



Full wwPDB EM Validation Report ⓘ

Nov 6, 2024 – 03:02 pm GMT

PDB ID : 6QCM
EMDB ID : EMD-4508
Title : Cryo em structure of the Listeria stressosome
Authors : Williams, A.H.; Redzej, A.; Waksman, G.; Cossart, P.
Deposited on : 2018-12-28
Resolution : 4.21 Å(reported)

This is a Full wwPDB EM Validation 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

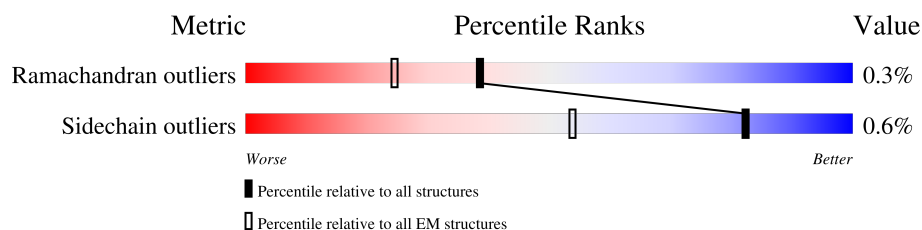
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.21 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	207382	16835
Sidechain outliers	206894	16415

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	AB	128	88% 10%
1	BC	128	89% 10%
1	DC	128	88% 10%
1	EB	128	90% 10%
1	FA	128	87% 10%
1	FB	128	88% 10%
1	FC	128	88% 10%
1	GC	128	90% 10%
1	HC	128	88% 10%
1	IC	128	87% 10%

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Mol	Chain	Length	Quality of chain
1	K	128	 88% • 10%
1	KB	128	 88% • 10%
1	L	128	 88% • 10%
1	LB	128	 88% • 10%
1	M	128	 88% • 10%
1	OB	128	 87% • 10%
1	P	128	 88% • 10%
1	PB	128	 89% • 10%
1	Q	128	 88% • 10%
1	SB	128	 89% • 10%
1	T	128	 88% • 10%
1	TB	128	 88% • 10%
1	U	128	 89% • 10%
1	UB	128	 88% • 10%
1	V	128	 88% • 10%
1	VB	128	 88% • 10%
1	W	128	 88% •• 10%
1	X	128	 87% • 10%
1	Y	128	 88% • 10%
1	Z	128	 89% • 10%
2	CB	129	 88% •• 10%
2	DB	129	 88% • 10%
2	E	129	 88% • 10%
2	F	129	 88% • 10%
2	GB	129	 87% • 10%

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Mol	Chain	Length	Quality of chain
2	IB	129	89% 10%
3	A	118	99%
3	B	118	100%
3	C	118	98%
3	D	118	98%
3	I	118	100%
3	J	118	99%
3	N	118	100%
3	O	118	100%
3	R	118	100%
3	S	118	100%
3	a	118	98%
3	b	118	100%
3	c	118	100%
3	d	118	99%
3	e	118	98%
3	f	118	99%
3	g	118	98%
3	h	118	99%
3	i	118	97%
3	j	118	99%
4	AD	123	99%
5	CD	136	88% 10%
5	FD	136	88% 10%
5	HD	136	89% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52697 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 RsbR protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	BC	115	Total	C	N	O	S	0	0
			871	555	150	160	6		
1	DC	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	EB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	FA	115	Total	C	N	O	S	0	0
			871	555	150	160	6		
1	FB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	FC	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	GC	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	HC	115	Total	C	N	O	S	0	0
			871	555	150	160	6		
1	IC	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	K	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	KB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	L	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	LB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	M	115	Total	C	N	O	S	0	0
			871	555	150	160	6		
1	OB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	P	115	Total	C	N	O	S	0	0
			875	557	150	162	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	PB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	Q	115	Total	C	N	O	S	0	0
			871	554	149	162	6		
1	SB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	T	115	Total	C	N	O	S	0	0
			867	551	148	162	6		
1	TB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	U	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	UB	115	Total	C	N	O	S	0	0
			869	554	147	162	6		
1	V	115	Total	C	N	O	S	0	0
			871	554	149	162	6		
1	VB	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	W	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	X	115	Total	C	N	O	S	0	0
			865	552	147	160	6		
1	Y	115	Total	C	N	O	S	0	0
			875	557	150	162	6		
1	Z	115	Total	C	N	O	S	0	0
			875	557	150	162	6		

