



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:13 PM UTC

PDB ID : 6Z5U / pdb_00006z5u
EMDB ID : EMD-11082
Title : Cryo-EM structure of the A. baumannii MlaBDEF complex bound to APPNHP
Authors : Mann, D.; Bergeron, J.R.C.
Deposited on : 2020-05-27
Resolution : 3.90 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:

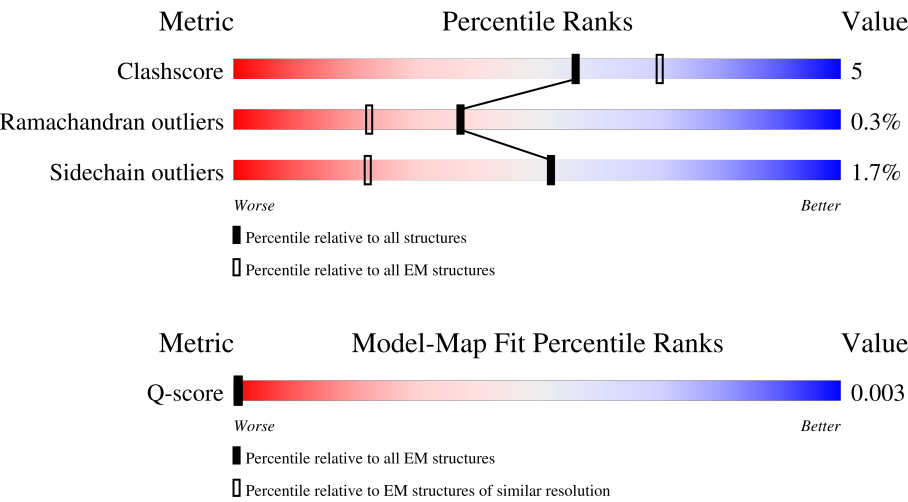
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	258	69% 93% 5% ..
1	B	258	70% 88% 10% ..
2	C	95	92% 79% 11% 8%
2	D	95	92% 85% 5% 8%

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Mol	Chain	Length	Quality of chain
3	E	226	
3	F	226	
3	G	226	
3	H	226	
3	I	226	
3	J	226	
4	K	276	
4	L	276	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17880 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 ABC transporter permease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	254	Total	C	N	O	S	0	0
			1886	1235	306	330	15		
1	B	254	Total	C	N	O	S	0	0
			1886	1235	306	330	15		

- Molecule 2 is a protein called Anti-sigma factor antagonist.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	87	Total	C	N	O	S	0	0
			696	449	120	125	2		
2	D	87	Total	C	N	O	S	0	0
			696	449	120	125	2		

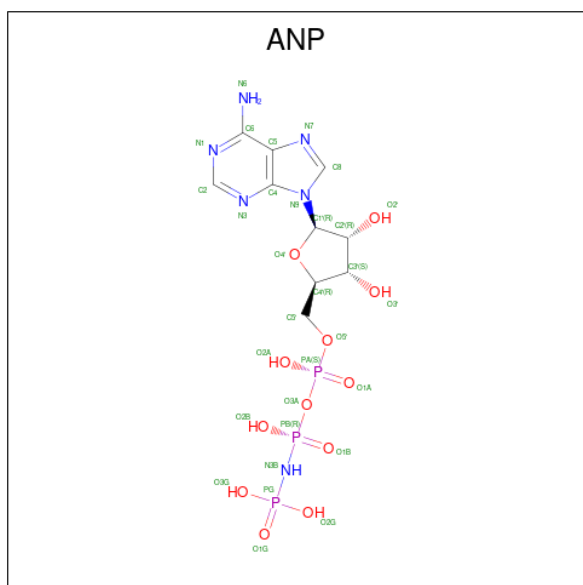
- Molecule 3 is a protein called MCE family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	190	Total	C	N	O	S	0	0
			1450	918	236	289	7		
3	G	191	Total	C	N	O	S	0	0
			1461	924	240	290	7		
3	H	189	Total	C	N	O	S	0	0
			1443	914	235	287	7		
3	I	193	Total	C	N	O	S	0	0
			1476	933	243	293	7		
3	J	190	Total	C	N	O	S	0	0
			1450	918	236	289	7		
3	F	193	Total	C	N	O	S	0	0
			1476	933	243	293	7		

- Molecule 4 is a protein called ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	253	Total	C	N	O	S	0	0
			1948	1233	335	372	8		
4	L	253	Total	C	N	O	S	0	0
			1948	1233	335	372	8		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
5	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	L	1	Total	C	N	O	P	0
			31	10	6	12	3	

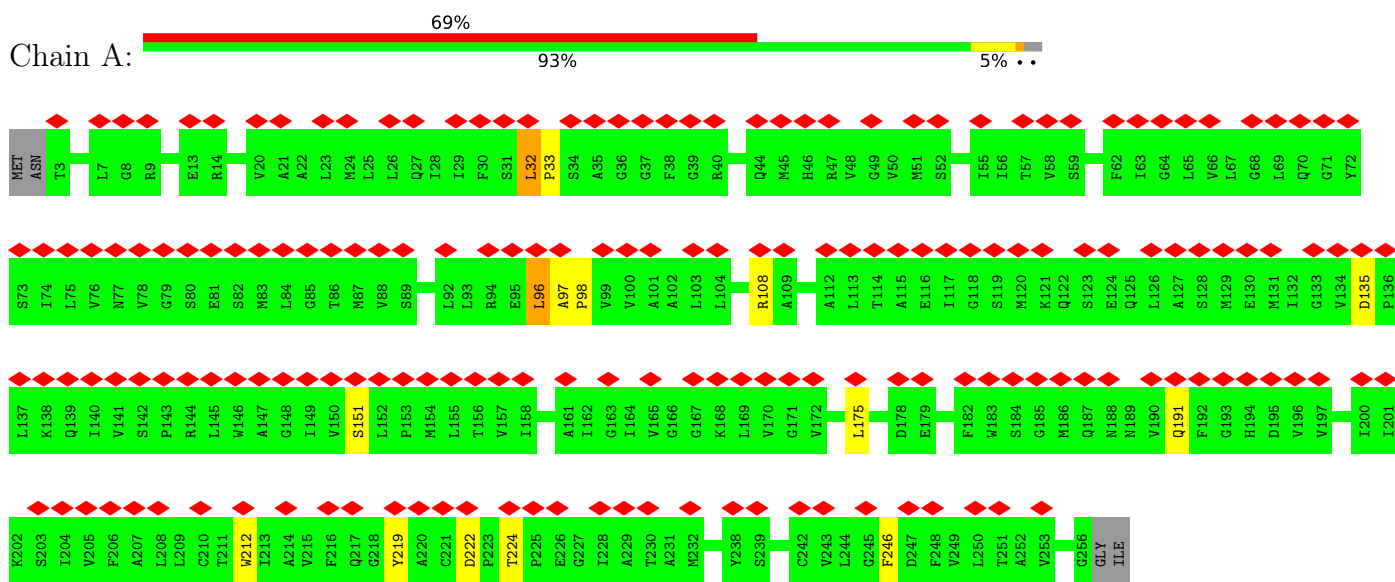
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	K	1	Total	Mg	0
			1	1	
6	L	1	Total	Mg	0
			1	1	

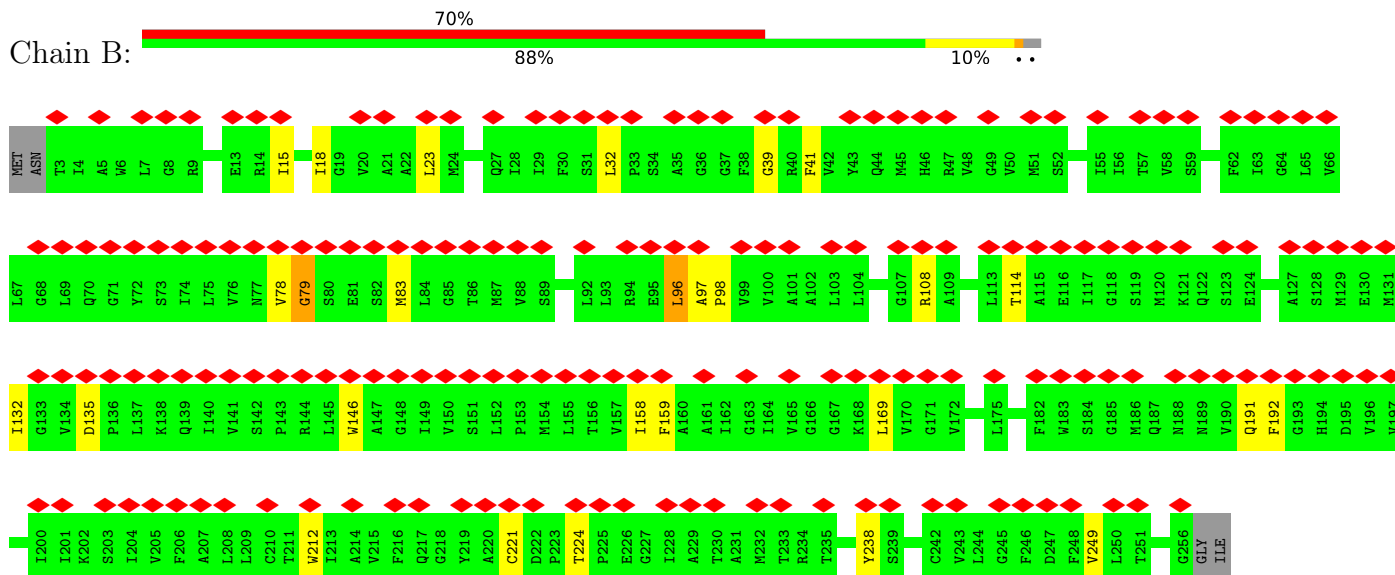
3 Residue-property plots

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

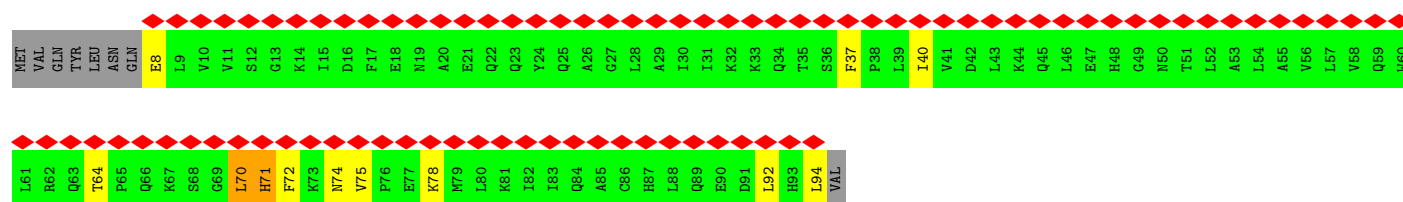
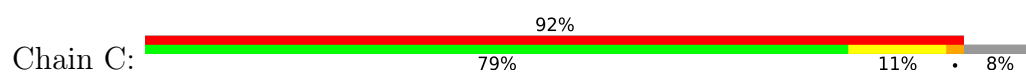
- Molecule 1: ABC transporter permease



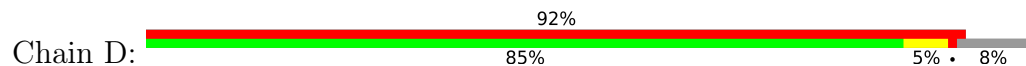
- Molecule 1: ABC transporter permease



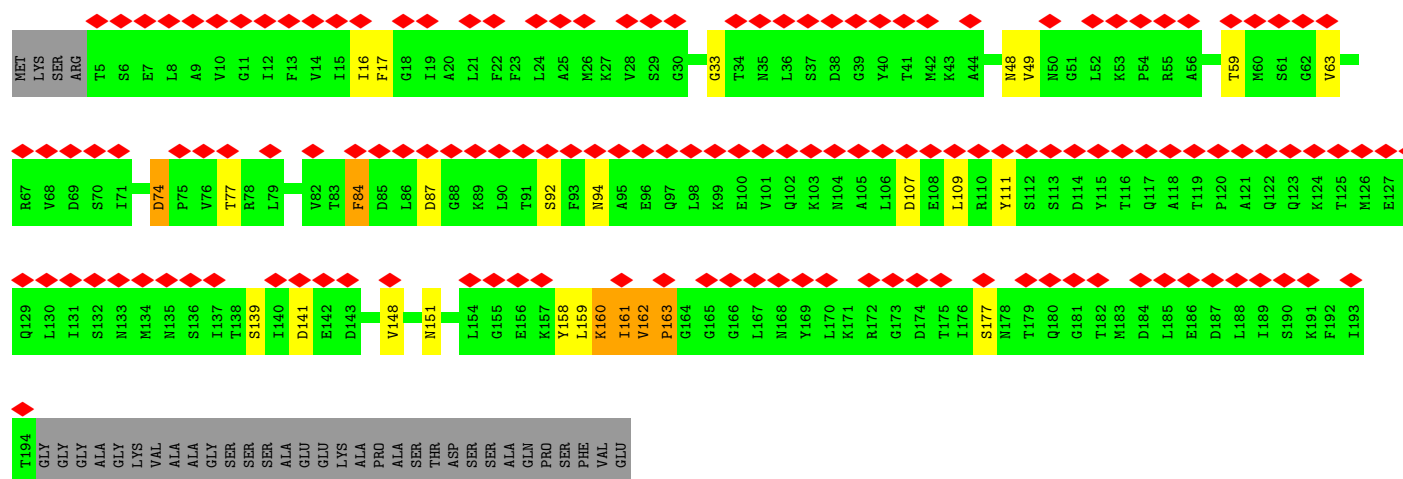
- Molecule 2: Anti-sigma factor antagonist



