



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:45 AM UTC

PDB ID : 3JA6 / pdb_00003ja6
EMDB ID : EMD-6319
Title : Cryo-electron Tomography and All-atom Molecular Dynamics Simulations Reveal a Novel Kinase Conformational Switch in Bacterial Chemotaxis Signaling
Authors : Cassidy, C.K.; Himes, B.A.; Alvarez, F.J.; Ma, J.; Zhao, G.; Perilla, J.R.; Schulten, K.; Zhang, P.
Deposited on : 2015-04-21
Resolution : 12.70 Å (reported)
Based on initial model : 1QU7

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:

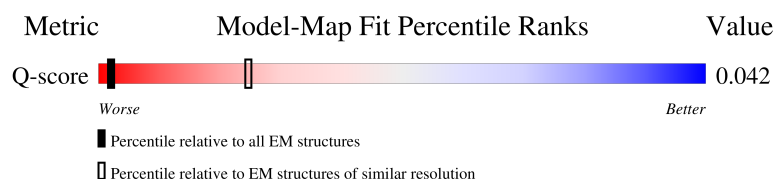
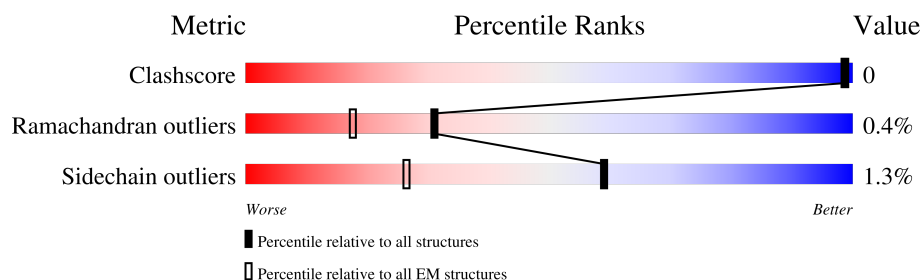
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 12.70 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	98 (10.80 - 11.80)

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	139	29% 93% 6% ..
1	B	139	45% 92% 6% .
1	D	139	55% 96% ..
1	F	139	49% 96% .

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Mol	Chain	Length	Quality of chain
2	C	379	
2	E	379	
3	G	309	
3	I	309	
3	K	309	
3	M	309	
3	O	309	
3	Q	309	
4	H	307	
4	J	307	
4	L	307	
4	N	307	
4	P	307	
4	R	307	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 77014 atoms, of which 38700 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 Chemotaxis protein CheW.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	139	Total	C	H	N	O	S	0	0
			2274	710	1169	183	210	2		
1	B	139	Total	C	H	N	O	S	0	0
			2274	710	1169	183	210	2		
1	D	139	Total	C	H	N	O	S	0	0
			2274	710	1169	183	210	2		
1	F	139	Total	C	H	N	O	S	0	0
			2274	710	1169	183	210	2		

- Molecule 2 is a protein called Chemotaxis protein CheA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	379	Total	C	H	N	O	S	0	0
			6110	1889	3131	513	567	10		
2	E	379	Total	C	H	N	O	S	0	0
			6110	1889	3131	513	567	10		

- Molecule 3 is a protein called Methyl-accepting chemotaxis protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	I	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	K	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	M	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	O	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		
3	Q	309	Total	C	H	N	O	S	0	0
			4656	1411	2322	407	510	6		

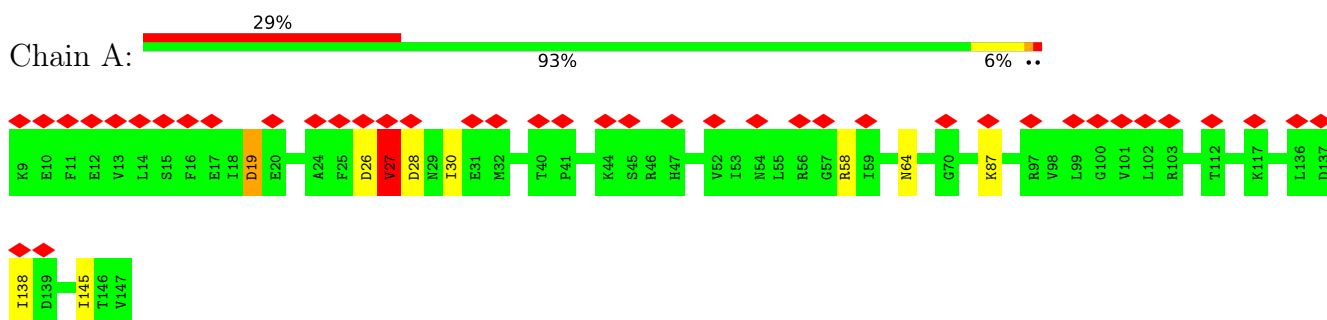
- Molecule 4 is a protein called Methyl-accepting chemotaxis protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	J	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	L	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	N	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	P	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0
4	R	307	Total 4627	C 1403	H 2305	N 405	O 508	S 6	0	0

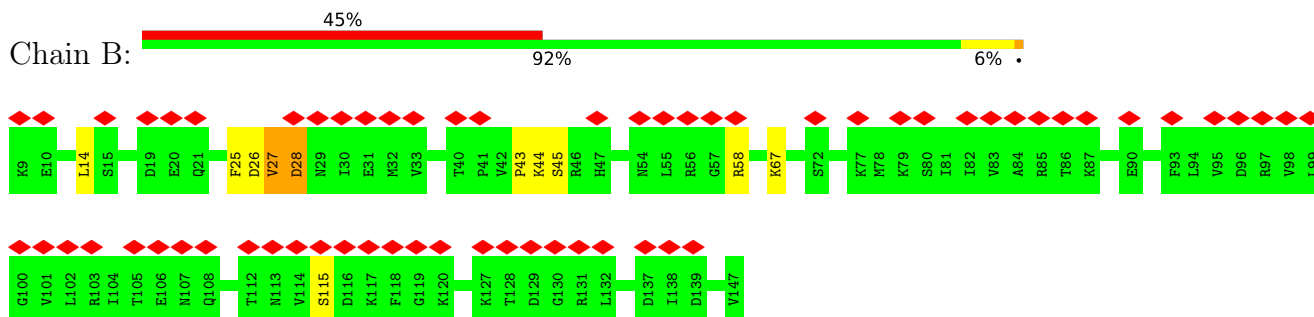
3 Residue-property plots [i](#)

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 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.