- Molecule 2 is a protein called RsbR protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CB	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	DB	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	E	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	F	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	GB	116	Total	C	N	O	S	0	0
			884	563	152	163	6		
2	IB	116	Total	C	N	O	S	0	0
			884	563	152	163	6		

- Molecule 3 is a protein called RsbS protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	B	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	C	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	D	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	I	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	J	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	N	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	O	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	R	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	S	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	a	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	b	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	c	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	d	118	Total	C	N	O	S	0	0
			872	557	136	175	4		
3	e	118	Total	C	N	O	S	0	0
			868	555	135	173	5		
3	f	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	g	118	Total	C	N	O	S	0	0
			875	559	136	175	5		
3	h	118	Total	C	N	O	S	0	0
			871	556	135	175	5		
3	i	118	Total	C	N	O	S	0	0
			872	556	136	175	5		
3	j	118	Total	C	N	O	S	0	0
			871	556	135	175	5		

- Molecule 4 is a protein called RsbR protein,RsbR protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	123	Total	C	N	O	S	0	0
			935	594	160	175	6		

- Molecule 5 is a protein called RsbR protein.

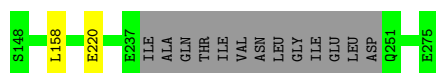
Mol	Chain	Residues	Atoms					AltConf	Trace
5	CD	123	Total	C	N	O	S	0	0
			935	595	161	173	6		
5	FD	123	Total	C	N	O	S	0	0
			927	589	159	173	6		
5	HD	123	Total	C	N	O	S	0	0
			931	591	159	175	6		

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.

