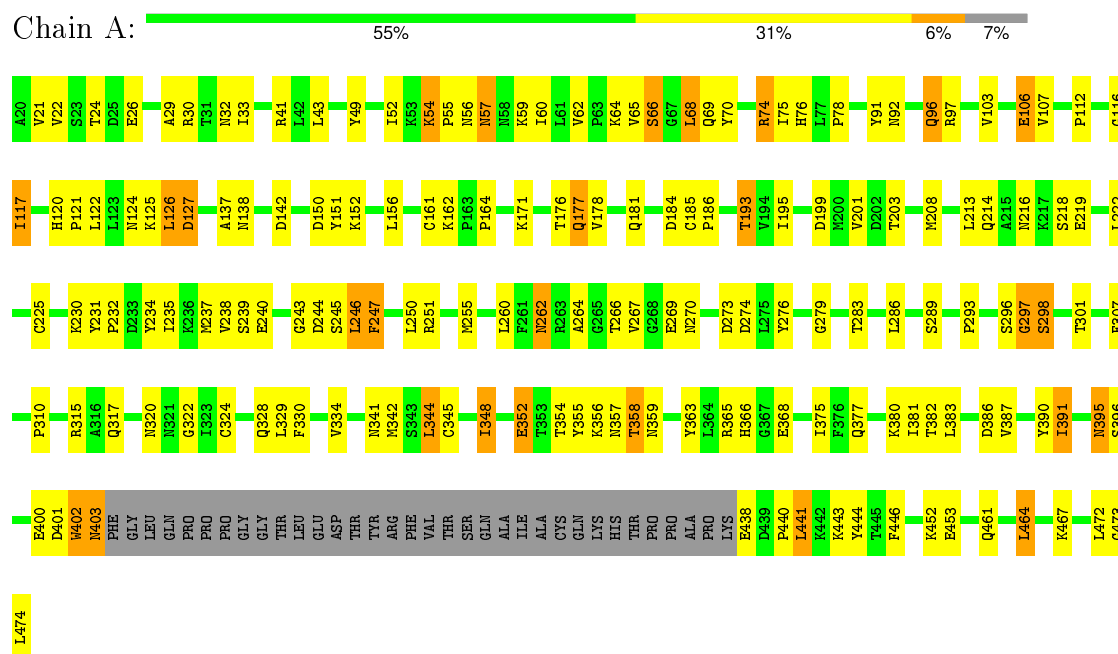
- Molecule 3 is a protein called H16.14J heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	119	Total	C	H	N	O	S	0	0
			1783	578	868	153	179	5		
3	F	119	Total	C	H	N	O	S	0	0
			1783	578	868	153	179	5		
3	G	119	Total	C	H	N	O	S	0	0
			1783	578	868	153	179	5		
3	I	119	Total	C	H	N	O	S	0	0
			1783	578	868	153	179	5		

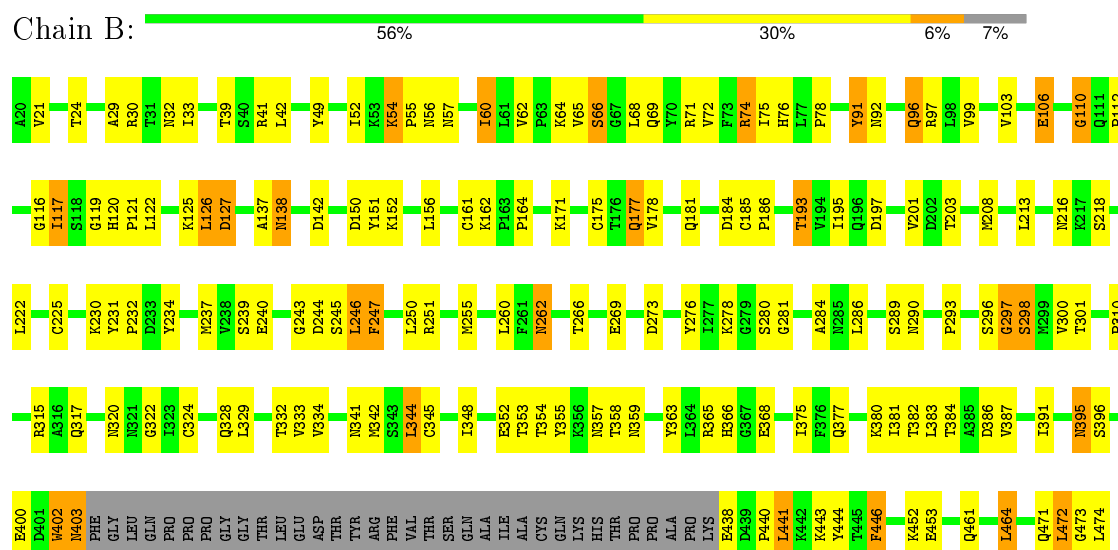
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: L1