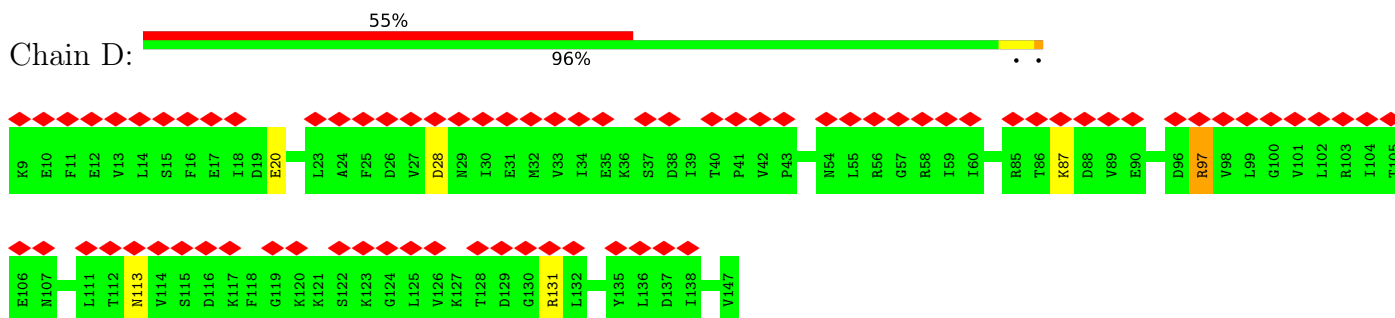
- Molecule 1: Chemotaxis protein CheW



- Molecule 1: Chemotaxis protein CheW

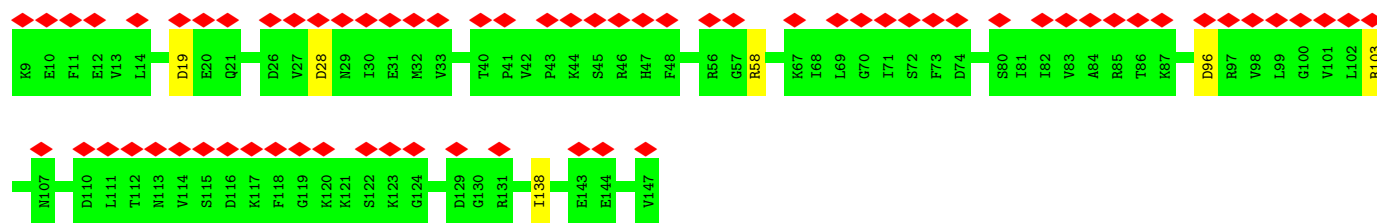


- Molecule 1: Chemotaxis protein CheW

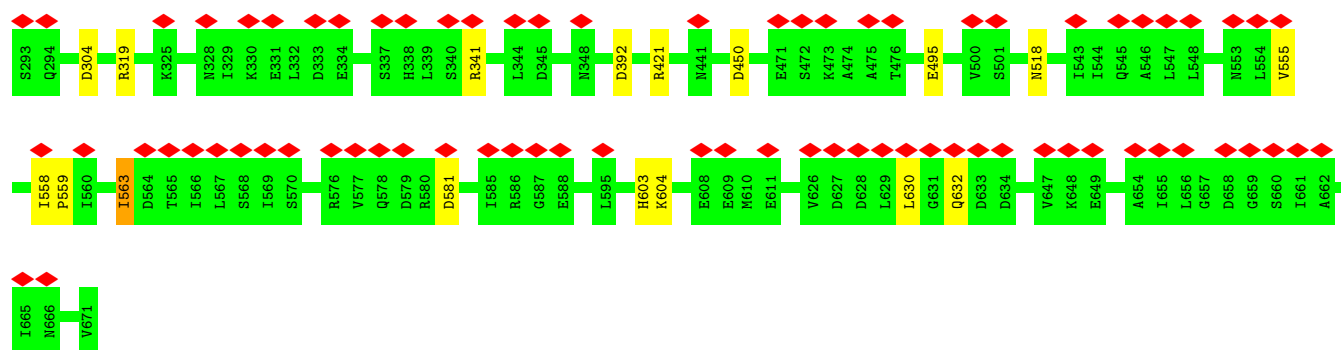


- Molecule 1: Chemotaxis protein CheW

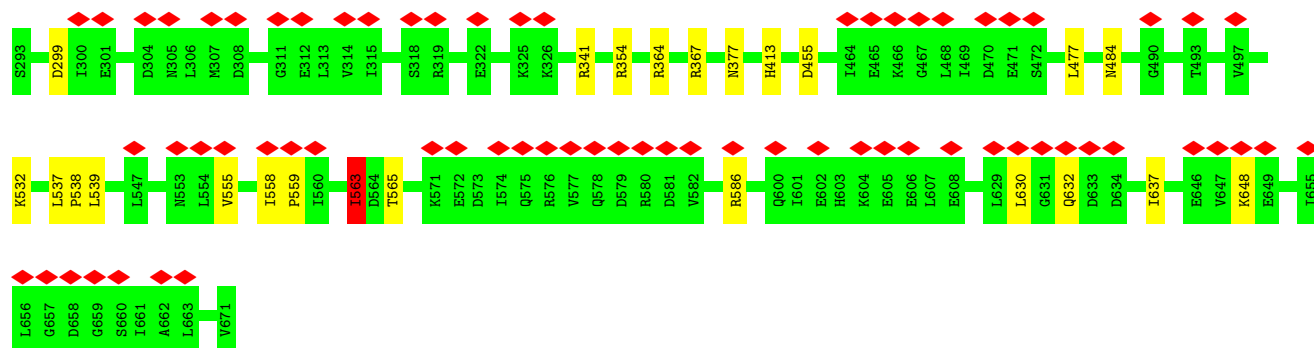




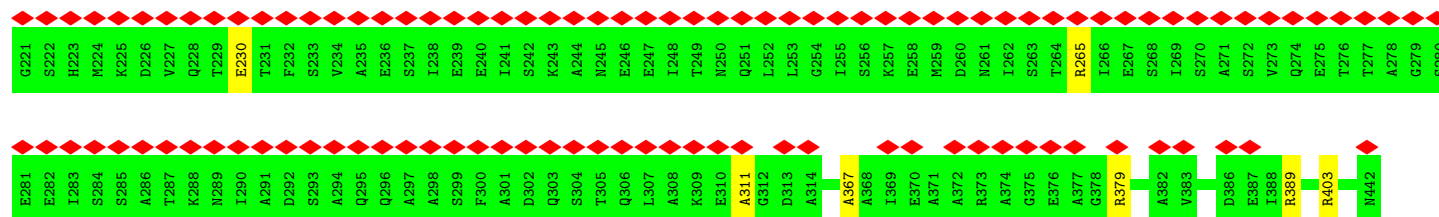
• Molecule 2: Chemotaxis protein CheA

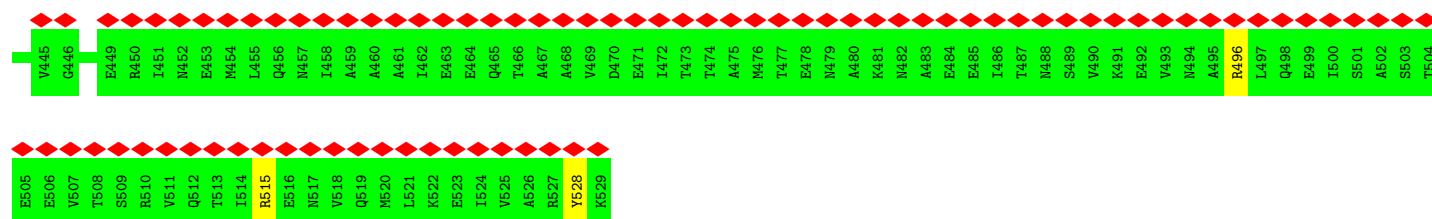


• Molecule 2: Chemotaxis protein CheA

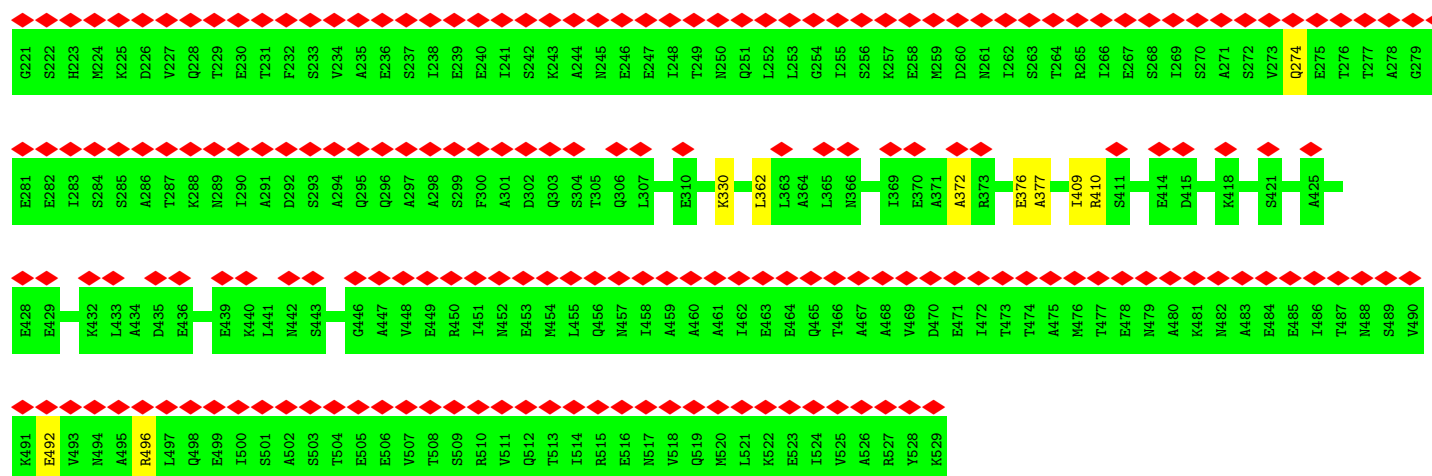


• Molecule 3: Methyl-accepting chemotaxis protein 2

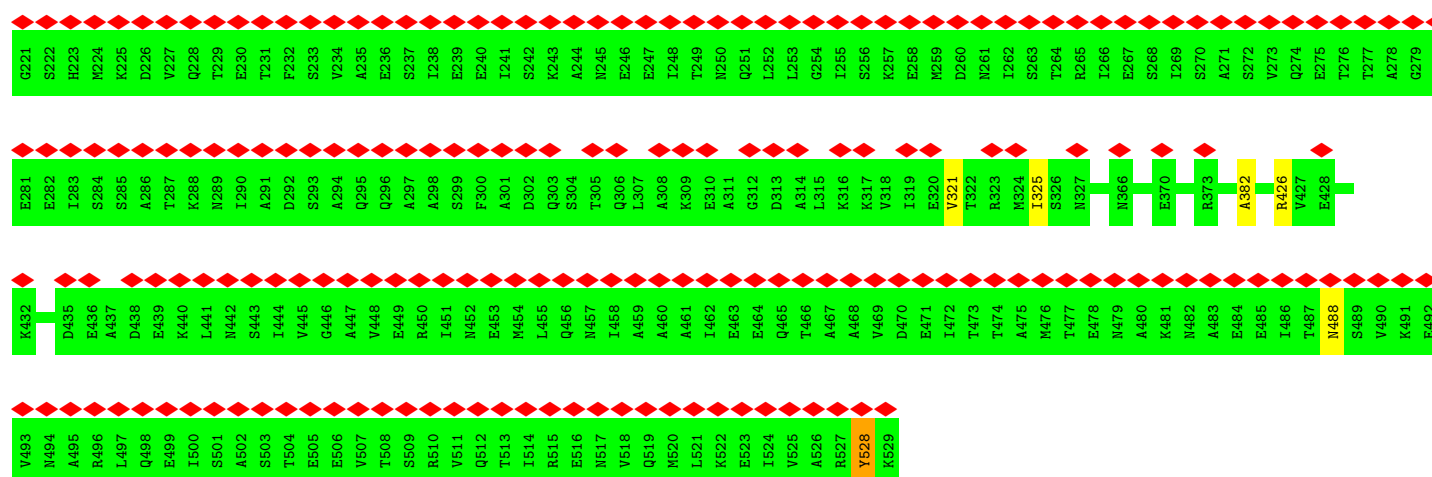




• Molecule 3: Methyl-accepting chemotaxis protein 2

