



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 08:09 AM EST

PDB ID : 3JA6
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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

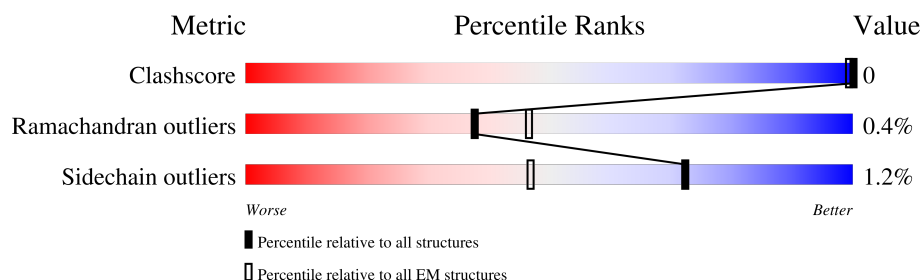
1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>29%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	B	139	<div> <div>45%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
1	D	139	<div> <div>55%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
1	F	139	<div> <div>49%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
2	C	379	<div> <div>20%</div> <div>95%</div> <div>5%</div> </div>
2	E	379	<div> <div>18%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
3	G	309	<div> <div>61%</div> <div>96%</div> <div>.</div> <div>.</div> </div>
3	I	309	<div> <div>63%</div> <div>95%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	K	309	<div>64%</div> <div>95%</div> <div>5%</div>
3	M	309	<div>66%</div> <div>95%</div> <div>.</div>
3	O	309	<div>61%</div> <div>96%</div> <div>.</div>
3	Q	309	<div>60%</div> <div>97%</div> <div>.</div>
4	H	307	<div>58%</div> <div>95%</div> <div>.</div>
4	J	307	<div>60%</div> <div>96%</div> <div>.</div>
4	L	307	<div>63%</div> <div>96%</div> <div>.</div>
4	N	307	<div>61%</div> <div>96%</div> <div>.</div>
4	P	307	<div>63%</div> <div>95%</div> <div>.</div>
4	R	307	<div>61%</div> <div>96%</div> <div>.</div>

2 Entry composition

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		

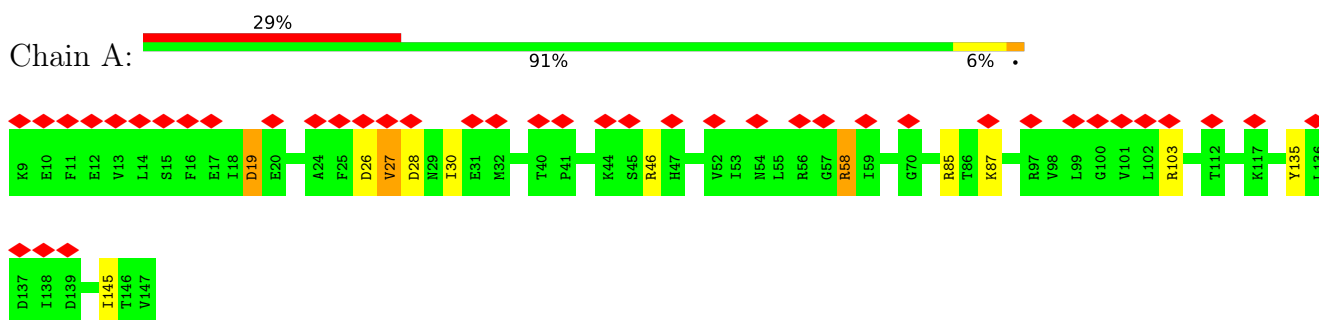
- Molecule 4 is a protein called Methyl-accepting chemotaxis protein 2.

