



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Oct 16, 2017 – 06:51 AM EDT

PDB ID : 6B1T  
EMDB ID: : EMD-7034  
Title : Improved cryoEM structure of human adenovirus type 5 with atomic details  
of minor proteins VI and VII  
Authors : Dai, X.H.; Wu, L.; Sun, R.; Zhou, Z.H.  
Deposited on : unknown  
Resolution : 3.20 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

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>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345



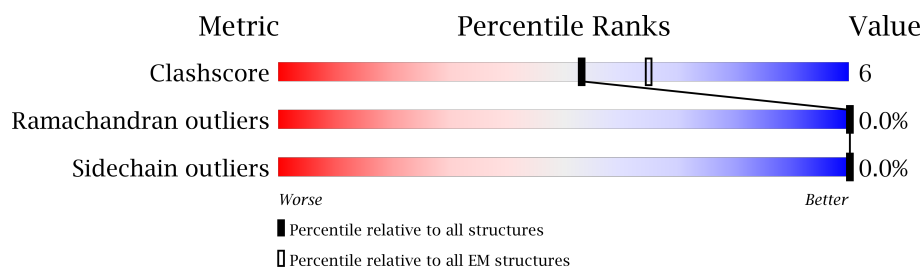
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026













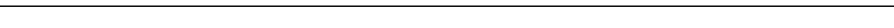



The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of 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	A	952	79% 16% 5%
1	B	952	80% 15% .
1	C	952	79% 16% .
1	D	952	80% 15% 5%
1	E	952	80% 16% .
1	F	952	79% 16% .
1	G	952	80% 16% 5%
1	H	952	81% 14% .
1	I	952	81% 14% .

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Mol	Chain	Length	Quality of chain
1	J	952	 79% 17%
1	K	952	 78% 17%
1	L	952	 81% 14%
2	M	571	 69% 11% 20%
3	N	585	 45% 51%
4	O	227	 73% 7% 21%
4	P	227	 70% 8% 21%
5	Q	140	 69% 16% 15%
5	R	140	 60% 6% 34%
5	S	140	 56% 5% 39%
5	T	140	 53% 10% 37%
6	U	33	 39% 48% 12%
6	V	33	 42% 45% 12%
6	Y	33	 42% 42% 15%
7	W	11	 64% 36%
8	X	217	 8% 7% 85%



## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 100134 atoms, of which 0 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	908	Total	C	N	O	S	0	0
			7286	4639	1231	1380	36		
1	B	910	Total	C	N	O	S	0	0
			7299	4647	1233	1383	36		
1	C	910	Total	C	N	O	S	0	0
			7302	4650	1232	1383	37		
1	D	906	Total	C	N	O	S	0	0
			7273	4631	1229	1378	35		
1	E	914	Total	C	N	O	S	0	0
			7325	4662	1237	1390	36		
1	F	910	Total	C	N	O	S	0	0
			7300	4647	1233	1384	36		
1	G	909	Total	C	N	O	S	0	0
			7293	4643	1232	1382	36		
1	H	913	Total	C	N	O	S	0	0
			7319	4659	1236	1387	37		
1	I	910	Total	C	N	O	S	0	0
			7300	4647	1233	1384	36		
1	J	913	Total	C	N	O	S	0	0
			7318	4658	1236	1388	36		
1	K	910	Total	C	N	O	S	0	0
			7299	4646	1233	1384	36		
1	L	912	Total	C	N	O	S	0	0
			7311	4654	1235	1386	36		

- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	455	Total	C	N	O	S	0	0
			3642	2309	630	691	12		

- Molecule 3 is a protein called Pre-hexon-linking protein IIIa.



Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	288	Total	C	N	O	S	0	0
			2236	1385	410	437	4		

- Molecule 4 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	180	Total	C	N	O	S	0	0
			1383	870	244	264	5		
4	P	180	Total	C	N	O	S	0	0
			1383	870	244	264	5		

- Molecule 5 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	119	Total	C	N	O	S	0	0
			874	541	155	176	2		
5	R	93	Total	C	N	O	S	0	0
			698	432	123	141	2		
5	S	86	Total	C	N	O	S	0	0
			647	397	115	133	2		
5	T	88	Total	C	N	O	S	0	0
			663	409	118	134	2		

- Molecule 6 is a protein called Pre-protein VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	29	Total	C	N	O	S	0	0
			216	132	42	40	2		
6	V	29	Total	C	N	O	S	0	0
			216	132	42	40	2		
6	Y	28	Total	C	N	O	S	0	0
			208	128	40	38	2		

- Molecule 7 is a protein called Pre-histone-like nucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	11	Total	C	N	O	S	0	0
			83	55	15	12	1		

- Molecule 8 is a protein called Pre-protein VI.