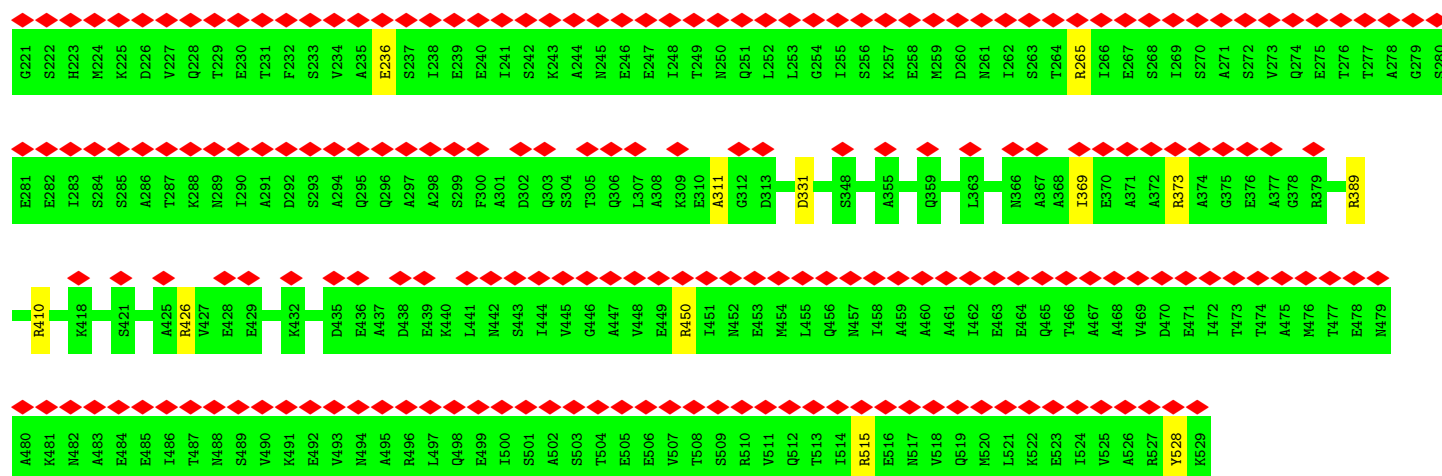


• Molecule 3: Methyl-accepting chemotaxis protein 2

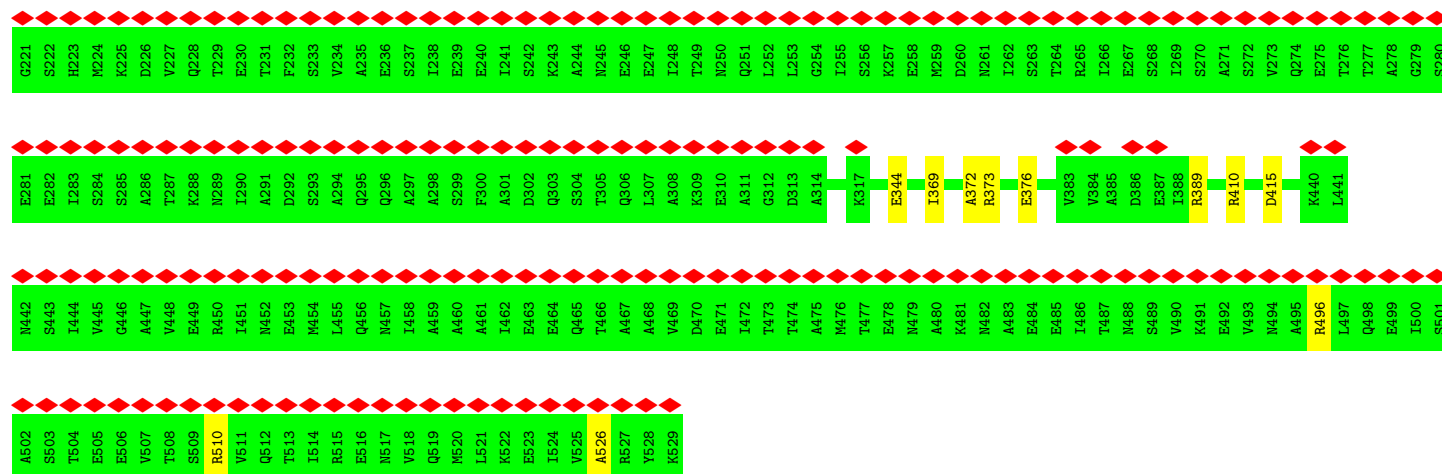


• Molecule 3: Methyl-accepting chemotaxis protein 2

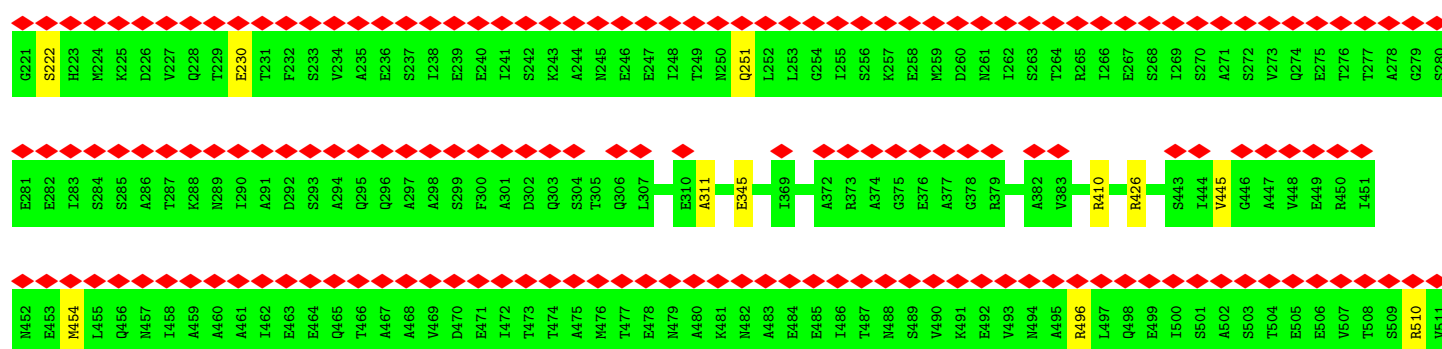


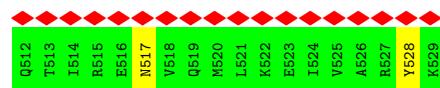


• Molecule 3: Methyl-accepting chemotaxis protein 2

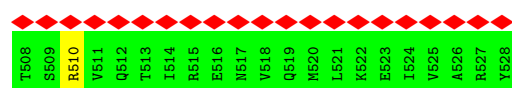
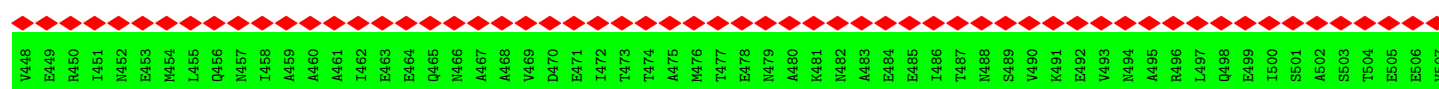
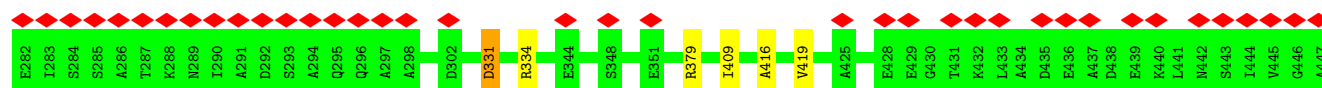
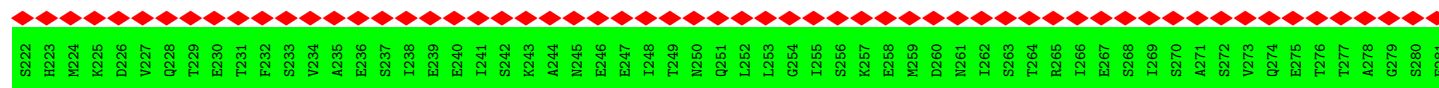


• Molecule 3: Methyl-accepting chemotaxis protein 2

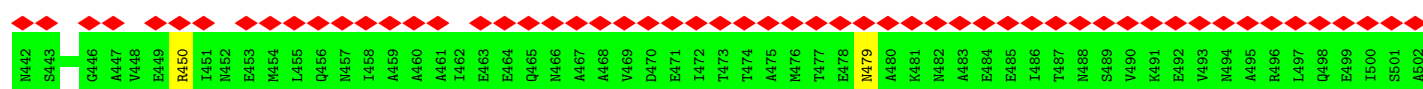
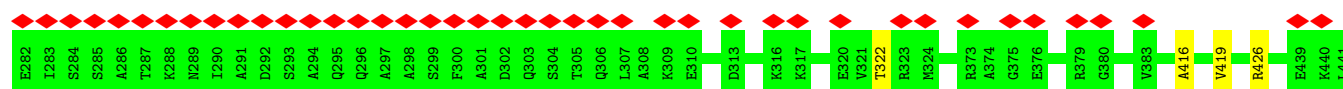
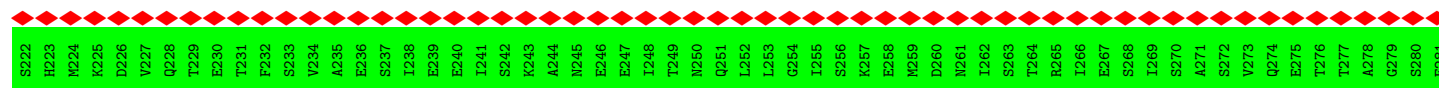




