



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 01:10 AM EST

PDB ID : 6W4P
EMDB ID : EMD-21536
Title : CaMKII alpha-30 Cryo-EM reconstruction - Class B
Authors : Chao, L.H.; Stratton, M.M.
Deposited on : 2020-03-11
Resolution : 6.60 Å(reported)
Based on initial models : 3SOA, 5IG3

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

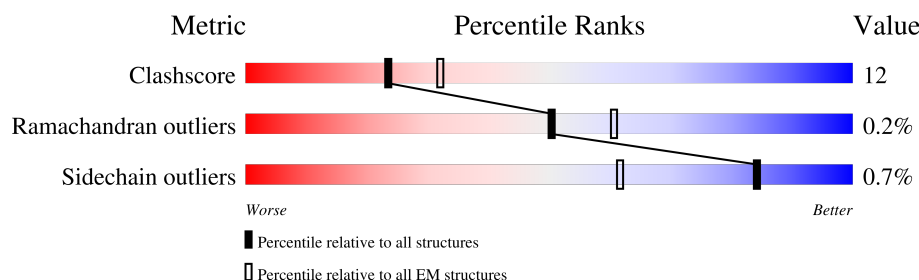
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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	473	24% 73%
1	B	473	22% 73%
1	C	473	22% 73%
1	D	473	22% 74%
1	E	473	22% 74%
1	F	473	22% 74%
1	G	473	25% 73%
1	I	473	23% 73%
1	J	473	22% 73%

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Mol	Chain	Length	Quality of chain
1	K	473	<div><div></div><div>22%</div><div></div><div></div><div>74%</div></div>
1	L	473	<div><div></div><div>22%</div><div></div><div></div><div>74%</div></div>
1	M	473	<div><div></div><div>22%</div><div></div><div></div><div>74%</div></div>
2	H	473	<div><div></div><div>27%</div><div></div><div>33%</div><div></div><div></div><div>38%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14476 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 Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	128	Total	C	N	O	S	0	0
			1041	658	187	191	5		
1	B	126	Total	C	N	O	S	0	0
			1023	650	181	187	5		
1	C	126	Total	C	N	O	S	0	0
			1022	648	181	188	5		
1	D	123	Total	C	N	O	S	0	0
			994	630	176	183	5		
1	E	123	Total	C	N	O	S	0	0
			994	630	176	183	5		
1	F	122	Total	C	N	O	S	0	0
			988	625	176	182	5		
1	G	128	Total	C	N	O	S	0	0
			1041	658	187	191	5		
1	I	126	Total	C	N	O	S	0	0
			1023	650	181	187	5		
1	J	126	Total	C	N	O	S	0	0
			1022	648	181	188	5		
1	K	123	Total	C	N	O	S	0	0
			994	630	176	183	5		
1	L	123	Total	C	N	O	S	0	0
			994	630	176	183	5		
1	M	122	Total	C	N	O	S	0	0
			988	625	176	182	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-322	SER	-	expression tag	UNP Q9UQM7
B	-337	SER	-	expression tag	UNP Q9UQM7
C	-332	SER	-	expression tag	UNP Q9UQM7
D	-334	SER	-	expression tag	UNP Q9UQM7
E	-336	SER	-	expression tag	UNP Q9UQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-337	SER	-	expression tag	UNP Q9UQM7
G	-322	SER	-	expression tag	UNP Q9UQM7
I	-337	SER	-	expression tag	UNP Q9UQM7
J	-332	SER	-	expression tag	UNP Q9UQM7
K	-334	SER	-	expression tag	UNP Q9UQM7
L	-336	SER	-	expression tag	UNP Q9UQM7
M	-337	SER	-	expression tag	UNP Q9UQM7

- Molecule 2 is a protein called Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	293	Total	C	N	O	S	0	0
			2352	1503	415	423	11		