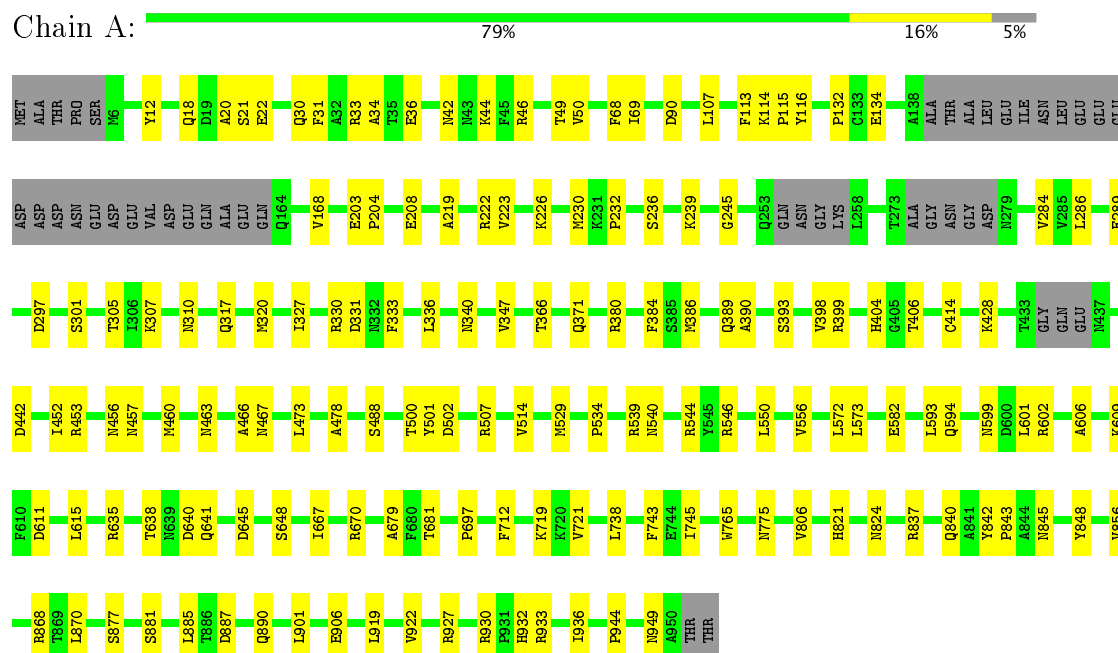
Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	33	Total	C	N	O	0	0
			260	158	49	53		