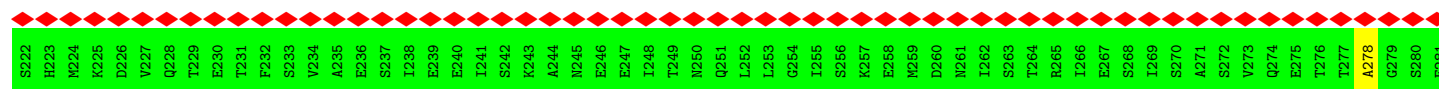
- Molecule 4: Methyl-accepting chemotaxis protein 2

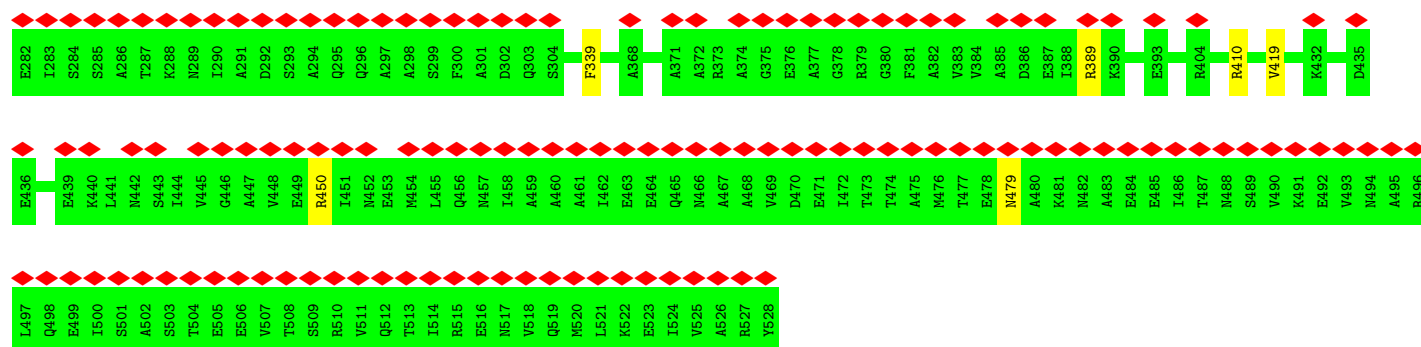


- Molecule 4: Methyl-accepting chemotaxis protein 2

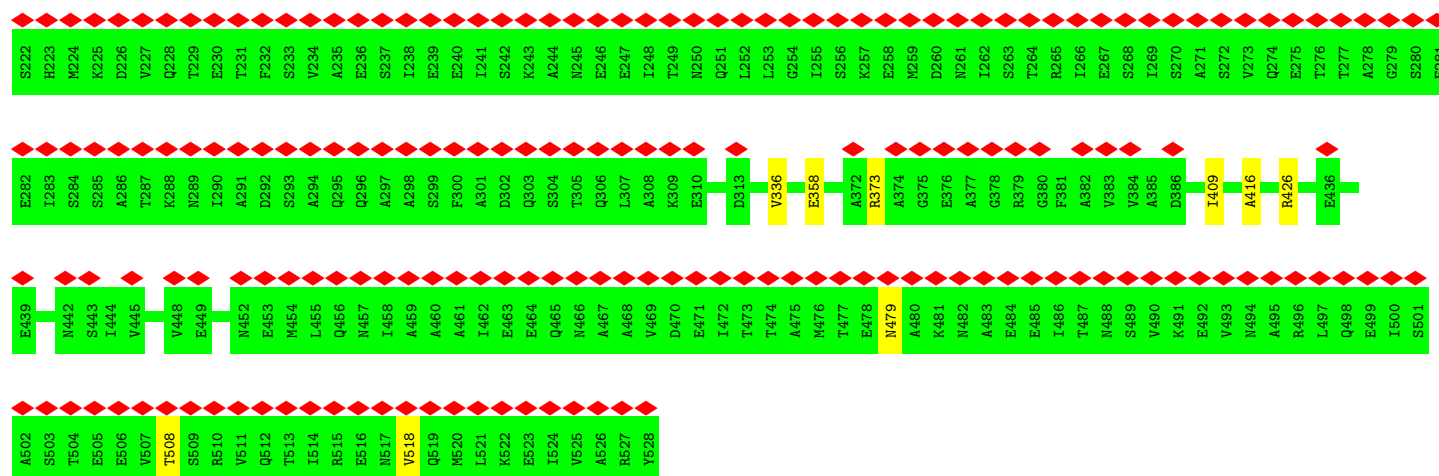


- Molecule 4: Methyl-accepting chemotaxis protein 2

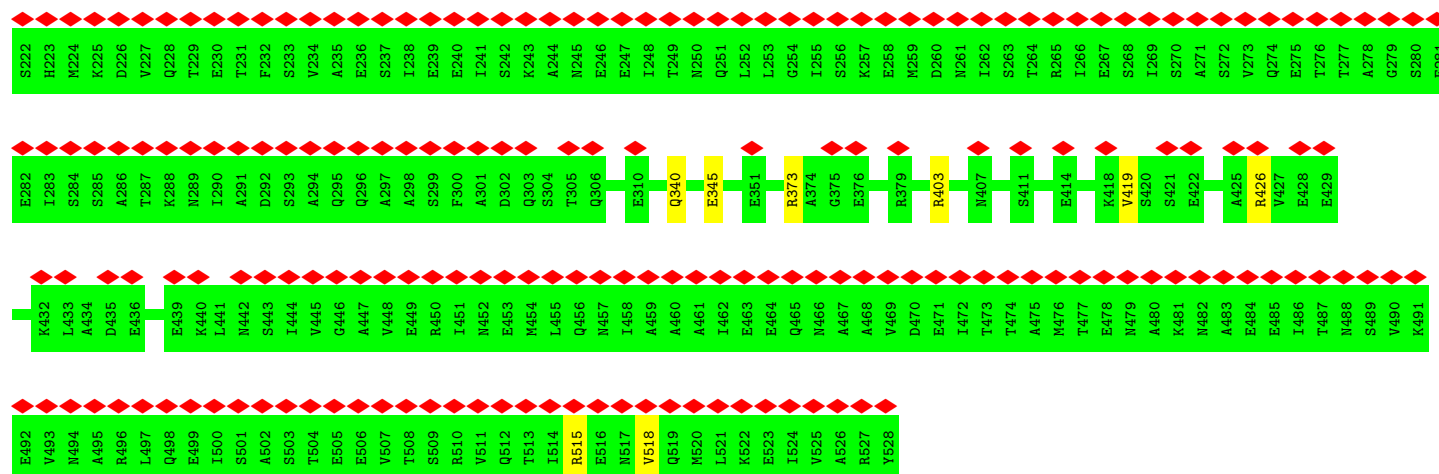




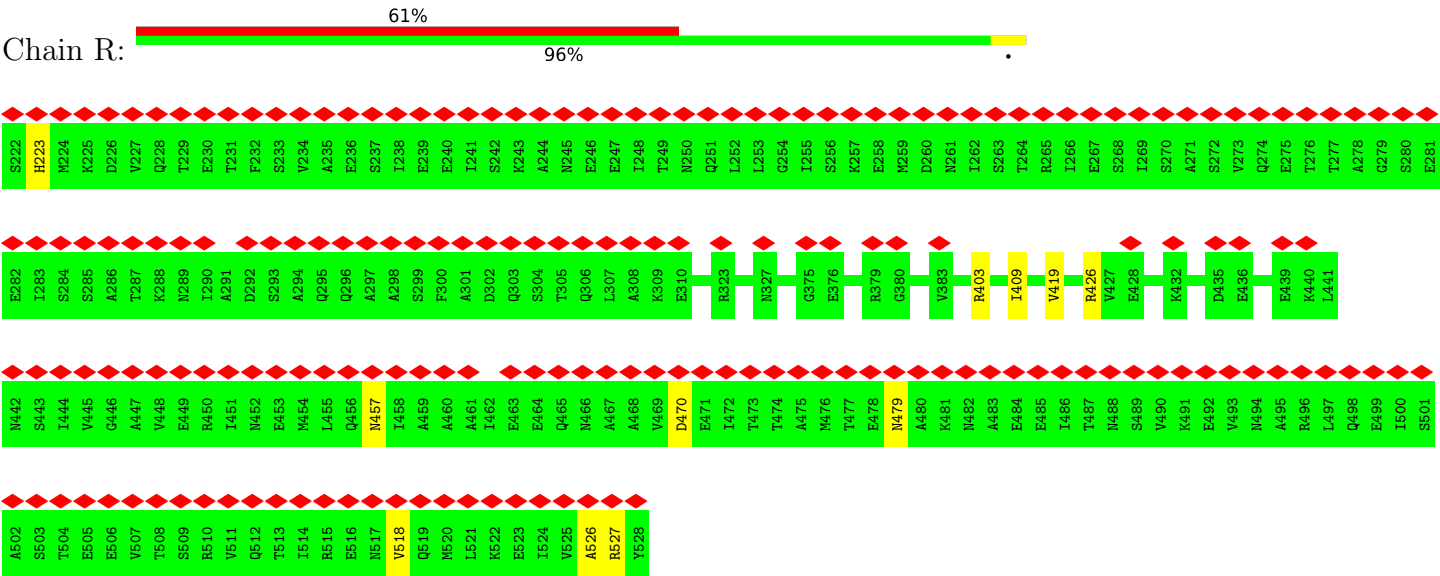
- Molecule 4: Methyl-accepting chemotaxis protein 2