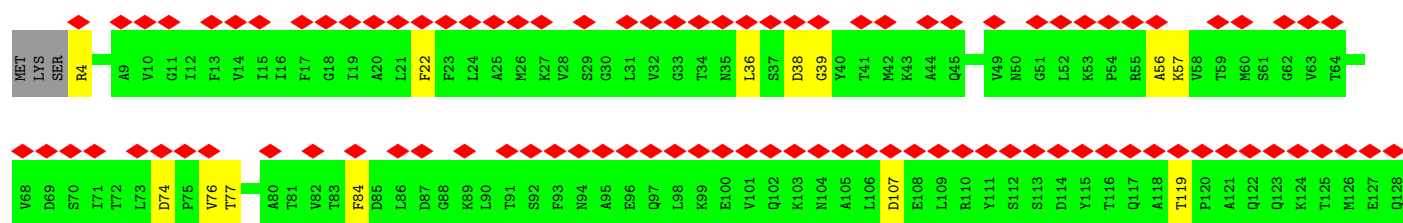
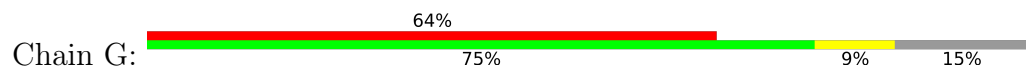
- Molecule 2: Anti-sigma factor antagonist

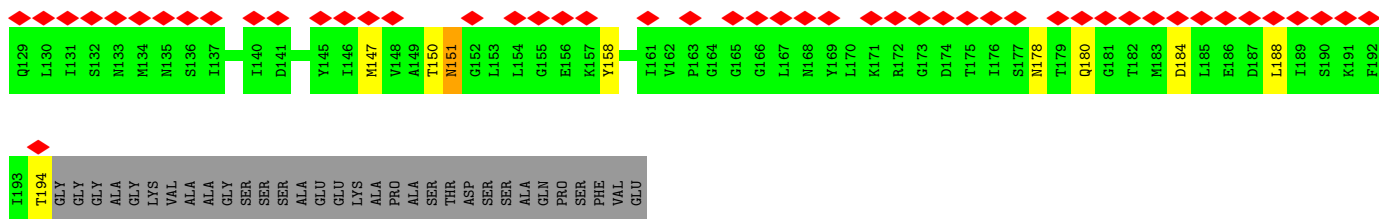


- Molecule 3: MCE family protein

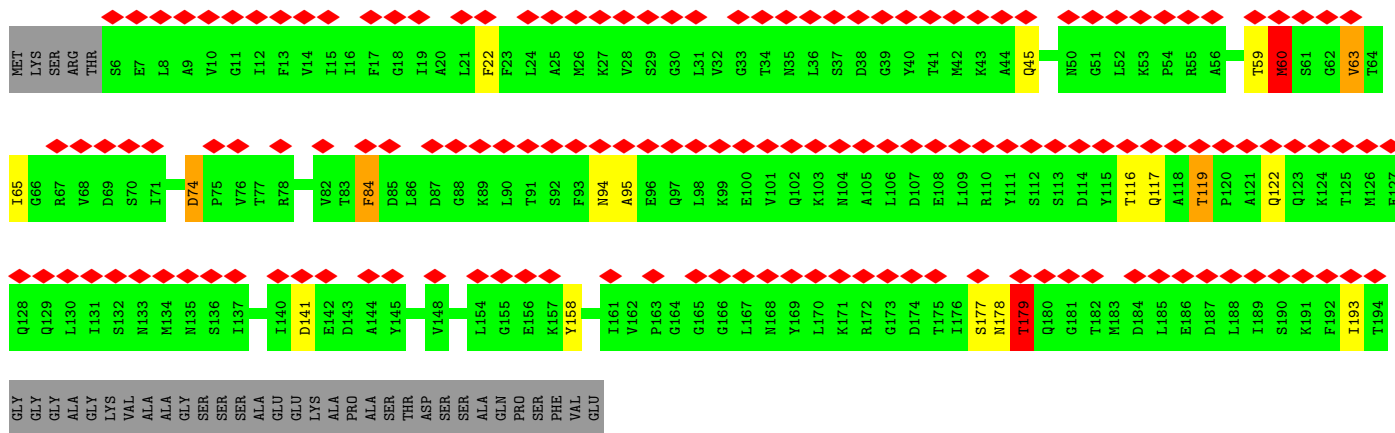
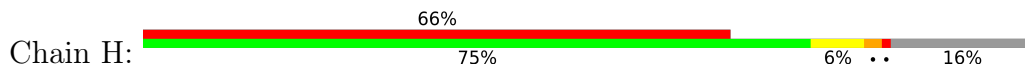


- Molecule 3: MCE family protein

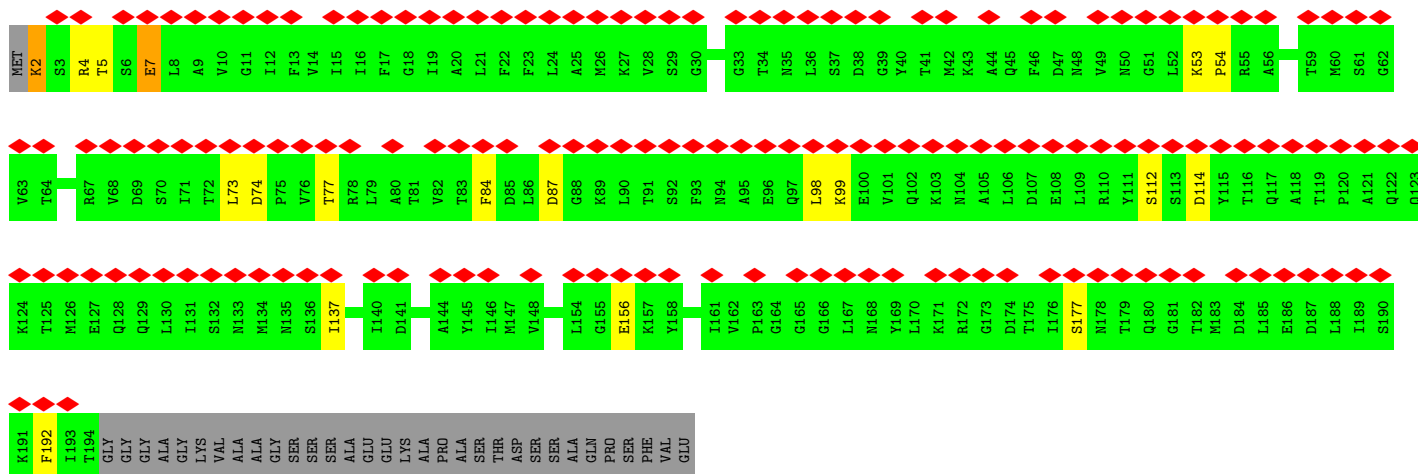
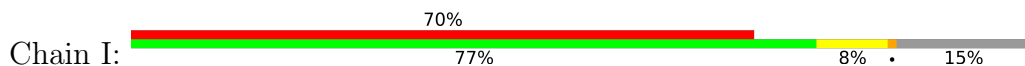




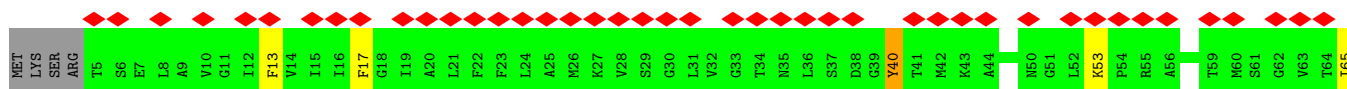
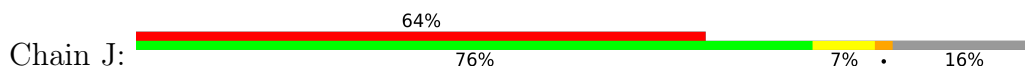
• Molecule 3: MCE family protein

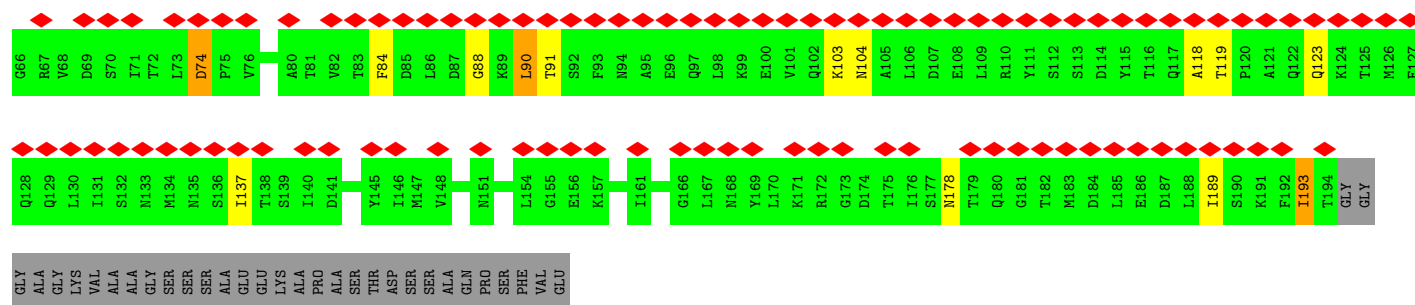


• Molecule 3: MCE family protein

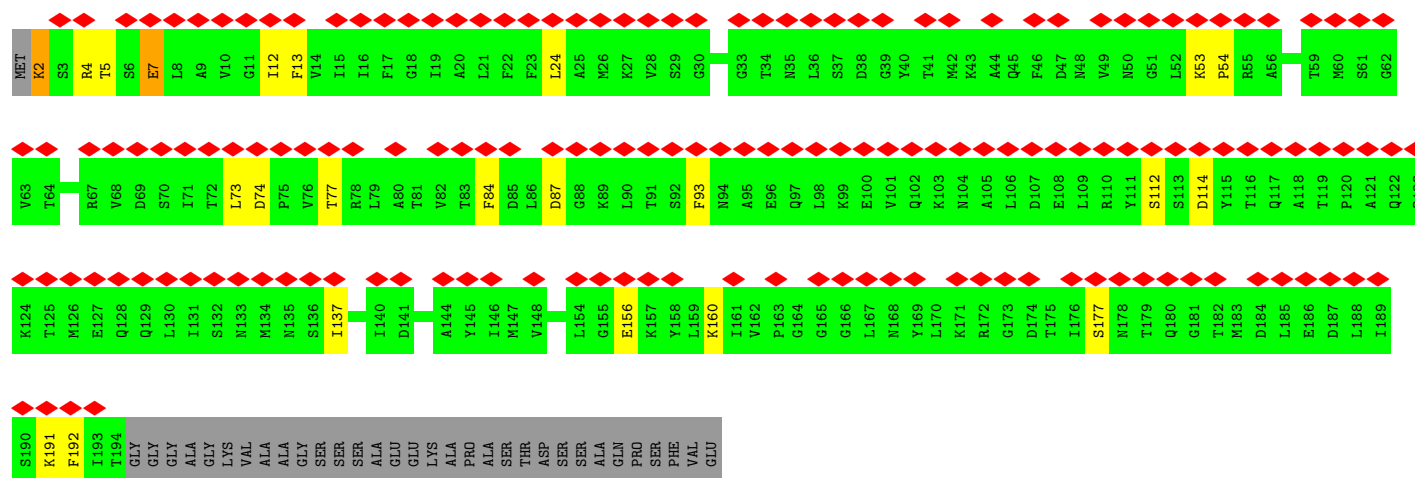
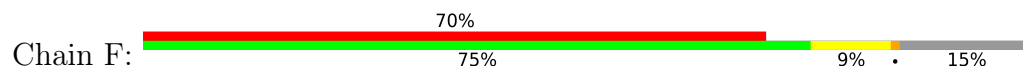


