



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 01:16 AM EST

PDB ID : 6OJ4
EMDB ID : EMD-20087
Title : In situ structure of rotavirus VP1 RNA-dependent RNA polymerase (DLP)
Authors : Jenni, S.; Salgado, E.N.; Herrmann, T.; Li, Z.; Grant, T.; Grigorieff, N.;
Trapani, S.; Estrozi, L.F.; Harrison, S.C.
Deposited on : 2019-04-10
Resolution : 3.30 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)	:	2.31.2

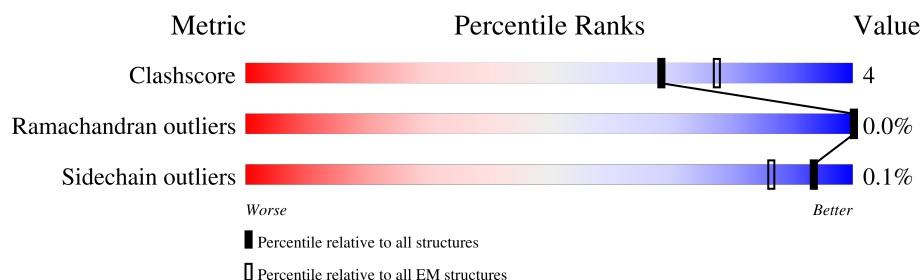
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	887	78% 10% 12%
1	B	887	79% 9% 12%
1	C	887	78% 9% 12%
1	D	887	82% 11% 7%
1	E	887	81% 9% 10%
1	F	887	81% 9% 10%
1	G	887	82% 9% 10%
1	H	887	81% 10% 10%
1	I	887	82% 8% 10%

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Mol	Chain	Length	Quality of chain
1	J	887	 82% 10% 8%
2	P	1088	 87% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 148556 atoms, of which 74461 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	781	Total	C	H	N	O	S	0	0
			12787	4052	6408	1101	1190	36		
1	B	781	Total	C	H	N	O	S	0	0
			12787	4052	6408	1101	1190	36		
1	C	780	Total	C	H	N	O	S	0	0
			12772	4047	6400	1100	1189	36		
1	D	827	Total	C	H	N	O	S	0	0
			13574	4297	6809	1163	1269	36		
1	E	795	Total	C	H	N	O	S	0	0
			13028	4132	6529	1118	1213	36		
1	F	802	Total	C	H	N	O	S	0	0
			13151	4170	6588	1130	1227	36		
1	G	802	Total	C	H	N	O	S	0	0
			13151	4170	6588	1130	1227	36		
1	H	802	Total	C	H	N	O	S	0	0
			13151	4170	6588	1130	1227	36		
1	I	800	Total	C	H	N	O	S	0	0
			13114	4159	6569	1127	1223	36		
1	J	816	Total	C	H	N	O	S	0	0
			13391	4242	6713	1149	1251	36		