- Molecule 4: Methyl-accepting chemotaxis protein 2



- Molecule 4: Methyl-accepting chemotaxis protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, γ =Not provided°, space group=Not provided	Depositor
Number of tilted images used	4000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	TomoCTF (strip-based periodogram)	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	8000	Depositor
Magnification	49834	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum voxel value	9.139	Depositor
Minimum voxel value	-8.682	Depositor
Average voxel value	0.000	Depositor
Voxel value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Tomogram size (Å)	391.3, 391.3, 252.84	wwPDB
Tomogram dimensions	130, 130, 84	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	3.01, 3.01, 3.01	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	0.84	0/1116	1.40	9/1501 (0.6%)
1	B	0.85	0/1116	1.37	10/1501 (0.7%)
1	D	0.84	0/1116	1.35	4/1501 (0.3%)
1	F	0.85	0/1116	1.36	3/1501 (0.2%)
2	C	0.84	0/3009	1.45	10/4051 (0.2%)
2	E	0.83	0/3009	1.45	16/4051 (0.4%)
3	G	0.81	0/2340	1.51	9/3153 (0.3%)
3	I	0.82	0/2340	1.54	5/3153 (0.2%)
3	K	0.81	0/2340	1.54	6/3153 (0.2%)
3	M	0.82	0/2340	1.52	5/3153 (0.2%)
3	O	0.83	0/2340	1.53	6/3153 (0.2%)
3	Q	0.83	0/2340	1.53	10/3153 (0.3%)
4	H	0.82	0/2328	1.56	6/3138 (0.2%)
4	J	0.81	0/2328	1.55	8/3138 (0.3%)
4	L	0.82	0/2328	1.55	5/3138 (0.2%)
4	N	0.82	0/2328	1.53	3/3138 (0.1%)
4	P	0.82	0/2328	1.52	4/3138 (0.1%)
4	R	0.81	0/2328	1.53	7/3138 (0.2%)
All	All	0.82	0/38490	1.50	126/51852 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	2
1	F	0	2
2	C	0	1
2	E	0	4
3	G	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	2
3	K	0	1
3	M	0	5
3	O	0	3
3	Q	0	2
4	H	0	2
4	J	0	1
4	L	0	3
4	N	0	1
4	P	0	2
All	All	0	35

There are no bond length outliers.

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	VAL	N-CA-C	7.37	124.67	109.34
3	Q	222	SER	N-CA-C	7.11	119.03	111.28
1	A	27	VAL	CA-C-N	6.99	134.88	121.54
1	A	27	VAL	C-N-CA	6.99	134.88	121.54
3	O	344	GLU	CA-C-N	6.97	129.84	120.65
3	O	344	GLU	C-N-CA	6.97	129.84	120.65
1	A	26	ASP	CA-C-N	6.93	134.44	121.97
1	A	26	ASP	C-N-CA	6.93	134.44	121.97
4	J	419	VAL	CA-C-N	6.66	129.49	120.44
4	J	419	VAL	C-N-CA	6.66	129.49	120.44
3	Q	528	TYR	N-CA-C	6.42	119.97	111.75
1	B	26	ASP	CA-C-N	6.41	133.51	121.97
1	B	26	ASP	C-N-CA	6.41	133.51	121.97
4	R	518	VAL	N-CA-C	-6.34	107.07	113.47
4	J	322	THR	N-CA-CB	6.34	119.20	110.01
2	E	632	GLN	N-CA-C	6.33	118.47	110.24
3	Q	517	ASN	CA-CB-CG	-6.31	106.29	112.60
1	F	96	ASP	CA-CB-CG	6.29	118.89	112.60
4	J	504	THR	N-CA-CB	6.23	119.39	110.16
1	A	27	VAL	N-CA-C	6.12	122.07	109.34
1	B	28	ASP	N-CA-C	6.10	123.79	110.80
4	J	416	ALA	CA-C-N	6.06	126.84	119.99
4	J	416	ALA	C-N-CA	6.06	126.84	119.99
4	R	419	VAL	CA-C-N	6.05	128.30	120.44
4	R	419	VAL	C-N-CA	6.05	128.30	120.44
4	H	416	ALA	CA-C-N	6.04	126.81	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	416	ALA	C-N-CA	6.04	126.81	119.99
4	P	419	VAL	CA-C-N	6.00	128.60	120.44
4	P	419	VAL	C-N-CA	6.00	128.60	120.44
3	G	379	ARG	N-CA-C	5.96	117.45	111.07
1	A	138	ILE	CA-C-N	5.96	129.07	120.79
1	A	138	ILE	C-N-CA	5.96	129.07	120.79
4	R	403	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	F	138	ILE	CA-C-N	5.92	129.02	120.79
1	F	138	ILE	C-N-CA	5.92	129.02	120.79
3	M	528	TYR	N-CA-C	5.87	118.46	111.71
4	H	334	ARG	NE-CZ-NH2	5.84	124.45	119.20
2	C	495	GLU	N-CA-C	5.72	119.14	111.24
2	C	392	ASP	CA-C-N	5.72	128.22	120.38
2	C	392	ASP	C-N-CA	5.72	128.22	120.38
3	G	389	ARG	NE-CZ-NH2	5.70	124.33	119.20
2	E	455	ASP	CA-C-N	5.64	128.10	120.38
2	E	455	ASP	C-N-CA	5.64	128.10	120.38
3	G	311	ALA	CA-C-N	5.59	126.03	119.94
3	G	311	ALA	C-N-CA	5.59	126.03	119.94
4	H	419	VAL	N-CA-C	5.59	116.99	110.62
4	J	518	VAL	N-CA-C	-5.58	107.83	113.47
3	M	311	ALA	CA-C-N	5.58	126.02	119.94
3	M	311	ALA	C-N-CA	5.58	126.02	119.94
4	L	278	ALA	CA-C-N	5.53	126.12	119.98
4	L	278	ALA	C-N-CA	5.53	126.12	119.98
3	G	403	ARG	NE-CZ-NH2	5.49	124.14	119.20
3	I	274	GLN	CA-C-N	5.48	127.57	120.44
3	I	274	GLN	C-N-CA	5.48	127.57	120.44
2	C	632	GLN	N-CA-C	5.48	117.37	110.24
2	E	558	ILE	CA-C-N	5.46	126.66	119.84
2	E	558	ILE	C-N-CA	5.46	126.66	119.84
2	E	648	LYS	CA-C-N	5.44	127.84	120.38
2	E	648	LYS	C-N-CA	5.44	127.84	120.38
2	C	563	ILE	N-CA-C	5.44	120.65	109.34
3	Q	251	GLN	N-CA-C	5.43	117.20	111.28
2	E	563	ILE	N-CA-C	5.42	120.61	109.34
3	K	488	ASN	CA-CB-CG	-5.42	107.19	112.60
2	C	555	VAL	N-CA-C	5.41	115.99	108.84
2	E	477	LEU	N-CA-C	5.39	117.68	110.35
4	L	339	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	64	ASN	CA-C-N	5.38	128.89	120.82
1	A	64	ASN	C-N-CA	5.38	128.89	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	518	VAL	N-CA-C	-5.38	108.26	113.53
3	G	528	TYR	N-CA-C	5.36	117.87	111.71
2	E	299	ASP	CA-CB-CG	-5.33	107.27	112.60
3	K	325	ILE	CA-C-N	5.33	127.88	120.63
3	K	325	ILE	C-N-CA	5.33	127.88	120.63
2	E	537	LEU	CA-C-N	5.32	126.50	119.84
2	E	537	LEU	C-N-CA	5.32	126.50	119.84
1	B	44	LYS	N-CA-C	5.32	118.73	111.39
1	D	113	ASN	CA-C-N	5.32	127.75	120.46
1	D	113	ASN	C-N-CA	5.32	127.75	120.46
3	O	526	ALA	CA-C-N	5.30	127.38	120.28
3	O	526	ALA	C-N-CA	5.30	127.38	120.28
4	L	419	VAL	CA-C-N	5.28	127.63	120.44
4	L	419	VAL	C-N-CA	5.28	127.63	120.44
3	M	515	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	I	377	ALA	N-CA-C	5.27	118.49	111.75
4	N	416	ALA	CA-C-N	5.26	125.94	119.99
4	N	416	ALA	C-N-CA	5.26	125.94	119.99
1	B	45	SER	N-CA-C	5.23	117.81	110.23
3	Q	445	VAL	CA-C-N	5.23	125.75	119.94
3	Q	445	VAL	C-N-CA	5.23	125.75	119.94
4	H	331	ASP	CA-CB-CG	-5.21	107.39	112.60
3	M	373	ARG	NE-CZ-NH1	-5.20	116.30	121.50
4	R	526	ALA	CA-C-N	5.19	128.61	120.82
4	R	526	ALA	C-N-CA	5.19	128.61	120.82
2	C	518	ASN	CA-CB-CG	-5.18	107.42	112.60
2	E	413	HIS	N-CA-C	5.17	116.72	111.14
4	J	510	ARG	NE-CZ-NH2	5.17	123.85	119.20
4	H	334	ARG	NE-CZ-NH1	-5.15	116.35	121.50
2	C	581	ASP	N-CA-C	5.13	117.54	110.35
2	E	555	VAL	N-CA-C	5.13	115.85	108.93
2	C	558	ILE	CA-C-N	5.12	126.24	119.84
2	C	558	ILE	C-N-CA	5.12	126.24	119.84
1	D	87	LYS	CA-C-N	5.11	127.54	120.29
1	D	87	LYS	C-N-CA	5.11	127.54	120.29
3	K	528	TYR	N-CA-C	5.08	118.25	111.75
3	G	389	ARG	NE-CZ-NH1	-5.08	116.42	121.50
3	O	373	ARG	NE-CZ-NH2	5.07	123.77	119.20
3	Q	345	GLU	CA-C-N	5.07	127.41	120.46
3	Q	345	GLU	C-N-CA	5.07	127.41	120.46
3	Q	311	ALA	CA-C-N	5.07	125.47	119.94
3	Q	311	ALA	C-N-CA	5.07	125.47	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	SER	CA-C-N	5.07	127.38	120.54
1	B	115	SER	C-N-CA	5.07	127.38	120.54
4	R	527	ARG	N-CA-C	5.06	119.72	111.37
2	E	539	LEU	N-CA-C	5.05	116.48	111.07
4	P	403	ARG	NE-CZ-NH2	5.04	123.74	119.20
3	K	382	ALA	CA-C-N	5.04	127.00	120.70
3	K	382	ALA	C-N-CA	5.04	127.00	120.70
3	O	389	ARG	NE-CZ-NH2	5.04	123.73	119.20
3	I	492	GLU	CA-C-N	5.04	126.91	120.56
3	I	492	GLU	C-N-CA	5.04	126.91	120.56
2	E	637	ILE	N-CA-C	5.03	115.59	109.30
3	G	367	ALA	CA-C-N	5.02	127.32	120.54
3	G	367	ALA	C-N-CA	5.02	127.32	120.54
1	B	43	PRO	CA-C-N	5.02	129.49	122.36
1	B	43	PRO	C-N-CA	5.02	129.49	122.36
4	N	518	VAL	N-CA-C	-5.00	108.42	113.47