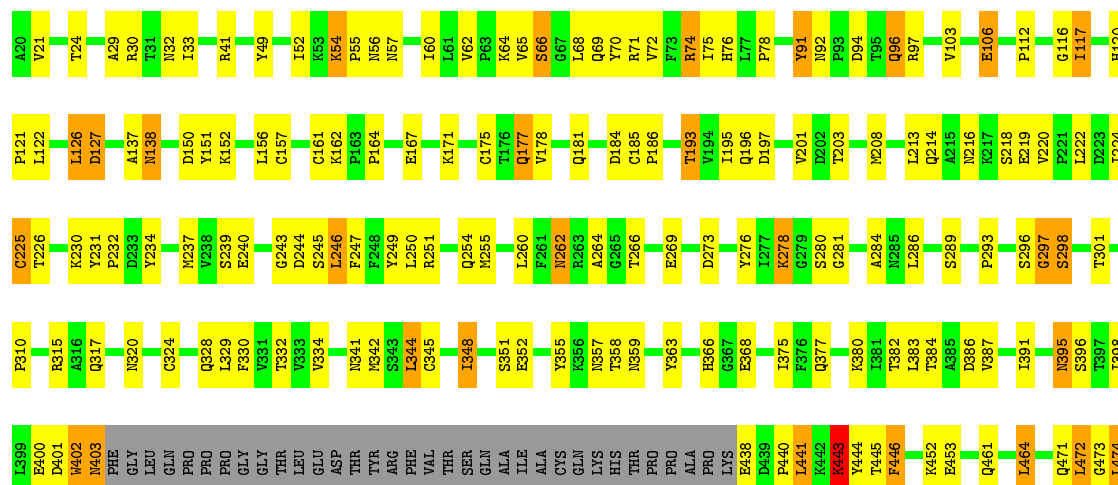


• Molecule 1: L1



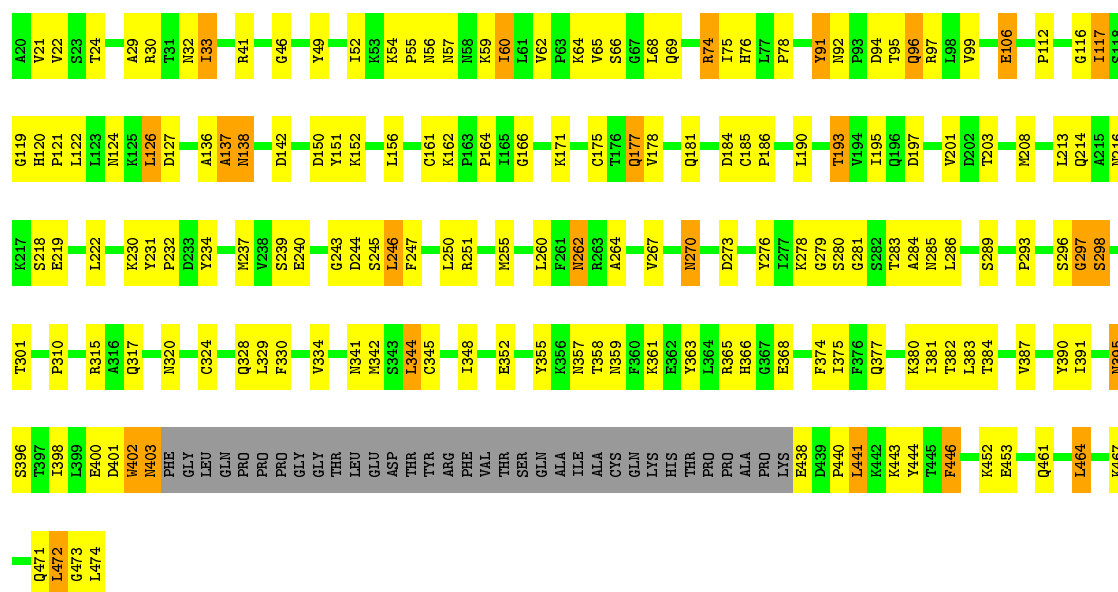
- Molecule 1: L1

Chain C: 



