



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jan 22, 2018 – 07:03 PM EST

PDB ID : 5NZR
EMDB ID: : EMD-3720
Title : The structure of the COPI coat leaf
Authors : Dodonova, S.O.; Aderhold, P.; Kopp, J.; Ganeva, I.; Roehling, S.; Hagen, W.J.H.; Sinning, I.; Wieland, F.; Briggs, J.A.G.
Deposited on : 2017-05-15
Resolution : 9.20 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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-20030736

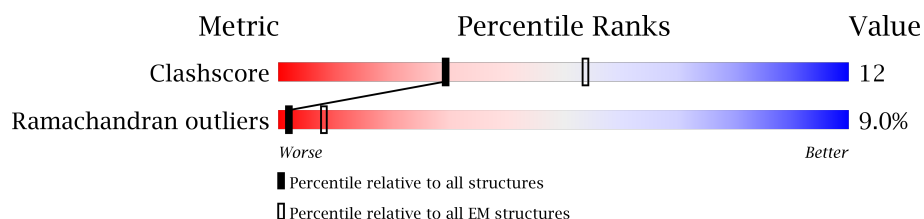
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










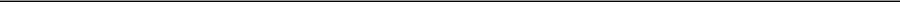

The reported resolution of this entry is 9.20 Å.

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

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	1262	 49% 14% • 36%
2	B	968	 66% 13% • 17%
3	C	905	 77% 14% • 7%
4	D	511	 29% 5% • 65%
5	F	181	 77% 8% • 12%
5	M	181	 65% 19% • 12%
5	R	181	 54% 27% 7% 12%
6	G	874	 75% 14% • 9%
6	K	874	 52% 9% • 36%
7	L	177	 66% 12% • 21%
7	Z	177	 66% 12% • 21%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18970 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	813	Total	C	N	O	0	0
			3251	1626	813	812		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1225	LEU	-	expression tag	UNP Q8CIE6
A	1226	GLU	-	expression tag	UNP Q8CIE6
A	1227	VAL	-	expression tag	UNP Q8CIE6
A	1228	LEU	-	expression tag	UNP Q8CIE6
A	1229	PHE	-	expression tag	UNP Q8CIE6
A	1230	GLN	-	expression tag	UNP Q8CIE6
A	1231	GLY	-	expression tag	UNP Q8CIE6
A	1232	PRO	-	expression tag	UNP Q8CIE6
A	1233	SER	-	expression tag	UNP Q8CIE6
A	1234	ALA	-	expression tag	UNP Q8CIE6
A	1235	TRP	-	expression tag	UNP Q8CIE6
A	1236	SER	-	expression tag	UNP Q8CIE6
A	1237	HIS	-	expression tag	UNP Q8CIE6
A	1238	PRO	-	expression tag	UNP Q8CIE6
A	1239	GLN	-	expression tag	UNP Q8CIE6
A	1240	PHE	-	expression tag	UNP Q8CIE6
A	1241	GLU	-	expression tag	UNP Q8CIE6
A	1242	LYS	-	expression tag	UNP Q8CIE6
A	1243	GLY	-	expression tag	UNP Q8CIE6
A	1244	GLY	-	expression tag	UNP Q8CIE6
A	1245	GLY	-	expression tag	UNP Q8CIE6
A	1246	SER	-	expression tag	UNP Q8CIE6
A	1247	GLY	-	expression tag	UNP Q8CIE6
A	1248	GLY	-	expression tag	UNP Q8CIE6
A	1249	GLY	-	expression tag	UNP Q8CIE6
A	1250	SER	-	expression tag	UNP Q8CIE6
A	1251	GLY	-	expression tag	UNP Q8CIE6
A	1252	GLY	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1253	SER	-	expression tag	UNP Q8CIE6
A	1254	ALA	-	expression tag	UNP Q8CIE6
A	1255	TRP	-	expression tag	UNP Q8CIE6
A	1256	SER	-	expression tag	UNP Q8CIE6
A	1257	HIS	-	expression tag	UNP Q8CIE6
A	1258	PRO	-	expression tag	UNP Q8CIE6
A	1259	GLN	-	expression tag	UNP Q8CIE6
A	1260	PHE	-	expression tag	UNP Q8CIE6
A	1261	GLU	-	expression tag	UNP Q8CIE6
A	1262	LYS	-	expression tag	UNP Q8CIE6