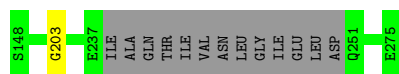
- Molecule 1: RsbR protein

Chain AB:  88% 10%



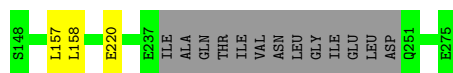
- Molecule 1: RsbR protein

Chain BC:  89% 10%



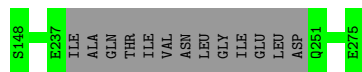
- Molecule 1: RsbR protein

Chain DC:  88% 10%




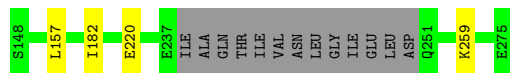
- Molecule 1: RsbR protein

Chain EB:  90% 10%




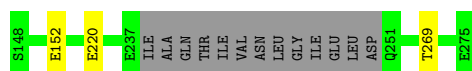
- Molecule 1: RsbR protein

Chain FA:  87% 10%



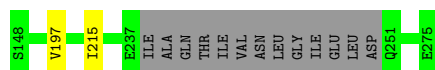
- Molecule 1: RsbR protein

Chain FB:  88% 10%



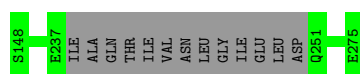
- Molecule 1: RsbR protein

Chain FC: 88% 10%



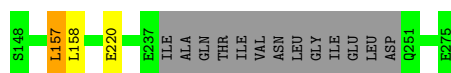
- Molecule 1: RsbR protein

Chain GC: 90% 10%



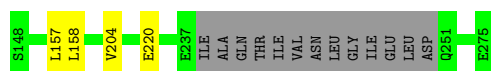
- Molecule 1: RsbR protein

Chain HC: 88% 10%



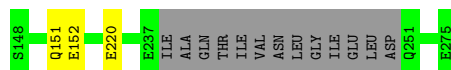
- Molecule 1: RsbR protein

Chain IC: 87% 10%



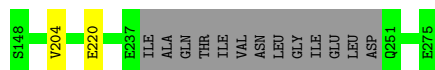
- Molecule 1: RsbR protein

Chain K: 88% 10%



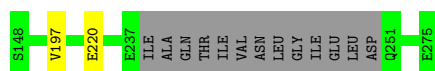
- Molecule 1: RsbR protein

Chain KB: 88% 10%



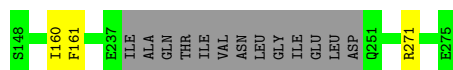
- Molecule 1: RsbR protein

Chain L: 88% 10%



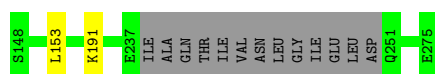
- Molecule 1: RsbR protein

Chain LB:
88% 10%



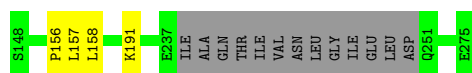
- Molecule 1: RsbR protein

Chain M:
88% 10%



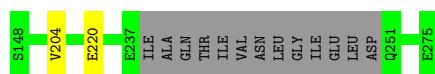
- Molecule 1: RsbR protein

Chain OB:
87% 10%



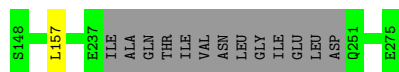
- Molecule 1: RsbR protein

Chain P:
88% 10%



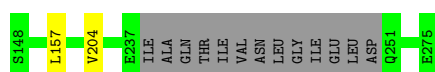
- Molecule 1: RsbR protein

Chain PB:
89% 10%



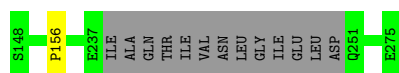
- Molecule 1: RsbR protein

Chain Q:
88% 10%



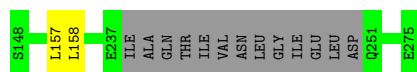
- Molecule 1: RsbR protein

Chain SB:
89% 10%



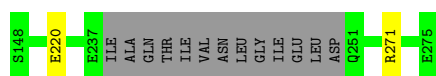
- Molecule 1: RsbR protein

Chain T: 88% 10%



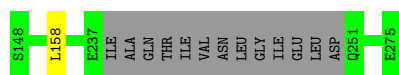
- Molecule 1: RsbR protein

Chain TB: 88% 10%



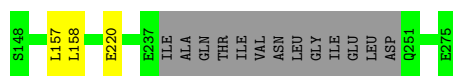
- Molecule 1: RsbR protein

Chain U: 89% 10%



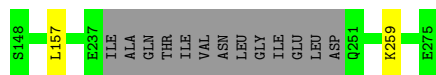
- Molecule 1: RsbR protein

Chain UB: 88% 10%



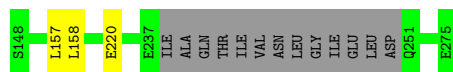
- Molecule 1: RsbR protein

Chain V: 88% 10%



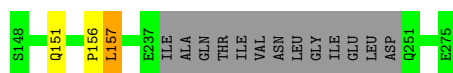
- Molecule 1: RsbR protein

Chain VB: 88% 10%



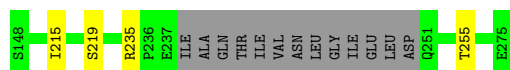
- Molecule 1: RsbR protein

Chain W: 88% 10%



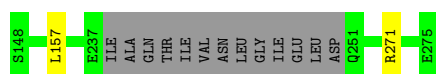
- Molecule 1: RsbR protein

Chain X: 87% 10%



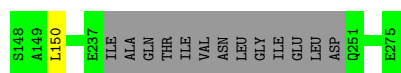
- Molecule 1: RsbR protein

Chain Y: 88% 10%



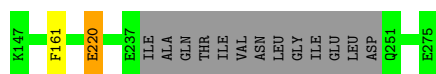
- Molecule 1: RsbR protein

Chain Z: 89% 10%



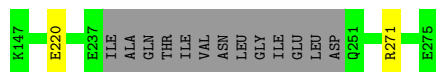
- Molecule 2: RsbR protein

Chain CB: 88% 10%



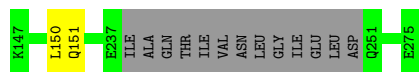
- Molecule 2: RsbR protein

Chain DB: 88% 10%