• Molecule 3: MCE family protein

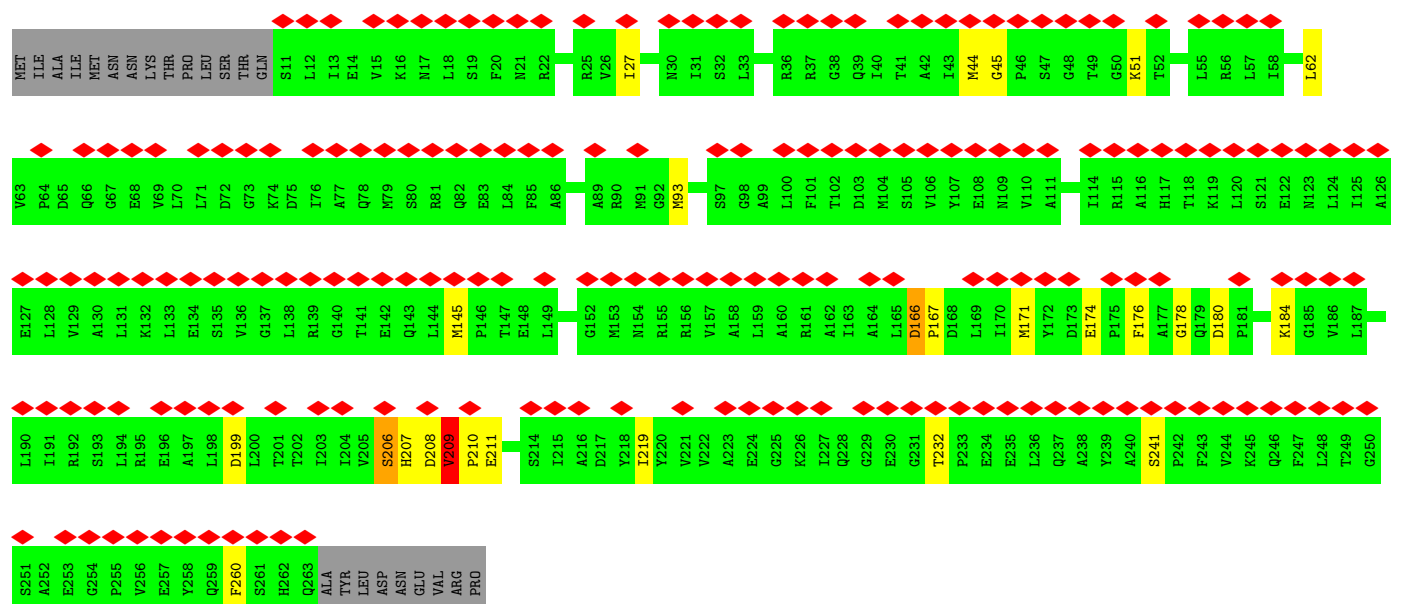
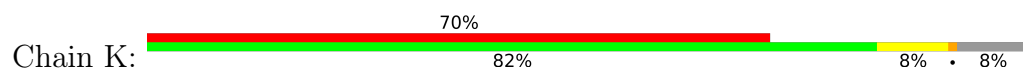




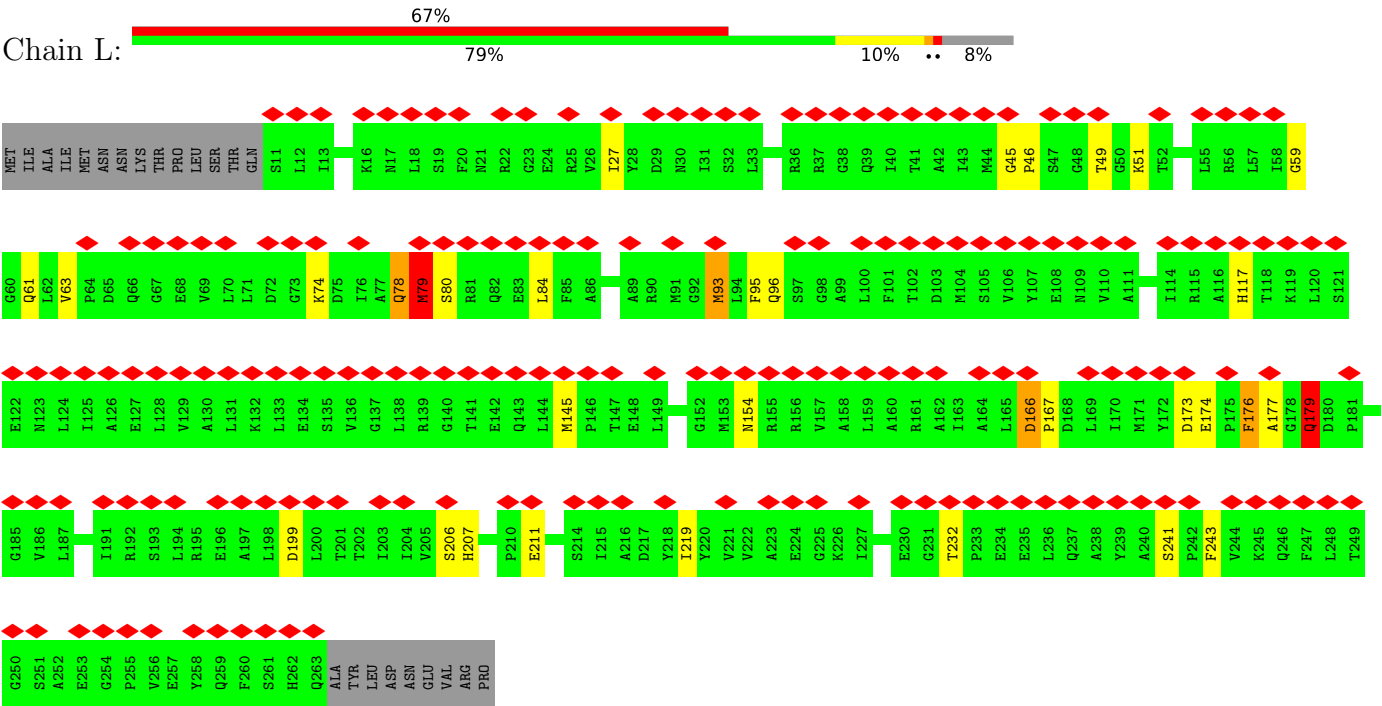
• Molecule 3: MCE family protein



• Molecule 4: ABC transporter ATP-binding protein



● Molecule 4: ABC transporter ATP-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93295	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.100	Depositor
Minimum map value	-2.040	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.458	Depositor
Map size ($\text{\AA}$)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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	1.24	1/1920 (0.1%)	1.36	16/2606 (0.6%)
1	B	1.26	3/1920 (0.2%)	1.36	15/2606 (0.6%)
2	C	0.92	1/708 (0.1%)	1.21	6/956 (0.6%)
2	D	0.95	1/708 (0.1%)	1.14	3/956 (0.3%)
3	E	1.06	0/1467	1.39	12/1983 (0.6%)
3	F	1.01	0/1493	1.31	9/2016 (0.4%)
3	G	1.03	1/1478 (0.1%)	1.34	10/1997 (0.5%)
3	H	1.10	2/1460 (0.1%)	1.37	11/1973 (0.6%)
3	I	1.01	0/1493	1.31	9/2016 (0.4%)
3	J	1.04	1/1467 (0.1%)	1.28	13/1983 (0.7%)
4	K	1.21	0/1977	1.33	19/2674 (0.7%)
4	L	1.22	4/1977 (0.2%)	1.36	23/2674 (0.9%)
All	All	1.12	14/18068 (0.1%)	1.33	146/24440 (0.6%)

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
3	E	0	1
3	F	0	1
3	H	0	2
3	I	0	1
4	L	0	1
All	All	0	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	207	HIS	CB-CG	-8.40	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	4	ARG	NE-CZ	6.84	1.40	1.33
3	J	40	TYR	CB-CG	-6.77	1.36	1.51
4	L	154	ASN	CB-CG	-5.76	1.37	1.52
1	B	238	TYR	CB-CG	-5.71	1.39	1.51
3	H	179	THR	CA-C	-5.63	1.45	1.52
4	L	117	HIS	CB-CG	-5.55	1.42	1.50
2	C	94	LEU	CB-CG	5.44	1.64	1.53
1	A	212	TRP	NE1-CE2	-5.38	1.31	1.37
2	D	94	LEU	CB-CG	5.34	1.64	1.53
3	H	141	ASP	CB-CG	-5.31	1.38	1.52
4	L	174	GLU	C-N	5.24	1.40	1.34
1	B	146	TRP	NE1-CE2	-5.16	1.31	1.37
1	B	212	TRP	NE1-CE2	-5.07	1.31	1.37