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	ARG	Sidechain
1	B	58	ARG	Sidechain
2	C	319	ARG	Sidechain
1	D	131	ARG	Sidechain
1	D	97	ARG	Sidechain
2	E	354	ARG	Sidechain
2	E	364	ARG	Sidechain
2	E	367	ARG	Sidechain
2	E	586	ARG	Sidechain
1	F	103	ARG	Sidechain
1	F	58	ARG	Sidechain
3	G	265	ARG	Sidechain
3	G	515	ARG	Sidechain
4	H	379	ARG	Sidechain
4	H	510	ARG	Sidechain
3	I	410	ARG	Sidechain
3	I	496	ARG	Sidechain
4	J	450	ARG	Sidechain
3	K	528	TYR	Sidechain
4	L	389	ARG	Sidechain
4	L	410	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	L	450	ARG	Sidechain
3	M	265	ARG	Sidechain
3	M	389	ARG	Sidechain
3	M	410	ARG	Sidechain
3	M	426	ARG	Sidechain
3	M	450	ARG	Sidechain
4	N	373	ARG	Sidechain
3	O	410	ARG	Sidechain
3	O	496	ARG	Sidechain
3	O	510	ARG	Sidechain
4	P	373	ARG	Sidechain
4	P	515	ARG	Sidechain
3	Q	410	ARG	Sidechain
3	Q	510	ARG	Sidechain

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	1105	1169	1166	0	0
1	B	1105	1169	1166	0	0
1	D	1105	1169	1166	1	0
1	F	1105	1169	1166	0	0
2	C	2979	3131	3128	3	0
2	E	2979	3131	3128	0	0
3	G	2334	2322	2319	0	0
3	I	2334	2322	2319	0	0
3	K	2334	2322	2319	0	0
3	M	2334	2322	2319	0	0
3	O	2334	2322	2319	0	0
3	Q	2334	2322	2319	0	0
4	H	2322	2305	2302	0	0
4	J	2322	2305	2302	0	0
4	L	2322	2305	2302	0	0
4	N	2322	2305	2302	0	0
4	P	2322	2305	2302	0	0
4	R	2322	2305	2302	0	0
All	All	38314	38700	38646	4	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 0.

All (4) 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:C:603:HIS:CG	2:C:604:LYS:H	2.35	0.44
2:C:421:ARG:HH22	2:C:450:ASP:CG	2.26	0.42
1:D:20:GLU:CD	1:D:97:ARG:HH22	2.27	0.41
2:C:603:HIS:CG	2:C:604:LYS:N	2.89	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	137/139 (99%)	120 (88%)	13 (10%)	4 (3%)	3	23
1	B	137/139 (99%)	118 (86%)	17 (12%)	2 (2%)	8	40
1	D	137/139 (99%)	122 (89%)	14 (10%)	1 (1%)	18	56
1	F	137/139 (99%)	123 (90%)	13 (10%)	1 (1%)	18	56
2	C	377/379 (100%)	355 (94%)	19 (5%)	3 (1%)	16	54
2	E	377/379 (100%)	354 (94%)	19 (5%)	4 (1%)	11	46
3	G	307/309 (99%)	305 (99%)	2 (1%)	0	100	100
3	I	307/309 (99%)	301 (98%)	4 (1%)	2 (1%)	18	56
3	K	307/309 (99%)	305 (99%)	2 (1%)	0	100	100
3	M	307/309 (99%)	306 (100%)	1 (0%)	0	100	100
3	O	307/309 (99%)	301 (98%)	4 (1%)	2 (1%)	18	56
3	Q	307/309 (99%)	305 (99%)	2 (1%)	0	100	100
4	H	305/307 (99%)	301 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	J	305/307 (99%)	300 (98%)	5 (2%)	0	100	100
4	L	305/307 (99%)	300 (98%)	5 (2%)	0	100	100
4	N	305/307 (99%)	301 (99%)	4 (1%)	0	100	100
4	P	305/307 (99%)	300 (98%)	5 (2%)	0	100	100
4	R	305/307 (99%)	299 (98%)	6 (2%)	0	100	100
All	All	4974/5010 (99%)	4816 (97%)	139 (3%)	19 (0%)	31	67

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	28	ASP
1	B	27	VAL
1	B	28	ASP
2	C	563	ILE
2	E	563	ILE
3	I	372	ALA
3	I	376	GLU
3	O	372	ALA
1	A	87	LYS
1	D	28	ASP
3	O	376	GLU
1	A	19	ASP
2	C	630	LEU
2	E	630	LEU
1	F	28	ASP
2	E	538	PRO
2	E	559	PRO
2	C	559	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	127/127 (100%)	123 (97%)	4 (3%)	35	56
1	B	127/127 (100%)	124 (98%)	3 (2%)	43	64
1	D	127/127 (100%)	127 (100%)	0	100	100
1	F	127/127 (100%)	126 (99%)	1 (1%)	73	80
2	C	337/337 (100%)	335 (99%)	2 (1%)	78	83
2	E	337/337 (100%)	331 (98%)	6 (2%)	51	68
3	G	253/253 (100%)	251 (99%)	2 (1%)	73	80
3	I	253/253 (100%)	250 (99%)	3 (1%)	63	75
3	K	253/253 (100%)	251 (99%)	2 (1%)	73	80
3	M	253/253 (100%)	250 (99%)	3 (1%)	63	75
3	O	253/253 (100%)	251 (99%)	2 (1%)	73	80
3	Q	253/253 (100%)	249 (98%)	4 (2%)	55	70
4	H	252/252 (100%)	250 (99%)	2 (1%)	73	80
4	J	252/252 (100%)	249 (99%)	3 (1%)	63	75
4	L	252/252 (100%)	251 (100%)	1 (0%)	84	84
4	N	252/252 (100%)	246 (98%)	6 (2%)	43	64
4	P	252/252 (100%)	249 (99%)	3 (1%)	63	75
4	R	252/252 (100%)	246 (98%)	6 (2%)	43	64
All	All	4212/4212 (100%)	4159 (99%)	53 (1%)	59	74

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	27	VAL
1	A	30	ILE
1	A	145	ILE
1	B	14	LEU
1	B	25	PHE
1	B	67	LYS
2	C	304	ASP
2	C	341	ARG
2	E	341	ARG
2	E	377	ASN
2	E	484	ASN
2	E	532	LYS
2	E	563	ILE

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Mol	Chain	Res	Type
2	E	565	THR
1	F	19	ASP
3	G	230	GLU
3	G	496	ARG
4	H	331	ASP
4	H	409	ILE
3	I	330	LYS
3	I	362	LEU
3	I	409	ILE
4	J	426	ARG
4	J	479	ASN
4	J	508	THR
3	K	321	VAL
3	K	426	ARG
4	L	479	ASN
3	M	236	GLU
3	M	331	ASP
3	M	369	ILE
4	N	336	VAL
4	N	358	GLU
4	N	409	ILE
4	N	426	ARG
4	N	479	ASN
4	N	508	THR
3	O	369	ILE
3	O	415	ASP
4	P	340	GLN
4	P	345	GLU
4	P	426	ARG
3	Q	230	GLU
3	Q	426	ARG
3	Q	454	MET
3	Q	496	ARG
4	R	223	HIS
4	R	409	ILE
4	R	426	ARG
4	R	457	ASN
4	R	470	ASP
4	R	479	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	438	HIS
1	D	47	HIS
1	F	54	ASN
3	G	223	HIS
3	G	488	ASN
3	I	223	HIS
3	I	245	ASN
3	I	361	ASN
3	I	512	GLN
4	J	274	GLN
4	J	401	ASN
4	J	465	GLN
3	K	245	ASN
3	K	261	ASN
3	K	289	ASN
3	K	465	GLN
3	K	488	ASN
4	L	457	ASN
4	L	465	GLN
4	L	479	ASN
4	L	482	ASN
3	M	223	HIS
3	M	245	ASN
3	M	306	GLN
3	M	401	ASN
4	N	223	HIS
4	N	261	ASN
4	N	359	GLN
3	O	245	ASN
3	O	303	GLN
3	O	517	ASN
4	P	245	ASN
4	P	396	GLN
4	P	482	ASN
3	Q	354	ASN
3	Q	442	ASN
3	Q	457	ASN
3	Q	465	GLN
4	R	228	GLN
4	R	245	ASN
4	R	465	GLN
4	R	479	ASN

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.