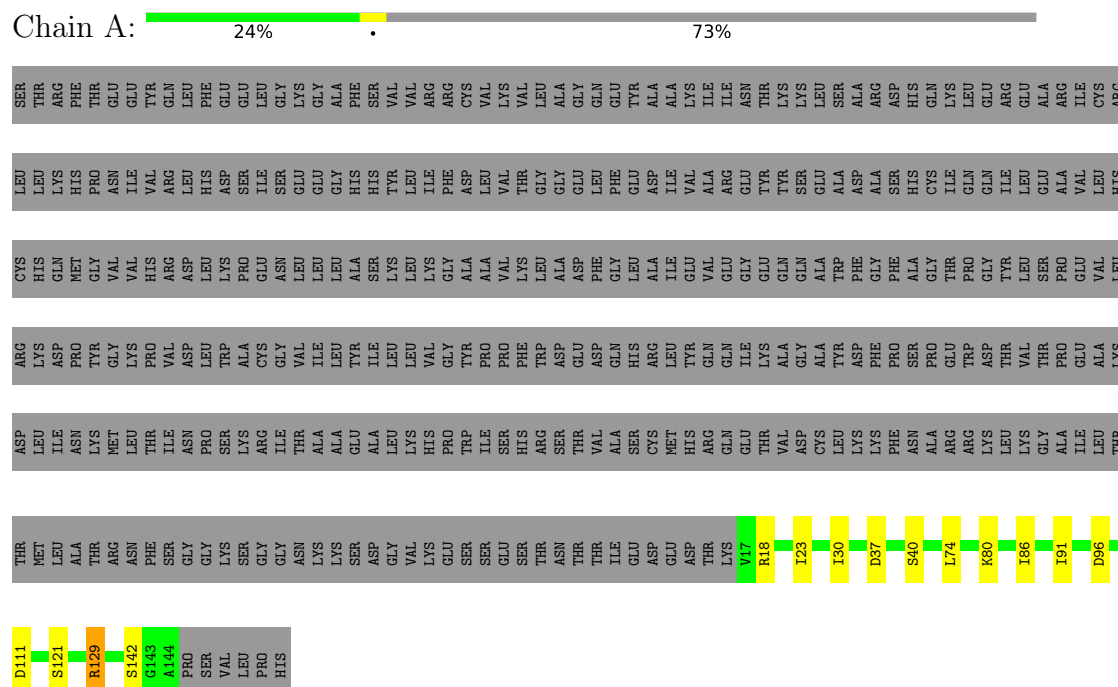
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	SER	-	expression tag	UNP Q9UQM7
H	34	MET	LYS	engineered mutation	UNP Q9UQM7
H	127	ASN	ASP	conflict	UNP Q9UQM7

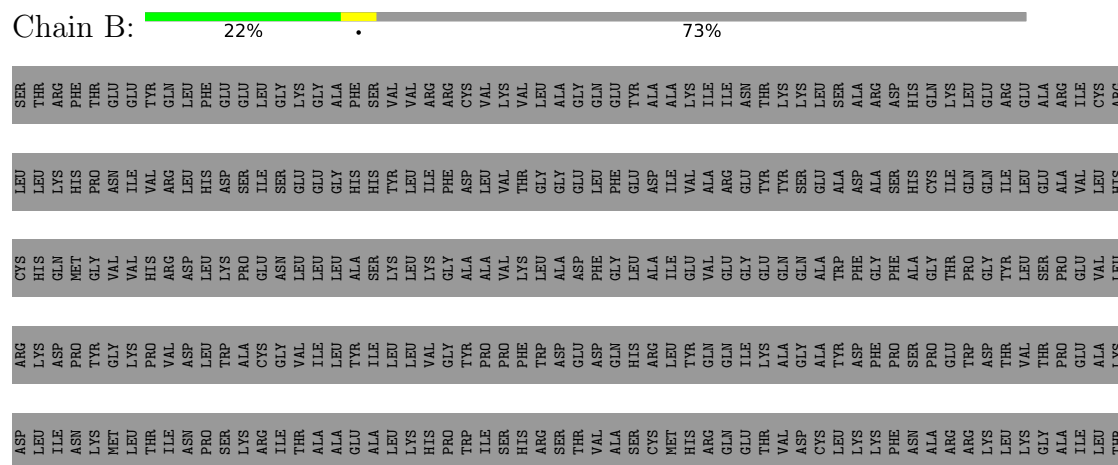
3 Residue-property plots [i](#)