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	206	SER	N-CA-C	10.88	122.23	108.19
3	H	74	ASP	CA-C-N	8.86	128.59	119.56
3	H	74	ASP	C-N-CA	8.86	128.59	119.56
3	G	77	THR	N-CA-C	-8.50	103.34	114.31
4	L	27	ILE	N-CA-C	-8.20	104.76	111.81
3	H	22	PHE	CA-CB-CG	-8.16	105.64	113.80
1	A	32	LEU	CA-C-N	8.04	127.76	119.56
1	A	32	LEU	C-N-CA	8.04	127.76	119.56
3	G	84	PHE	CA-CB-CG	8.02	121.82	113.80
4	L	232	THR	N-CA-C	-7.97	98.43	110.07
1	B	41	PHE	CA-CB-CG	7.85	121.65	113.80
3	E	74	ASP	CA-C-N	7.78	127.96	119.87
3	E	74	ASP	C-N-CA	7.78	127.96	119.87
3	I	114	ASP	N-CA-C	7.66	121.22	112.57
3	F	114	ASP	N-CA-C	7.66	121.22	112.57
3	H	117	GLN	N-CA-C	-7.62	104.51	113.88
3	J	123	GLN	N-CA-C	-7.59	102.36	111.69
3	H	177	SER	N-CA-C	7.49	122.15	112.26
1	A	219	TYR	N-CA-C	7.47	119.06	111.07
3	H	179	THR	N-CA-C	7.36	120.25	109.07
4	L	241	SER	N-CA-C	-7.34	100.31	109.64
4	L	174	GLU	CA-C-N	7.19	126.82	119.56
4	L	174	GLU	C-N-CA	7.19	126.82	119.56
3	G	74	ASP	CA-C-N	7.14	127.30	119.87
3	G	74	ASP	C-N-CA	7.14	127.30	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	119	THR	CA-C-N	7.14	126.84	119.56
3	J	119	THR	C-N-CA	7.14	126.84	119.56
3	I	137	ILE	CB-CA-C	-7.08	102.08	111.70
3	F	137	ILE	CB-CA-C	-7.08	102.08	111.70
3	J	74	ASP	CA-C-N	7.06	127.22	119.87
3	J	74	ASP	C-N-CA	7.06	127.22	119.87
4	L	166	ASP	CA-C-N	7.02	126.98	120.03
4	L	166	ASP	C-N-CA	7.02	126.98	120.03
3	G	22	PHE	N-CA-C	-6.98	103.61	111.14
3	E	139	SER	N-CA-C	6.89	121.27	112.86
4	L	145	MET	CA-C-N	6.89	126.58	119.56
4	L	145	MET	C-N-CA	6.89	126.58	119.56
2	D	64	THR	CA-C-N	6.83	127.39	119.47
2	D	64	THR	C-N-CA	6.83	127.39	119.47
3	E	92	SER	N-CA-C	6.80	121.80	112.90
3	E	77	THR	N-CA-C	-6.78	105.57	114.31
3	I	77	THR	N-CA-C	-6.78	105.57	114.31
3	F	77	THR	N-CA-C	-6.78	105.57	114.31
4	K	219	ILE	N-CA-C	6.76	118.53	108.46
4	K	145	MET	CA-C-N	6.70	126.39	119.56
4	K	145	MET	C-N-CA	6.70	126.39	119.56
4	K	166	ASP	CA-C-N	6.68	126.64	120.03
4	K	166	ASP	C-N-CA	6.68	126.64	120.03
3	J	17	PHE	CA-CB-CG	-6.66	107.14	113.80
4	K	45	GLY	CA-C-N	6.66	126.64	119.78
4	K	45	GLY	C-N-CA	6.66	126.64	119.78
4	K	178	GLY	N-CA-C	-6.63	104.30	111.93
4	L	177	ALA	N-CA-C	6.63	118.16	111.07
3	G	151	ASN	N-CA-C	6.60	119.30	111.71
4	L	45	GLY	CA-C-N	6.59	126.57	119.78
4	L	45	GLY	C-N-CA	6.59	126.57	119.78
2	C	75	VAL	CA-C-N	6.57	126.55	119.78
2	C	75	VAL	C-N-CA	6.57	126.55	119.78
2	C	64	THR	CA-C-N	6.55	126.18	119.56
2	C	64	THR	C-N-CA	6.55	126.18	119.56
3	G	84	PHE	N-CA-CB	-6.47	101.00	110.84
4	K	232	THR	N-CA-C	-6.47	100.62	110.07
3	H	193	ILE	CA-C-N	6.33	133.10	121.70
3	H	193	ILE	C-N-CA	6.33	133.10	121.70
1	B	132	ILE	N-CA-C	-6.31	106.58	112.83
1	A	246	PHE	CA-CB-CG	-6.29	107.51	113.80
3	I	74	ASP	CA-C-N	6.25	126.38	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	74	ASP	C-N-CA	6.25	126.38	119.87
3	F	74	ASP	CA-C-N	6.25	126.38	119.87
3	F	74	ASP	C-N-CA	6.25	126.38	119.87
4	L	179	GLN	N-CA-C	6.24	116.09	107.73
3	J	137	ILE	N-CA-C	6.22	117.77	109.37
3	H	60	MET	N-CA-C	-6.20	98.30	108.41
3	J	53	LYS	CA-C-N	6.11	125.79	119.56
3	J	53	LYS	C-N-CA	6.11	125.79	119.56
3	E	109	LEU	N-CA-C	-6.10	102.32	110.55
4	L	176	PHE	CB-CA-C	-6.09	100.26	110.56
4	K	62	LEU	CA-C-N	-6.08	118.21	122.59
4	K	62	LEU	C-N-CA	-6.08	118.21	122.59
2	C	37	PHE	CA-C-N	6.08	126.04	119.78
2	C	37	PHE	C-N-CA	6.08	126.04	119.78
4	L	173	ASP	CA-C-N	6.05	128.91	123.10
4	L	173	ASP	C-N-CA	6.05	128.91	123.10
4	L	206	SER	N-CA-C	5.97	118.20	108.76
1	B	108	ARG	N-CA-C	5.94	117.75	111.28
3	I	137	ILE	N-CA-C	5.94	117.72	109.29
3	F	137	ILE	N-CA-C	5.94	117.72	109.29
3	H	84	PHE	CA-CB-CG	5.92	119.72	113.80
4	K	174	GLU	CA-C-N	5.91	125.53	119.56
4	K	174	GLU	C-N-CA	5.91	125.53	119.56
4	L	219	ILE	N-CA-C	5.90	116.36	108.11
1	A	222	ASP	CA-C-N	5.82	127.12	119.84
1	A	222	ASP	C-N-CA	5.82	127.12	119.84
4	L	63	VAL	CA-C-N	5.80	125.77	120.03
4	L	63	VAL	C-N-CA	5.80	125.77	120.03
1	A	135	ASP	CA-C-N	5.77	125.44	119.56
1	A	135	ASP	C-N-CA	5.77	125.44	119.56
3	E	48	ASN	N-CA-C	5.73	117.30	107.28
1	B	221	CYS	N-CA-C	5.71	117.31	111.14
1	B	224	THR	CA-C-N	5.66	126.03	119.47
1	B	224	THR	C-N-CA	5.66	126.03	119.47
1	A	224	THR	CA-C-N	5.64	126.01	119.47
1	A	224	THR	C-N-CA	5.64	126.01	119.47
3	E	107	ASP	CA-CB-CG	5.63	118.23	112.60
4	K	241	SER	N-CA-C	-5.61	102.04	109.84
2	D	48	HIS	N-CA-C	5.59	118.10	110.55
4	K	209	VAL	N-CA-C	5.59	120.96	108.88
1	A	191	GLN	N-CA-C	5.50	118.52	109.72
3	E	84	PHE	CA-CB-CG	5.48	119.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	178	ASN	N-CA-C	5.48	119.19	111.52
3	E	111	TYR	N-CA-C	-5.45	104.89	112.30
3	E	151	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	175	LEU	N-CA-C	5.39	119.49	113.02
3	G	107	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	135	ASP	CA-C-N	5.38	125.04	119.56
1	B	135	ASP	C-N-CA	5.38	125.04	119.56
1	B	39	GLY	N-CA-C	-5.37	108.76	114.67
4	K	260	PHE	N-CA-C	5.36	117.11	108.32
4	L	49	THR	CB-CA-C	-5.36	102.81	111.28
3	J	84	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	32	LEU	CA-C-N	5.33	125.02	119.64
1	B	32	LEU	C-N-CA	5.33	125.02	119.64
1	A	151	SER	N-CA-C	5.33	116.77	111.07
4	L	93	MET	N-CA-C	5.31	117.46	109.23
3	I	177	SER	N-CA-C	5.29	118.90	112.23
3	F	177	SER	N-CA-C	5.29	118.90	112.23
1	B	96	LEU	CA-C-N	-5.27	113.51	120.09
1	B	96	LEU	C-N-CA	-5.27	113.51	120.09
3	E	177	SER	N-CA-C	5.17	117.91	111.24
3	G	188	LEU	N-CA-C	-5.16	105.77	111.71
3	G	150	THR	O-C-N	-5.14	117.18	123.30
3	H	116	THR	N-CA-C	5.13	119.69	113.38
4	L	243	PHE	CA-CB-CG	-5.12	108.68	113.80
3	J	118	ALA	CA-C-N	5.10	130.88	121.70
3	J	118	ALA	C-N-CA	5.10	130.88	121.70
4	K	176	PHE	CA-CB-CG	-5.09	108.70	113.80
3	I	112	SER	N-CA-C	-5.08	105.83	112.23
3	F	112	SER	N-CA-C	-5.08	105.83	112.23
4	K	27	ILE	N-CA-C	-5.07	106.86	111.67
3	I	54	PRO	N-CA-C	-5.06	103.17	111.21
3	F	54	PRO	N-CA-C	-5.06	103.17	111.21
1	A	96	LEU	CA-C-N	-5.04	113.79	120.09
1	A	96	LEU	C-N-CA	-5.04	113.79	120.09
1	B	169	LEU	CA-C-N	-5.04	114.19	121.65
1	B	169	LEU	C-N-CA	-5.04	114.19	121.65
1	A	108	ARG	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	84	PHE	Sidechain
3	F	84	PHE	Sidechain
3	H	158	TYR	Sidechain
3	H	84	PHE	Sidechain
3	I	84	PHE	Sidechain
4	L	79	MET	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	1886	0	1976	5	0
1	B	1886	0	1976	39	0
2	C	696	0	723	6	0
2	D	696	0	723	3	0
3	E	1450	0	1477	18	0
3	F	1476	0	1508	49	0
3	G	1461	0	1489	9	0
3	H	1443	0	1470	19	0
3	I	1476	0	1508	15	0
3	J	1450	0	1477	15	0
4	K	1948	0	1985	15	0
4	L	1948	0	1985	31	0
5	K	31	0	13	0	0
5	L	31	0	13	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
All	All	17880	0	18323	177	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 5.