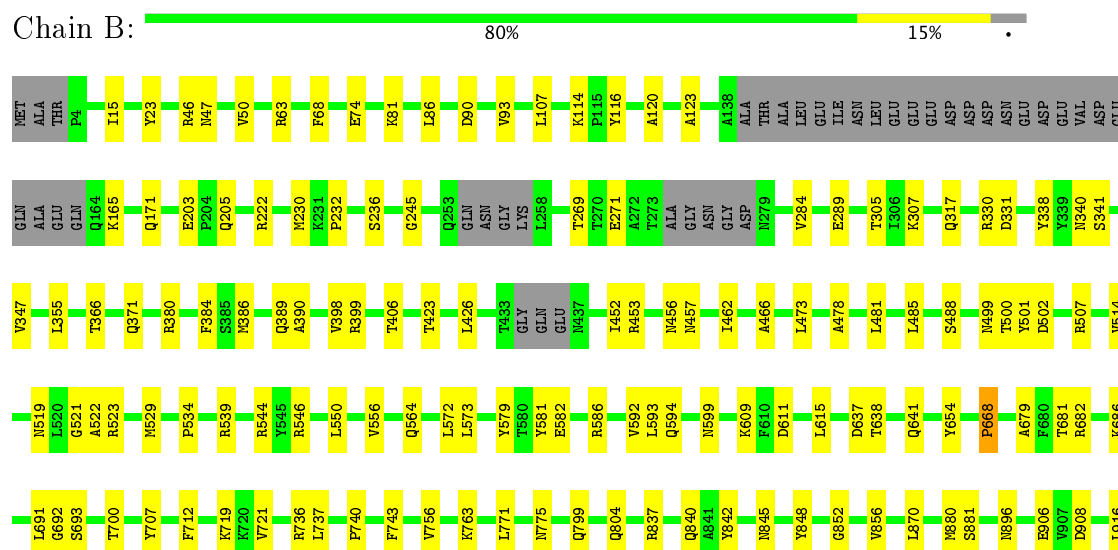
### 3 Residue-property plots

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

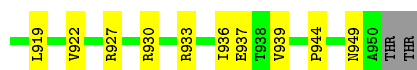
- Molecule 1: Hexon protein



- Molecule 1: Hexon protein

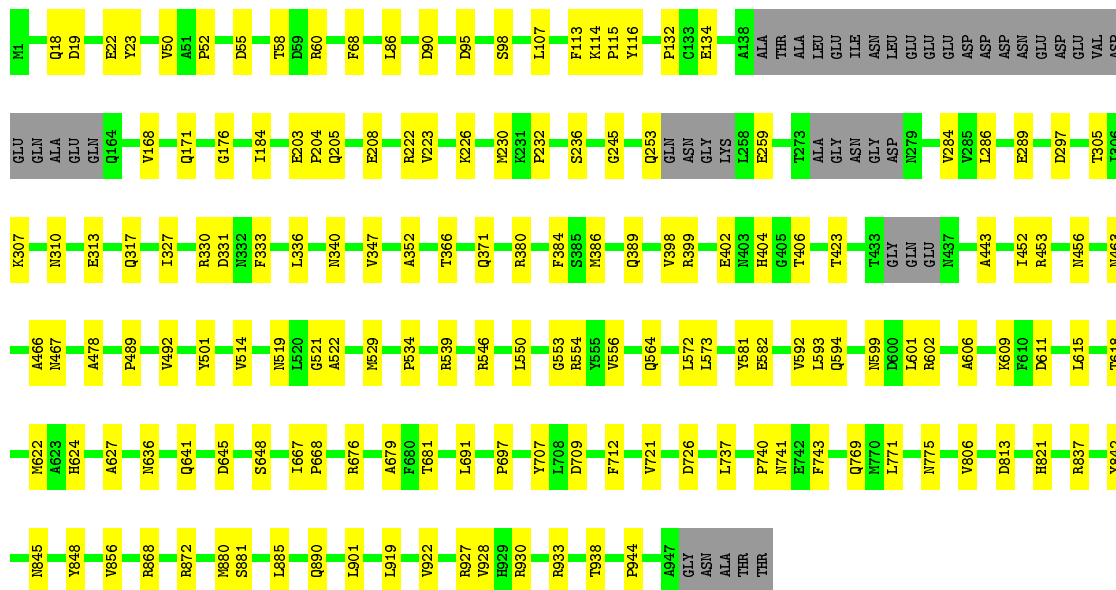






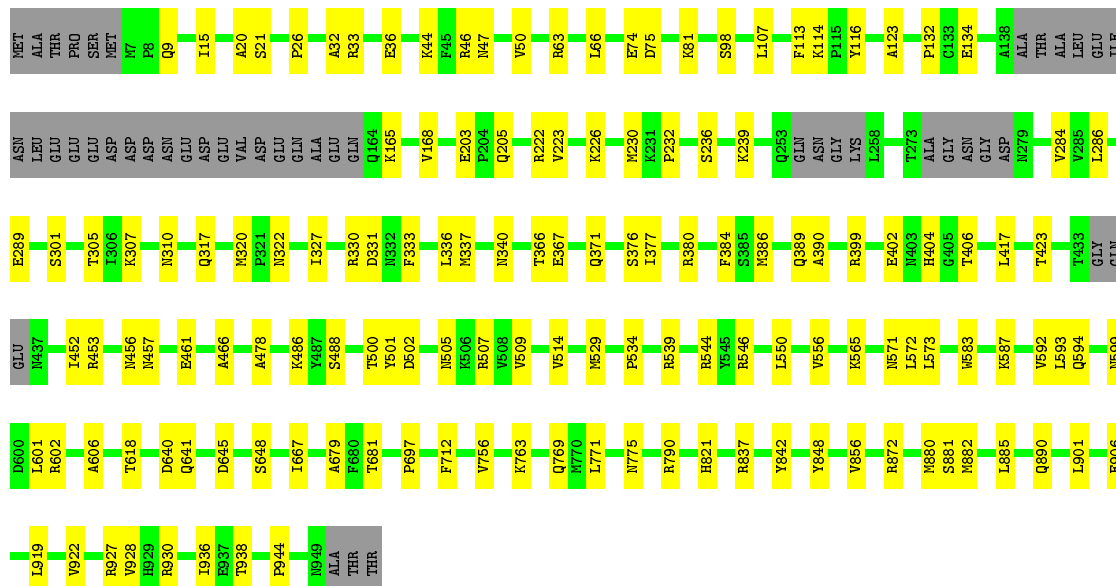
• Molecule 1: Hexon protein

Chain C: 79% 16% .