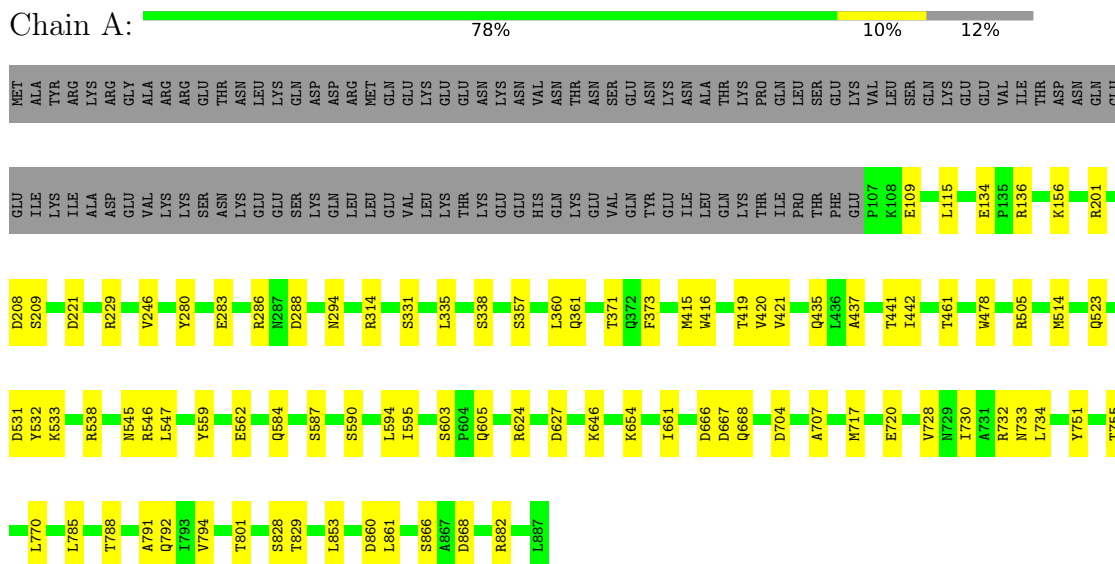
- Molecule 2 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	1086	Total	C	H	N	O	S	0	0
			17650	5633	8861	1455	1662	39		

