



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:08 PM BST

PDB ID : 4USN
EMDB ID: : EMD-2706
Title : The structure of the immature HIV-1 capsid in intact virus particles at sub-nm resolution
Authors : Schur, F.K.M.; Hagen, W.J.H.; Rumlova, M.; Ruml, T.; Mueller, B.; Kraeuslich, H.-G.; Briggs, J.A.G.
Deposited on : 2014-07-11
Resolution : 8.80 Å(reported)
Based on PDB ID : 1L6N,3DS2

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

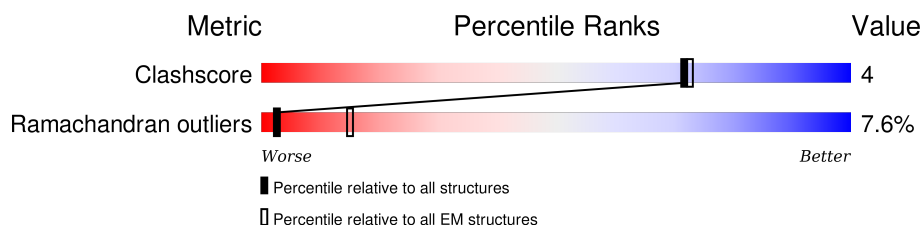
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 8.80 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

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	210	 75% 22% .
1	B	210	 81% 18% .
1	C	210	 86% 13% .
1	D	210	 76% 23% .
1	E	210	 78% 21% .
1	F	210	 84% 14% .
1	G	210	 85% 14%
1	H	210	 79% 19% .
1	I	210	 85% 14% .
1	J	210	 82% 14% .
1	K	210	 80% 18% .

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Mol	Chain	Length	Quality of chain
1	L	210	<div><div></div><div>85%</div><div>12%</div><div></div></div>
1	M	210	<div><div></div><div>81%</div><div>17%</div><div></div></div>
1	N	210	<div><div></div><div>89%</div><div>9%</div><div></div></div>
1	O	210	<div><div></div><div>88%</div><div>10%</div><div></div></div>
1	P	210	<div><div></div><div>84%</div><div>13%</div><div></div></div>
1	Q	210	<div><div></div><div>84%</div><div>15%</div><div></div></div>
1	R	210	<div><div></div><div>82%</div><div>15%</div><div></div></div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 22662 atoms, of which 7542 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 P24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	B	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	C	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	D	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	E	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	F	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	G	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	H	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	I	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	J	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	K	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	L	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	M	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	N	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	O	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	P	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		
1	Q	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	210	Total	C	H	N	O	0	0
			1259	420	419	210	210		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	GLU	ASP	CONFLICT	UNP Q9IVM8
A	301	ALA	TYR	CONFLICT	UNP Q9IVM8
A	340	GLY	ALA	CONFLICT	UNP Q9IVM8
B	207	GLU	ASP	CONFLICT	UNP Q9IVM8
B	301	ALA	TYR	CONFLICT	UNP Q9IVM8
B	340	GLY	ALA	CONFLICT	UNP Q9IVM8
C	207	GLU	ASP	CONFLICT	UNP Q9IVM8
C	301	ALA	TYR	CONFLICT	UNP Q9IVM8
C	340	GLY	ALA	CONFLICT	UNP Q9IVM8
D	207	GLU	ASP	CONFLICT	UNP Q9IVM8
D	301	ALA	TYR	CONFLICT	UNP Q9IVM8
D	340	GLY	ALA	CONFLICT	UNP Q9IVM8
E	207	GLU	ASP	CONFLICT	UNP Q9IVM8
E	301	ALA	TYR	CONFLICT	UNP Q9IVM8
E	340	GLY	ALA	CONFLICT	UNP Q9IVM8
F	207	GLU	ASP	CONFLICT	UNP Q9IVM8
F	301	ALA	TYR	CONFLICT	UNP Q9IVM8
F	340	GLY	ALA	CONFLICT	UNP Q9IVM8
G	207	GLU	ASP	CONFLICT	UNP Q9IVM8
G	301	ALA	TYR	CONFLICT	UNP Q9IVM8
G	340	GLY	ALA	CONFLICT	UNP Q9IVM8
H	207	GLU	ASP	CONFLICT	UNP Q9IVM8
H	301	ALA	TYR	CONFLICT	UNP Q9IVM8
H	340	GLY	ALA	CONFLICT	UNP Q9IVM8
I	207	GLU	ASP	CONFLICT	UNP Q9IVM8
I	301	ALA	TYR	CONFLICT	UNP Q9IVM8
I	340	GLY	ALA	CONFLICT	UNP Q9IVM8
J	207	GLU	ASP	CONFLICT	UNP Q9IVM8
J	301	ALA	TYR	CONFLICT	UNP Q9IVM8
J	340	GLY	ALA	CONFLICT	UNP Q9IVM8
K	207	GLU	ASP	CONFLICT	UNP Q9IVM8
K	301	ALA	TYR	CONFLICT	UNP Q9IVM8
K	340	GLY	ALA	CONFLICT	UNP Q9IVM8
L	207	GLU	ASP	CONFLICT	UNP Q9IVM8
L	301	ALA	TYR	CONFLICT	UNP Q9IVM8
L	340	GLY	ALA	CONFLICT	UNP Q9IVM8