• Molecule 1: Hexon protein

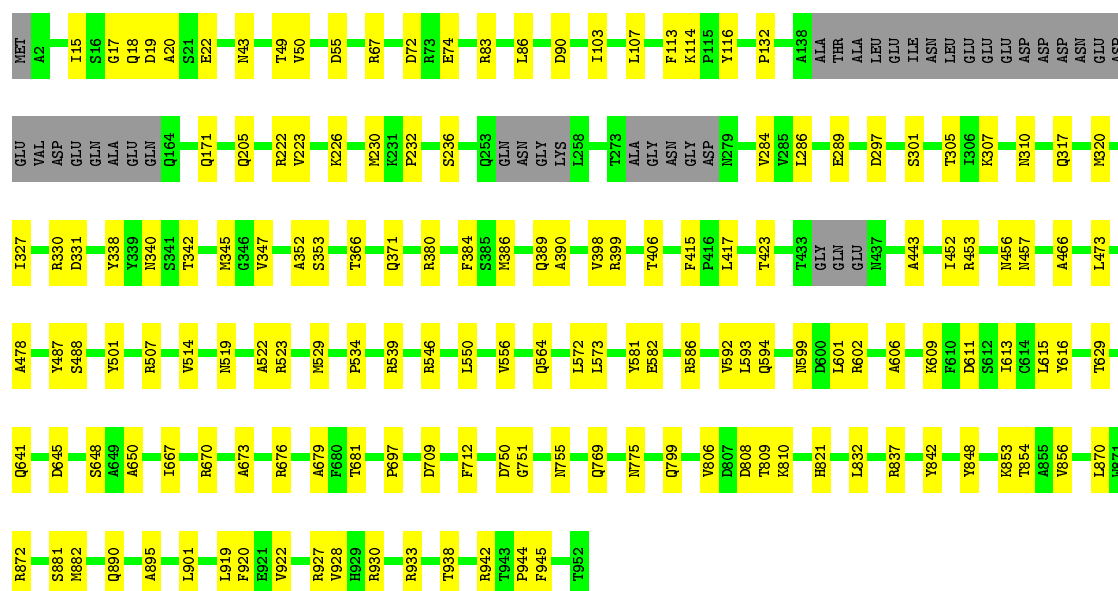
Chain D: 80% 15% 5%



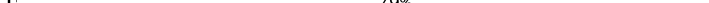
• Molecule 1: Hexon protein

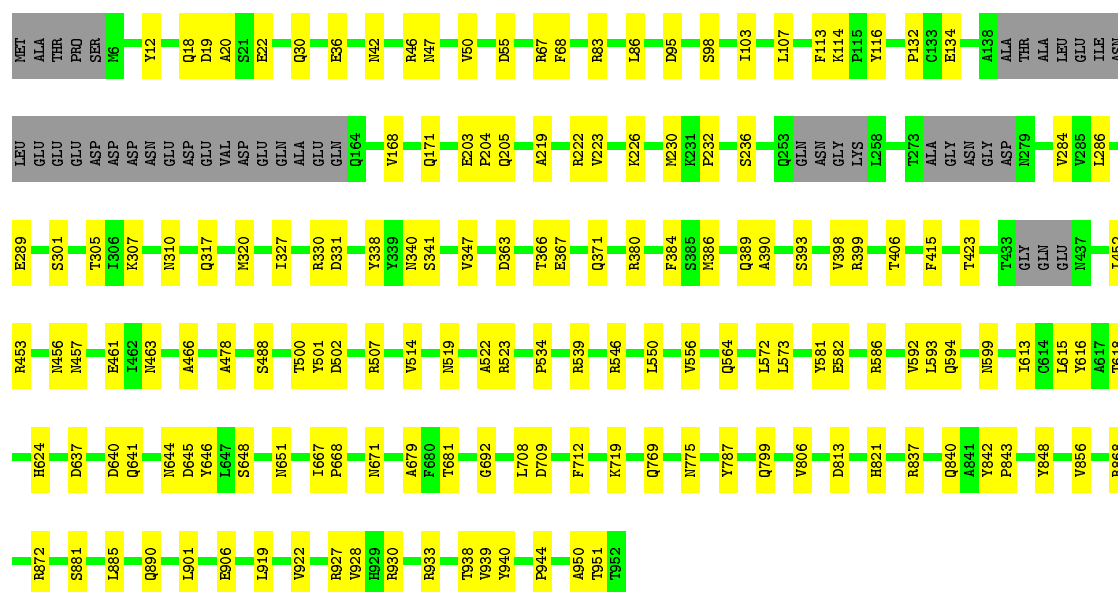
Chain E: 80% 16% .



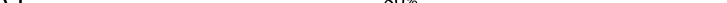


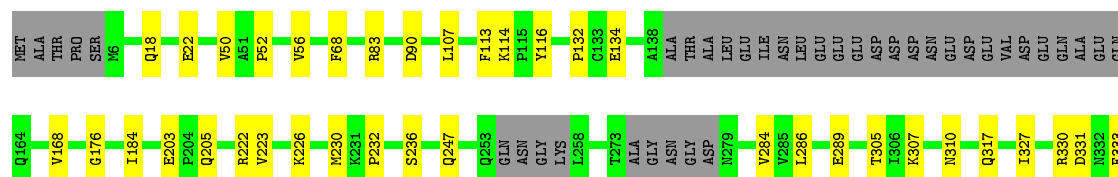
- Molecule 1: Hexon protein

Chain F:  79% 16% .