- Molecule 2 is a protein called Coatomer subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	800	Total	C	N	O	0	0
			3198	1600	800	798		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9JIF7
B	2	HIS	-	expression tag	UNP Q9JIF7
B	3	HIS	-	expression tag	UNP Q9JIF7
B	4	HIS	-	expression tag	UNP Q9JIF7
B	5	HIS	-	expression tag	UNP Q9JIF7
B	6	HIS	-	expression tag	UNP Q9JIF7
B	7	HIS	-	expression tag	UNP Q9JIF7
B	8	GLU	-	expression tag	UNP Q9JIF7
B	9	ASN	-	expression tag	UNP Q9JIF7
B	10	LEU	-	expression tag	UNP Q9JIF7
B	11	TYR	-	expression tag	UNP Q9JIF7
B	12	PHE	-	expression tag	UNP Q9JIF7
B	13	GLN	-	expression tag	UNP Q9JIF7
B	14	GLY	-	expression tag	UNP Q9JIF7
B	15	HIS	-	expression tag	UNP Q9JIF7

- Molecule 3 is a protein called Coatomer subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	843	Total	C	N	O	0	0
			3371	1686	843	842		

- Molecule 4 is a protein called Coatomer subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	177	Total	C	N	O	0	0
			706	354	177	175		

- Molecule 5 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	159	Total	C	N	O	0	0
			635	318	159	158		
5	R	159	Total	C	N	O	0	0
			635	318	159	158		
5	M	159	Total	C	N	O	0	0
			635	318	159	158		

- Molecule 6 is a protein called Coatomer subunit gamma-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	798	Total	C	N	O	0	0
			3190	1596	798	796		
6	K	560	Total	C	N	O	0	0
			2239	1120	560	559		

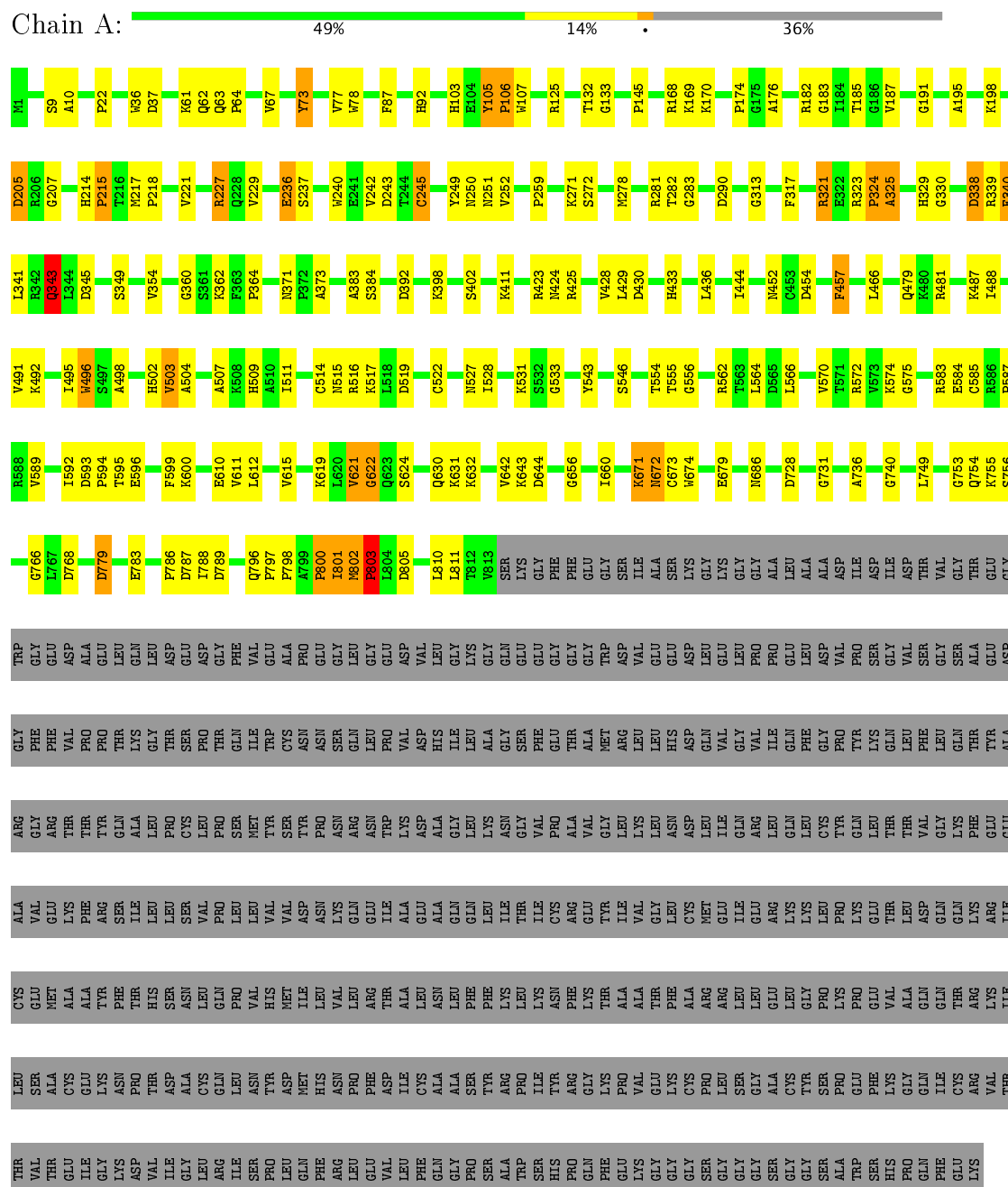
- Molecule 7 is a protein called Coatomer subunit zeta-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Z	139	Total	C	N	O	0	0
			555	278	139	138		
7	L	139	Total	C	N	O	0	0
			555	278	139	138		