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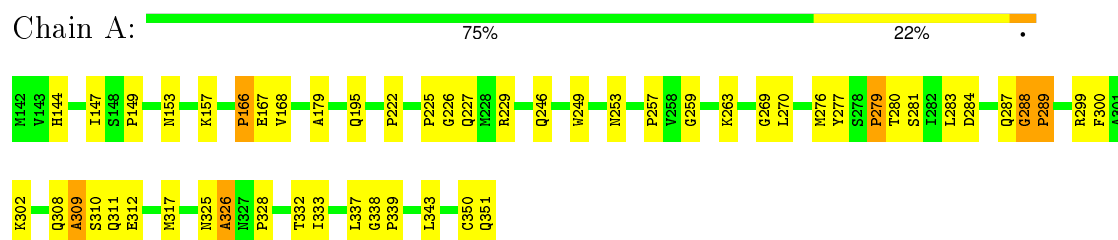
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Chain	Residue	Modelled	Actual	Comment	Reference
M	207	GLU	ASP	CONFLICT	UNP Q9IVM8
M	301	ALA	TYR	CONFLICT	UNP Q9IVM8
M	340	GLY	ALA	CONFLICT	UNP Q9IVM8
N	207	GLU	ASP	CONFLICT	UNP Q9IVM8
N	301	ALA	TYR	CONFLICT	UNP Q9IVM8
N	340	GLY	ALA	CONFLICT	UNP Q9IVM8
O	207	GLU	ASP	CONFLICT	UNP Q9IVM8
O	301	ALA	TYR	CONFLICT	UNP Q9IVM8
O	340	GLY	ALA	CONFLICT	UNP Q9IVM8
P	207	GLU	ASP	CONFLICT	UNP Q9IVM8
P	301	ALA	TYR	CONFLICT	UNP Q9IVM8
P	340	GLY	ALA	CONFLICT	UNP Q9IVM8
Q	207	GLU	ASP	CONFLICT	UNP Q9IVM8
Q	301	ALA	TYR	CONFLICT	UNP Q9IVM8
Q	340	GLY	ALA	CONFLICT	UNP Q9IVM8
R	207	GLU	ASP	CONFLICT	UNP Q9IVM8
R	301	ALA	TYR	CONFLICT	UNP Q9IVM8
R	340	GLY	ALA	CONFLICT	UNP Q9IVM8

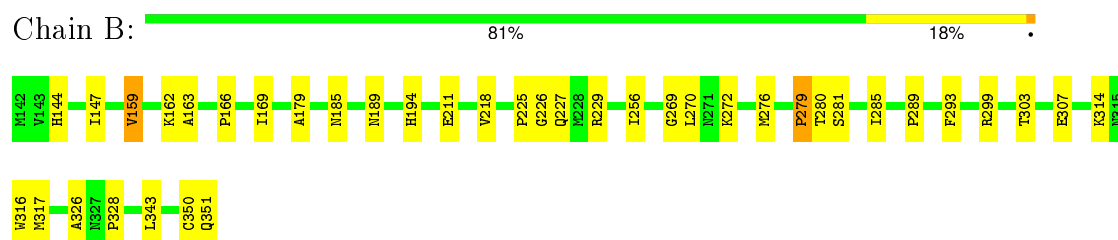
3 Residue-property plots

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.