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

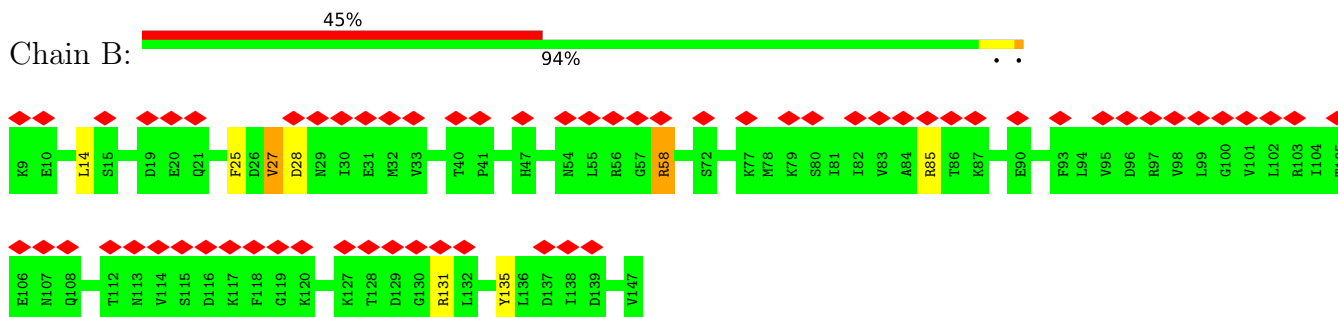
3 Residue-property plots [i](#)

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.