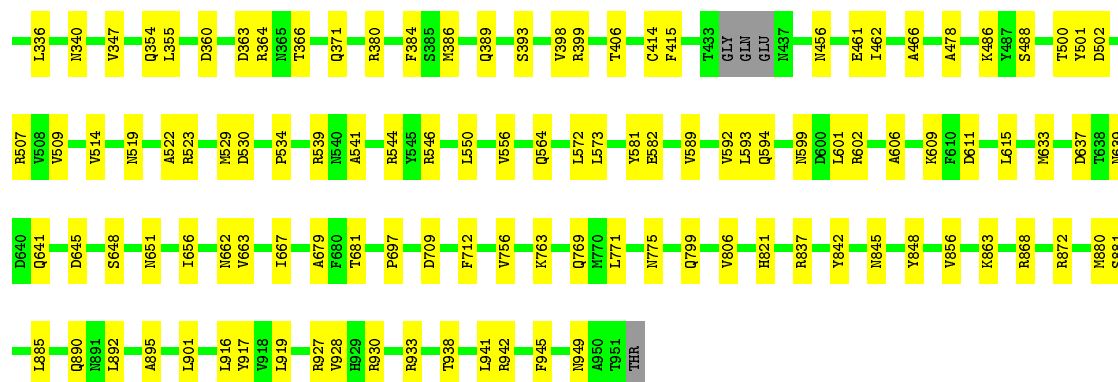


- Molecule 1: Hexon protein

Chain G:  80% 16% 5%

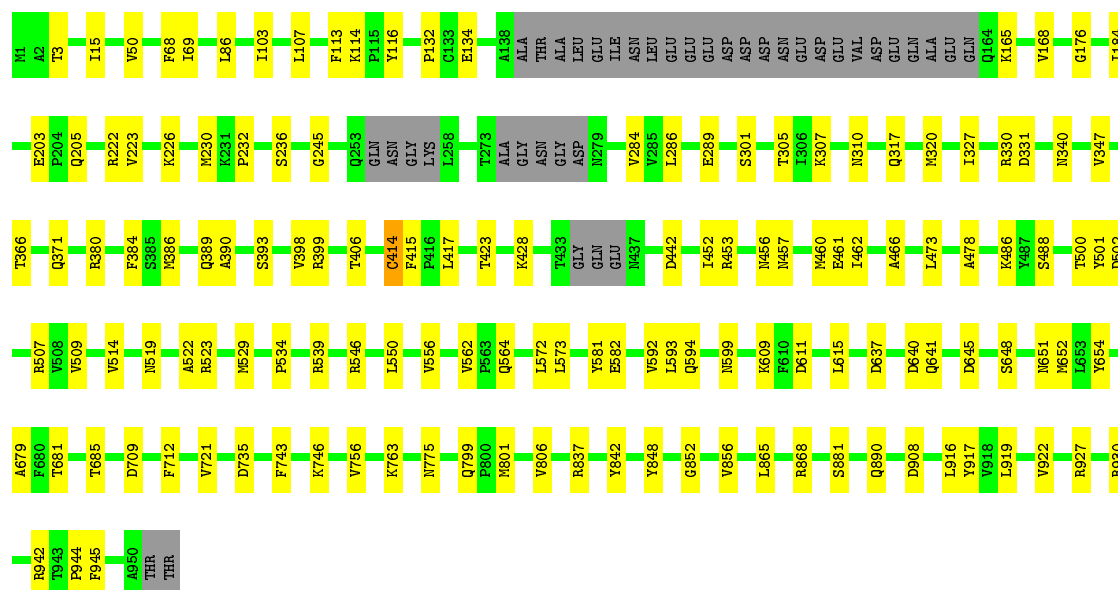






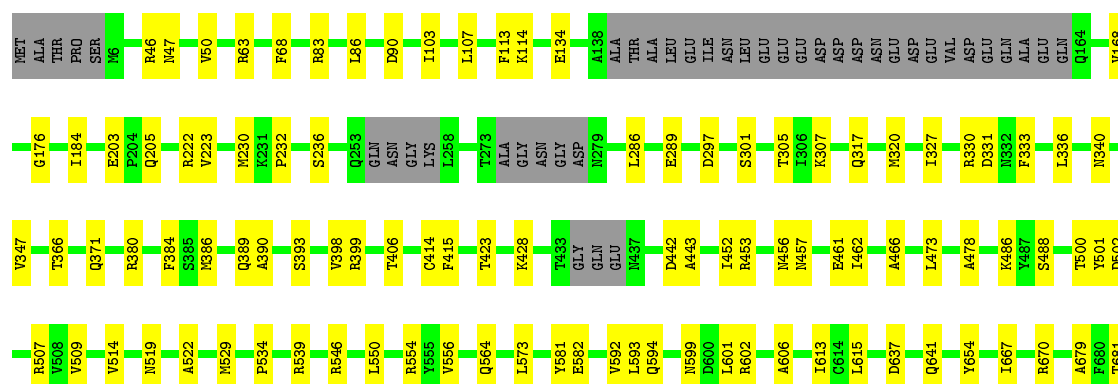
• Molecule 1: Hexon protein

Chain H: 81% 14%

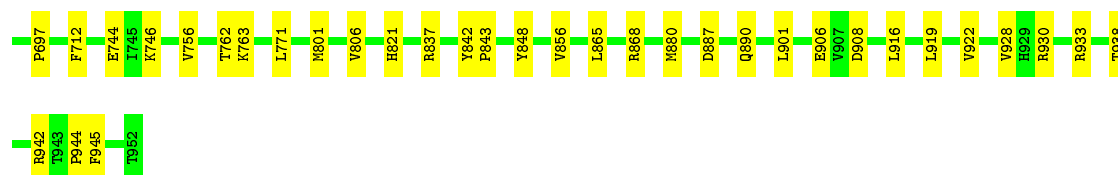


• Molecule 1: Hexon protein

Chain I: 81% 14%

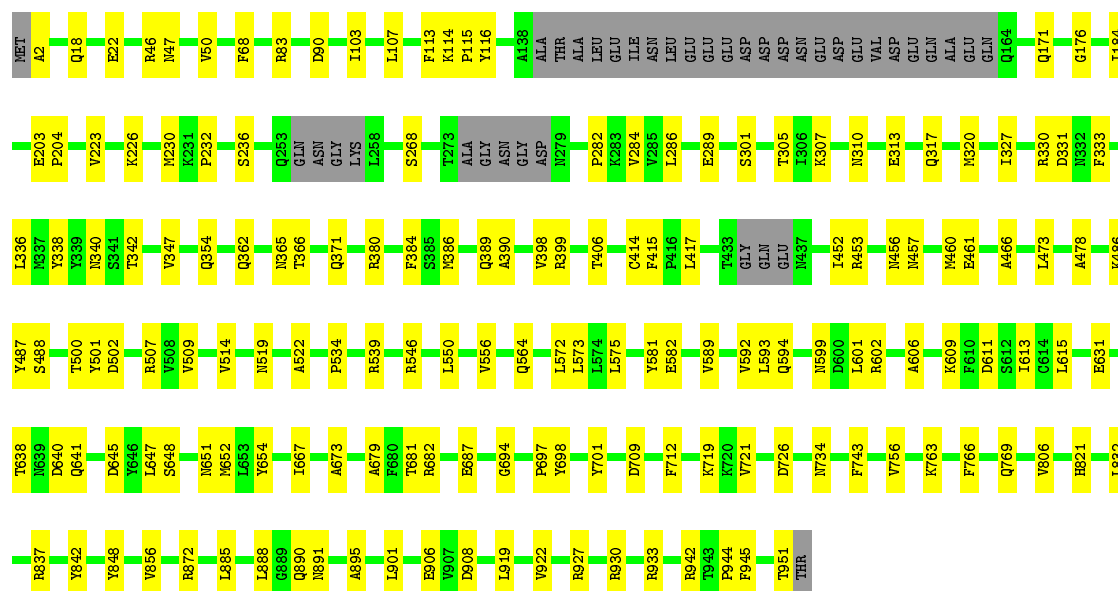






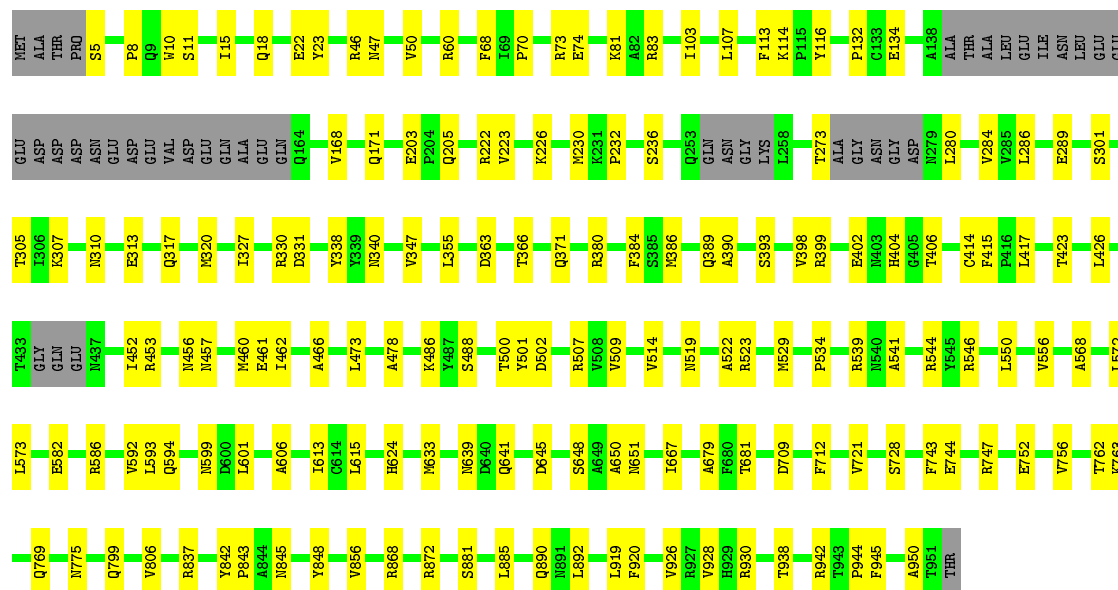
- Molecule 1: Hexon protein