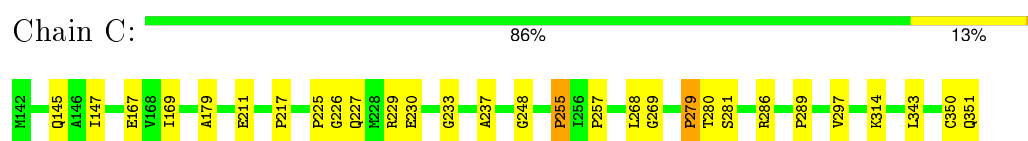
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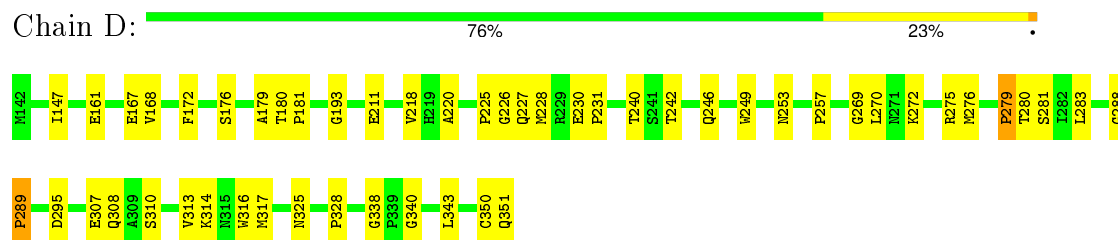
• Molecule 1: P24