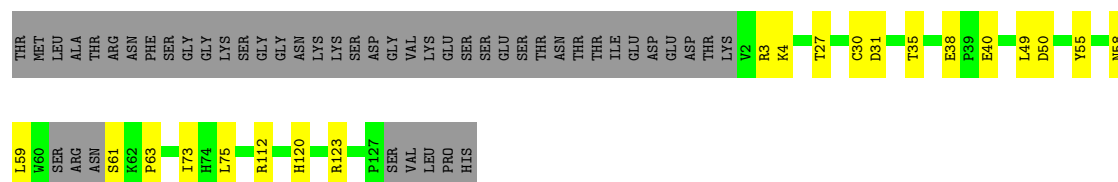
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Calcium/calmodulin-dependent protein kinase type II subunit alpha



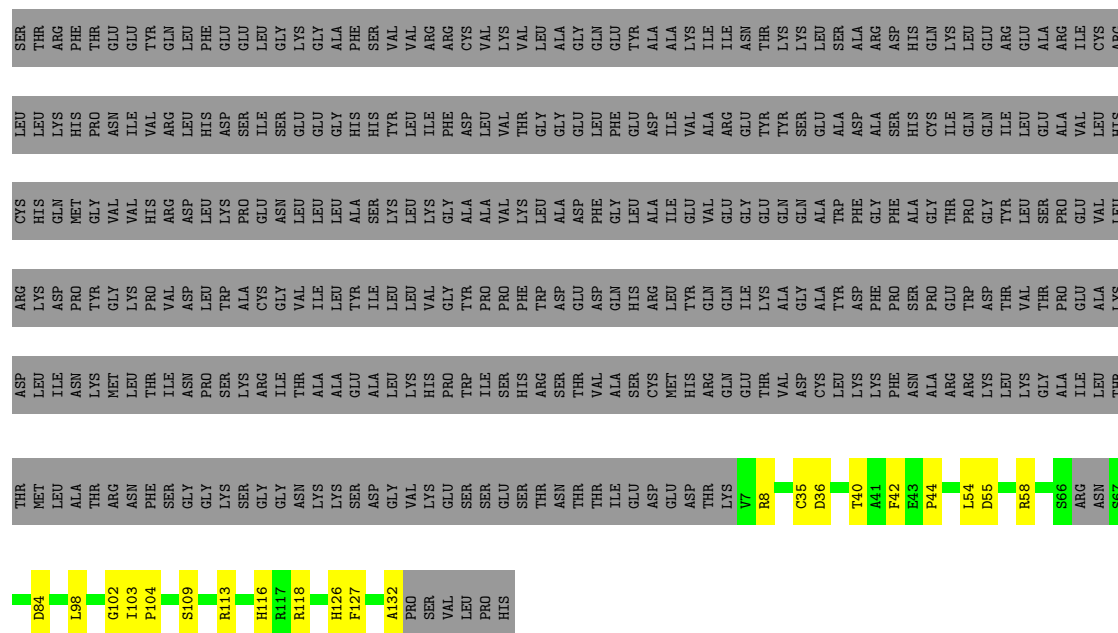
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha





