



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 10:47 AM EST

PDB ID : 7RD1
EMDB ID : EMD-24408
Title : The Capsid Structure of the ChAdOx1 viral vector/chimpanzee adenovirus Y25
Authors : Baker, A.T.; Boyd, R.J.; Sarkar, D.; Vermaas, J.V.; Williams, D.; Singharoy, A.
Deposited on : 2021-07-08
Resolution : 3.07 Å(reported)

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 ⓘ 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:

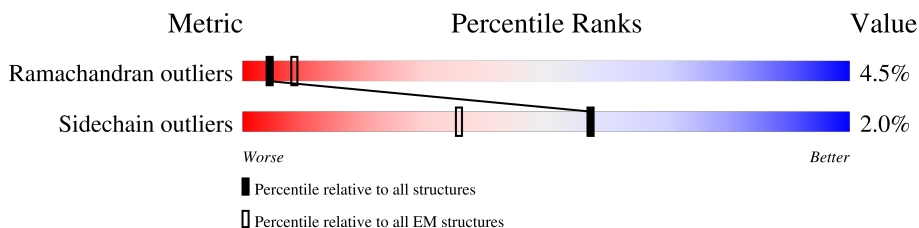
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 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 3.07 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.




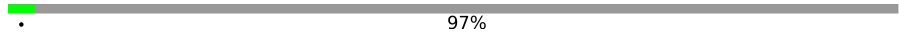
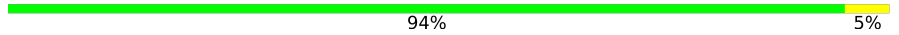

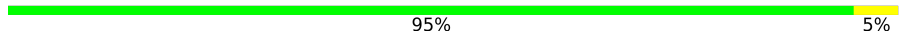
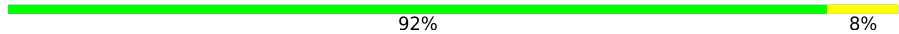
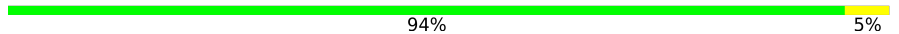
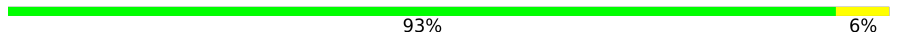
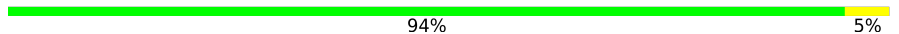
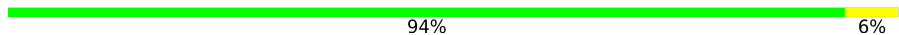
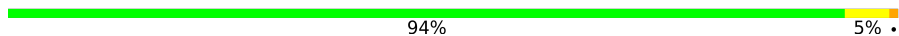
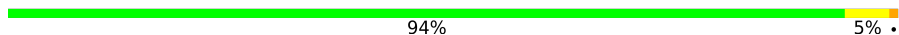
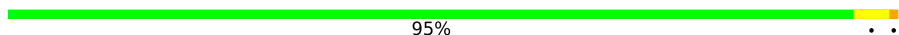
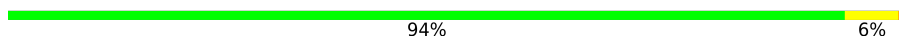