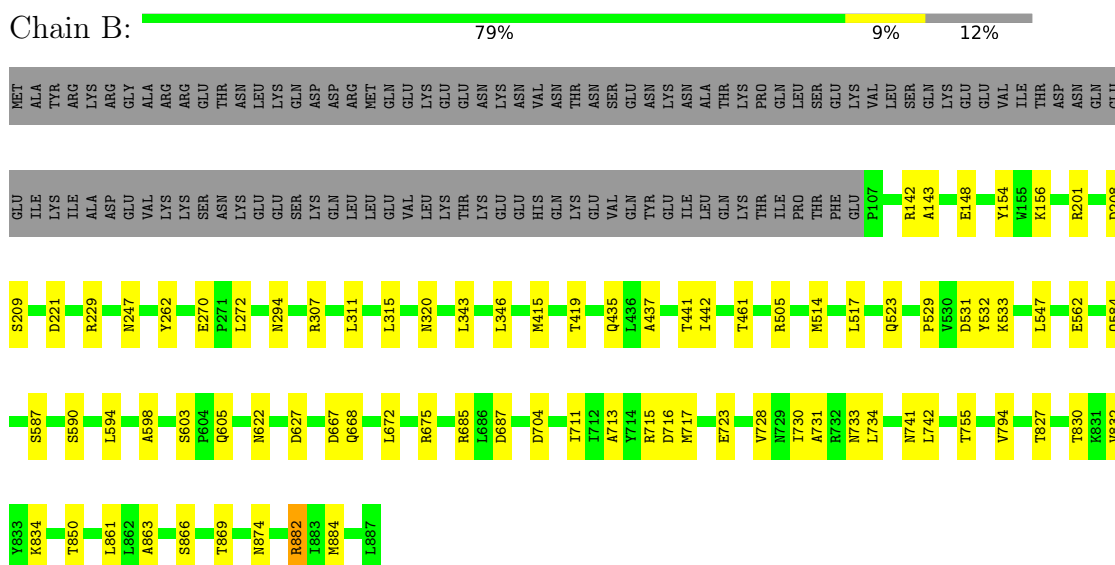
3 Residue-property plots

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: Inner capsid protein VP2

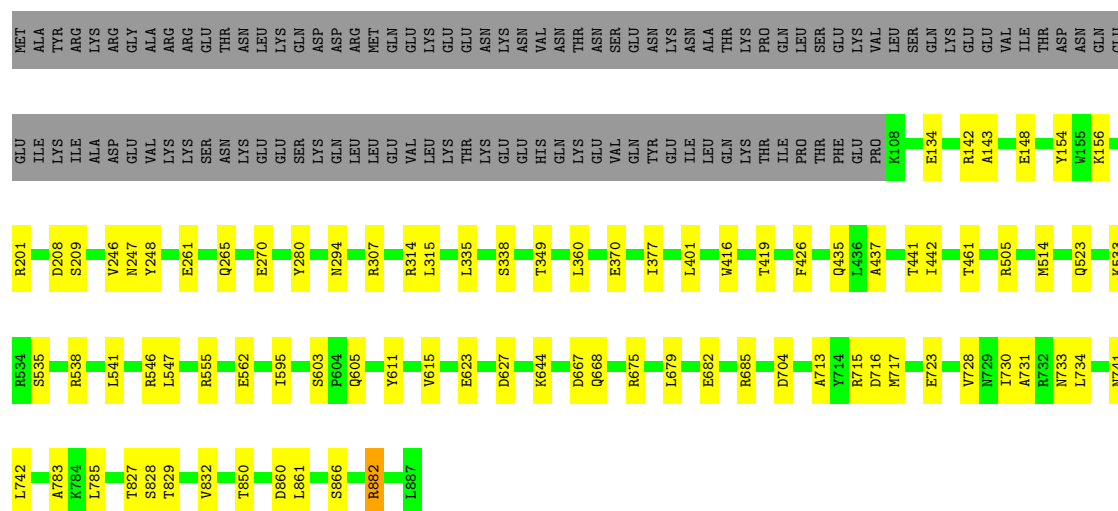


- Molecule 1: Inner capsid protein VP2



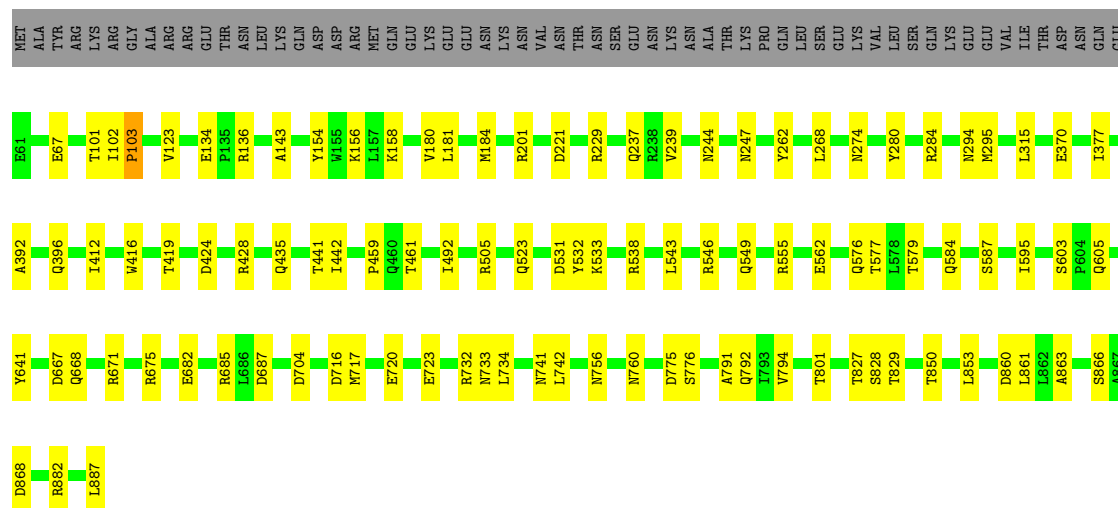
- Molecule 1: Inner capsid protein VP2

78% 9% 12%



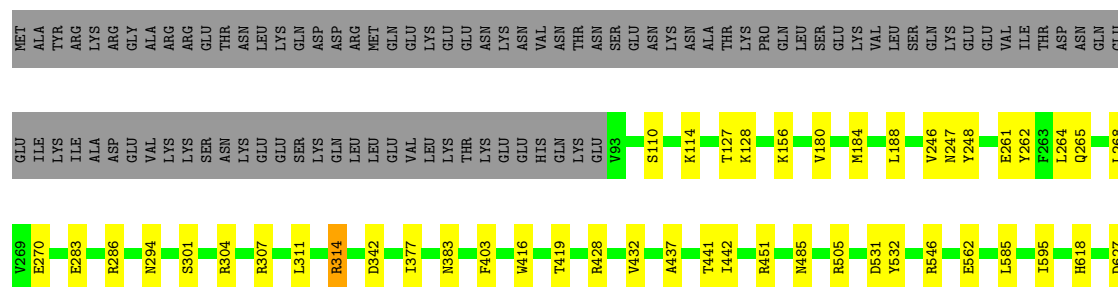
- Molecule 1: Inner capsid protein VP2

82% 11% 7%



- Molecule 1: Inner capsid protein VP2

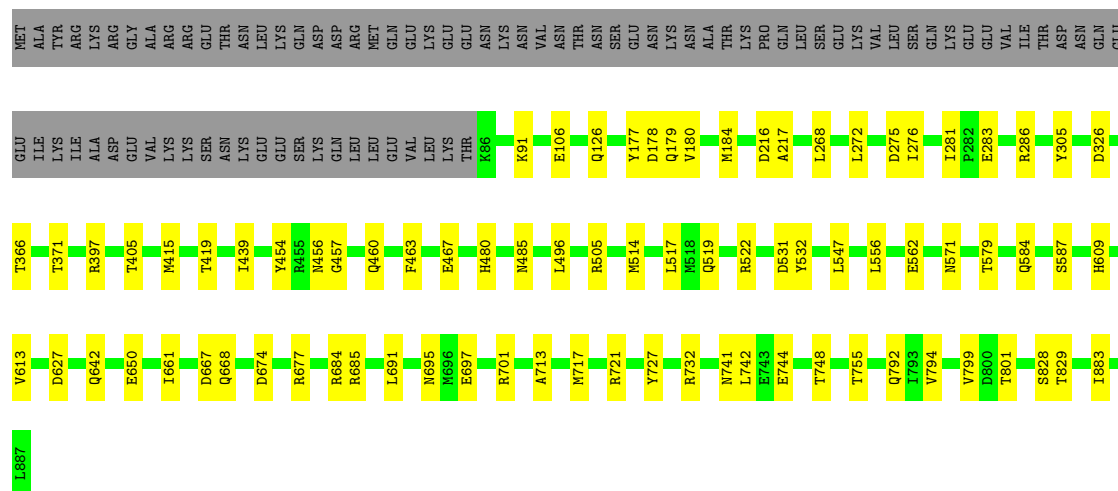
81% 9% 10%





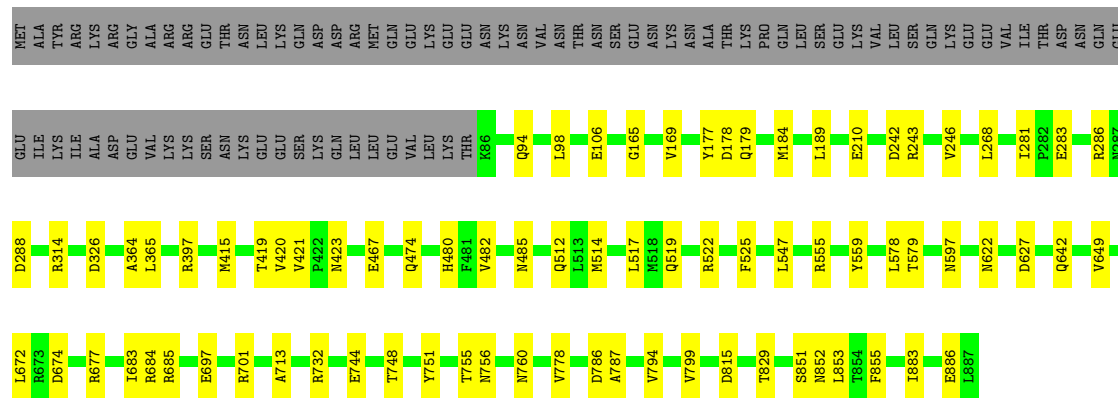