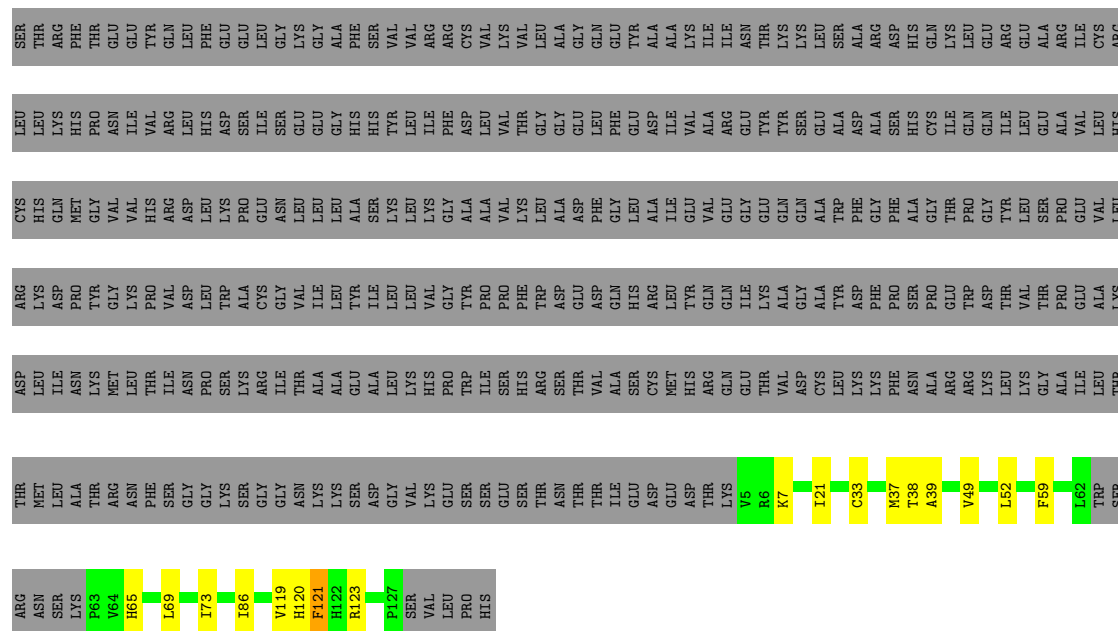
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain C: 22% 73%