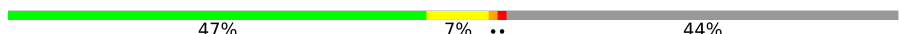





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	243	97%
1	1	243	93%
1	2	243	91%
1	3	243	89%
1	4	243	91%
1	8	243	90%
1	U	243	95%
1	V	243	92%
1	W	243	90%
1	X	243	89%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Y	243	 10% . 89%
1	Z	243	 . 97%
2	A	942	 94% 5%
2	B	942	 90% 9% .
2	C	942	 95% 5%
2	D	942	 92% 8%
2	E	942	 94% 5%
2	F	942	 93% 6%
2	G	942	 94% 5%
2	H	942	 94% 6%
2	I	942	 94% 5% .
2	J	942	 94% 5% .
2	K	942	 95% . .
2	L	942	 94% 6% .
3	M	532	 78% . 18%
4	N	142	 52% 9% . 37%
4	O	142	 47% 7% . . 44%
4	P	142	 58% 8% . 32%
4	Q	142	 47% . . 49%
5	R	589	 18% . 81%
6	S	227	 70% 7% . 23%
6	T	227	 69% 8% . 22%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 197782 atoms, of which 96589 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 Pre-protein VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	0	7	106	35	51	8	12	0	0
1	U	11	171	55	83	17	16	0	0
1	1	17	245	77	118	23	27	0	0
1	V	20	286	96	136	22	31	1	0
1	2	21	323	106	156	31	29	1	0
1	W	24	361	118	174	34	34	1	0
1	3	26	386	125	186	36	38	1	0
1	X	26	386	125	186	36	38	1	0
1	4	22	335	110	160	32	32	1	0
1	Y	26	386	125	186	36	38	1	0
1	8	24	363	118	177	34	33	1	0
1	Z	7	106	35	51	8	12	0	0

- Molecule 2 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			
2	A	942	14601	4743	7121	1259	1442	36	0	0
2	B	942	14601	4743	7121	1259	1442	36	0	0
2	C	942	14601	4743	7121	1259	1442	36	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	E	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	F	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	G	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	H	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	I	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	J	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	K	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		
2	L	942	Total	C	H	N	O	S	0	0
			14601	4743	7121	1259	1442	36		

- Molecule 3 is a protein called Penton protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	435	Total	C	H	N	O	S	0	0
			6923	2219	3423	596	672	13		

- Molecule 4 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	N	89	Total	C	H	N	O	S	0	0
			1328	412	664	114	135	3		
4	O	79	Total	C	H	N	O	S	0	0
			1187	368	595	102	119	3		
4	P	96	Total	C	H	N	O	S	0	0
			1435	443	720	125	144	3		
4	Q	73	Total	C	H	N	O	S	0	0
			1108	342	560	99	104	3		

- Molecule 5 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	114	Total	C	H	N	O	S	0	0
			1767	539	885	167	173	3		

- Molecule 6 is a protein called Pre-hexon-linking protein VIII.

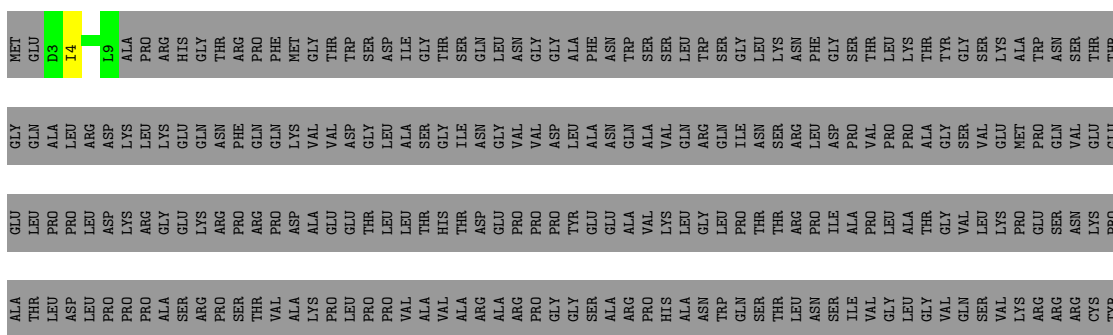
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	S	175	Total	C	H	N	O	S	0	0
			2673	861	1308	234	265	5		
6	T	177	Total	C	H	N	O	S	0	0
			2695	867	1318	236	269	5		

3 Residue-property plots

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.