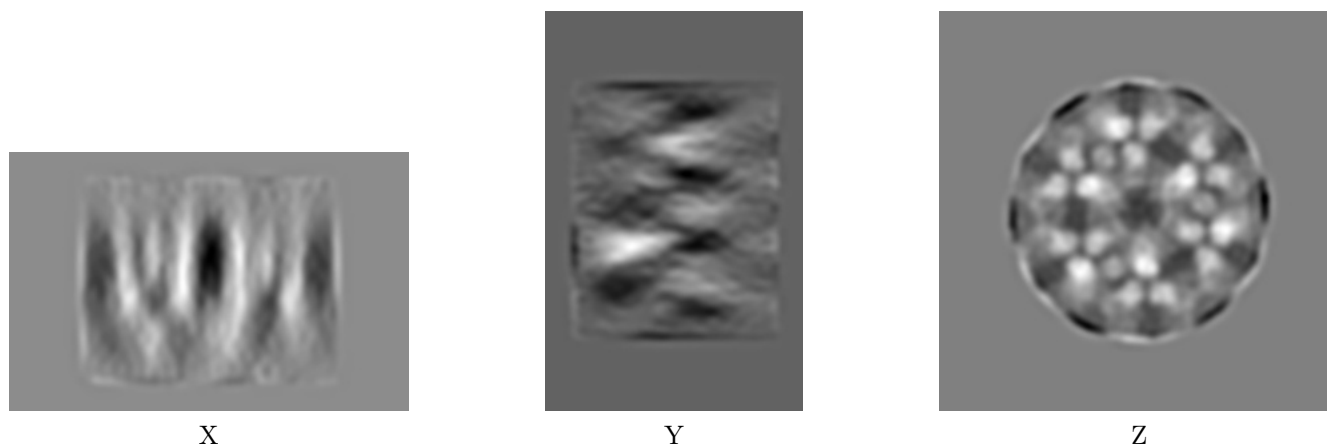
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

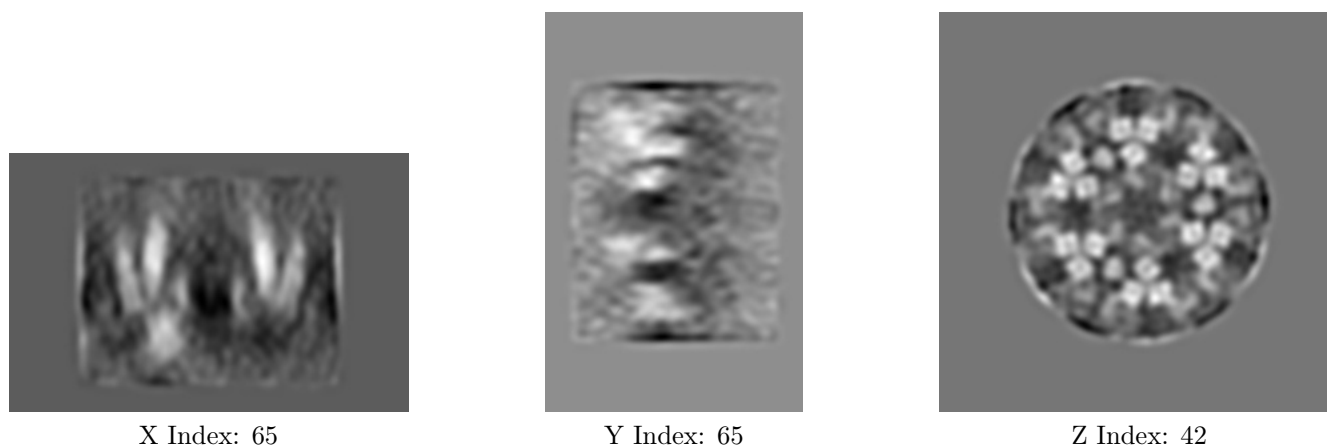
This section contains visualisations of the EMDB entry EMD-6319. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



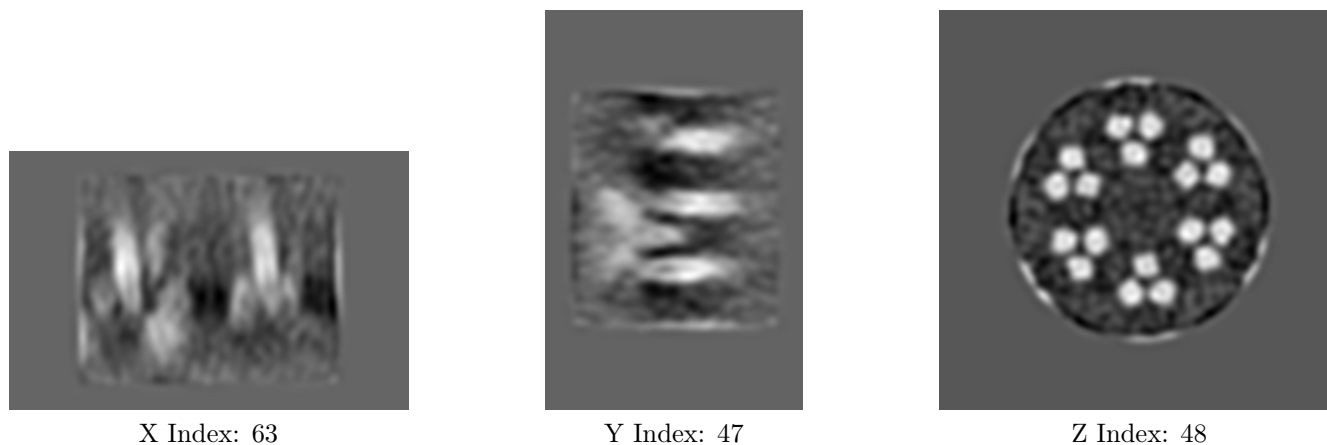
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



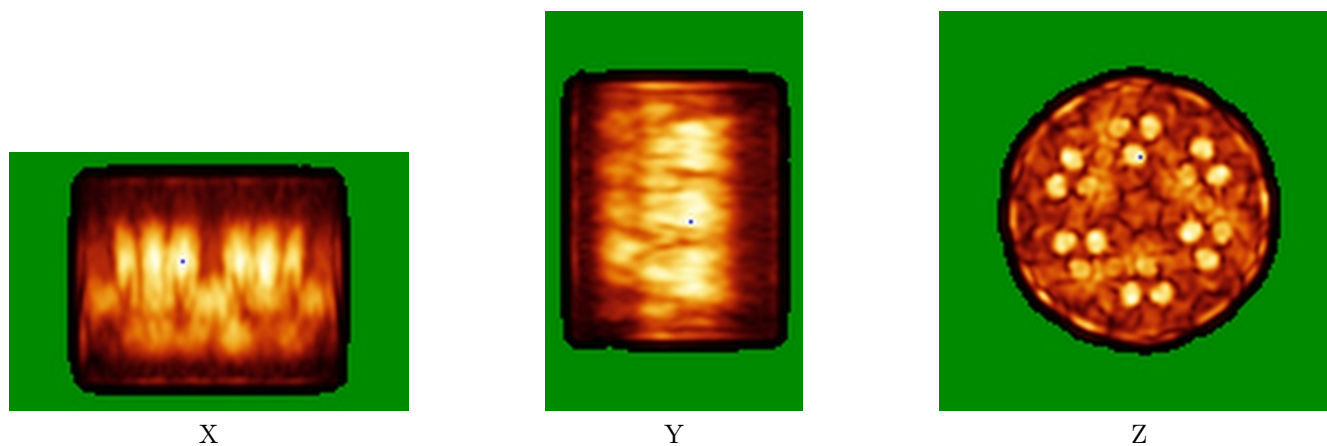
The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