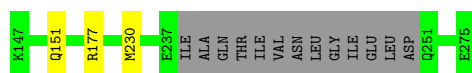
- Molecule 2: RsbR protein

Chain E: 88% 10%



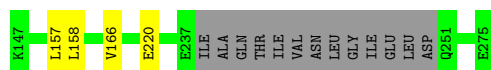
- Molecule 2: RsbR protein

Chain F: 88% 10%



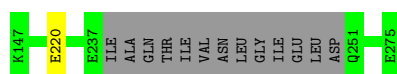
- Molecule 2: RsbR protein

Chain GB: 87% 10%



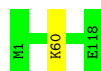
- Molecule 2: RsbR protein

Chain IB: 89% 10%



- Molecule 3: RsbS protein

Chain A: 99%



- Molecule 3: RsbS protein

Chain B: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain C: 98%



- Molecule 3: RsbS protein

Chain D: 98%



- Molecule 3: RsbS protein

Chain I: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain J:  99% .



- Molecule 3: RsbS protein

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain R:  100%

There are no outlier residues recorded for this chain.

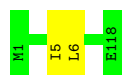
- Molecule 3: RsbS protein

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain a:  98% .



- Molecule 3: RsbS protein

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: RsbS protein

Chain d:  99% .



- Molecule 3: RsbS protein

Chain e:  98%



- Molecule 3: RsbS protein

Chain f:  99%



- Molecule 3: RsbS protein

Chain g:  98%



- Molecule 3: RsbS protein

Chain h:  99%



- Molecule 3: RsbS protein

Chain i:  97%



- Molecule 3: RsbS protein

Chain j:  99%

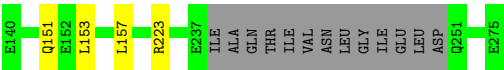
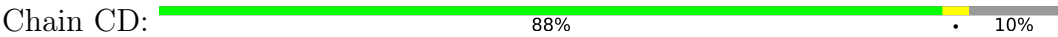


- Molecule 4: RsbR protein,RsbR protein

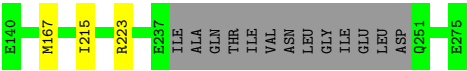
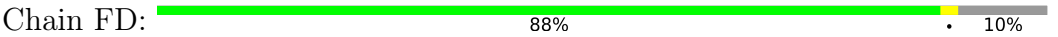
Chain AD:  99%



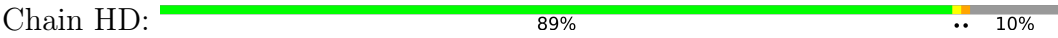
- Molecule 5: RsbR protein



- Molecule 5: RsbR protein



- Molecule 5: RsbR protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78000	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 ($e^-/\text{\AA}^2$)	2.25	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	AB	0.30	0/881	0.65	0/1193
1	BC	0.28	0/877	0.65	0/1188
1	DC	0.28	0/881	0.66	1/1193 (0.1%)
1	EB	0.29	0/881	0.63	0/1193
1	FA	0.30	0/877	0.60	1/1188 (0.1%)
1	FB	0.29	0/881	0.61	0/1193
1	FC	0.27	0/881	0.64	0/1193
1	GC	0.27	0/881	0.61	0/1193
1	HC	0.29	0/877	0.63	1/1188 (0.1%)
1	IC	0.28	0/881	0.64	1/1193 (0.1%)
1	K	0.28	0/881	0.64	0/1193
1	KB	0.30	0/881	0.61	0/1193
1	L	0.27	0/881	0.58	0/1193
1	LB	0.28	0/881	0.63	0/1193
1	M	0.27	0/877	0.66	1/1188 (0.1%)
1	OB	0.30	0/881	0.66	2/1193 (0.2%)
1	P	0.27	0/881	0.60	0/1193
1	PB	0.27	0/881	0.60	0/1193
1	Q	0.31	0/877	0.63	1/1189 (0.1%)
1	SB	0.28	0/881	0.60	0/1193
1	T	0.30	0/873	0.64	1/1185 (0.1%)
1	TB	0.29	0/881	0.65	0/1193
1	U	0.29	0/881	0.63	0/1193
1	UB	0.30	0/875	0.64	1/1186 (0.1%)
1	V	0.29	0/877	0.58	0/1189
1	VB	0.28	0/881	0.66	1/1193 (0.1%)
1	W	0.28	0/881	0.62	0/1193
1	X	0.29	0/871	0.68	1/1181 (0.1%)
1	Y	0.29	0/881	0.62	0/1193
1	Z	0.29	0/881	0.63	1/1193 (0.1%)
2	CB	0.29	0/890	0.63	0/1204
2	DB	0.27	0/890	0.62	0/1204
2	E	0.27	0/890	0.61	0/1204
2	F	0.27	0/890	0.61	0/1204