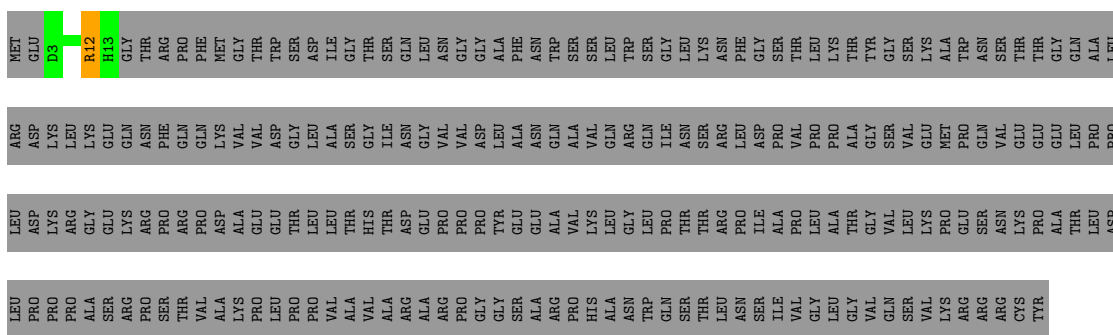
- Molecule 1: Pre-protein VI

Chain 0:  97%



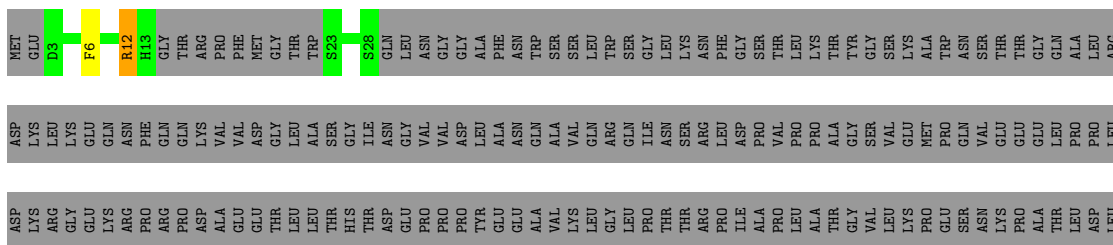
- Molecule 1: Pre-protein VI

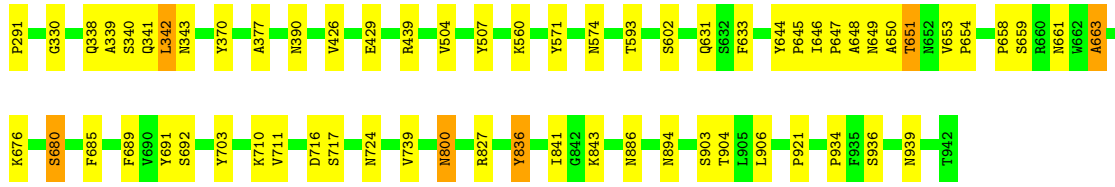
Chain U:  95%



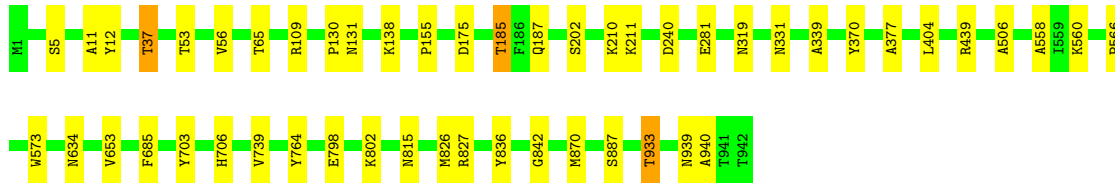
- Molecule 1: Pre-protein VI

Chain 1:  93%

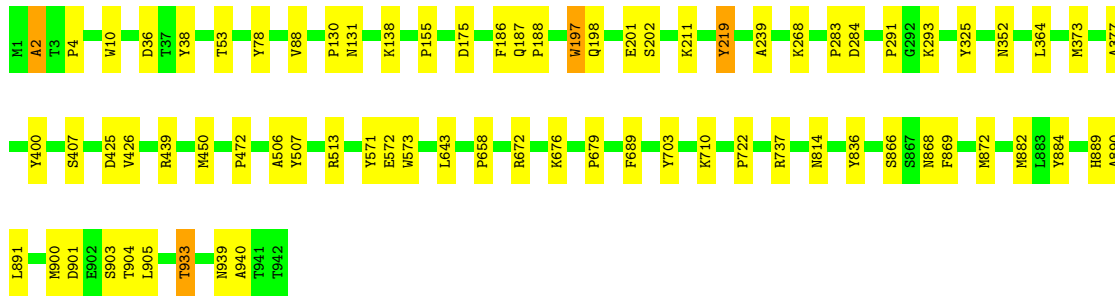




• Molecule 2: Hexon protein



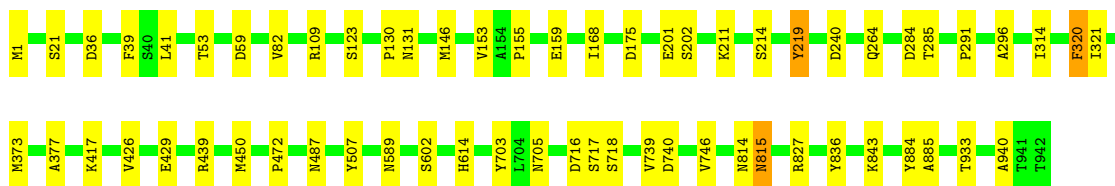
• Molecule 2: Hexon protein