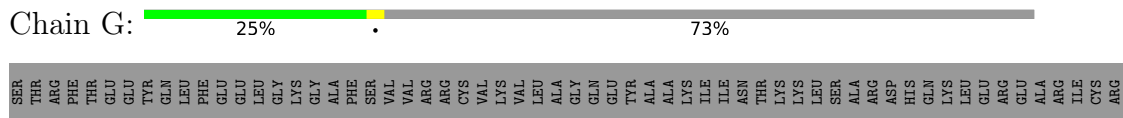


- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain D: 22% 74%

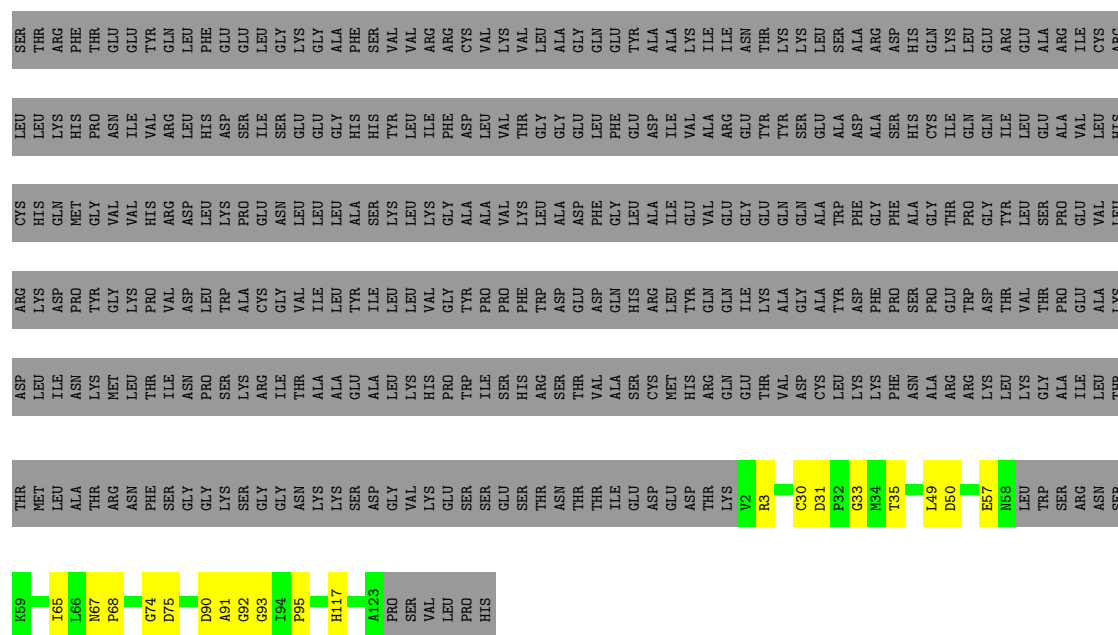


Chain E: 22% . 74%

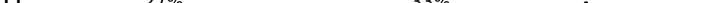


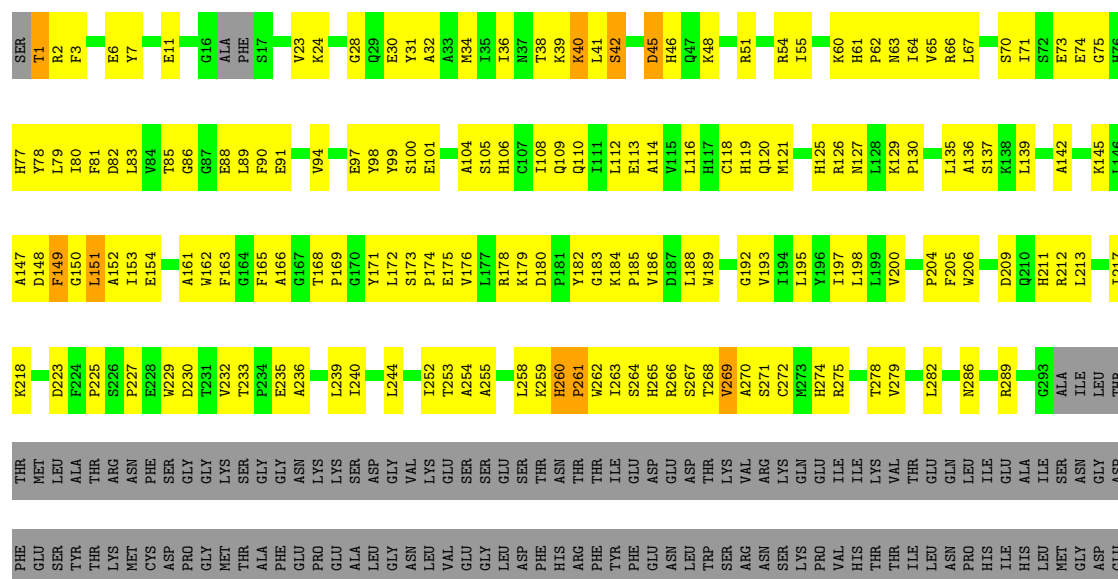
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain M: 22% 1% 74%



- Molecule 2: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain H:  27% 33% . 38%



SER	ALA	CYS	ILE	ALA	TYR	ILE	ARG	ILE	THR	GLN	TYR	LEU	ASP	ALA	GLY	GLY	ILE	PRO	ARG	THR	ALA	GLN	SER	GLU	GLU	THR	ARG	VAL	TRP	HIS	ARG	ARG	ASP	GLY	LYS	TRP	GLN	ILE	VAL	HIS	PHE	HIS	ARG	SER	GLY	ALA	PRO	SER	VAL	LEU	PRO	HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40329	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	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	0.25	0/1068	0.42	0/1445
1	B	0.25	0/1050	0.42	0/1421
1	C	0.25	0/1048	0.42	0/1417
1	D	0.25	0/1019	0.41	0/1378
1	E	0.26	0/1019	0.42	0/1378
1	F	0.25	0/1012	0.41	0/1367
1	G	0.25	0/1068	0.42	0/1445
1	I	0.26	0/1050	0.42	0/1421
1	J	0.25	0/1048	0.42	0/1417
1	K	0.25	0/1019	0.41	0/1378
1	L	0.26	0/1019	0.42	0/1378
1	M	0.25	0/1012	0.41	0/1367
2	H	0.37	0/2407	0.65	2/3254 (0.1%)
All	All	0.27	0/14839	0.46	2/20066 (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
2	H	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	269	VAL	N-CA-C	5.69	126.35	111.00
2	H	151	LEU	N-CA-C	-5.10	97.22	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	149	PHE	Peptide
2	H	150	GLY	Peptide
2	H	40	LYS	Peptide