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	GB	0.29	0/890	0.65	0/1204
2	IB	0.27	0/890	0.59	0/1204
3	A	0.27	0/881	0.55	0/1188
3	B	0.26	0/881	0.51	0/1188
3	C	0.26	0/881	0.49	0/1188
3	D	0.28	0/881	0.59	1/1188 (0.1%)
3	I	0.27	0/881	0.56	0/1188
3	J	0.26	0/881	0.51	0/1188
3	N	0.27	0/881	0.56	0/1188
3	O	0.26	0/881	0.51	0/1188
3	R	0.26	0/877	0.52	0/1184
3	S	0.26	0/877	0.51	0/1184
3	a	0.26	0/877	0.53	0/1184
3	b	0.25	0/877	0.49	0/1184
3	c	0.26	0/881	0.51	0/1188
3	d	0.26	0/878	0.56	1/1185 (0.1%)
3	e	0.26	0/874	0.51	0/1180
3	f	0.27	0/881	0.55	1/1188 (0.1%)
3	g	0.27	0/881	0.51	0/1188
3	h	0.27	0/877	0.52	0/1184
3	i	0.27	0/878	0.56	0/1184
3	j	0.26	0/877	0.52	1/1184 (0.1%)
4	AD	0.28	0/941	0.64	0/1274
5	CD	0.27	0/941	0.63	1/1273 (0.1%)
5	FD	0.27	0/933	0.62	0/1265
5	HD	0.27	0/935	0.68	1/1264 (0.1%)
All	All	0.28	0/53055	0.60	19/71756 (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	AB	0	2
1	DC	0	1
1	FA	0	1
1	FB	0	2
1	FC	0	1
1	HC	0	2
1	IC	0	1
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	KB	0	2
1	L	0	1
1	P	0	2
1	PB	0	1
1	Q	0	1
1	TB	0	1
1	U	0	1
1	UB	0	1
1	VB	0	1
1	W	0	2
2	CB	0	1
2	DB	0	1
2	E	0	1
2	F	0	1
2	GB	0	3
2	IB	0	1
3	a	0	1
3	e	0	1
4	AD	0	1
5	CD	0	2
5	HD	0	1
All	All	0	39

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	100	LEU	CA-CB-CG	7.72	133.06	115.30
5	CD	153	LEU	CA-CB-CG	7.59	132.77	115.30
5	HD	158	LEU	CA-CB-CG	7.58	132.72	115.30
1	UB	158	LEU	CA-CB-CG	7.10	131.64	115.30
1	OB	157	LEU	CA-CB-CG	6.34	129.88	115.30
1	X	219	SER	C-N-CA	5.78	136.16	121.70
1	Q	157	LEU	CA-CB-CG	5.77	128.57	115.30
1	VB	157	LEU	CA-CB-CG	5.72	128.46	115.30
3	D	92	LEU	CA-CB-CG	5.71	128.42	115.30
1	DC	157	LEU	CA-CB-CG	5.63	128.26	115.30
1	HC	157	LEU	CA-CB-CG	5.61	128.21	115.30
3	j	20	LEU	CA-CB-CG	5.60	128.18	115.30
1	M	153	LEU	CA-CB-CG	5.46	127.85	115.30
1	IC	157	LEU	CA-CB-CG	5.36	127.64	115.30
1	OB	156	PRO	C-N-CA	5.24	134.79	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	150	LEU	CA-CB-CG	5.15	127.14	115.30
3	f	6	LEU	CA-CB-CG	5.10	127.04	115.30
1	T	157	LEU	CA-CB-CG	5.04	126.88	115.30
1	FA	182	ILE	CG1-CB-CG2	-5.03	100.33	111.40