• Molecule 1: P24



• Molecule 1: P24



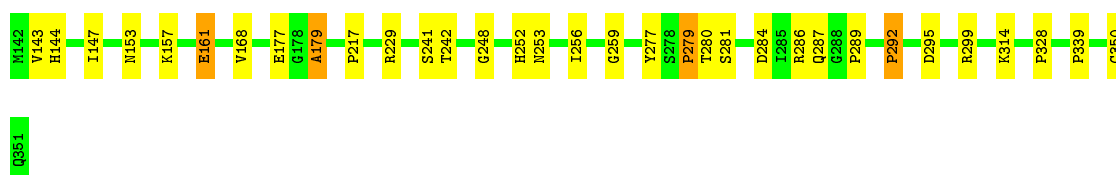
• Molecule 1: P24





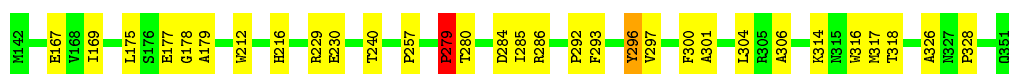
- Molecule 1: P24

Chain F: 84% 14%



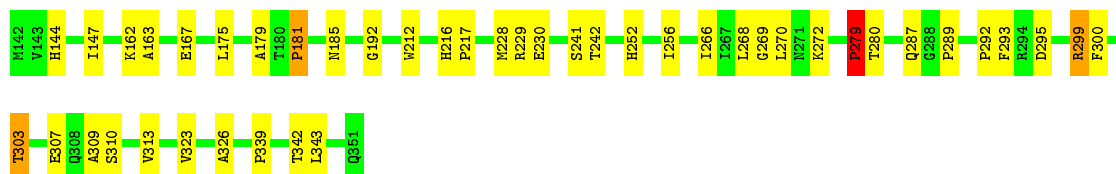
- Molecule 1: P24

Chain G: 85% 14%



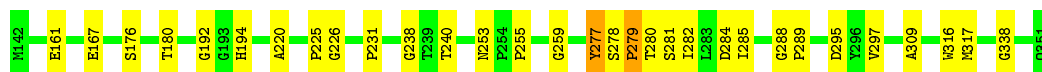
- Molecule 1: P24

Chain H: 79% 19%



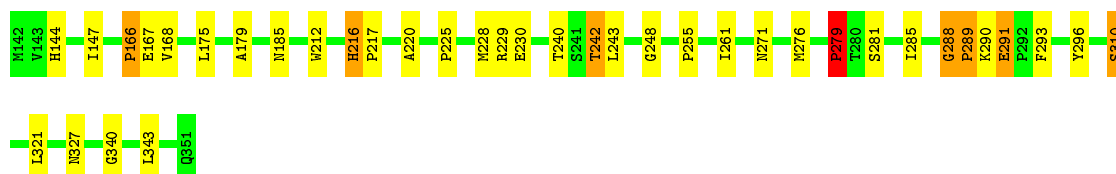
- Molecule 1: P24

Chain I: 85% 14%

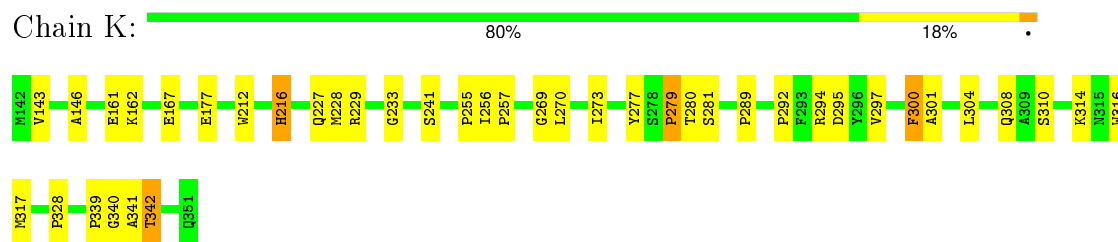


- Molecule 1: P24

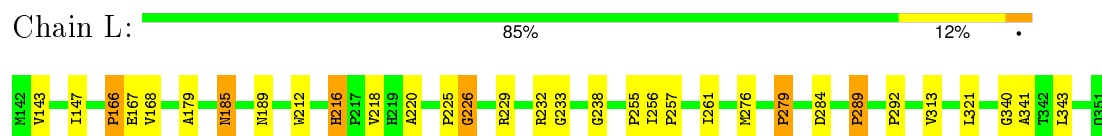
Chain J: 82% 14%



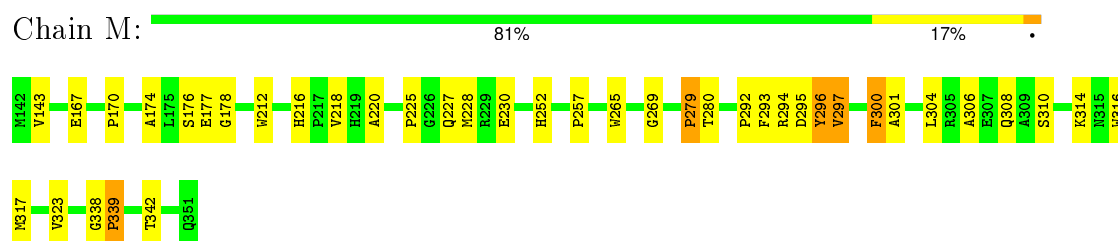
- Molecule 1: P24



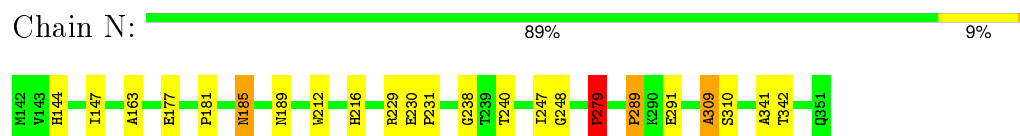
- Molecule 1: P24



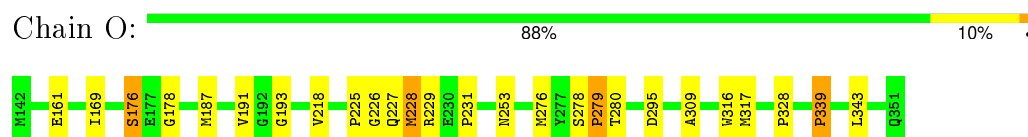
- Molecule 1: P24



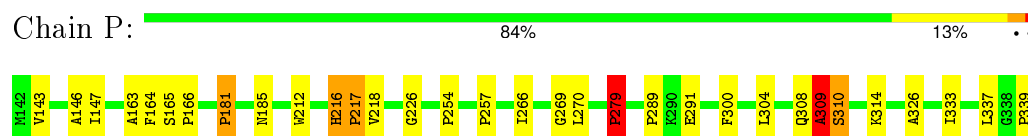
- Molecule 1: P24



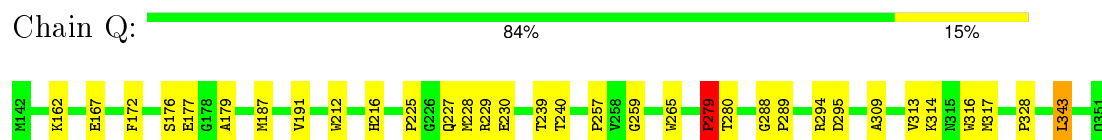
- Molecule 1: P24



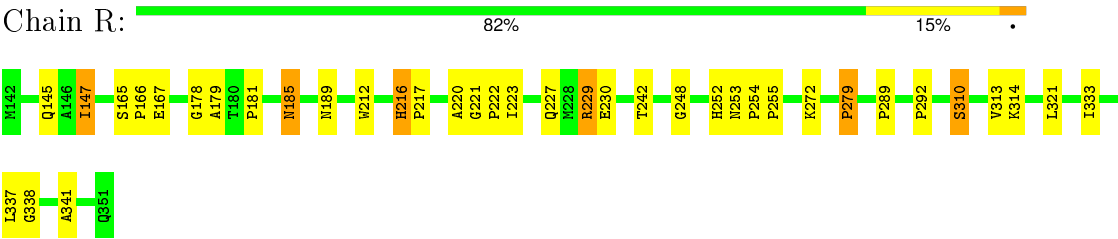
- Molecule 1: P24



- Molecule 1: P24



● Molecule 1: P24



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING OF INDIVIDUAL TILTS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	42000	Depositor