• Molecule 1: Inner capsid protein VP2

Chain F: 81% 9% 10%



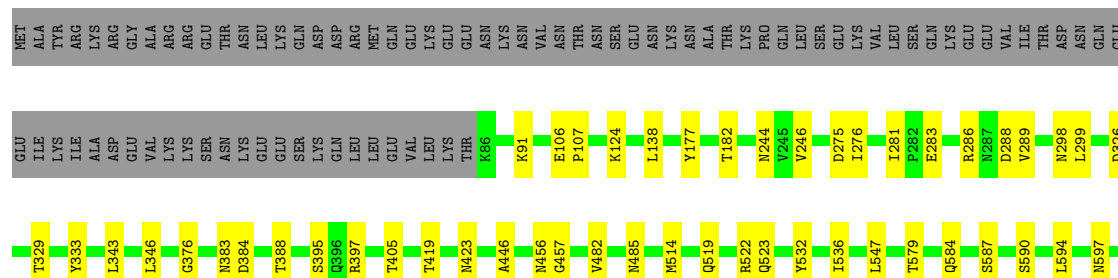
• Molecule 1: Inner capsid protein VP2

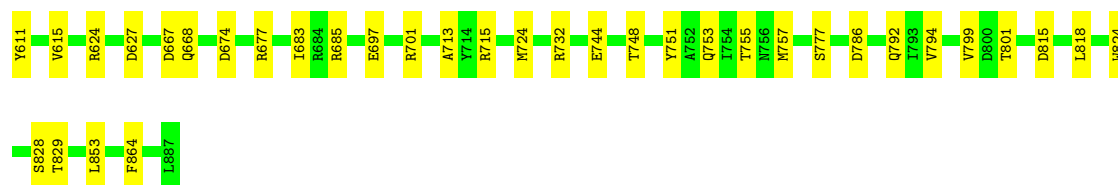
Chain G: 82% 9% 10%



• Molecule 1: Inner capsid protein VP2

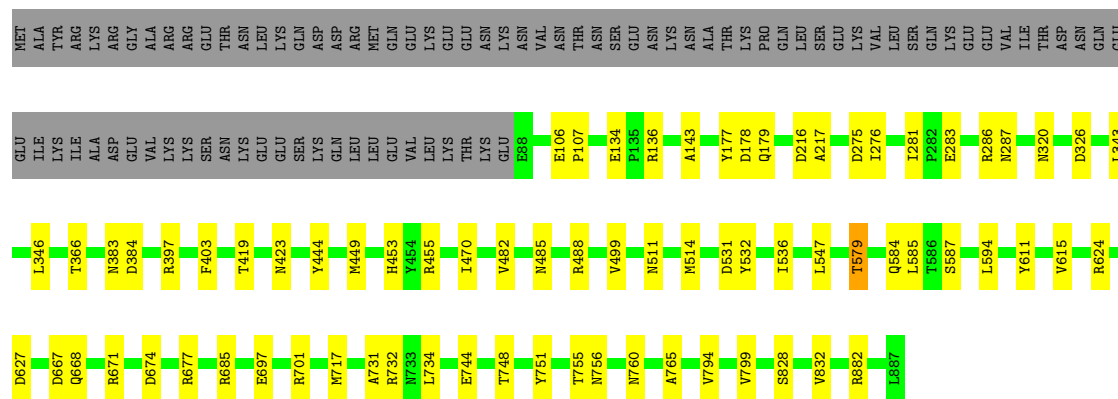
Chain H: 81% 10% 10%





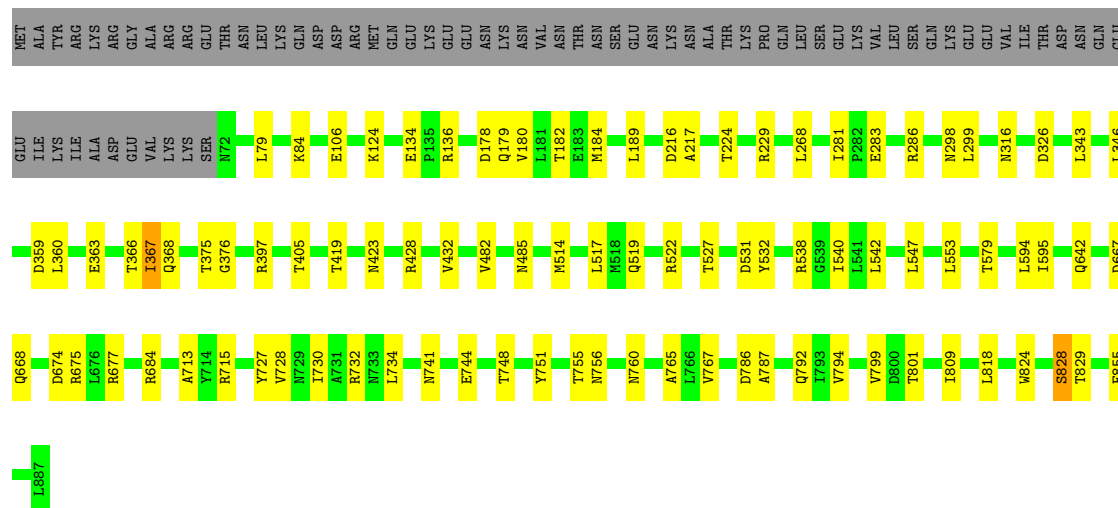
• Molecule 1: Inner capsid protein VP2

Chain I: 82% 8% 10%



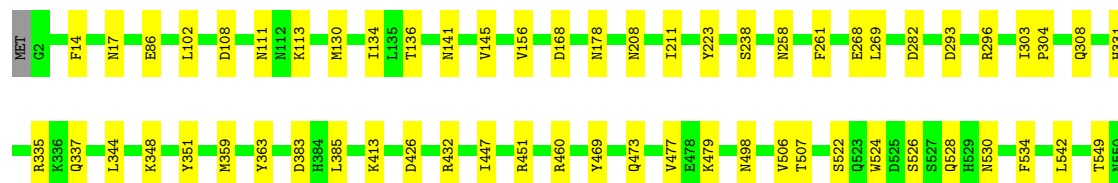
• Molecule 1: Inner capsid protein VP2

Chain J: 82% 10% 8%



• Molecule 2: RNA-directed RNA polymerase