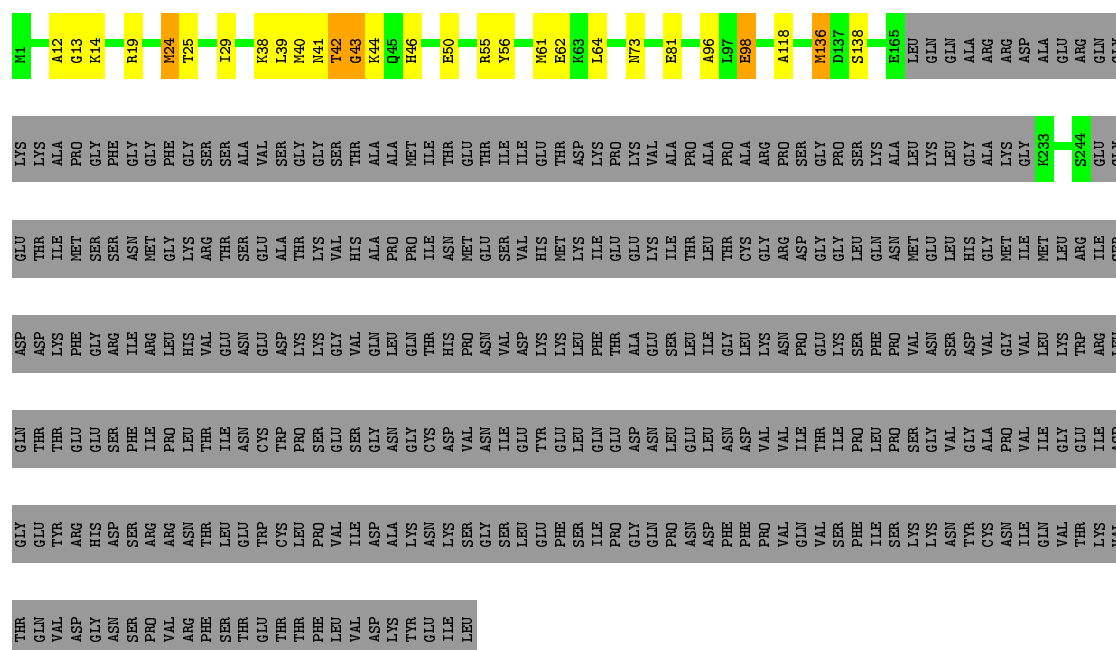
3 Residue-property plots

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.