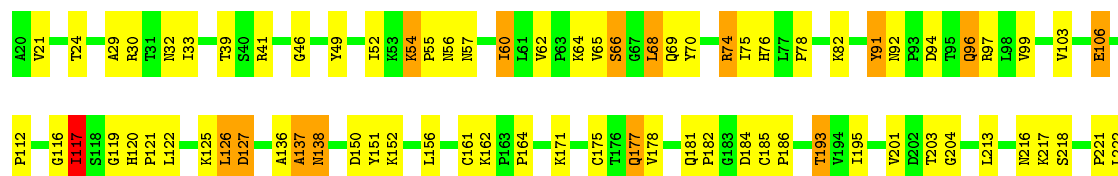
- Molecule 1: L1

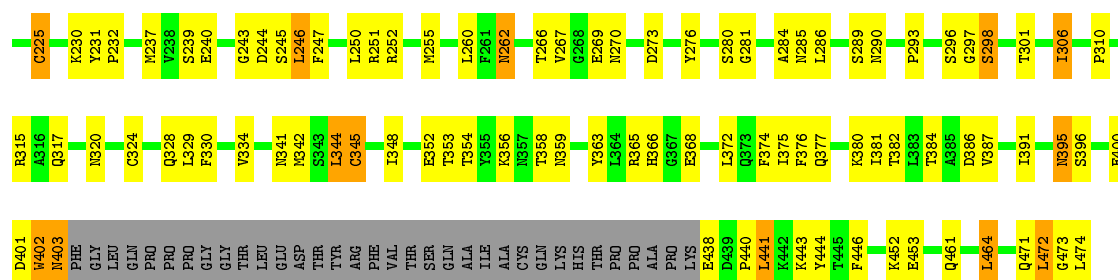
Chain D: 



- Molecule 1: L1

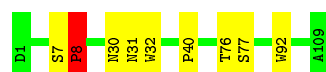
Chain E: 





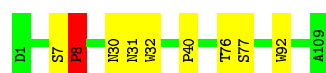
- Molecule 2: H16.14J light chain

Chain L: 92% 7% .



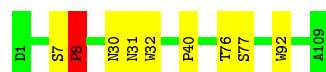
- Molecule 2: H16.14J light chain

Chain J: 92% 7% .



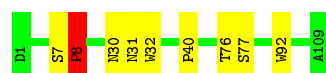
- Molecule 2: H16.14J light chain

Chain K: 92% 7% .



- Molecule 2: H16.14J light chain

Chain M: 92% 7% .



- Molecule 3: H16.14J heavy chain

Chain H: 88% 11% .




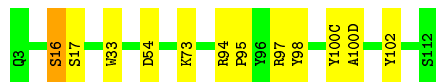
- Molecule 3: H16.14J heavy chain

Chain F: 90% 9% .




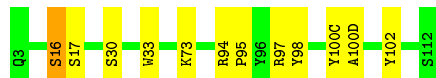
- Molecule 3: H16.14J heavy chain

Chain G:  90% 9% .



- Molecule 3: H16.14J heavy chain

Chain I:  90% 9% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	5642	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)	620	Depositor
Maximum defocus (nm)	4690	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	A	0.58	6/3407 (0.2%)	0.72	3/4632 (0.1%)
1	B	0.49	0/3407	0.70	2/4632 (0.0%)
1	C	0.53	2/3407 (0.1%)	0.71	1/4632 (0.0%)
1	D	0.55	3/3407 (0.1%)	0.71	3/4632 (0.1%)
1	E	0.52	1/3407 (0.0%)	0.72	0/4632
2	J	0.69	1/850 (0.1%)	0.70	1/1155 (0.1%)
2	K	0.69	1/850 (0.1%)	0.70	1/1155 (0.1%)
2	L	0.70	1/850 (0.1%)	0.70	1/1155 (0.1%)
2	M	0.69	1/850 (0.1%)	0.70	1/1155 (0.1%)
3	F	0.74	2/939 (0.2%)	0.68	0/1269
3	G	0.74	2/939 (0.2%)	0.68	0/1269
3	H	0.74	2/939 (0.2%)	0.68	0/1269
3	I	0.74	2/939 (0.2%)	0.68	0/1269
All	All	0.60	24/24191 (0.1%)	0.71	13/32856 (0.0%)