All (177) 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)
3:J:40:TYR:CE2	3:J:91:THR:HG21	1.25	1.62
3:J:40:TYR:HE2	3:J:91:THR:CG2	1.34	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:CG	3:F:12:ILE:HD13	1.68	1.23
1:B:23:LEU:HD21	3:F:12:ILE:CD1	1.67	1.22
1:B:18:ILE:CG2	3:F:13:PHE:HD1	1.55	1.19
3:G:184:ASP:OD2	3:F:160:LYS:NZ	1.74	1.19
1:B:23:LEU:HD11	3:F:12:ILE:CD1	1.75	1.16
1:B:23:LEU:HD11	3:F:12:ILE:HD12	1.22	1.14
3:H:60:MET:HB3	3:H:65:ILE:HD13	1.30	1.13
1:B:23:LEU:CG	3:F:12:ILE:CD1	2.26	1.11
1:B:23:LEU:CD2	3:F:12:ILE:CD1	2.29	1.11
1:B:23:LEU:HG	3:F:12:ILE:HD13	1.28	1.11
4:K:184:LYS:HD3	4:K:211:GLU:OE2	1.49	1.11
1:B:23:LEU:HD21	3:F:12:ILE:HD11	1.20	1.09
3:H:63:VAL:HG11	3:I:73:LEU:HB2	1.12	1.08
1:B:23:LEU:CD2	3:F:12:ILE:HD13	1.83	1.08
3:E:162:VAL:HG12	3:E:163:PRO:HD2	1.33	1.04
1:B:23:LEU:CD1	3:F:12:ILE:CD1	2.35	1.03
4:L:93:MET:CE	4:L:95:PHE:HE1	1.72	1.02
4:L:93:MET:HE2	4:L:95:PHE:HE1	1.21	1.01
3:H:119:THR:CG2	3:H:122:GLN:HG2	1.90	1.01
1:B:15:ILE:HG12	3:F:13:PHE:CE2	1.93	1.01
3:J:40:TYR:CE2	3:J:91:THR:CG2	2.21	1.01
1:B:18:ILE:CG2	3:F:13:PHE:CD1	2.44	1.00
3:H:119:THR:HG21	3:H:122:GLN:CG	1.91	1.00
3:J:189:ILE:O	3:J:193:ILE:HG22	1.60	1.00
3:J:40:TYR:CZ	3:J:91:THR:HG21	1.98	0.98
3:J:88:GLY:HA2	3:J:91:THR:HG22	1.45	0.97
3:H:63:VAL:HG11	3:I:73:LEU:CB	1.93	0.97
4:L:93:MET:HE2	4:L:95:PHE:CE1	1.99	0.96
1:B:23:LEU:CD1	3:F:12:ILE:HD12	1.95	0.96
3:E:59:THR:O	3:E:161:ILE:HG22	1.65	0.96
1:B:18:ILE:HG21	3:F:13:PHE:HD1	1.32	0.94
4:K:51:LYS:NZ	4:K:207:HIS:HE1	1.66	0.93
3:H:119:THR:CG2	3:H:122:GLN:CG	2.45	0.93
3:H:63:VAL:CG1	3:I:73:LEU:HB2	1.97	0.92
3:H:119:THR:HG22	3:H:122:GLN:HG2	1.50	0.92
1:B:249:VAL:CG2	3:F:24:LEU:HD13	2.01	0.90
3:J:88:GLY:O	3:J:91:THR:O	1.89	0.89
1:B:15:ILE:CG1	3:F:13:PHE:CE2	2.56	0.89
1:B:18:ILE:HG21	3:F:13:PHE:CD1	2.08	0.88
3:H:119:THR:HG21	3:H:122:GLN:HG3	1.53	0.88
4:L:93:MET:CE	4:L:95:PHE:CE1	2.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:LYS:O	3:F:2:LYS:NZ	2.08	0.87
4:L:176:PHE:HE2	4:L:211:GLU:HB3	1.39	0.87
3:I:2:LYS:O	3:I:2:LYS:NZ	2.08	0.85
1:B:23:LEU:CD2	3:F:12:ILE:HD11	1.98	0.84
1:B:18:ILE:HG22	3:F:13:PHE:HD1	1.43	0.83
1:B:18:ILE:HG22	3:F:13:PHE:CD1	2.14	0.83
1:B:249:VAL:CG2	3:F:24:LEU:CD1	2.57	0.83
4:L:176:PHE:CE2	4:L:211:GLU:HB3	2.15	0.82
3:J:65:ILE:HD12	3:J:90:LEU:HB2	1.61	0.82
1:B:249:VAL:HG22	3:F:24:LEU:CD1	2.10	0.82
1:B:15:ILE:HG13	3:F:13:PHE:CG	2.13	0.81
1:B:249:VAL:HG21	3:F:24:LEU:HD13	1.61	0.81
4:K:51:LYS:NZ	4:K:207:HIS:CE1	2.50	0.80
3:H:60:MET:HB3	3:H:65:ILE:CD1	2.11	0.78
4:L:93:MET:SD	4:L:95:PHE:HE1	2.08	0.76
4:K:208:ASP:OD2	4:K:210:PRO:HD2	1.87	0.74
3:H:45:GLN:O	3:H:179:THR:HG21	1.87	0.74
4:L:74:LYS:HE2	4:L:79:MET:HB3	1.68	0.74
3:J:189:ILE:O	3:J:193:ILE:CG2	2.36	0.73
4:L:93:MET:SD	4:L:95:PHE:CE1	2.81	0.73
4:K:51:LYS:HZ3	4:K:207:HIS:HE1	1.36	0.73
3:E:160:LYS:NZ	3:E:160:LYS:HB3	2.02	0.73
4:L:79:MET:O	4:L:84:LEU:HD11	1.90	0.72
4:K:51:LYS:HZ1	4:K:207:HIS:HE1	1.37	0.71
3:I:2:LYS:HB2	3:I:2:LYS:HZ3	1.56	0.70
4:K:51:LYS:HZ3	4:K:207:HIS:CE1	2.08	0.70
1:B:23:LEU:HG	3:F:12:ILE:CD1	2.07	0.68
3:F:2:LYS:HB2	3:F:2:LYS:HZ3	1.57	0.68
3:E:162:VAL:HG12	3:E:163:PRO:CD	2.19	0.67
1:B:15:ILE:CG1	3:F:13:PHE:CD2	2.78	0.66
3:E:160:LYS:HB3	3:E:160:LYS:HZ1	1.60	0.65
3:I:192:PHE:CE2	3:J:193:ILE:O	2.50	0.65
4:L:179:GLN:HE21	4:L:179:GLN:HA	1.63	0.64
1:B:15:ILE:HG13	3:F:13:PHE:CD2	2.32	0.64
4:K:51:LYS:HZ1	4:K:207:HIS:CE1	2.15	0.63
4:L:176:PHE:CE2	4:L:211:GLU:CB	2.82	0.63
3:H:60:MET:CB	3:H:65:ILE:HD13	2.20	0.62
2:D:78:LYS:NZ	4:K:199:ASP:OD2	2.32	0.61
4:L:179:GLN:HA	4:L:179:GLN:NE2	2.15	0.61
1:A:32:LEU:N	1:A:33:PRO:CD	2.64	0.60
3:E:63:VAL:HG21	3:F:73:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HD11	3:F:12:ILE:HD11	1.76	0.59
2:C:78:LYS:NZ	4:L:199:ASP:OD2	2.34	0.59
3:E:162:VAL:CG1	3:E:163:PRO:HD2	2.21	0.59
1:B:15:ILE:CG1	3:F:13:PHE:CG	2.87	0.58
3:E:148:VAL:HA	3:E:159:LEU:HD23	1.85	0.58
3:G:147:MET:HG2	3:G:180:GLN:HG2	1.86	0.58
4:L:78:GLN:HB2	4:L:79:MET:HE3	1.84	0.58
3:E:161:ILE:O	3:E:161:ILE:HG12	2.02	0.58
3:H:119:THR:HG22	3:H:122:GLN:CG	2.22	0.58
3:H:119:THR:HG21	3:H:122:GLN:HG2	1.62	0.57
3:H:119:THR:HB	3:H:122:GLN:HB2	1.86	0.57
3:I:2:LYS:NZ	3:I:2:LYS:HB2	2.20	0.57
3:F:2:LYS:NZ	3:F:2:LYS:HB2	2.20	0.56
3:I:53:LYS:HE2	3:I:156:GLU:CB	2.36	0.56
2:C:72:PHE:HB2	2:C:92:LEU:O	2.06	0.55
3:E:161:ILE:O	3:E:161:ILE:HG23	2.04	0.55
3:F:53:LYS:HE2	3:F:156:GLU:CB	2.36	0.55
3:J:40:TYR:HE2	3:J:91:THR:CB	2.14	0.54
4:L:79:MET:HE3	4:L:79:MET:N	2.23	0.53
3:F:53:LYS:HE2	3:F:156:GLU:HB3	1.90	0.53
3:I:53:LYS:HE2	3:I:156:GLU:HB3	1.90	0.53
1:B:249:VAL:HG22	3:F:24:LEU:HD12	1.89	0.53
4:L:176:PHE:CD2	4:L:211:GLU:CB	2.91	0.53
1:A:32:LEU:H	1:A:33:PRO:HD3	1.75	0.52
3:G:57:LYS:HE2	3:G:151:ASN:ND2	2.24	0.52
3:I:7:GLU:HA	3:I:7:GLU:OE1	2.10	0.52
4:L:74:LYS:HE2	4:L:79:MET:CB	2.39	0.52
4:L:176:PHE:CD2	4:L:211:GLU:HB2	2.45	0.51
3:F:2:LYS:NZ	3:F:2:LYS:CB	2.73	0.51
3:F:7:GLU:HA	3:F:7:GLU:OE1	2.10	0.51
1:B:23:LEU:CD1	3:F:12:ILE:HD11	2.36	0.51
4:L:176:PHE:N	4:L:176:PHE:CD1	2.79	0.50
3:I:2:LYS:NZ	3:I:2:LYS:CB	2.73	0.50
3:I:7:GLU:N	3:I:7:GLU:CD	2.71	0.49
4:K:208:ASP:OD2	4:K:210:PRO:CD	2.60	0.49
3:E:160:LYS:NZ	3:E:160:LYS:CB	2.72	0.49
4:L:176:PHE:N	4:L:176:PHE:HD1	2.10	0.49
4:K:208:ASP:OD2	4:K:210:PRO:HG2	2.12	0.49
3:F:7:GLU:N	3:F:7:GLU:CD	2.71	0.49
4:K:44:MET:SD	4:K:209:VAL:CG2	3.01	0.48
4:L:176:PHE:HD2	4:L:211:GLU:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:194:THR:CG2	3:F:191:LYS:HG2	2.44	0.48
3:H:74:ASP:OD1	3:H:74:ASP:C	2.57	0.48
1:B:97:ALA:N	1:B:98:PRO:CD	2.79	0.46
3:E:87:ASP:OD1	3:E:87:ASP:C	2.58	0.46
2:C:70:LEU:HD13	2:C:92:LEU:C	2.41	0.46
2:D:64:THR:HB	2:D:65:PRO:HD3	1.97	0.46
1:A:32:LEU:N	1:A:33:PRO:HD3	2.31	0.46
3:G:194:THR:HG23	3:F:192:PHE:N	2.31	0.46
4:L:78:GLN:HB2	4:L:79:MET:CE	2.46	0.45
4:L:61:GLN:CD	4:L:61:GLN:N	2.75	0.45
1:B:96:LEU:O	1:B:97:ALA:C	2.56	0.45
4:K:180:ASP:C	4:K:180:ASP:OD1	2.59	0.45
4:L:80:SER:O	4:L:84:LEU:HG	2.17	0.45
3:J:13:PHE:CD1	3:J:13:PHE:C	2.88	0.45
3:J:74:ASP:C	3:J:74:ASP:OD1	2.60	0.45
2:D:65:PRO:HB3	2:D:70:LEU:HB2	1.98	0.44
2:C:70:LEU:HD13	2:C:92:LEU:HA	1.99	0.44
3:G:147:MET:HG2	3:G:180:GLN:CG	2.47	0.44
1:A:97:ALA:N	1:A:98:PRO:CD	2.80	0.44
1:B:15:ILE:HG12	3:F:13:PHE:CD2	2.45	0.44
3:E:94:ASN:OD1	3:E:94:ASN:C	2.61	0.44
3:F:87:ASP:OD1	3:F:87:ASP:C	2.57	0.44
3:E:162:VAL:HA	3:E:163:PRO:HD3	1.76	0.43
3:G:76:VAL:HG12	3:F:93:PHE:CE2	2.54	0.43
3:E:74:ASP:OD1	3:E:74:ASP:C	2.61	0.43
3:G:56:ALA:HB1	3:G:158:TYR:HA	1.99	0.43
3:H:119:THR:O	3:H:122:GLN:N	2.46	0.43
3:E:16:ILE:O	3:E:17:PHE:C	2.60	0.43
3:E:160:LYS:HZ1	3:E:162:VAL:HG22	1.83	0.43
4:L:166:ASP:N	4:L:167:PRO:CD	2.82	0.42
3:I:87:ASP:OD1	3:I:87:ASP:C	2.57	0.42
4:L:96:GLN:OE1	4:L:96:GLN:HA	2.19	0.42
1:B:79:GLY:O	1:B:83:MET:HB2	2.19	0.42
1:A:96:LEU:O	1:A:97:ALA:C	2.57	0.42
4:K:93:MET:HG2	4:K:171:MET:HB2	2.02	0.42
4:L:46:PRO:O	4:L:51:LYS:NZ	2.54	0.41
3:H:119:THR:CG2	3:H:122:GLN:CB	2.98	0.41
3:G:194:THR:HG22	3:F:191:LYS:CG	2.51	0.41
1:B:158:ILE:O	1:B:159:PHE:C	2.63	0.41
1:B:191:GLN:O	1:B:192:PHE:C	2.62	0.41
4:L:93:MET:SD	4:L:95:PHE:CZ	3.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:HG21	3:F:24:LEU:CD1	2.32	0.41
3:E:158:TYR:HE1	3:E:160:LYS:HG2	1.86	0.41
2:C:8:GLU:N	2:C:40:ILE:O	2.55	0.40
3:H:94:ASN:O	3:H:95:ALA:C	2.61	0.40
4:L:79:MET:O	4:L:84:LEU:CD1	2.65	0.40
3:I:98:LEU:O	3:I:99:LYS:C	2.64	0.40
3:I:192:PHE:HE2	3:J:193:ILE:O	2.01	0.40
3:J:103:LYS:O	3:J:104:ASN:C	2.61	0.40
2:C:71:HIS:HB2	2:C:74:ASN:HD22	1.86	0.40
4:K:166:ASP:N	4:K:167:PRO:CD	2.84	0.40
4:L:79:MET:HE3	4:L:79:MET:H	1.85	0.40

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	252/258 (98%)	248 (98%)	4 (2%)	0	100	100
1	B	252/258 (98%)	248 (98%)	3 (1%)	1 (0%)	30	64
2	C	85/95 (90%)	84 (99%)	1 (1%)	0	100	100
2	D	85/95 (90%)	83 (98%)	1 (1%)	1 (1%)	10	41
3	E	188/226 (83%)	179 (95%)	7 (4%)	2 (1%)	11	43
3	F	191/226 (84%)	188 (98%)	3 (2%)	0	100	100
3	G	189/226 (84%)	179 (95%)	8 (4%)	2 (1%)	11	43
3	H	187/226 (83%)	184 (98%)	3 (2%)	0	100	100
3	I	191/226 (84%)	188 (98%)	3 (2%)	0	100	100
3	J	188/226 (83%)	182 (97%)	6 (3%)	0	100	100
4	K	251/276 (91%)	246 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	251/276 (91%)	247 (98%)	3 (1%)	1 (0%)	30	64
All	All	2310/2614 (88%)	2256 (98%)	47 (2%)	7 (0%)	37	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	GLY
3	E	163	PRO
3	G	39	GLY
2	D	64	THR
3	E	33	GLY
3	G	119	THR
4	L	59	GLY

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	202/205 (98%)	202 (100%)	0	100	100
1	B	202/205 (98%)	200 (99%)	2 (1%)	68	75
2	C	77/85 (91%)	75 (97%)	2 (3%)	40	60
2	D	77/85 (91%)	77 (100%)	0	100	100
3	E	162/186 (87%)	157 (97%)	5 (3%)	35	57
3	F	165/186 (89%)	161 (98%)	4 (2%)	43	63
3	G	163/186 (88%)	160 (98%)	3 (2%)	51	67
3	H	161/186 (87%)	155 (96%)	6 (4%)	30	53
3	I	165/186 (89%)	161 (98%)	4 (2%)	43	63
3	J	162/186 (87%)	160 (99%)	2 (1%)	63	72
4	K	210/231 (91%)	208 (99%)	2 (1%)	68	75
4	L	210/231 (91%)	207 (99%)	3 (1%)	59	71
All	All	1956/2158 (91%)	1923 (98%)	33 (2%)	52	68

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	78	VAL
1	B	114	THR
2	C	70	LEU
2	C	71	HIS
3	E	49	VAL
3	E	141	ASP
3	E	160	LYS
3	E	161	ILE
3	E	162	VAL
3	G	36	LEU
3	G	38	ASP
3	G	178	ASN
3	H	59	THR
3	H	60	MET
3	H	63	VAL
3	H	119	THR
3	H	178	ASN
3	H	179	THR
3	I	2	LYS
3	I	4	ARG
3	I	5	THR
3	I	7	GLU
3	J	90	LEU
3	J	193	ILE
4	K	206	SER
4	K	209	VAL
4	L	78	GLN
4	L	79	MET
4	L	179	GLN
3	F	2	LYS
3	F	4	ARG
3	F	5	THR
3	F	7	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
2	C	74	ASN
2	C	93	HIS
3	G	178	ASN

Continued on next page...