Chain J: 79% 17%




- Molecule 1: Hexon protein

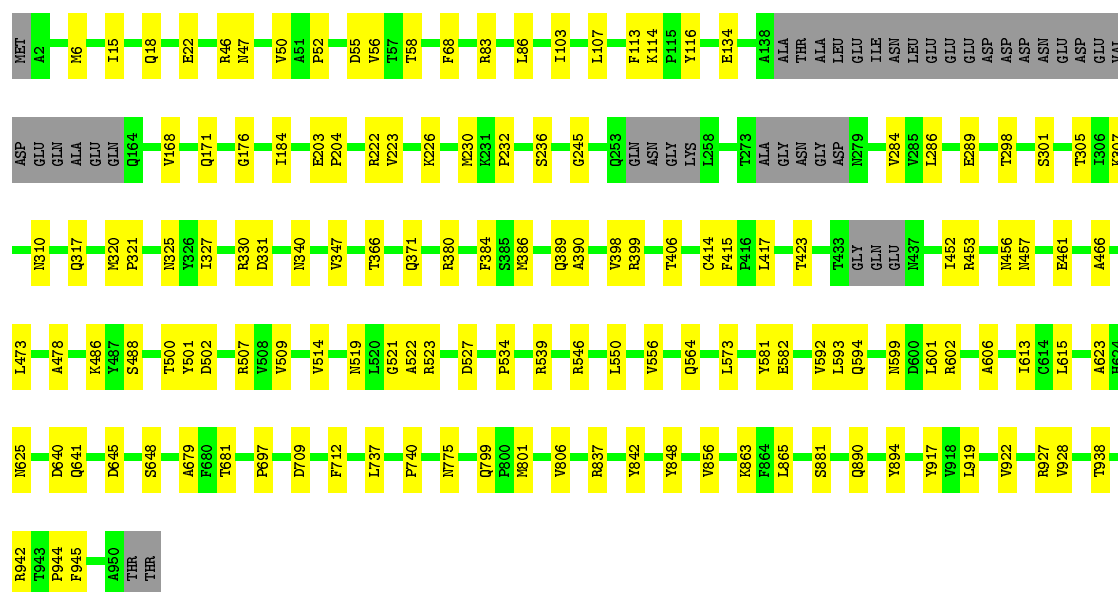
Chain K: 78% 17%



- Molecule 1: Hexon protein

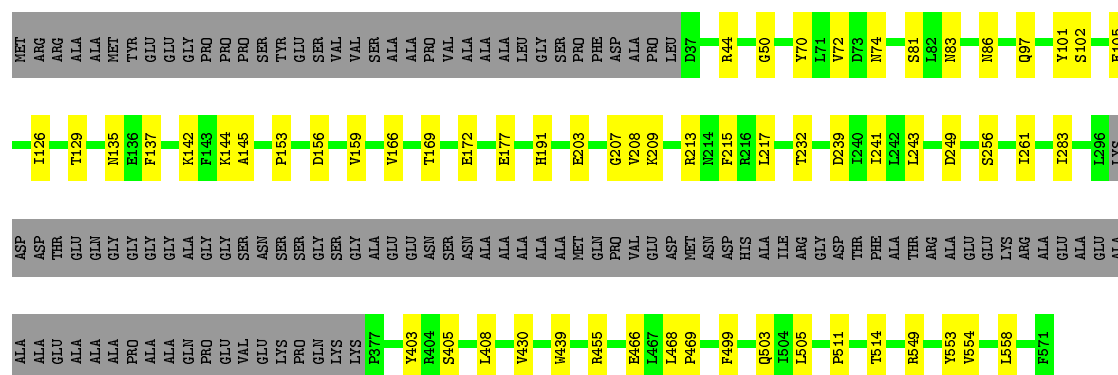


Chain L:  81% 14% .



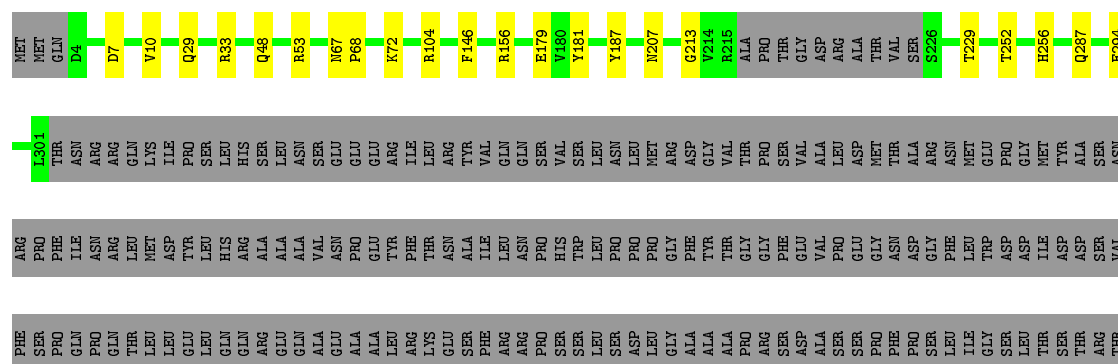
• Molecule 2: Penton protein

Chain M:  69% 11% 20%



• Molecule 3: Pre-hexon-linking protein IIIa

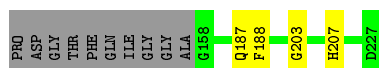
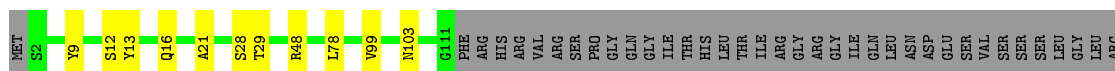
Chain N:  45% 51%