Image detector	GATAN MULTISCAN	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1.98	7/839 (0.8%)	1.74	9/1047 (0.9%)
1	B	1.96	3/839 (0.4%)	1.73	9/1047 (0.9%)
1	C	1.95	3/839 (0.4%)	1.67	4/1047 (0.4%)
1	D	1.95	4/839 (0.5%)	1.67	11/1047 (1.1%)
1	E	1.98	11/839 (1.3%)	1.66	8/1047 (0.8%)
1	F	1.98	6/839 (0.7%)	1.64	6/1047 (0.6%)
1	G	1.91	5/839 (0.6%)	1.63	4/1047 (0.4%)
1	H	1.91	6/839 (0.7%)	1.71	9/1047 (0.9%)
1	I	1.89	2/839 (0.2%)	1.67	7/1047 (0.7%)
1	J	1.84	4/839 (0.5%)	1.71	11/1047 (1.1%)
1	K	1.84	5/839 (0.6%)	1.66	5/1047 (0.5%)
1	L	1.83	4/839 (0.5%)	1.68	10/1047 (1.0%)
1	M	1.94	7/839 (0.8%)	1.65	8/1047 (0.8%)
1	N	1.91	3/839 (0.4%)	1.71	8/1047 (0.8%)
1	O	1.91	2/839 (0.2%)	1.66	5/1047 (0.5%)
1	P	1.90	2/839 (0.2%)	1.68	8/1047 (0.8%)
1	Q	1.91	6/839 (0.7%)	1.61	4/1047 (0.4%)
1	R	1.94	5/839 (0.6%)	1.69	5/1047 (0.5%)
All	All	1.92	85/15102 (0.6%)	1.68	131/18846 (0.7%)

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	A	0	9
1	B	0	6
1	C	0	6
1	D	0	12
1	E	0	2
1	F	0	9
1	G	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	14
1	I	0	5
1	J	0	12
1	K	0	5
1	L	0	6
1	M	0	5
1	N	0	5
1	O	0	6
1	P	0	5
1	Q	0	2
1	R	0	6
All	All	0	118