Chain P: 87% 13%



D551	S792	Y992	D552	G797	L996	Y561	E801	S816	L820	K823	V827	A843	P844	E848	Q853	T873	I874	N875	R879	D880	I894	N906	V907	Q908	Q912	R917	E922	S926	K941	P942	S943	I944	Y948	I951	E955	K979	I980	Y981	K985	D779	Q785																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
T564	Y561	L996	S998	Y992	Y1001	Y564	N1000	S816	Y1004	V1029	E1040	N1043	M1063	K1069	M1070	S1075	Q1087	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50176	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 ($e^-/\text{\AA}^2$)	64	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	A	0.52	0/6495	0.64	0/8810
1	B	0.52	0/6495	0.63	1/8810 (0.0%)
1	C	0.52	0/6487	0.63	1/8799 (0.0%)
1	D	0.52	0/6885	0.63	1/9332 (0.0%)
1	E	0.52	0/6618	0.64	0/8979
1	F	0.53	0/6683	0.61	0/9064
1	G	0.52	0/6683	0.62	0/9064
1	H	0.53	0/6683	0.61	0/9064
1	I	0.52	0/6665	0.62	0/9041
1	J	0.52	0/6798	0.61	0/9217
2	P	0.44	0/8963	0.59	0/12120
All	All	0.51	0/75455	0.62	3/102300 (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	B	0	1
1	C	0	1
1	D	0	2
1	F	0	1
1	G	0	2
1	H	0	1
1	I	0	3
1	J	0	3
2	P	0	1
All	All	0	15