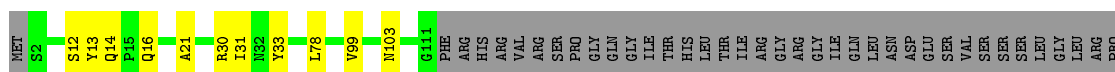




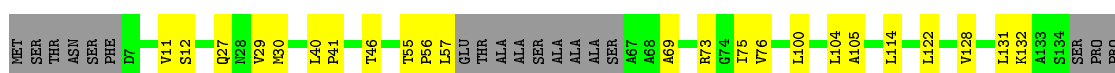
Chain O:  73% 7% 21%



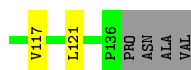
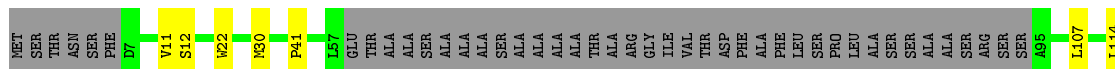
Chain P:  70% 8% 21%



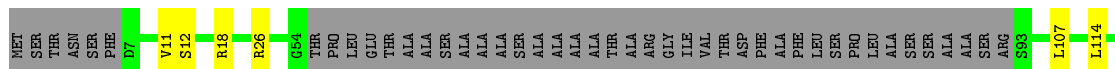
Chain Q:  69% 16% 15%



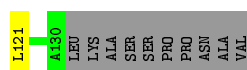
Chain R:  60% 6% 34%



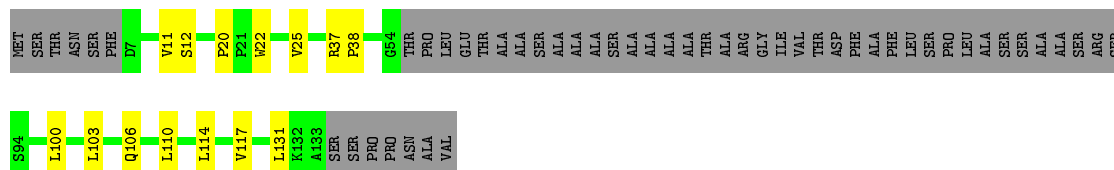
Chain S:  56% 5% 39%







- Molecule 5: Hexon-interlacing protein



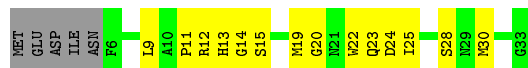
- Molecule 6: Pre-protein VI



- Molecule 6: Pre-protein VI



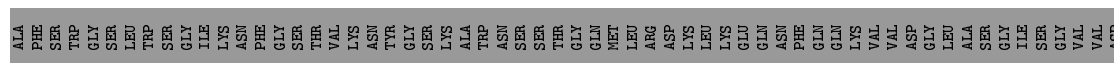
- Molecule 6: Pre-protein VI



- Molecule 7: Pre-histone-like nucleoprotein



- Molecule 8: Pre-protein VI





THR	THR	ARG	PRO	ILE	ALA	PRO	MET	ALA	THR	THR	GLY	VAL	LEU	GLY	GLN	HIS	THR	PRO	VAL	THR	THR	LEU	ASP	PRO	PRO	ALA	ALA	ASP	GLN	LYS	PRO	VAL	VAL	PRO	PRO	GLY	THR	THR	ALA	ALA	VAL	VAL	VAL	THR	THR	ARG	PRO	PRO	SER	ARG	ALA	SER	ALA	LEU	LEU	ARG	ARG	ALA	ALA	ALA	GLY	PRO	THR	SER	ARG	SER
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LEU ARG PRO VAL ALA SER GLY ASN TRP GLN SER THR LEU ASN SER ILE VAL GLY LEU GLY VAL GLN SER LEU LYS ARG ARG ARG CYS PHE



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.33	0/7481	0.52	0/10170
1	B	0.32	0/7495	0.52	0/10189
1	C	0.33	0/7498	0.52	0/10194
1	D	0.35	0/7468	0.52	0/10153
1	E	0.34	0/7521	0.53	0/10227
1	F	0.35	0/7495	0.53	0/10190
1	G	0.36	0/7488	0.54	0/10180
1	H	0.36	0/7515	0.54	0/10217
1	I	0.35	0/7495	0.53	0/10190
1	J	0.35	0/7514	0.53	0/10217
1	K	0.35	0/7494	0.53	0/10188
1	L	0.34	0/7507	0.53	0/10207
2	M	0.30	0/3734	0.51	0/5091
3	N	0.30	0/2271	0.52	0/3090
4	O	0.37	0/1422	0.52	0/1942
4	P	0.36	0/1422	0.53	0/1942
5	Q	0.27	0/884	0.55	0/1204
5	R	0.26	0/706	0.52	0/962
5	S	0.26	0/653	0.52	0/888
5	T	0.26	0/669	0.49	0/909
6	U	0.39	0/222	0.55	0/298
6	V	0.33	0/222	0.50	0/298
6	Y	0.32	0/214	0.51	0/287
7	W	0.33	0/85	0.40	0/110
8	X	0.33	0/265	0.52	0/359
All	All	0.34	0/102740	0.53	0/139702

There are no bond length outliers.