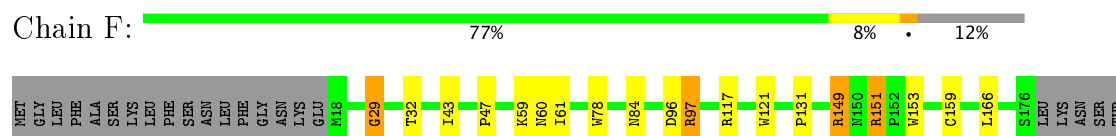
• Molecule 1: Coatomer subunit alpha



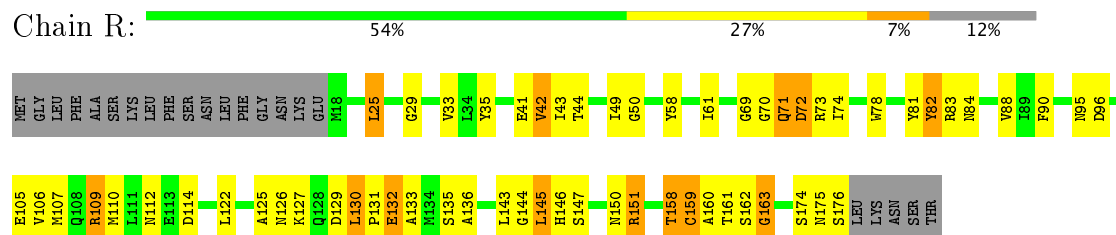




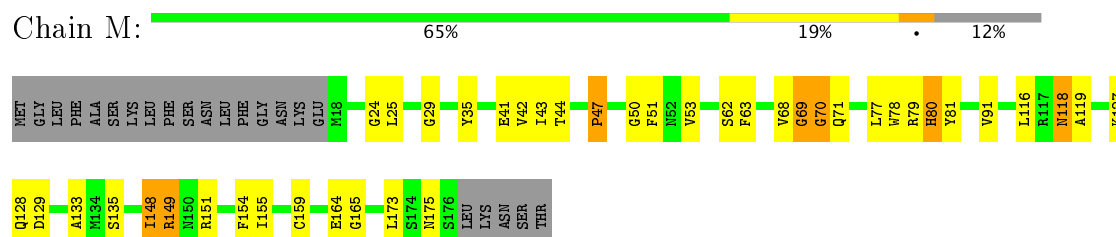
- Molecule 5: ADP-ribosylation factor 1



- Molecule 5: ADP-ribosylation factor 1

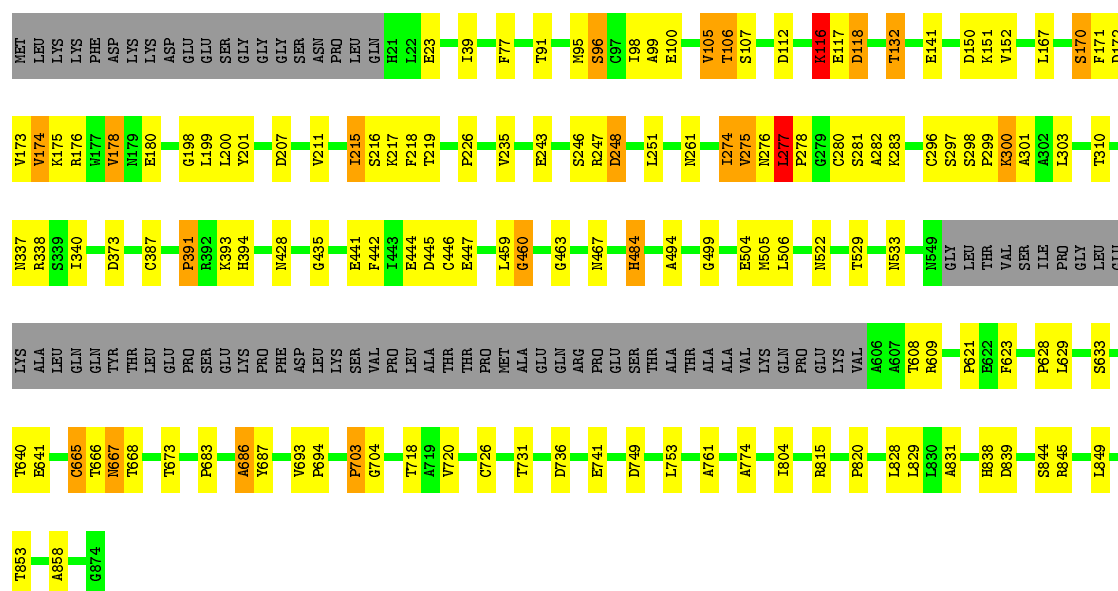


- Molecule 5: ADP-ribosylation factor 1

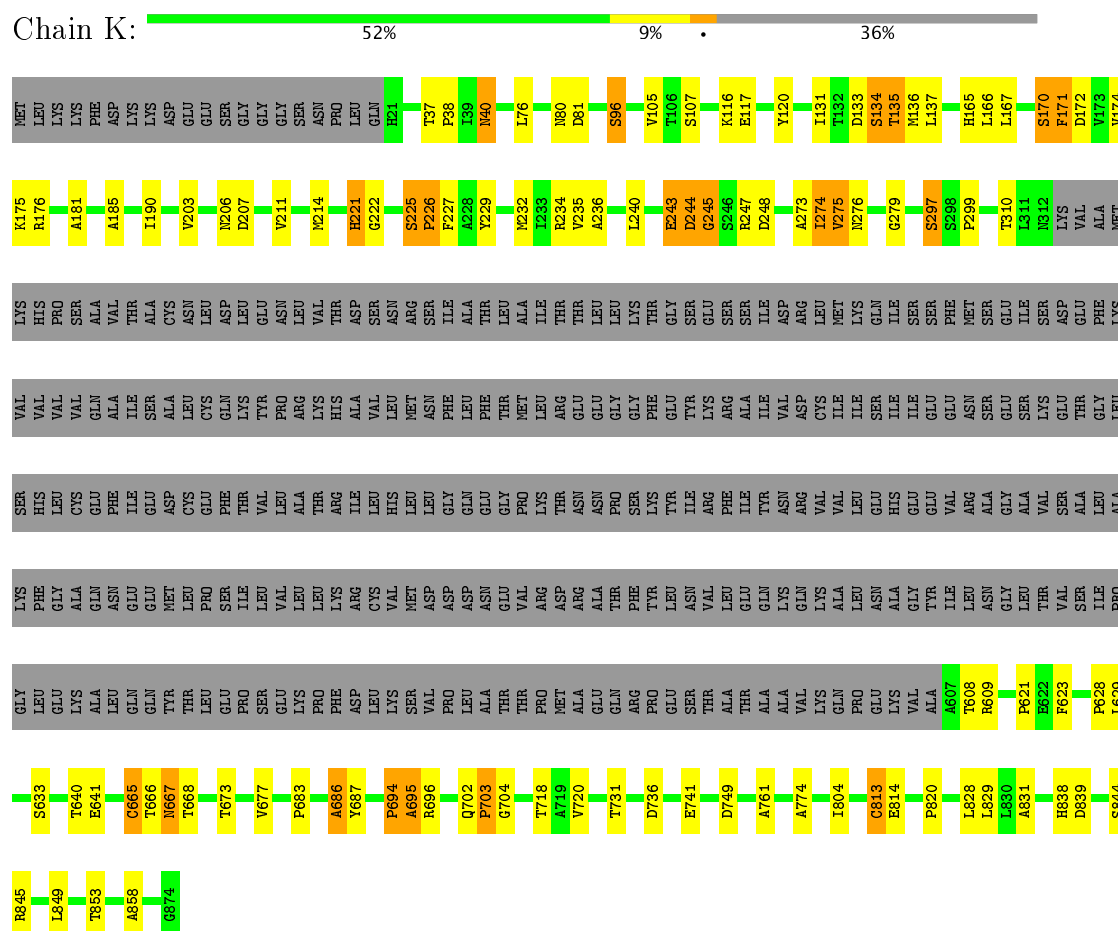


- Molecule 6: Coatomer subunit gamma-1



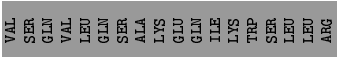


• Molecule 6: Coatomer subunit gamma-1



• Molecule 7: Coatomer subunit zeta-1





● Molecule 7: Coatomer subunit zeta-1



4 Experimental information

Property	Value	Source
Reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	38498	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF-determination for each individual tilt image was performed using CTFFIND4. Strip-based CTF-correction and tomogram reconstruction was performed in Imod.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (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	1.56	15/3250 (0.5%)	1.81	74/4061 (1.8%)
2	B	1.71	19/3193 (0.6%)	1.55	45/3983 (1.1%)
3	C	1.76	23/3370 (0.7%)	1.70	60/4211 (1.4%)
4	D	1.67	3/704 (0.4%)	1.65	10/877 (1.1%)
5	F	1.56	1/634 (0.2%)	1.71	9/791 (1.1%)
5	M	1.60	4/634 (0.6%)	1.65	10/791 (1.3%)