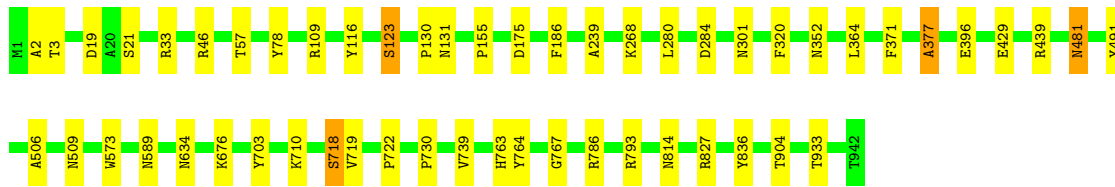
• Molecule 2: Hexon protein



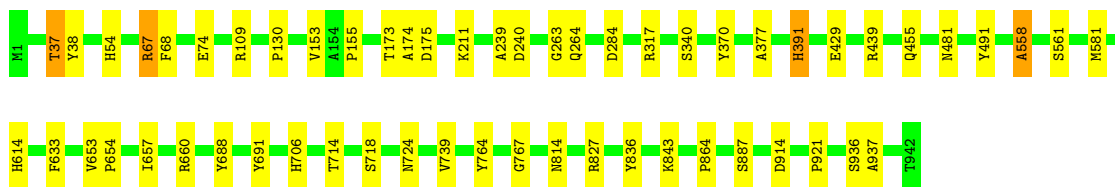
• Molecule 2: Hexon protein



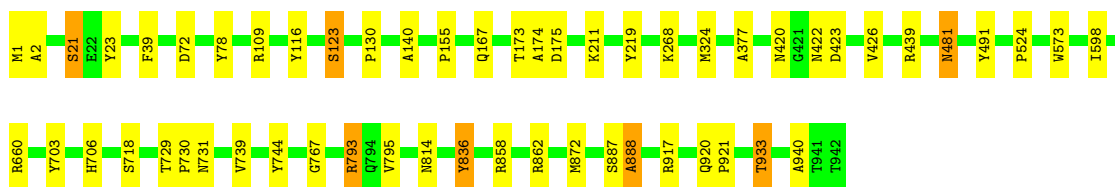
• Molecule 2: Hexon protein



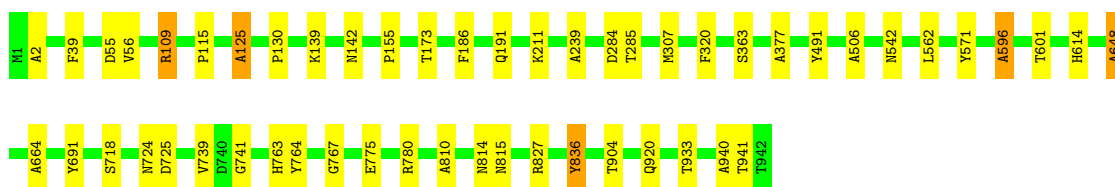
• Molecule 2: Hexon protein



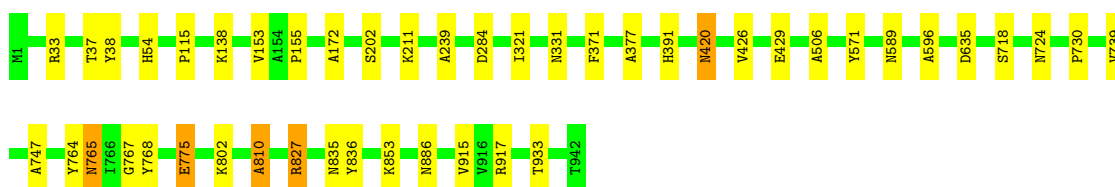
• Molecule 2: Hexon protein

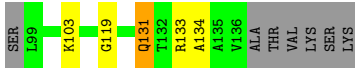


• Molecule 2: Hexon protein