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	158	LEU	Peptide
1	AB	220	GLU	Peptide
4	AD	220	GLU	Peptide
2	CB	220	GLU	Peptide
5	CD	151	GLN	Peptide
5	CD	157	LEU	Peptide
2	DB	220	GLU	Peptide
1	DC	220	GLU	Peptide
2	E	150	LEU	Peptide
2	F	151	GLN	Peptide
1	FA	220	GLU	Peptide
1	FB	152	GLU	Peptide
1	FB	220	GLU	Peptide
1	FC	215	ILE	Peptide
2	GB	157	LEU	Peptide
2	GB	166	VAL	Peptide
2	GB	220	GLU	Peptide
1	HC	157	LEU	Peptide
1	HC	220	GLU	Peptide
5	HD	158	LEU	Peptide
2	IB	220	GLU	Peptide
1	IC	220	GLU	Peptide
1	K	151	GLN	Peptide
1	K	220	GLU	Peptide
1	KB	204	VAL	Peptide
1	KB	220	GLU	Peptide
1	L	220	GLU	Peptide
1	P	204	VAL	Peptide
1	P	220	GLU	Peptide
1	PB	157	LEU	Peptide
1	Q	204	VAL	Peptide
1	TB	220	GLU	Peptide
1	U	158	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	UB	220	GLU	Peptide
1	VB	220	GLU	Peptide
1	W	151	GLN	Peptide
1	W	156	PRO	Peptide
3	a	5	ILE	Peptide
3	e	5	ILE	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	AB	111/128 (87%)	95 (86%)	16 (14%)	0	100	100
1	BC	111/128 (87%)	91 (82%)	19 (17%)	1 (1%)	14	50
1	DC	111/128 (87%)	93 (84%)	17 (15%)	1 (1%)	14	50
1	EB	111/128 (87%)	90 (81%)	21 (19%)	0	100	100
1	FA	111/128 (87%)	83 (75%)	27 (24%)	1 (1%)	14	50
1	FB	111/128 (87%)	89 (80%)	22 (20%)	0	100	100
1	FC	111/128 (87%)	87 (78%)	23 (21%)	1 (1%)	14	50
1	GC	111/128 (87%)	98 (88%)	13 (12%)	0	100	100
1	HC	111/128 (87%)	90 (81%)	20 (18%)	1 (1%)	14	50
1	IC	111/128 (87%)	88 (79%)	22 (20%)	1 (1%)	14	50
1	K	111/128 (87%)	88 (79%)	23 (21%)	0	100	100
1	KB	111/128 (87%)	93 (84%)	18 (16%)	0	100	100
1	L	111/128 (87%)	90 (81%)	21 (19%)	0	100	100
1	LB	111/128 (87%)	91 (82%)	18 (16%)	2 (2%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	111/128 (87%)	88 (79%)	23 (21%)	0	100	100
1	OB	111/128 (87%)	94 (85%)	16 (14%)	1 (1%)	14	50
1	P	111/128 (87%)	96 (86%)	15 (14%)	0	100	100
1	PB	111/128 (87%)	93 (84%)	18 (16%)	0	100	100
1	Q	111/128 (87%)	89 (80%)	22 (20%)	0	100	100
1	SB	111/128 (87%)	94 (85%)	16 (14%)	1 (1%)	14	50
1	T	111/128 (87%)	93 (84%)	17 (15%)	1 (1%)	14	50
1	TB	111/128 (87%)	92 (83%)	19 (17%)	0	100	100
1	U	111/128 (87%)	94 (85%)	17 (15%)	0	100	100
1	UB	111/128 (87%)	92 (83%)	18 (16%)	1 (1%)	14	50
1	V	111/128 (87%)	91 (82%)	19 (17%)	1 (1%)	14	50
1	VB	111/128 (87%)	89 (80%)	21 (19%)	1 (1%)	14	50
1	W	111/128 (87%)	92 (83%)	18 (16%)	1 (1%)	14	50
1	X	111/128 (87%)	93 (84%)	18 (16%)	0	100	100
1	Y	111/128 (87%)	93 (84%)	18 (16%)	0	100	100
1	Z	111/128 (87%)	92 (83%)	19 (17%)	0	100	100
2	CB	112/129 (87%)	96 (86%)	16 (14%)	0	100	100
2	DB	112/129 (87%)	91 (81%)	21 (19%)	0	100	100
2	E	112/129 (87%)	87 (78%)	24 (21%)	1 (1%)	14	50
2	F	112/129 (87%)	93 (83%)	19 (17%)	0	100	100
2	GB	112/129 (87%)	97 (87%)	14 (12%)	1 (1%)	14	50
2	IB	112/129 (87%)	93 (83%)	19 (17%)	0	100	100
3	A	116/118 (98%)	100 (86%)	16 (14%)	0	100	100
3	B	116/118 (98%)	103 (89%)	13 (11%)	0	100	100
3	C	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	D	116/118 (98%)	101 (87%)	15 (13%)	0	100	100
3	I	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
3	J	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
3	N	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
3	O	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
3	R	116/118 (98%)	105 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	116/118 (98%)	100 (86%)	16 (14%)	0	100	100
3	a	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
3	b	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
3	c	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	d	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	e	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
3	f	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	g	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
3	h	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
3	i	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
3	j	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
4	AD	119/123 (97%)	99 (83%)	20 (17%)	0	100	100
5	CD	119/136 (88%)	104 (87%)	15 (13%)	0	100	100
5	FD	119/136 (88%)	98 (82%)	21 (18%)	0	100	100
5	HD	115/136 (85%)	93 (81%)	21 (18%)	1 (1%)	14	50
All	All	6794/7505 (90%)	5785 (85%)	991 (15%)	18 (0%)	38	72