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	8	PRO	N-CD	9.84	1.61	1.47
2	L	8	PRO	N-CD	9.77	1.61	1.47
2	M	8	PRO	N-CD	9.77	1.61	1.47
2	J	8	PRO	N-CD	9.77	1.61	1.47
3	H	102	TYR	C-N	9.13	1.55	1.34

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	8	PRO	CA-N-CD	-6.87	101.89	111.50
2	M	8	PRO	CA-N-CD	-6.86	101.90	111.50
2	J	8	PRO	CA-N-CD	-6.86	101.90	111.50
2	K	8	PRO	CA-N-CD	-6.84	101.92	111.50
1	A	443	LYS	CD-CE-NZ	-6.41	96.96	111.70

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	3322	0	3227	141	0
1	B	3322	0	3227	190	0
1	C	3322	0	3226	190	0
1	D	3322	0	3227	190	0
1	E	3322	0	3227	196	0
2	J	831	820	820	26	0
2	K	831	820	820	30	0
2	L	831	820	820	29	0
2	M	831	820	820	22	0
3	F	915	868	865	45	0
3	G	915	868	864	40	0
3	H	915	868	865	53	0
3	I	915	868	865	30	0
All	All	23594	6752	22873	880	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 19.

The worst 5 of 880 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:B:280:SER:HB2	2:M:92:TRP:CZ2	1.26	1.59
1:C:358:THR:HG21	3:F:98:TYR:CZ	1.32	1.59
1:C:284:ALA:CB	2:K:32:TRP:HH2	1.24	1.50
1:E:181:GLN:CB	3:H:73:LYS:HZ3	1.25	1.48
1:B:181:GLN:CB	3:I:73:LYS:NZ	1.74	1.47

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	A	417/455 (92%)	378 (91%)	29 (7%)	10 (2%)	7	47
1	B	417/455 (92%)	378 (91%)	29 (7%)	10 (2%)	7	47
1	C	417/455 (92%)	375 (90%)	34 (8%)	8 (2%)	10	52
1	D	417/455 (92%)	377 (90%)	30 (7%)	10 (2%)	7	47
1	E	417/455 (92%)	378 (91%)	31 (7%)	8 (2%)	10	52
2	J	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
2	K	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
2	L	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
2	M	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
3	F	117/119 (98%)	112 (96%)	4 (3%)	1 (1%)	21	67
3	G	117/119 (98%)	112 (96%)	4 (3%)	1 (1%)	21	67
3	H	117/119 (98%)	112 (96%)	4 (3%)	1 (1%)	21	67
3	I	117/119 (98%)	112 (96%)	4 (3%)	1 (1%)	21	67
All	All	2981/3187 (94%)	2734 (92%)	197 (7%)	50 (2%)	16	55

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ALA
1	A	298	SER
1	A	402	TRP
1	B	137	ALA
1	B	298	SER

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	A	368/396 (93%)	334 (91%)	34 (9%)	11	43
1	B	368/396 (93%)	335 (91%)	33 (9%)	12	44
1	C	368/396 (93%)	329 (89%)	39 (11%)	8	36
1	D	368/396 (93%)	335 (91%)	33 (9%)	12	44
1	E	368/396 (93%)	330 (90%)	38 (10%)	9	37
2	J	92/92 (100%)	90 (98%)	2 (2%)	60	83
2	K	92/92 (100%)	90 (98%)	2 (2%)	60	83
2	L	92/92 (100%)	90 (98%)	2 (2%)	60	83
2	M	92/92 (100%)	90 (98%)	2 (2%)	60	83
3	F	95/95 (100%)	95 (100%)	0	100	100
3	G	95/95 (100%)	95 (100%)	0	100	100
3	H	95/95 (100%)	95 (100%)	0	100	100
3	I	95/95 (100%)	95 (100%)	0	100	100
All	All	2588/2728 (95%)	2403 (93%)	185 (7%)	23	55

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	247	PHE
1	C	464	LEU
1	E	438	GLU
1	C	278	LYS
1	C	351	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	262	ASN
1	C	461	GLN
1	E	366	HIS
1	C	285	ASN
1	C	341	ASN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.