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Mol	Chain	Res	Type
3	H	123	GLN
3	H	178	ASN
3	I	45	GLN
3	J	122	GLN
3	J	178	ASN
4	K	30	ASN
4	K	117	HIS
4	K	123	ASN
4	K	207	HIS
4	L	30	ASN
4	L	123	ASN
3	F	45	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ANP	L	302	6	33,33,33	2.76	13 (39%)	45,52,52	2.26	15 (33%)
5	ANP	K	301	6	33,33,33	2.34	13 (39%)	45,52,52	2.15	16 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	L	302	6	-	6/18/38/38	0/3/3/3
5	ANP	K	301	6	-	5/18/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302	ANP	PA-O3A	-8.15	1.50	1.59
5	L	302	ANP	PB-O3A	-8.00	1.49	1.59
5	K	301	ANP	PB-O3A	-5.58	1.52	1.59
5	L	302	ANP	C4-N3	4.64	1.43	1.34
5	K	301	ANP	PA-O3A	-4.39	1.54	1.59
5	K	301	ANP	C2-N3	4.38	1.41	1.33
5	K	301	ANP	C4-N3	4.22	1.42	1.34
5	L	302	ANP	C2-N3	4.22	1.41	1.33
5	K	301	ANP	C5-C4	4.16	1.46	1.39
5	L	302	ANP	C5-C4	3.87	1.46	1.39
5	K	301	ANP	C2-N1	3.53	1.40	1.33
5	L	302	ANP	C2-N1	3.01	1.39	1.33
5	K	301	ANP	C2'-C3'	2.94	1.61	1.53
5	L	302	ANP	C5-C6	2.72	1.48	1.41
5	L	302	ANP	C5-N7	-2.66	1.34	1.39
5	K	301	ANP	C5-N7	-2.57	1.34	1.39
5	L	302	ANP	PB-N3B	-2.56	1.56	1.63
5	K	301	ANP	PB-O2B	2.42	1.63	1.56
5	K	301	ANP	PG-N3B	-2.42	1.57	1.63
5	K	301	ANP	C5-C6	2.39	1.47	1.41
5	L	302	ANP	PG-N3B	-2.36	1.57	1.63
5	K	301	ANP	PG-O1G	2.34	1.49	1.46
5	K	301	ANP	PB-N3B	-2.31	1.57	1.63
5	L	302	ANP	O4'-C1'	2.23	1.47	1.42
5	L	302	ANP	C2'-C3'	2.12	1.59	1.53
5	L	302	ANP	C1'-N9	2.11	1.52	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	302	ANP	C5-C4-N3	-5.48	119.18	126.72
5	L	302	ANP	N3-C2-N1	-5.29	120.58	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	301	ANP	C5-C4-N3	-5.01	119.81	126.72
5	K	301	ANP	N3-C2-N1	-4.77	121.36	128.58
5	L	302	ANP	C4-N9-C1'	-4.58	115.92	126.63
5	K	301	ANP	O3G-PG-O1G	-4.11	103.14	113.45
5	L	302	ANP	O3A-PB-N3B	-3.97	95.58	106.59
5	K	301	ANP	N3-C4-N9	3.96	133.91	127.17
5	L	302	ANP	N3-C4-N9	3.84	133.69	127.17
5	L	302	ANP	C2-N3-C4	3.77	121.05	111.83
5	L	302	ANP	C4-C5-N7	-3.70	106.35	110.58
5	L	302	ANP	C5-N7-C8	3.58	109.08	103.45
5	K	301	ANP	C5-N7-C8	3.43	108.84	103.45
5	K	301	ANP	C2-N3-C4	3.36	120.05	111.83
5	K	301	ANP	C4-C5-N7	-3.35	106.75	110.58
5	K	301	ANP	C4-N9-C1'	-3.23	119.07	126.63
5	L	302	ANP	O4'-C1'-N9	3.11	114.06	108.09
5	K	301	ANP	O2B-PB-O3A	3.00	114.66	104.64
5	K	301	ANP	O4'-C1'-N9	2.89	113.64	108.09
5	K	301	ANP	O4'-C1'-C2'	-2.86	100.49	106.62
5	K	301	ANP	C1'-N9-C8	-2.85	120.77	127.09
5	K	301	ANP	O3A-PB-N3B	-2.81	98.80	106.59
5	L	302	ANP	C6-C5-N7	2.76	137.40	132.09
5	L	302	ANP	C1'-N9-C8	-2.63	121.27	127.09
5	K	301	ANP	O5'-C5'-C4'	2.54	117.65	108.99
5	L	302	ANP	O2B-PB-O3A	2.51	113.01	104.64
5	K	301	ANP	C6-C5-N7	2.31	136.55	132.09
5	L	302	ANP	PA-O5'-C5'	2.31	134.60	121.35
5	L	302	ANP	O3G-PG-O1G	-2.26	107.79	113.45
5	K	301	ANP	O4'-C4'-C3'	-2.15	100.89	105.15
5	L	302	ANP	C4-N9-C8	-2.08	103.55	105.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	301	ANP	PG-N3B-PB-O1B
5	K	301	ANP	PG-N3B-PB-O3A
5	L	302	ANP	PG-N3B-PB-O1B
5	L	302	ANP	PG-N3B-PB-O3A
5	L	302	ANP	C4'-C5'-O5'-PA
5	L	302	ANP	O4'-C4'-C5'-O5'
5	L	302	ANP	C3'-C4'-C5'-O5'
5	K	301	ANP	C4'-C5'-O5'-PA

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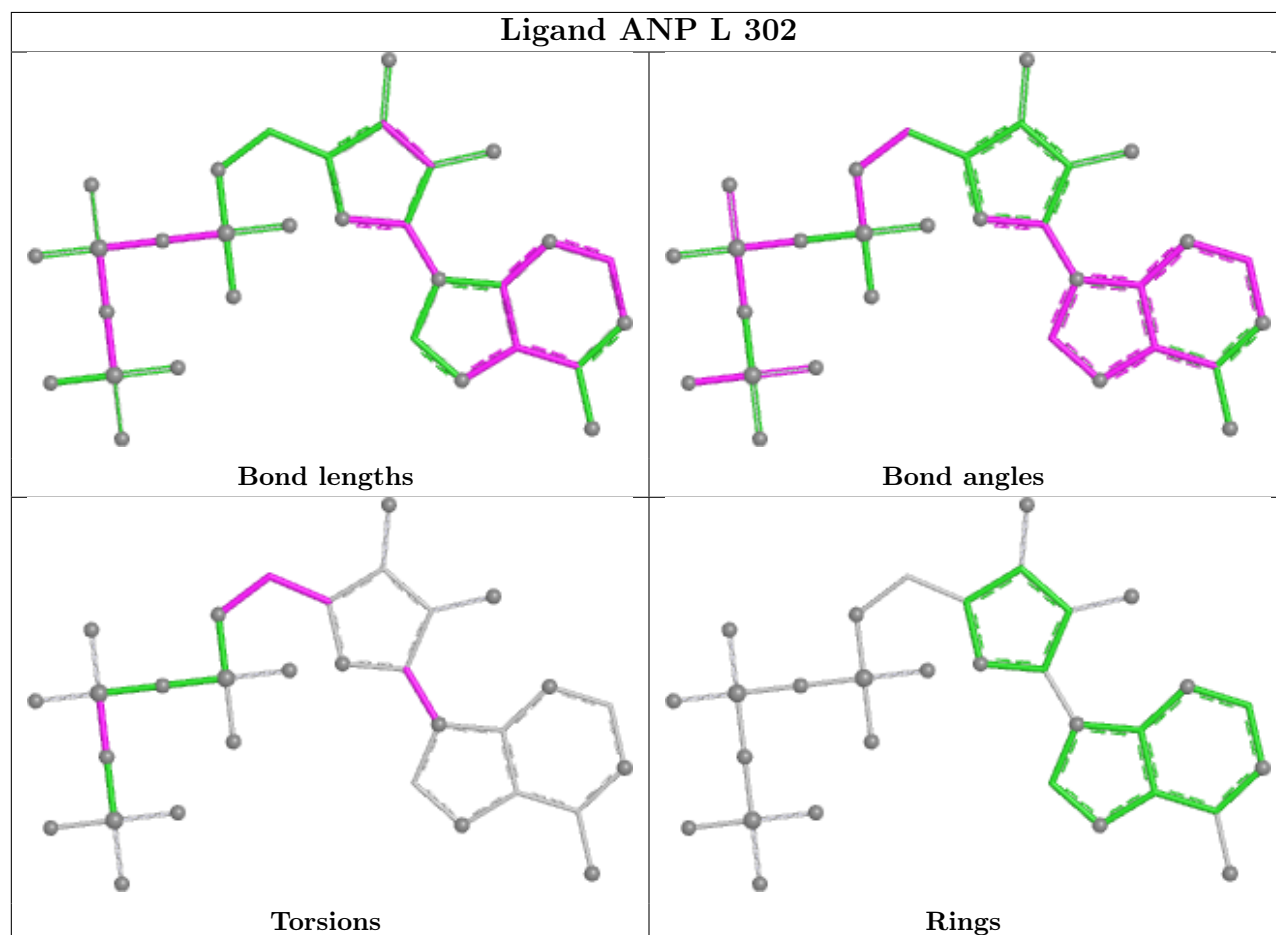
Continued from previous page...

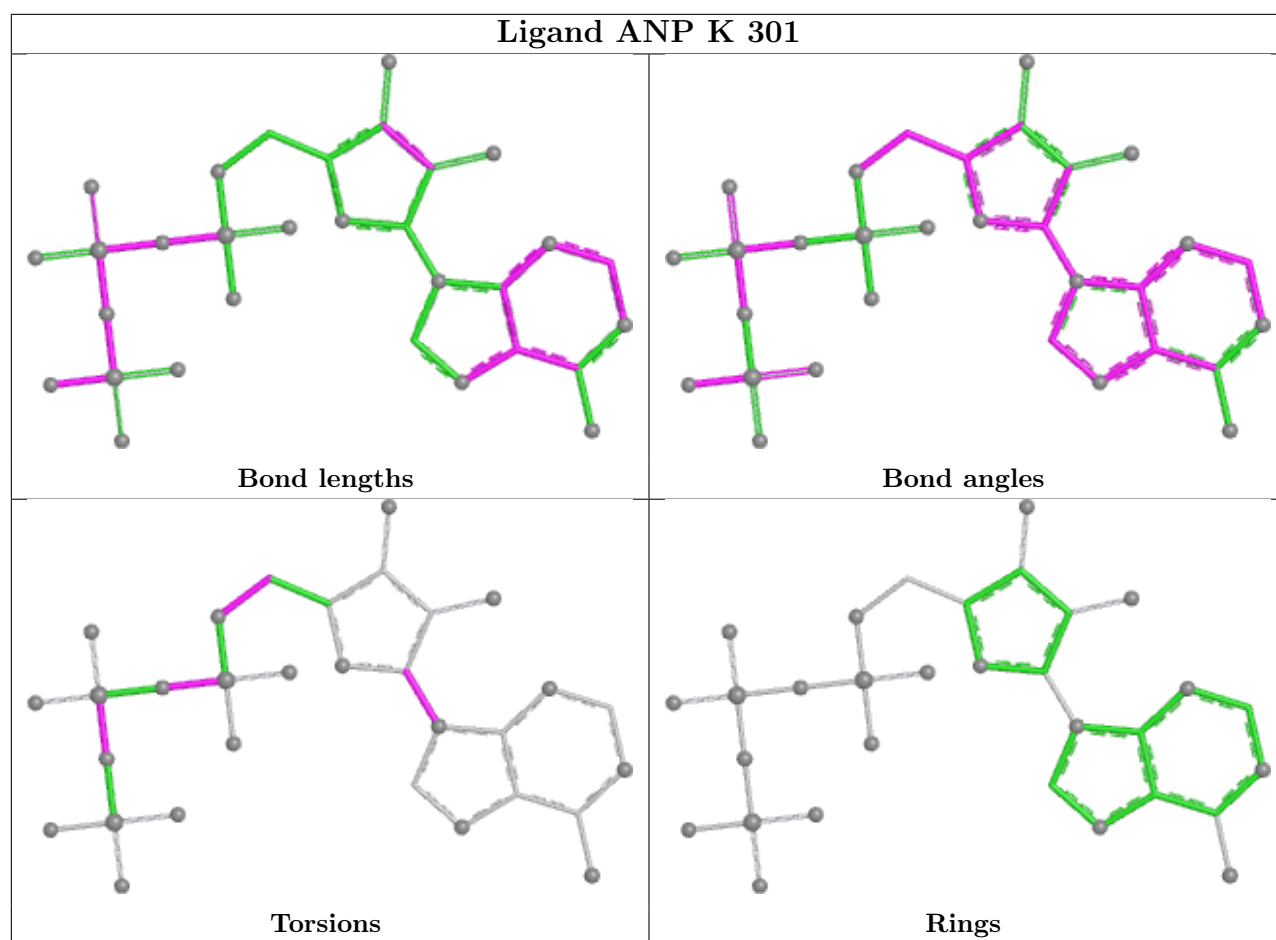
Mol	Chain	Res	Type	Atoms
5	L	302	ANP	C2'-C1'-N9-C4
5	K	301	ANP	PB-O3A-PA-O1A
5	K	301	ANP	C2'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

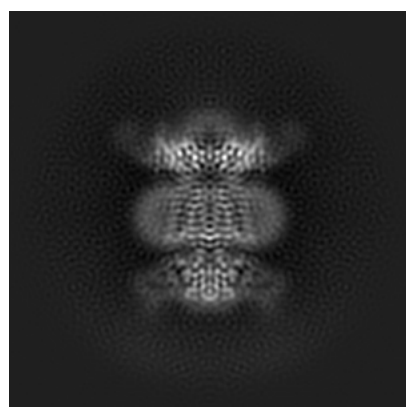
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11082. These allow visual inspection of the internal detail of the map and identification of artifacts.