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	HD	159	PRO
1	BC	203	GLY
1	FC	197	VAL
1	UB	157	LEU
1	W	157	LEU
1	FA	157	LEU
2	GB	158	LEU
1	LB	161	PHE
1	V	157	LEU
2	E	151	GLN
1	HC	158	LEU
1	LB	160	ILE
1	OB	158	LEU
1	SB	156	PRO
1	IC	158	LEU
1	DC	158	LEU
1	T	158	LEU

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Mol	Chain	Res	Type
1	VB	158	LEU

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	AB	100/111 (90%)	100 (100%)	0	100	100
1	BC	99/111 (89%)	99 (100%)	0	100	100
1	DC	100/111 (90%)	100 (100%)	0	100	100
1	EB	100/111 (90%)	100 (100%)	0	100	100
1	FA	99/111 (89%)	98 (99%)	1 (1%)	73	82
1	FB	100/111 (90%)	99 (99%)	1 (1%)	73	82
1	FC	100/111 (90%)	100 (100%)	0	100	100
1	GC	100/111 (90%)	100 (100%)	0	100	100
1	HC	99/111 (89%)	99 (100%)	0	100	100
1	IC	100/111 (90%)	99 (99%)	1 (1%)	73	82
1	K	100/111 (90%)	99 (99%)	1 (1%)	73	82
1	KB	100/111 (90%)	100 (100%)	0	100	100
1	L	100/111 (90%)	99 (99%)	1 (1%)	73	82
1	LB	100/111 (90%)	99 (99%)	1 (1%)	73	82
1	M	99/111 (89%)	98 (99%)	1 (1%)	73	82
1	OB	100/111 (90%)	99 (99%)	1 (1%)	73	82
1	P	100/111 (90%)	100 (100%)	0	100	100
1	PB	100/111 (90%)	100 (100%)	0	100	100
1	Q	99/111 (89%)	99 (100%)	0	100	100
1	SB	100/111 (90%)	100 (100%)	0	100	100
1	T	98/111 (88%)	98 (100%)	0	100	100
1	TB	100/111 (90%)	99 (99%)	1 (1%)	73	82
1	U	100/111 (90%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UB	99/111 (89%)	99 (100%)	0	100	100
1	V	99/111 (89%)	98 (99%)	1 (1%)	73	82
1	VB	100/111 (90%)	100 (100%)	0	100	100
1	W	100/111 (90%)	99 (99%)	1 (1%)	73	82
1	X	98/111 (88%)	95 (97%)	3 (3%)	35	56
1	Y	100/111 (90%)	98 (98%)	2 (2%)	50	69
1	Z	100/111 (90%)	100 (100%)	0	100	100
2	CB	101/112 (90%)	99 (98%)	2 (2%)	50	69
2	DB	101/112 (90%)	100 (99%)	1 (1%)	73	82
2	E	101/112 (90%)	101 (100%)	0	100	100
2	F	101/112 (90%)	99 (98%)	2 (2%)	50	69
2	GB	101/112 (90%)	101 (100%)	0	100	100
2	IB	101/112 (90%)	101 (100%)	0	100	100
3	A	99/100 (99%)	98 (99%)	1 (1%)	73	82
3	B	99/100 (99%)	99 (100%)	0	100	100
3	C	99/100 (99%)	97 (98%)	2 (2%)	50	69
3	D	99/100 (99%)	98 (99%)	1 (1%)	73	82
3	I	99/100 (99%)	99 (100%)	0	100	100
3	J	99/100 (99%)	98 (99%)	1 (1%)	73	82
3	N	99/100 (99%)	99 (100%)	0	100	100
3	O	99/100 (99%)	99 (100%)	0	100	100
3	R	98/100 (98%)	98 (100%)	0	100	100
3	S	98/100 (98%)	98 (100%)	0	100	100
3	a	98/100 (98%)	97 (99%)	1 (1%)	73	82
3	b	98/100 (98%)	98 (100%)	0	100	100
3	c	99/100 (99%)	99 (100%)	0	100	100
3	d	98/100 (98%)	98 (100%)	0	100	100
3	e	97/100 (97%)	96 (99%)	1 (1%)	73	82
3	f	99/100 (99%)	99 (100%)	0	100	100
3	g	99/100 (99%)	97 (98%)	2 (2%)	50	69
3	h	98/100 (98%)	97 (99%)	1 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	i	98/100 (98%)	95 (97%)	3 (3%)	35	56
3	j	98/100 (98%)	98 (100%)	0	100	100
4	AD	107/108 (99%)	107 (100%)	0	100	100
5	CD	107/119 (90%)	106 (99%)	1 (1%)	75	83
5	FD	105/119 (88%)	102 (97%)	3 (3%)	37	58
5	HD	106/119 (89%)	106 (100%)	0	100	100
All	All	5990/6467 (93%)	5952 (99%)	38 (1%)	82	88