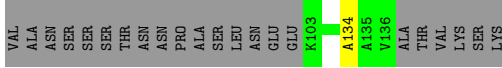
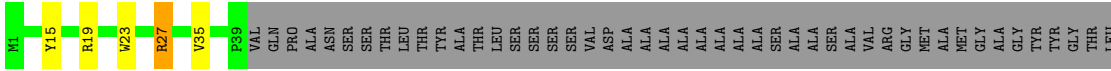


• Molecule 2: Hexon protein

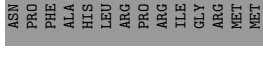
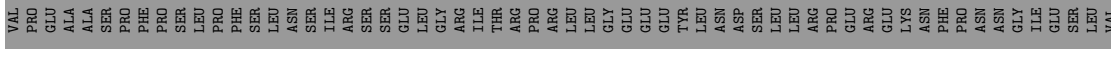
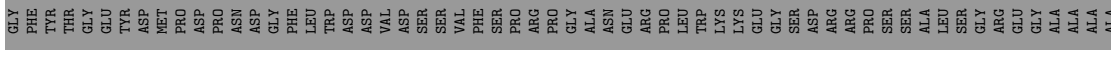
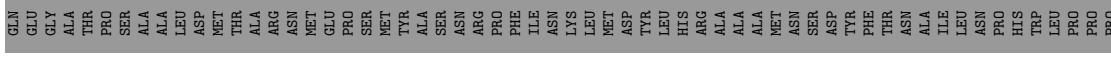
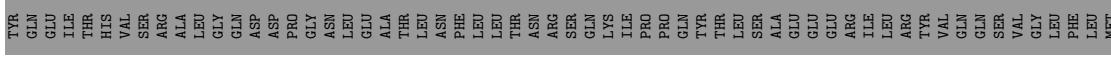
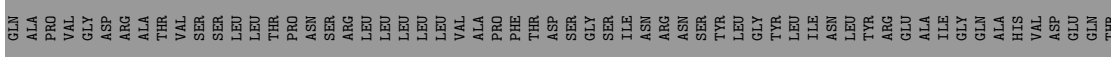
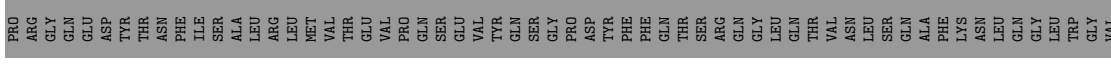
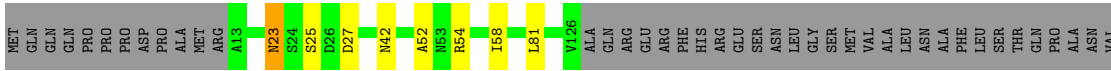