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	1041	0	1003	10	0
1	B	1023	0	985	20	0
1	C	1022	0	983	12	0
1	D	994	0	958	9	0
1	E	994	0	958	16	0
1	F	988	0	952	11	0
1	G	1041	0	1003	9	0
1	I	1023	0	985	12	0
1	J	1022	0	983	12	0
1	K	994	0	958	10	0
1	L	994	0	958	15	0
1	M	988	0	952	12	0
2	H	2352	0	2356	224	0
All	All	14476	0	14034	348	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 348 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:H:266:ARG:HB3	2:H:270:ALA:HB2	1.30	1.09
2:H:99:TYR:OH	2:H:198:LEU:O	1.69	1.09
1:J:36:ASP:OD2	1:J:118:ARG:NH1	1.90	1.05
1:C:36:ASP:OD2	1:C:118:ARG:NH1	1.90	1.02
1:B:31:ASP:OD1	1:B:112:ARG:NH1	1.93	1.01

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	126/473 (27%)	123 (98%)	3 (2%)	0	100	100
1	B	122/473 (26%)	119 (98%)	3 (2%)	0	100	100
1	C	122/473 (26%)	116 (95%)	6 (5%)	0	100	100
1	D	119/473 (25%)	116 (98%)	3 (2%)	0	100	100
1	E	119/473 (25%)	116 (98%)	3 (2%)	0	100	100
1	F	118/473 (25%)	117 (99%)	0	1 (1%)	19	60
1	G	126/473 (27%)	123 (98%)	3 (2%)	0	100	100
1	I	122/473 (26%)	119 (98%)	3 (2%)	0	100	100
1	J	122/473 (26%)	116 (95%)	6 (5%)	0	100	100
1	K	119/473 (25%)	116 (98%)	3 (2%)	0	100	100
1	L	119/473 (25%)	116 (98%)	3 (2%)	0	100	100
1	M	118/473 (25%)	117 (99%)	0	1 (1%)	19	60
2	H	289/473 (61%)	270 (93%)	17 (6%)	2 (1%)	22	63
All	All	1741/6149 (28%)	1684 (97%)	53 (3%)	4 (0%)	50	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	91	ALA
1	M	91	ALA
2	H	42	SER
2	H	261	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	111/405 (27%)	110 (99%)	1 (1%)	78	88
1	B	109/405 (27%)	109 (100%)	0	100	100
1	C	109/405 (27%)	108 (99%)	1 (1%)	78	88
1	D	106/405 (26%)	105 (99%)	1 (1%)	78	88
1	E	106/405 (26%)	105 (99%)	1 (1%)	78	88
1	F	105/405 (26%)	105 (100%)	0	100	100
1	G	111/405 (27%)	110 (99%)	1 (1%)	78	88
1	I	109/405 (27%)	109 (100%)	0	100	100
1	J	109/405 (27%)	108 (99%)	1 (1%)	78	88
1	K	106/405 (26%)	105 (99%)	1 (1%)	78	88
1	L	106/405 (26%)	105 (99%)	1 (1%)	78	88
1	M	105/405 (26%)	105 (100%)	0	100	100
2	H	250/405 (62%)	247 (99%)	3 (1%)	71	83
All	All	1542/5265 (29%)	1531 (99%)	11 (1%)	84	90

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	76	ASP
2	H	1	THR
2	H	260	HIS
2	H	45	ASP
1	G	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	140	HIS
1	I	72	HIS
2	H	286	ASN
1	L	120	HIS
1	E	120	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-21536. 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.