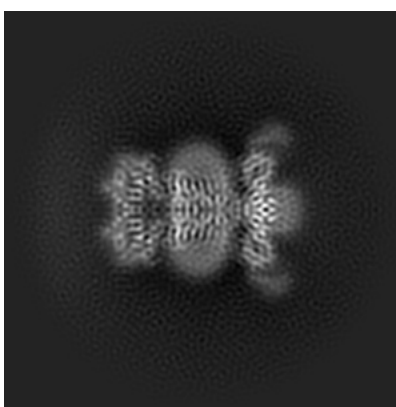
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

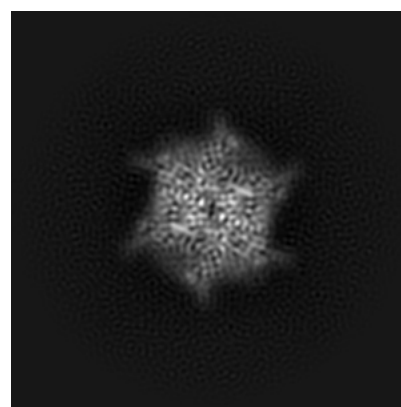
6.1.1 Primary map



X



Y

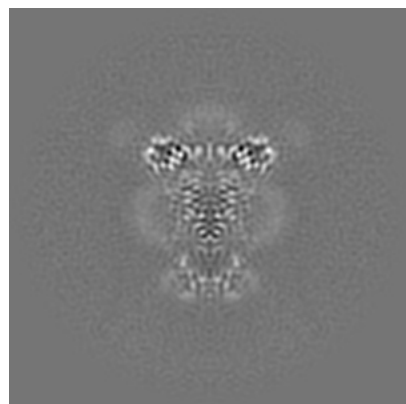


Z

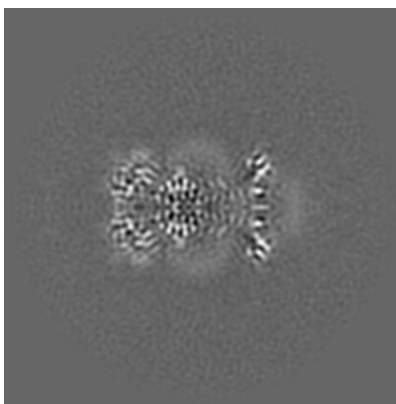
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

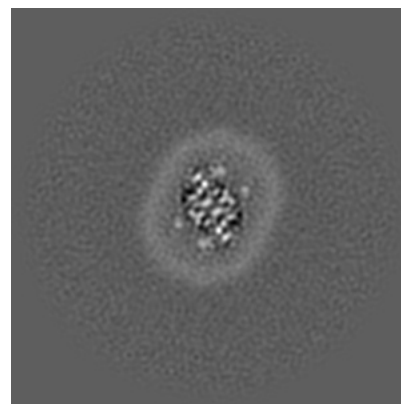
6.2.1 Primary map



X Index: 128



Y Index: 128

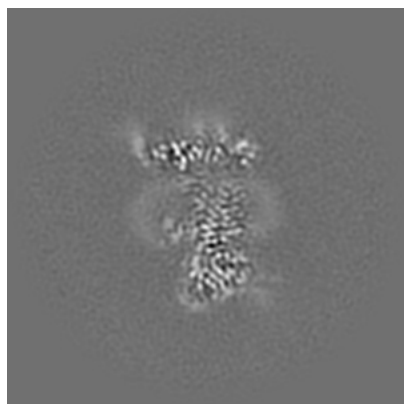


Z Index: 128

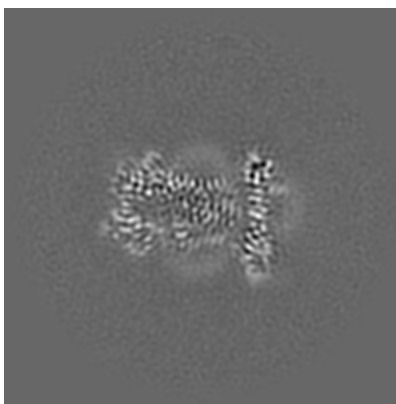
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

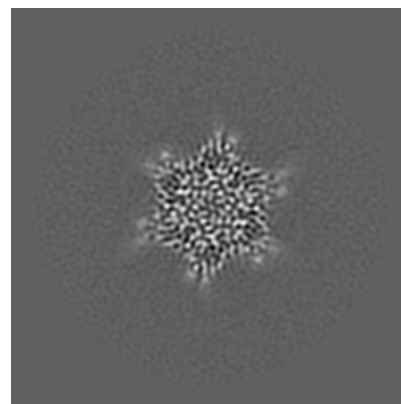
6.3.1 Primary map



X Index: 116



Y Index: 119

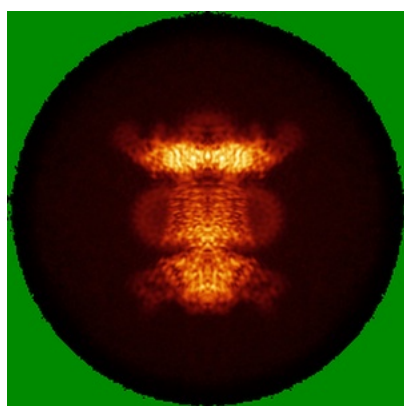


Z Index: 162

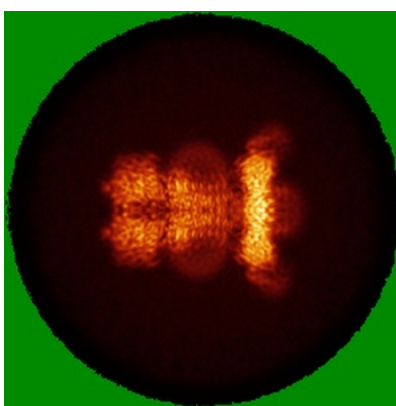
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

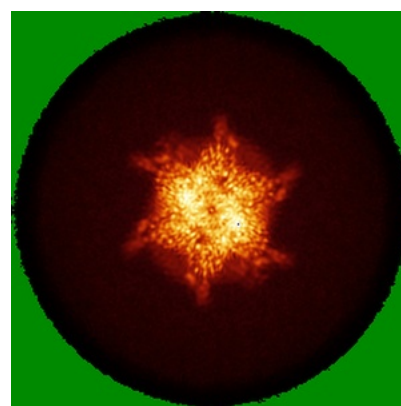
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

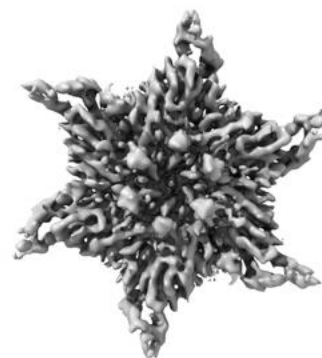
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.458. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

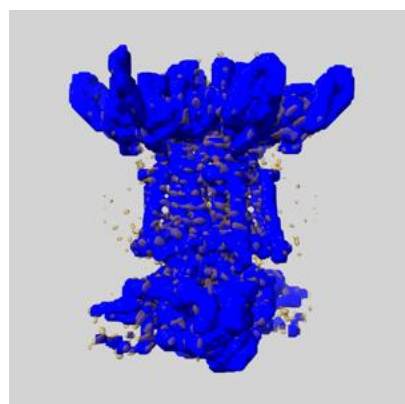
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

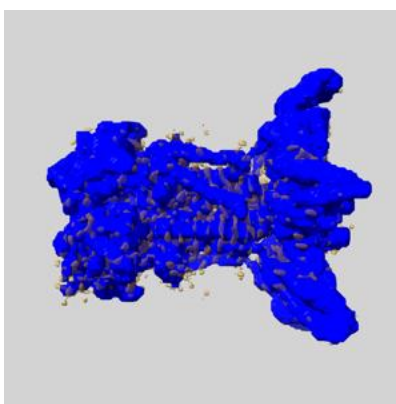
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

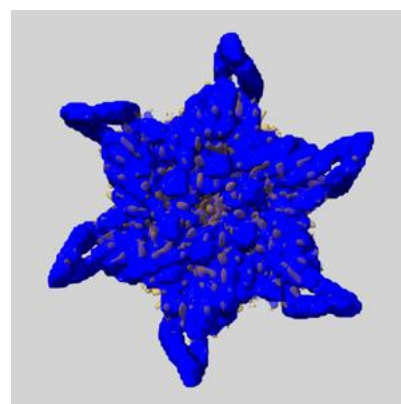
6.6.1 emd_11082_msk_1.map [i](#)



X



Y

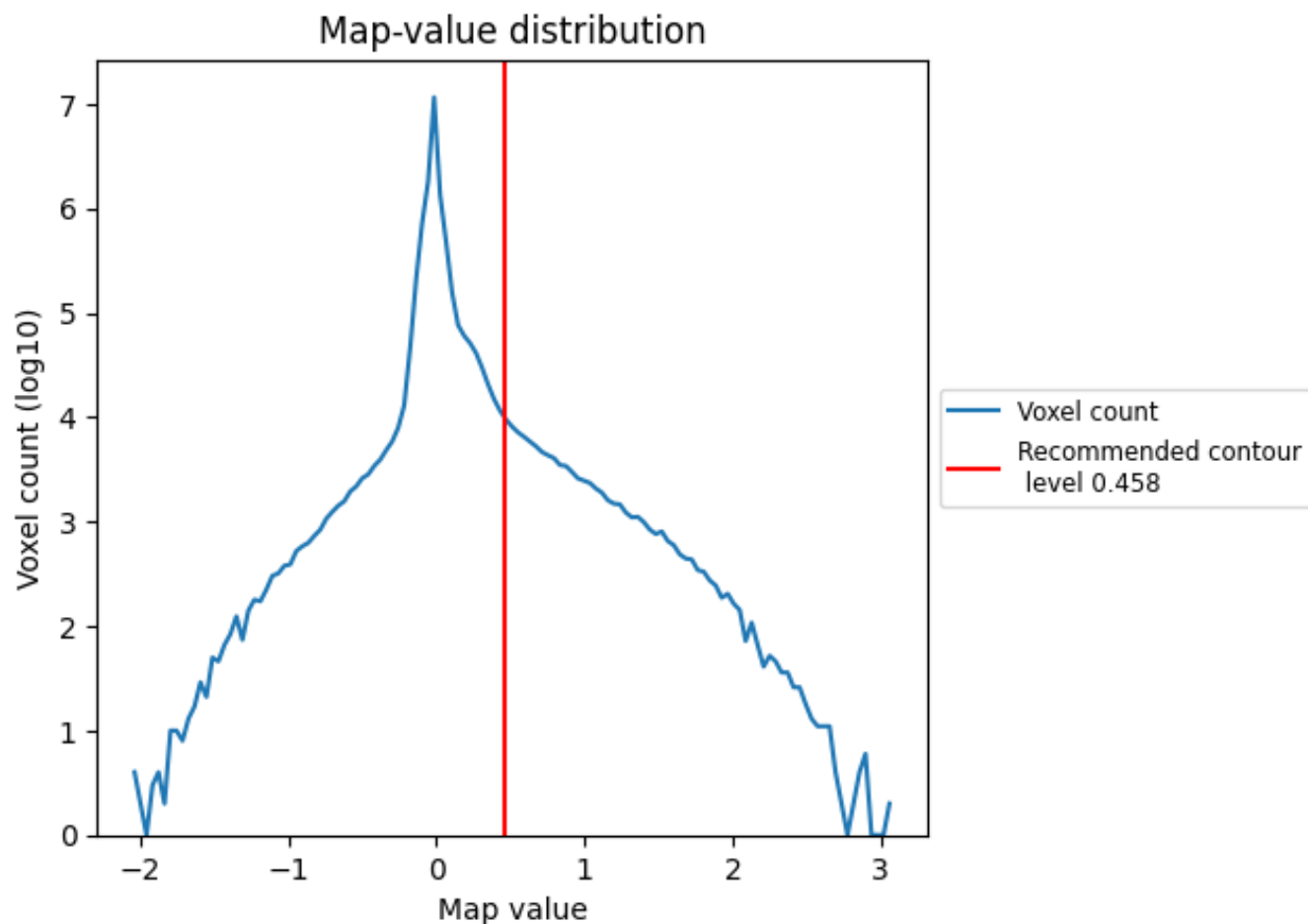


Z

7 Map analysis [i](#)

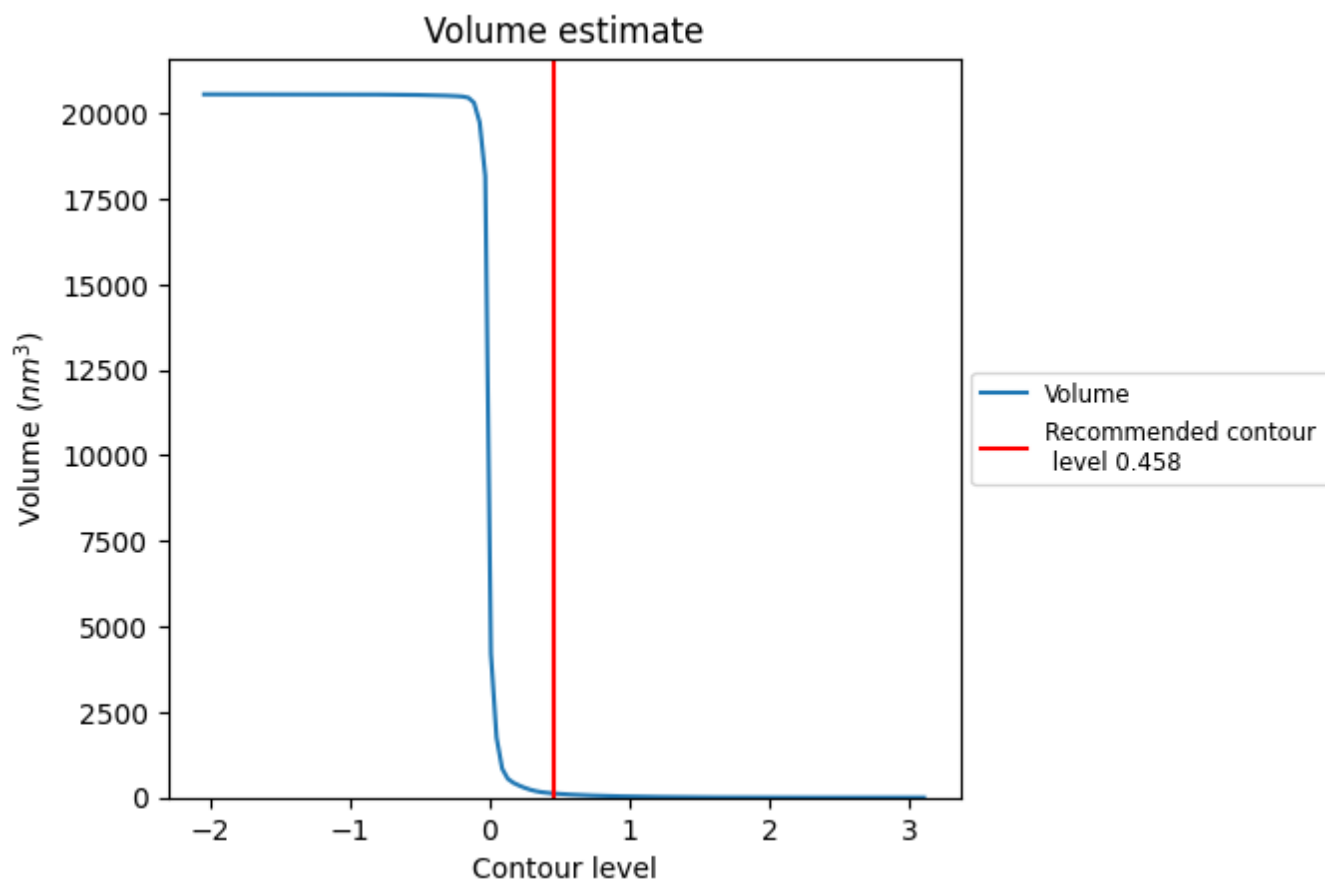
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