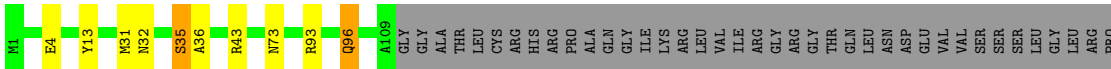
• Molecule 4: Hexon-interlacing protein



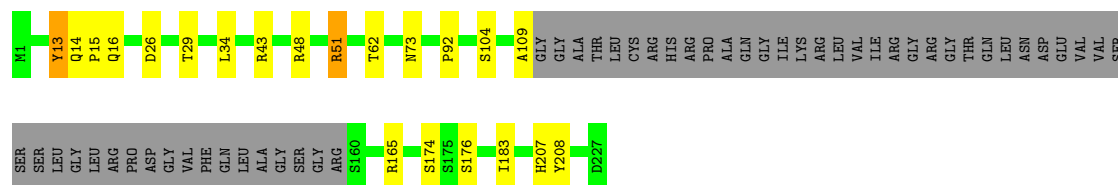
• Molecule 5: Pre-hexon-linking protein IIIa



• Molecule 6: Pre-hexon-linking protein VIII



• Molecule 6: Pre-hexon-linking protein VIII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5748	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.1802	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
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	0	0.95	0/55	1.06	0/73
1	1	0.81	0/128	1.22	1/171 (0.6%)
1	2	0.88	0/173	1.21	1/234 (0.4%)
1	3	0.79	0/206	1.30	1/279 (0.4%)
1	4	0.76	0/181	1.24	1/245 (0.4%)
1	8	0.91	0/192	1.18	0/260
1	U	0.85	0/90	1.27	1/121 (0.8%)
1	V	0.84	0/153	1.25	0/206
1	W	0.79	0/193	1.22	1/261 (0.4%)
1	X	0.93	0/206	1.17	1/279 (0.4%)
1	Y	0.75	0/206	1.26	1/279 (0.4%)
1	Z	0.91	0/55	0.79	0/73
2	A	0.90	0/7683	1.07	8/10460 (0.1%)
2	B	0.91	0/7683	1.11	10/10460 (0.1%)
2	C	0.90	0/7683	1.06	4/10460 (0.0%)
2	D	0.89	0/7683	1.11	8/10460 (0.1%)
2	E	0.90	0/7683	1.07	8/10460 (0.1%)
2	F	0.91	0/7683	1.07	4/10460 (0.0%)
2	G	0.91	0/7683	1.08	9/10460 (0.1%)
2	H	0.91	0/7683	1.07	4/10460 (0.0%)
2	I	0.90	0/7683	1.07	9/10460 (0.1%)
2	J	0.90	0/7683	1.08	13/10460 (0.1%)
2	K	0.91	0/7683	1.07	10/10460 (0.1%)
2	L	0.91	0/7683	1.08	9/10460 (0.1%)
3	M	0.91	0/3580	1.05	3/4872 (0.1%)
4	N	0.92	0/672	1.19	5/909 (0.6%)
4	O	0.87	0/597	1.18	4/803 (0.5%)
4	P	0.92	0/723	1.11	3/979 (0.3%)
4	Q	0.90	0/554	1.04	0/746
5	R	0.94	0/892	0.98	0/1213
6	S	0.87	0/1403	1.14	8/1917 (0.4%)
6	T	0.89	0/1415	1.14	5/1933 (0.3%)
All	All	0.90	0/103870	1.08	132/141373 (0.1%)

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
2	A	0	2
2	B	0	5
2	D	0	6
2	E	0	4
2	F	0	2
2	G	0	1
2	H	0	3
2	I	0	6
2	J	0	2
2	K	0	1
2	L	0	5
3	M	0	1
4	O	0	1
4	Q	0	1
5	R	0	1
6	T	0	2
All	All	0	43

There are no bond length outliers.