There are no bond angle outliers.

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	7286	0	6998	126	0
1	B	7299	0	7011	103	0
1	C	7302	0	7020	112	0
1	D	7273	0	6984	133	0
1	E	7325	0	7036	117	0
1	F	7300	0	7012	133	0
1	G	7293	0	7004	96	0
1	H	7319	0	7033	92	0
1	I	7300	0	7011	88	0
1	J	7318	0	7029	109	0
1	K	7299	0	7010	114	0
1	L	7311	0	7022	96	0
2	M	3642	0	3562	34	0
3	N	2236	0	2207	15	0
4	O	1383	0	1326	11	0
4	P	1383	0	1326	20	0
5	Q	874	0	890	17	0
5	R	698	0	713	7	0
5	S	647	0	652	6	0
5	T	663	0	676	13	0
6	U	216	0	196	38	0
6	V	216	0	196	44	0
6	Y	208	0	190	37	0
7	W	83	0	84	17	0
8	X	260	0	256	35	0
All	All	100134	0	96444	1256	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 6.

The worst 5 of 1256 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:30:GLN:NE2	6:Y:22:TRP:CZ3	1.83	1.43
1:D:790:ARG:HH21	8:X:137:ARG:NE	1.25	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLN:NE2	6:Y:22:TRP:HZ3	1.16	1.31
4:P:203:GLY:O	4:P:208:TYR:CE1	1.82	1.31
1:D:872:ARG:NH2	7:W:23:GLY:CA	1.94	1.30

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	898/952 (94%)	860 (96%)	38 (4%)	0	100	100
1	B	900/952 (94%)	856 (95%)	43 (5%)	1 (0%)	55	89
1	C	900/952 (94%)	859 (95%)	40 (4%)	1 (0%)	55	89
1	D	896/952 (94%)	856 (96%)	40 (4%)	0	100	100
1	E	904/952 (95%)	866 (96%)	38 (4%)	0	100	100
1	F	900/952 (94%)	865 (96%)	34 (4%)	1 (0%)	55	89
1	G	899/952 (94%)	859 (96%)	40 (4%)	0	100	100
1	H	903/952 (95%)	867 (96%)	36 (4%)	0	100	100
1	I	900/952 (94%)	865 (96%)	35 (4%)	0	100	100
1	J	903/952 (95%)	869 (96%)	34 (4%)	0	100	100
1	K	900/952 (94%)	864 (96%)	36 (4%)	0	100	100
1	L	902/952 (95%)	867 (96%)	35 (4%)	0	100	100
2	M	451/571 (79%)	426 (94%)	25 (6%)	0	100	100
3	N	284/585 (48%)	276 (97%)	8 (3%)	0	100	100
4	O	176/227 (78%)	171 (97%)	5 (3%)	0	100	100
4	P	176/227 (78%)	171 (97%)	4 (2%)	1 (1%)	28	72
5	Q	115/140 (82%)	109 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	89/140 (64%)	86 (97%)	3 (3%)	0	100	100
5	S	82/140 (59%)	79 (96%)	3 (4%)	0	100	100
5	T	84/140 (60%)	81 (96%)	3 (4%)	0	100	100
6	U	27/33 (82%)	27 (100%)	0	0	100	100
6	V	27/33 (82%)	27 (100%)	0	0	100	100
6	Y	26/33 (79%)	24 (92%)	2 (8%)	0	100	100
7	W	9/11 (82%)	9 (100%)	0	0	100	100
8	X	29/217 (13%)	28 (97%)	1 (3%)	0	100	100
All	All	12380/13921 (89%)	11867 (96%)	509 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	204	PRO
1	C	668	PRO
1	F	668	PRO
1	B	668	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	A	793/829 (96%)	793 (100%)	0	100	100
1	B	795/829 (96%)	794 (100%)	1 (0%)	94	99
1	C	796/829 (96%)	796 (100%)	0	100	100
1	D	792/829 (96%)	792 (100%)	0	100	100
1	E	798/829 (96%)	798 (100%)	0	100	100
1	F	795/829 (96%)	795 (100%)	0	100	100
1	G	794/829 (96%)	794 (100%)	0	100	100
1	H	797/829 (96%)	796 (100%)	1 (0%)	94	99

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	795/829 (96%)	795 (100%)	0	100	100
1	J	797/829 (96%)	797 (100%)	0	100	100
1	K	795/829 (96%)	795 (100%)	0	100	100
1	L	796/829 (96%)	796 (100%)	0	100	100
2	M	412/489 (84%)	412 (100%)	0	100	100
3	N	241/500 (48%)	241 (100%)	0	100	100
4	O	147/186 (79%)	147 (100%)	0	100	100
4	P	147/186 (79%)	147 (100%)	0	100	100
5	Q	97/112 (87%)	97 (100%)	0	100	100
5	R	81/112 (72%)	81 (100%)	0	100	100
5	S	75/112 (67%)	75 (100%)	0	100	100
5	T	76/112 (68%)	76 (100%)	0	100	100
6	U	22/26 (85%)	22 (100%)	0	100	100
6	V	22/26 (85%)	22 (100%)	0	100	100
6	Y	21/26 (81%)	21 (100%)	0	100	100
7	W	8/8 (100%)	8 (100%)	0	100	100
8	X	30/184 (16%)	30 (100%)	0	100	100
All	All	10922/12027 (91%)	10920 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
1	B	896	ASN
1	H	414	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	890	GLN
1	H	167	HIS
2	M	118	HIS
1	G	14	HIS
1	G	559	HIS



### 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.