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CB	161	PHE
2	CB	220	GLU
2	DB	271	ARG
2	F	177	ARG
2	F	230	MET
1	FA	259	LYS
1	FB	269	THR
1	IC	204	VAL
1	K	152	GLU
1	L	197	VAL
1	LB	271	ARG
1	M	191	LYS
1	OB	191	LYS
1	TB	271	ARG
1	V	259	LYS
1	W	157	LEU
1	X	215	ILE
1	X	235	ARG
1	X	255	THR
1	Y	157	LEU
1	Y	271	ARG
3	A	60	LYS
3	C	6	LEU
3	C	28	PHE
3	D	28	PHE
3	J	6	LEU
3	a	6	LEU
3	e	6	LEU
3	g	6	LEU

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Mol	Chain	Res	Type
3	g	28	PHE
3	h	6	LEU
3	i	6	LEU
3	i	23	HIS
3	i	60	LYS
5	CD	223	ARG
5	FD	167	MET
5	FD	215	ILE
5	FD	223	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	217	GLN
1	BC	228	GLN
1	DC	151	GLN
1	DC	217	GLN
2	F	151	GLN
1	FA	192	ASN
1	FA	214	HIS
1	FC	192	ASN
1	K	256	ASN
1	KB	228	GLN
1	KB	256	ASN
1	M	214	HIS
1	P	192	ASN
1	PB	256	ASN
1	SB	214	HIS
1	SB	256	ASN
1	TB	228	GLN
1	UB	192	ASN
1	W	256	ASN
1	X	214	HIS
1	X	228	GLN
1	Y	256	ASN
1	Z	151	GLN
3	A	17	GLN
3	A	29	GLN
3	I	17	GLN
3	b	82	GLN
3	d	37	HIS
3	e	29	GLN

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Mol	Chain	Res	Type
3	f	37	HIS
3	h	29	GLN
3	i	29	GLN
4	AD	146	GLN
5	CD	146	GLN
5	CD	192	ASN
5	CD	228	GLN
5	CD	256	ASN
5	FD	192	ASN
5	HD	146	GLN
5	HD	151	GLN
5	HD	228	GLN

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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	HD	2
4	AD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AD	237:GLU	C	238:GLN	N	11.07
1	HD	220:GLU	C	221:ALA	N	5.35
1	HD	222:VAL	C	223:ARG	N	3.25

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4508. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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 standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 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.