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	571	TYR	CB-CG-CD2	-7.83	116.30	121.00
2	L	116	TYR	CB-CG-CD2	-7.82	116.31	121.00
2	E	571	TYR	CB-CG-CD2	-7.53	116.48	121.00
1	U	12	ARG	NE-CZ-NH1	7.51	124.06	120.30
2	L	116	TYR	CB-CG-CD1	7.36	125.42	121.00

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	109	ARG	Sidechain
2	A	207	ARG	Sidechain
2	B	219	TYR	Sidechain
2	B	507	TYR	Sidechain
2	B	571	TYR	Sidechain

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	0	55	51	50	0	0
1	1	127	118	116	0	0
1	2	167	156	155	0	0
1	3	200	186	185	0	0
1	4	175	160	159	0	0
1	8	186	177	176	0	0
1	U	88	83	82	0	0
1	V	150	136	134	0	0
1	W	187	174	173	0	0
1	X	200	186	185	0	0
1	Y	200	186	185	0	0
1	Z	55	51	50	0	0
2	A	7480	7121	7121	0	0
2	B	7480	7121	7121	0	0
2	C	7480	7121	7121	0	0
2	D	7480	7121	7121	0	0
2	E	7480	7121	7121	0	0
2	F	7480	7121	7121	0	0
2	G	7480	7121	7121	0	0
2	H	7480	7121	7121	0	0
2	I	7480	7121	7121	0	0
2	J	7480	7121	7121	0	0
2	K	7480	7121	7121	0	0
2	L	7480	7121	7121	0	0
3	M	3500	3423	3420	0	0
4	N	664	664	663	0	0
4	O	592	595	593	0	0
4	P	715	720	719	0	0
4	Q	548	560	559	0	0
5	R	882	885	884	0	0
6	S	1365	1308	1307	0	0
6	T	1377	1318	1317	0	0
All	All	101193	96589	96564	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	0	5/243 (2%)	4 (80%)	0	1 (20%)	0	0
1	1	13/243 (5%)	9 (69%)	3 (23%)	1 (8%)	1	5
1	2	19/243 (8%)	15 (79%)	2 (10%)	2 (10%)	0	2
1	3	24/243 (10%)	16 (67%)	7 (29%)	1 (4%)	3	15
1	4	20/243 (8%)	14 (70%)	3 (15%)	3 (15%)	0	0
1	8	22/243 (9%)	13 (59%)	5 (23%)	4 (18%)	0	0
1	U	9/243 (4%)	7 (78%)	2 (22%)	0	100	100
1	V	16/243 (7%)	13 (81%)	2 (12%)	1 (6%)	1	7
1	W	22/243 (9%)	12 (54%)	8 (36%)	2 (9%)	1	3
1	X	24/243 (10%)	16 (67%)	3 (12%)	5 (21%)	0	0
1	Y	24/243 (10%)	18 (75%)	5 (21%)	1 (4%)	3	15
1	Z	5/243 (2%)	5 (100%)	0	0	100	100
2	A	940/942 (100%)	822 (87%)	80 (8%)	38 (4%)	3	15
2	B	940/942 (100%)	771 (82%)	99 (10%)	70 (7%)	1	5
2	C	940/942 (100%)	824 (88%)	85 (9%)	31 (3%)	4	19
2	D	940/942 (100%)	819 (87%)	75 (8%)	46 (5%)	2	12
2	E	940/942 (100%)	826 (88%)	79 (8%)	35 (4%)	3	17
2	F	940/942 (100%)	834 (89%)	67 (7%)	39 (4%)	3	15
2	G	940/942 (100%)	824 (88%)	82 (9%)	34 (4%)	3	18
2	H	940/942 (100%)	811 (86%)	89 (10%)	40 (4%)	2	14
2	I	940/942 (100%)	827 (88%)	79 (8%)	34 (4%)	3	18
2	J	940/942 (100%)	829 (88%)	75 (8%)	36 (4%)	3	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	940/942 (100%)	816 (87%)	95 (10%)	29 (3%)	4	21
2	L	940/942 (100%)	827 (88%)	75 (8%)	38 (4%)	3	15
3	M	429/532 (81%)	390 (91%)	28 (6%)	11 (3%)	5	24
4	N	85/142 (60%)	65 (76%)	9 (11%)	11 (13%)	0	1
4	O	73/142 (51%)	54 (74%)	9 (12%)	10 (14%)	0	1
4	P	92/142 (65%)	69 (75%)	11 (12%)	12 (13%)	0	1
4	Q	69/142 (49%)	57 (83%)	9 (13%)	3 (4%)	2	14
5	R	112/589 (19%)	94 (84%)	13 (12%)	5 (4%)	2	13
6	S	171/227 (75%)	141 (82%)	20 (12%)	10 (6%)	1	9
6	T	173/227 (76%)	143 (83%)	18 (10%)	12 (7%)	1	6
All	All	12687/16363 (78%)	10985 (87%)	1137 (9%)	565 (4%)	4	13