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

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



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

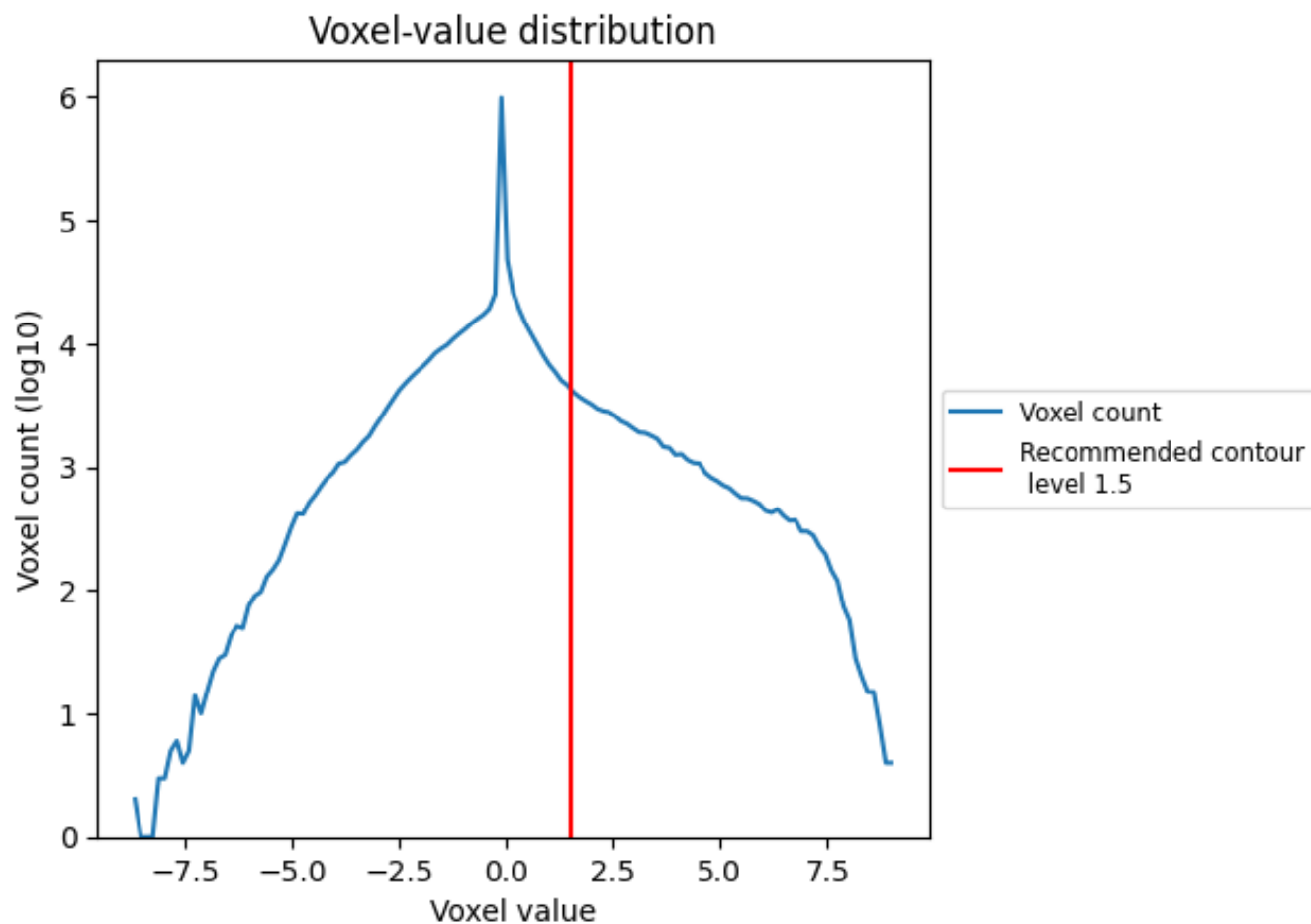
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

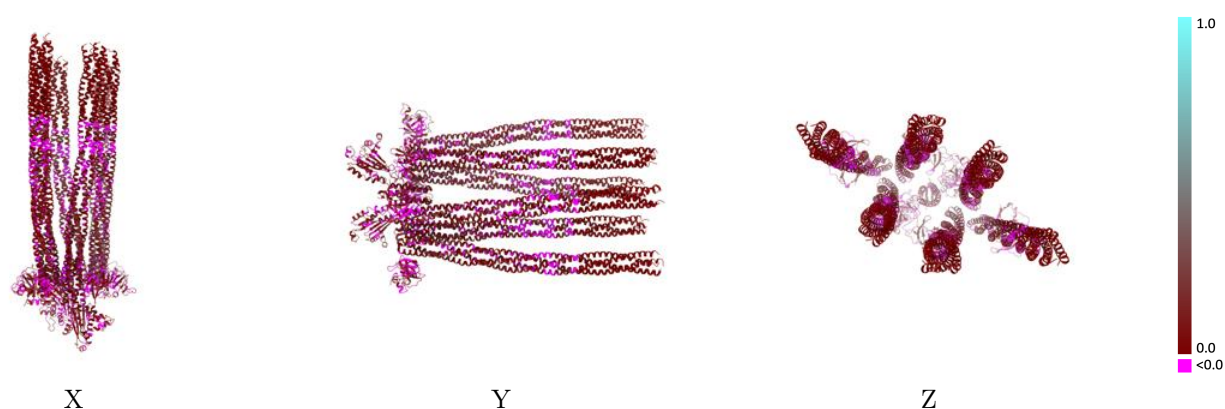
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6319 and PDB model 3JA6. Per-residue inclusion information can be found in section 3 on page 6.

8.1 Map-model overlay [i](#)

This section was not generated.

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

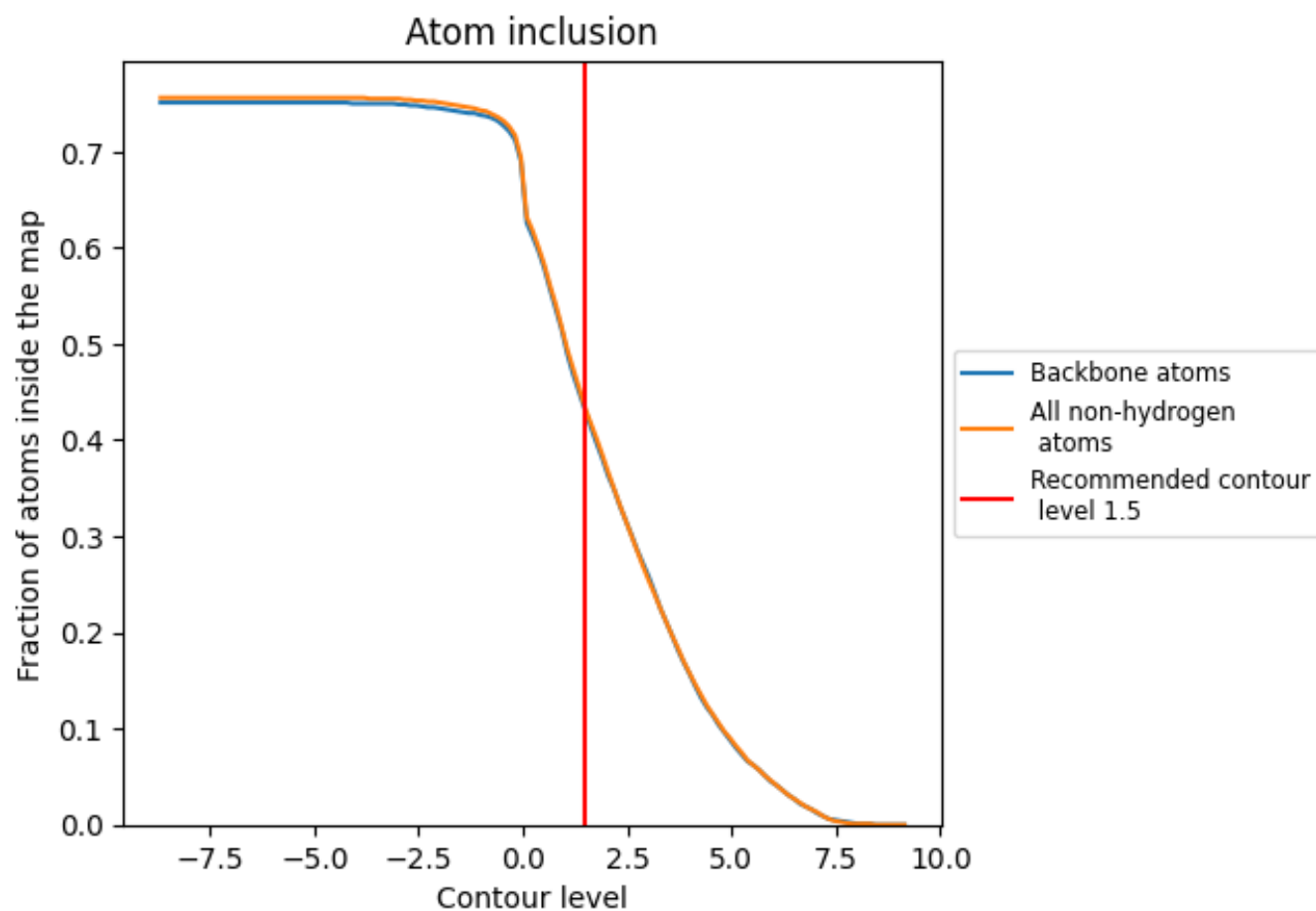


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 43% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4320	 0.0420
A	 0.6280	 0.0630
B	 0.5100	 0.0390
C	 0.7750	 0.0580
D	 0.4150	 0.0440
E	 0.7850	 0.0550
F	 0.4830	 0.0470
G	 0.3770	 0.0410
H	 0.3690	 0.0410
I	 0.3270	 0.0300
J	 0.3810	 0.0560
K	 0.3340	 0.0290
L	 0.3420	 0.0420
M	 0.3140	 0.0320
N	 0.3670	 0.0470
O	 0.3630	 0.0390
P	 0.3320	 0.0310
Q	 0.3730	 0.0370
R	 0.3630	 0.0350