5	R	1.88	10/634 (1.6%)	1.81	15/791 (1.9%)
6	G	1.62	11/3188 (0.3%)	1.59	45/3982 (1.1%)
6	K	1.72	9/2237 (0.4%)	1.69	44/2793 (1.6%)
7	L	2.05	3/554 (0.5%)	1.72	7/691 (1.0%)
7	Z	1.87	3/554 (0.5%)	1.69	10/691 (1.4%)
All	All	1.69	101/18952 (0.5%)	1.68	329/23662 (1.4%)

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	B	0	3

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	940	GLY	N-CA	-7.80	1.34	1.46
5	R	29	GLY	CA-C	-7.62	1.39	1.51
5	R	35	TYR	CA-C	-7.33	1.33	1.52
1	A	191	GLY	CA-C	-7.04	1.40	1.51
3	C	572	ARG	CA-C	-6.59	1.35	1.52

The worst 5 of 329 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLN	N-CA-C	-9.86	84.38	111.00
6	K	117	GLU	C-N-CA	9.76	146.10	121.70
2	B	326	HIS	N-CA-C	-9.59	85.12	111.00
6	G	96	SER	N-CA-C	9.10	135.56	111.00
2	B	940	GLY	N-CA-C	-9.03	90.52	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	898	ALA	Peptide
2	B	903	CYS	Peptide
2	B	938	VAL	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	3251	0	869	36	0
2	B	3198	0	810	58	0
3	C	3371	0	919	23	0
4	D	706	0	182	9	0
5	F	635	0	181	3	0
5	M	635	0	181	19	0
5	R	635	0	181	37	0
6	G	3190	0	822	57	0
6	K	2239	0	572	39	0
7	L	555	0	148	2	0
7	Z	555	0	147	15	0
All	All	18970	0	5012	279	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 12.

The worst 5 of 279 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)
6:K:107:SER:N	5:M:50:GLY:HA3	1.28	1.43
6:G:107:SER:N	5:R:50:GLY:HA3	1.16	1.43
6:G:107:SER:H	5:R:50:GLY:CA	1.31	1.41
6:K:167:LEU:CA	6:K:170:SER:O	1.73	1.35
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	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	811/1262 (64%)	590 (73%)	112 (14%)	109 (13%)	0	6
2	B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	1	14
3	C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	1	16
4	D	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1	18
5	F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	2	24
5	M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0	8
5	R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0	7
6	G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1	20
6	K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1	19
7	L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1	21
7	Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	2	26
All	All	4710/6291 (75%)	3832 (81%)	456 (10%)	422 (9%)	2	15

5 of 422 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	64	PRO

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Mol	Chain	Res	Type
1	A	92	HIS
1	A	106	PRO
1	A	125	ARG

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.