5 of 565 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	6	PHE
1	W	10	ALA
1	8	25	ILE
2	A	21	SER
2	A	76	ASN

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	0	7/203 (3%)	7 (100%)	0	100	100
1	1	15/203 (7%)	14 (93%)	1 (7%)	16	45
1	2	18/203 (9%)	17 (94%)	1 (6%)	21	51
1	3	22/203 (11%)	19 (86%)	3 (14%)	3	15
1	4	19/203 (9%)	18 (95%)	1 (5%)	22	53
1	8	20/203 (10%)	19 (95%)	1 (5%)	24	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	10/203 (5%)	9 (90%)	1 (10%)	7	27
1	V	17/203 (8%)	14 (82%)	3 (18%)	2	8
1	W	20/203 (10%)	19 (95%)	1 (5%)	24	55
1	X	22/203 (11%)	22 (100%)	0	100	100
1	Y	22/203 (11%)	22 (100%)	0	100	100
1	Z	7/203 (3%)	7 (100%)	0	100	100
2	A	810/810 (100%)	798 (98%)	12 (2%)	65	84
2	B	810/810 (100%)	787 (97%)	23 (3%)	43	71
2	C	810/810 (100%)	791 (98%)	19 (2%)	50	75
2	D	810/810 (100%)	790 (98%)	20 (2%)	47	74
2	E	810/810 (100%)	795 (98%)	15 (2%)	57	79
2	F	810/810 (100%)	790 (98%)	20 (2%)	47	74
2	G	810/810 (100%)	794 (98%)	16 (2%)	55	78
2	H	810/810 (100%)	796 (98%)	14 (2%)	60	82
2	I	810/810 (100%)	795 (98%)	15 (2%)	57	79
2	J	810/810 (100%)	800 (99%)	10 (1%)	71	87
2	K	810/810 (100%)	797 (98%)	13 (2%)	62	83
2	L	810/810 (100%)	798 (98%)	12 (2%)	65	84
3	M	393/461 (85%)	389 (99%)	4 (1%)	76	89
4	N	74/105 (70%)	72 (97%)	2 (3%)	44	72
4	O	64/105 (61%)	63 (98%)	1 (2%)	62	83
4	P	79/105 (75%)	76 (96%)	3 (4%)	33	64
4	Q	58/105 (55%)	55 (95%)	3 (5%)	23	54
5	R	96/502 (19%)	93 (97%)	3 (3%)	40	69
6	S	149/189 (79%)	146 (98%)	3 (2%)	55	78
6	T	151/189 (80%)	146 (97%)	5 (3%)	38	68
All	All	10983/13917 (79%)	10758 (98%)	225 (2%)	57	78

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	487	ASN
6	T	43	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	391	HIS
6	S	179	ARG
2	L	843	LYS

Sometimes 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 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-24408. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

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

9 Map-model fit

This section was not generated.