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	882	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	882	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	671	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	143	ALA	Peptide
1	C	143	ALA	Peptide
1	D	102	ILE	Peptide
1	D	143	ALA	Peptide
1	F	106	GLU	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	6379	6408	6408	53	0
1	B	6379	6408	6408	48	0
1	C	6372	6400	6400	50	0
1	D	6765	6809	6809	56	0
1	E	6499	6529	6529	47	0
1	F	6563	6588	6588	46	0
1	G	6563	6588	6588	45	0
1	H	6563	6588	6588	51	0
1	I	6545	6569	6569	43	0
1	J	6678	6713	6713	55	0
2	P	8789	8861	8861	84	0
All	All	74095	74461	74461	558	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 4.

The worst 5 of 558 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:P:874:ILE:HD11	2:P:996:LEU:HD13	1.62	0.81
1:A:294:ASN:OD1	1:A:866:SER:OG	2.01	0.78
1:B:201:ARG:O	1:F:642:GLN:NE2	2.17	0.77
1:E:294:ASN:OD1	1:E:866:SER:OG	2.02	0.77
1:J:124:LYS:NZ	1:J:182:THR:O	2.17	0.77

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	779/887 (88%)	713 (92%)	66 (8%)	0	100	100
1	B	779/887 (88%)	713 (92%)	66 (8%)	0	100	100
1	C	778/887 (88%)	705 (91%)	73 (9%)	0	100	100
1	D	825/887 (93%)	751 (91%)	73 (9%)	1 (0%)	51	81
1	E	793/887 (89%)	724 (91%)	69 (9%)	0	100	100
1	F	800/887 (90%)	713 (89%)	87 (11%)	0	100	100
1	G	800/887 (90%)	723 (90%)	77 (10%)	0	100	100
1	H	800/887 (90%)	716 (90%)	83 (10%)	1 (0%)	51	81
1	I	798/887 (90%)	725 (91%)	72 (9%)	1 (0%)	51	81
1	J	814/887 (92%)	736 (90%)	78 (10%)	0	100	100
2	P	1084/1088 (100%)	986 (91%)	97 (9%)	1 (0%)	51	81
All	All	9050/9958 (91%)	8205 (91%)	841 (9%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	942	PRO
1	H	107	PRO

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Mol	Chain	Res	Type
1	D	103	PRO
1	I	107	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	717/818 (88%)	716 (100%)	1 (0%)	93	97
1	B	717/818 (88%)	716 (100%)	1 (0%)	93	97
1	C	716/818 (88%)	716 (100%)	0	100	100
1	D	762/818 (93%)	762 (100%)	0	100	100
1	E	731/818 (89%)	730 (100%)	1 (0%)	93	97
1	F	738/818 (90%)	737 (100%)	1 (0%)	93	97
1	G	738/818 (90%)	737 (100%)	1 (0%)	93	97
1	H	738/818 (90%)	737 (100%)	1 (0%)	93	97
1	I	736/818 (90%)	735 (100%)	1 (0%)	93	97
1	J	752/818 (92%)	751 (100%)	1 (0%)	93	97
2	P	986/989 (100%)	985 (100%)	1 (0%)	93	97
All	All	8331/9169 (91%)	8322 (100%)	9 (0%)	93	97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	732	ARG
2	P	130	MET
1	F	732	ARG
1	G	732	ARG
1	H	732	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	792	GLN
2	P	1044	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 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-20087. 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.