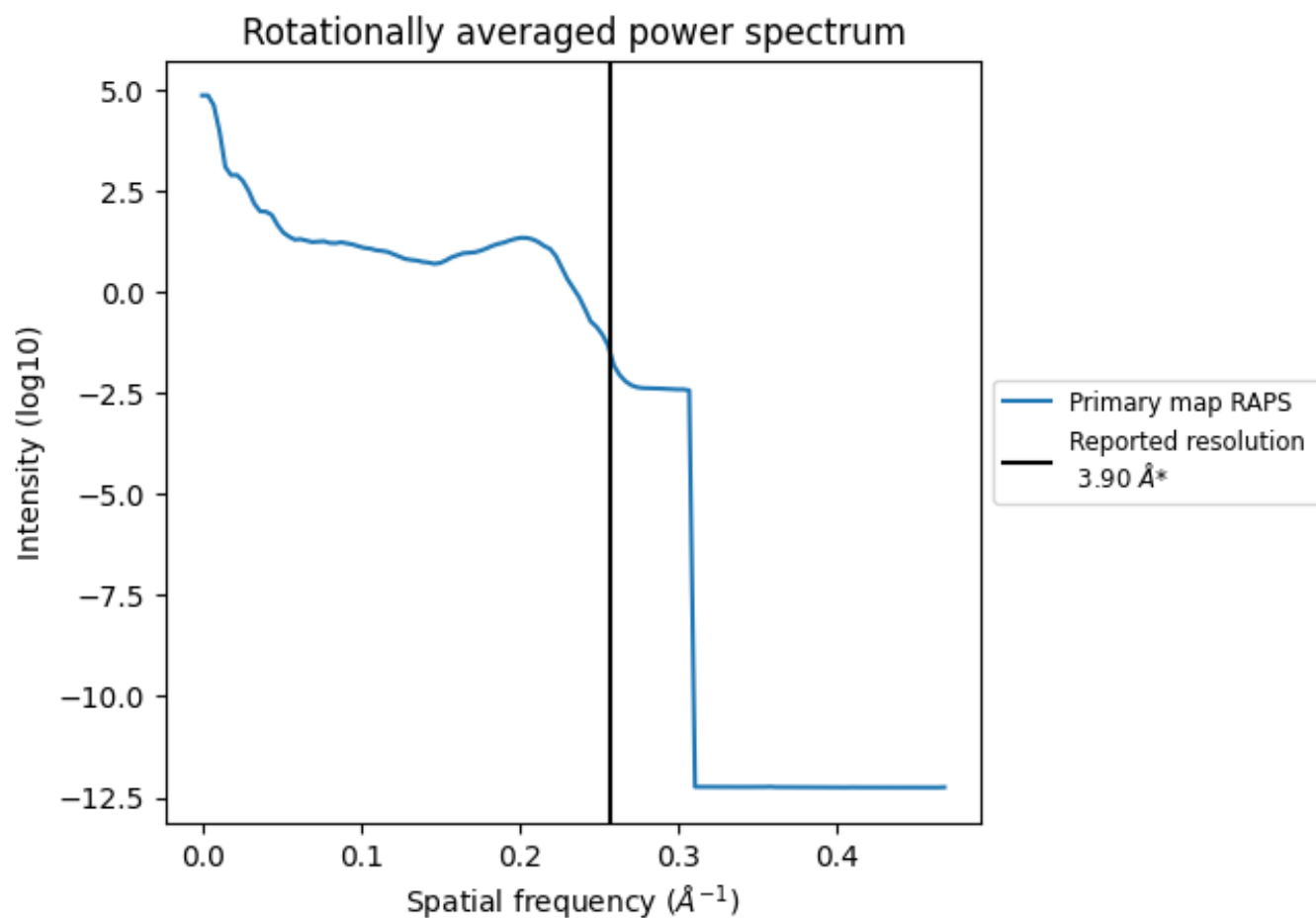
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm³; this corresponds to an approximate mass of 107 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

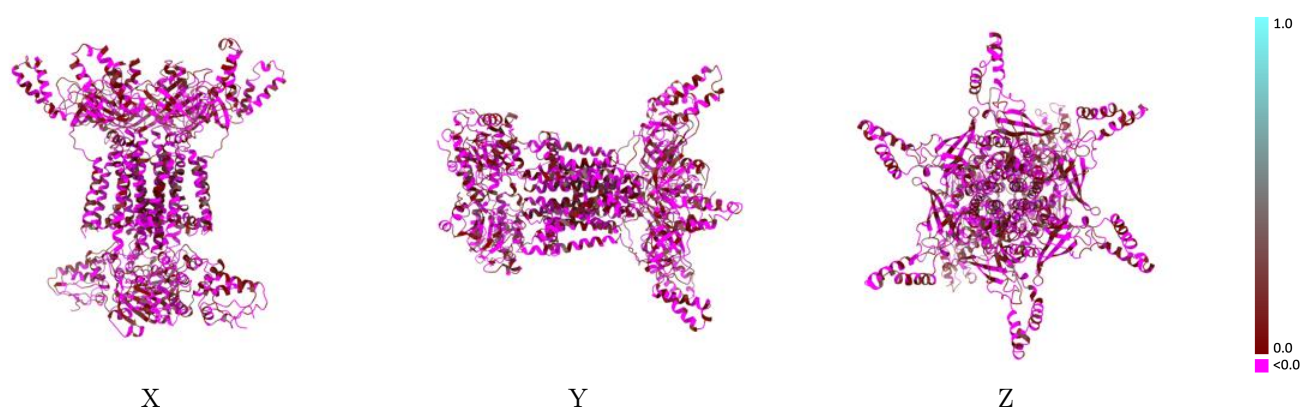
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-11082 and PDB model 6Z5U. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

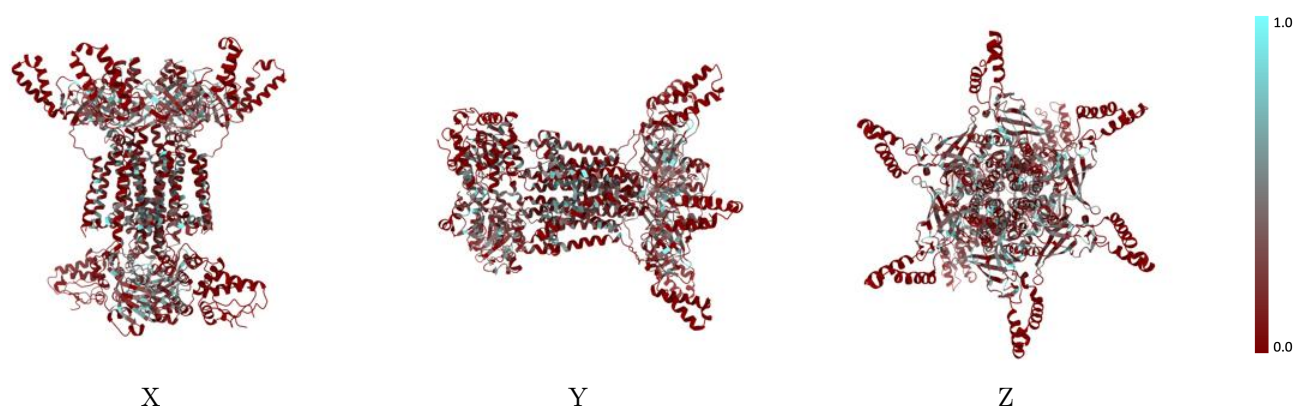
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



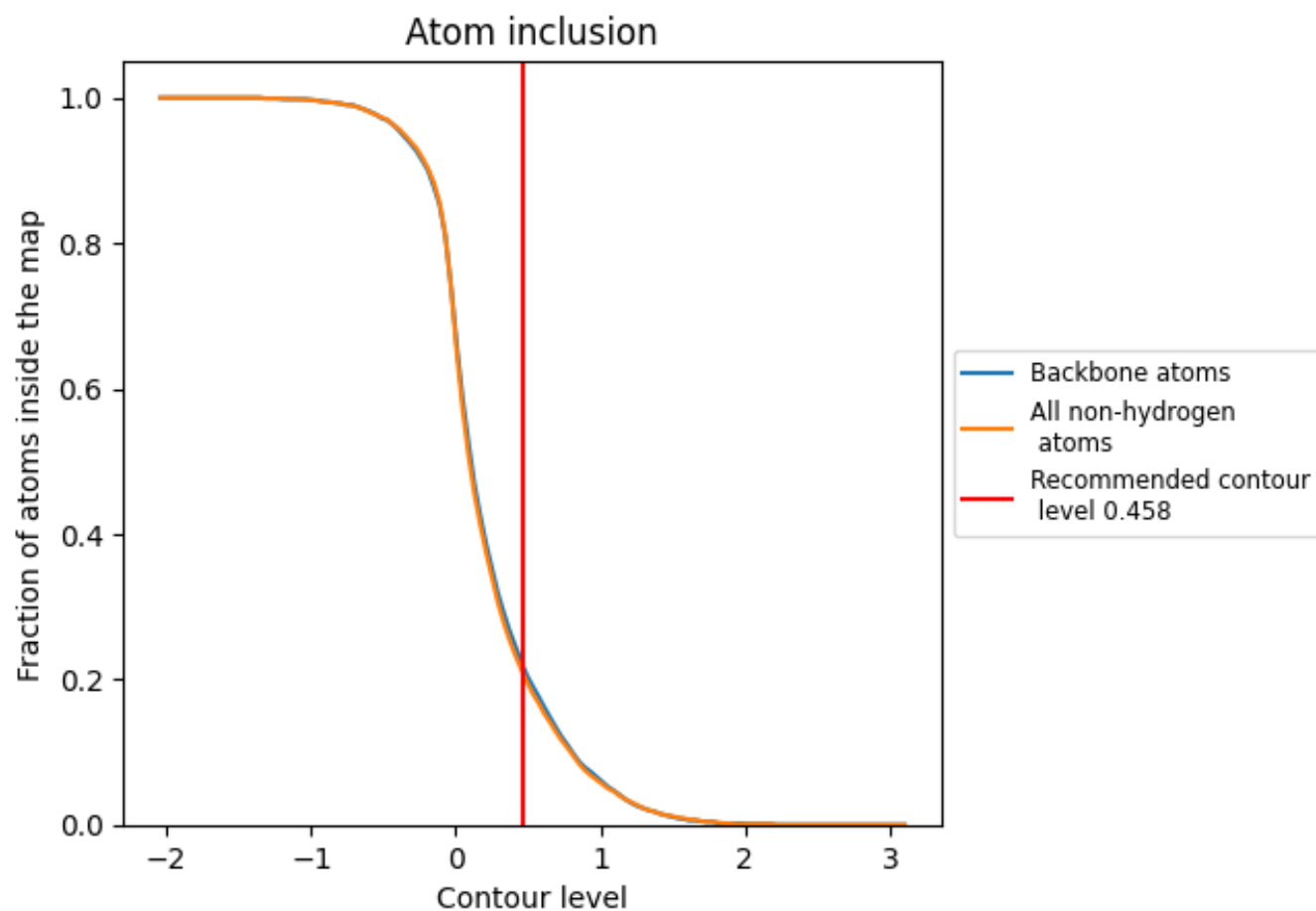
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.458).

9.4 Atom inclusion [i](#)



At the recommended contour level, 22% of all backbone atoms, 21% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.458) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2110	0.0030
A	0.2790	-0.0030
B	0.2810	0.0000
C	0.0000	-0.0060
D	0.0000	0.0010
E	0.2180	0.0110
F	0.1750	-0.0070
G	0.2180	0.0050
H	0.2120	0.0020
I	0.1750	-0.0060
J	0.2060	0.0100
K	0.2430	0.0080
L	0.2420	0.0120

1.0

0.0

<0.0