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	185	ASN	CA-C	-6.31	1.36	1.52
1	F	295	ASP	CA-C	-6.24	1.36	1.52
1	D	328	PRO	CA-C	-6.23	1.40	1.52
1	L	238	GLY	CA-C	-6.18	1.42	1.51
1	A	328	PRO	CA-C	-6.15	1.40	1.52

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	242	THR	CA-C-N	-8.27	99.01	117.20
1	A	289	PRO	N-CA-C	-7.78	91.86	112.10
1	J	166	PRO	N-CA-C	7.57	131.77	112.10
1	L	166	PRO	N-CA-C	7.45	131.46	112.10
1	D	351	GLN	N-CA-C	-7.17	91.64	111.00

There are no chirality outliers.

5 of 118 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	GLY	Mainchain
1	A	277	TYR	Mainchain
1	A	279	PRO	Peptide
1	A	284	ASP	Mainchain
1	A	288	GLY	Mainchain

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	840	419	218	8	0
1	B	840	419	218	5	0
1	C	840	419	219	1	0
1	D	840	419	217	4	0
1	E	840	419	218	7	0
1	F	840	419	219	3	0
1	G	840	419	219	6	0
1	H	840	419	218	4	0
1	I	840	419	219	4	0
1	J	840	419	219	3	0
1	K	840	419	217	6	0
1	L	840	419	219	2	0
1	M	840	419	218	6	0
1	N	840	419	219	3	0
1	O	840	419	219	3	0
1	P	840	419	218	5	0
1	Q	840	419	219	6	0
1	R	840	419	219	5	0
All	All	15120	7542	3932	81	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 81 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:F:179:ALA:O	1:F:259:GLY:HA3	2.08	0.54
1:Q:179:ALA:O	1:Q:259:GLY:HA2	2.10	0.52
1:R:181:PRO:O	1:R:185:ASN:N	2.45	0.50
1:G:175:LEU:C	1:G:177:GLU:H	2.17	0.48
1:H:303:THR:O	1:H:307:GLU:N	2.46	0.48

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	208/210 (99%)	168 (81%)	20 (10%)	20 (10%)	1	15
1	B	208/210 (99%)	170 (82%)	23 (11%)	15 (7%)	1	22
1	C	208/210 (99%)	167 (80%)	24 (12%)	17 (8%)	1	18
1	D	208/210 (99%)	169 (81%)	19 (9%)	20 (10%)	1	15
1	E	208/210 (99%)	169 (81%)	22 (11%)	17 (8%)	1	18
1	F	208/210 (99%)	170 (82%)	25 (12%)	13 (6%)	2	25
1	G	208/210 (99%)	176 (85%)	21 (10%)	11 (5%)	2	29
1	H	208/210 (99%)	174 (84%)	17 (8%)	17 (8%)	1	18
1	I	208/210 (99%)	169 (81%)	24 (12%)	15 (7%)	1	22
1	J	208/210 (99%)	173 (83%)	17 (8%)	18 (9%)	1	17
1	K	208/210 (99%)	171 (82%)	18 (9%)	19 (9%)	1	17
1	L	208/210 (99%)	173 (83%)	20 (10%)	15 (7%)	1	22
1	M	208/210 (99%)	176 (85%)	17 (8%)	15 (7%)	1	22
1	N	208/210 (99%)	179 (86%)	20 (10%)	9 (4%)	3	34
1	O	208/210 (99%)	168 (81%)	28 (14%)	12 (6%)	2	27
1	P	208/210 (99%)	177 (85%)	13 (6%)	18 (9%)	1	17
1	Q	208/210 (99%)	178 (86%)	15 (7%)	15 (7%)	1	22
1	R	208/210 (99%)	177 (85%)	11 (5%)	20 (10%)	1	15
All	All	3744/3780 (99%)	3104 (83%)	354 (10%)	286 (8%)	2	20

5 of 286 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	147	ILE
1	A	167	GLU
1	A	179	ALA

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Mol	Chain	Res	Type
1	A	225	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.