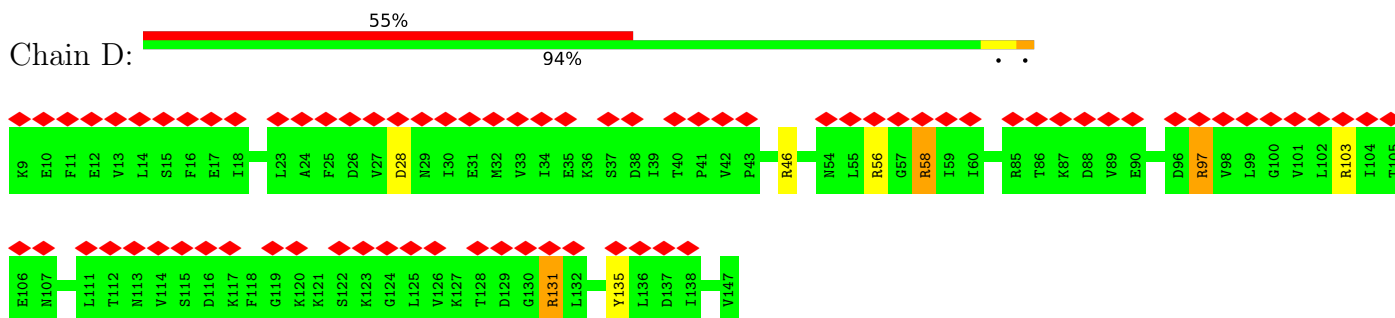
- Molecule 1: Chemotaxis protein CheW



- Molecule 1: Chemotaxis protein CheW

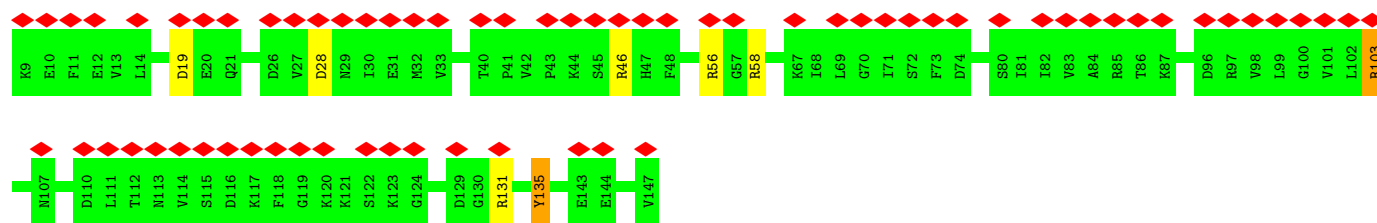


- Molecule 1: Chemotaxis protein CheW

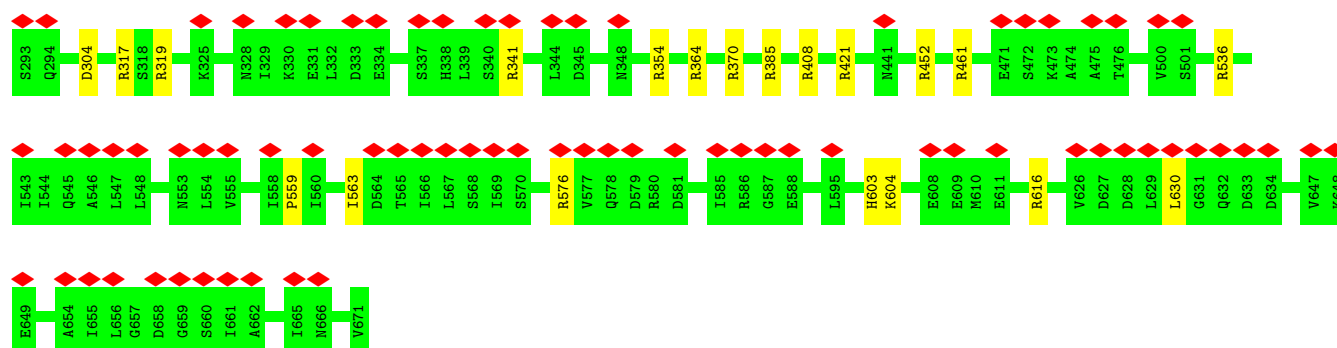


- Molecule 1: Chemotaxis protein CheW

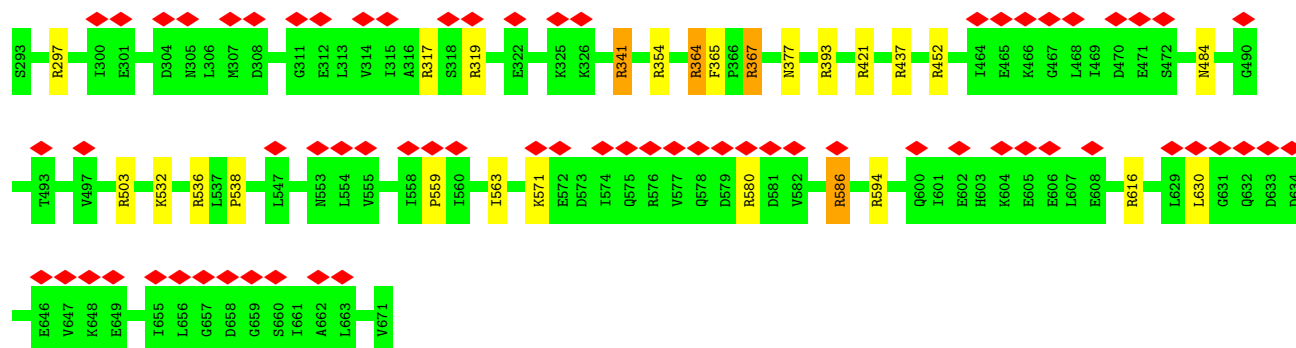




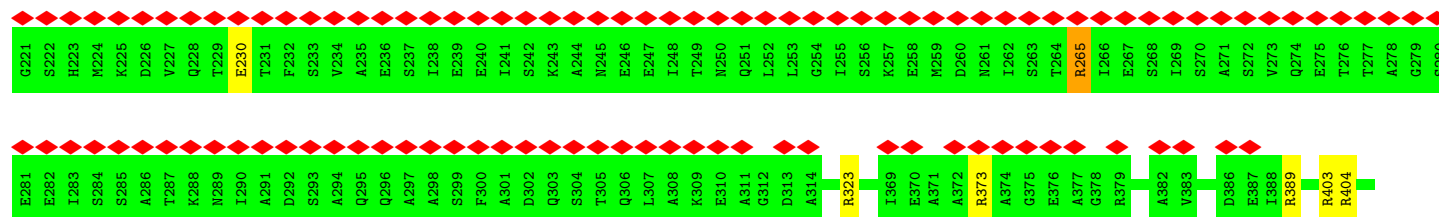
• Molecule 2: Chemotaxis protein CheA



• Molecule 2: Chemotaxis protein CheA

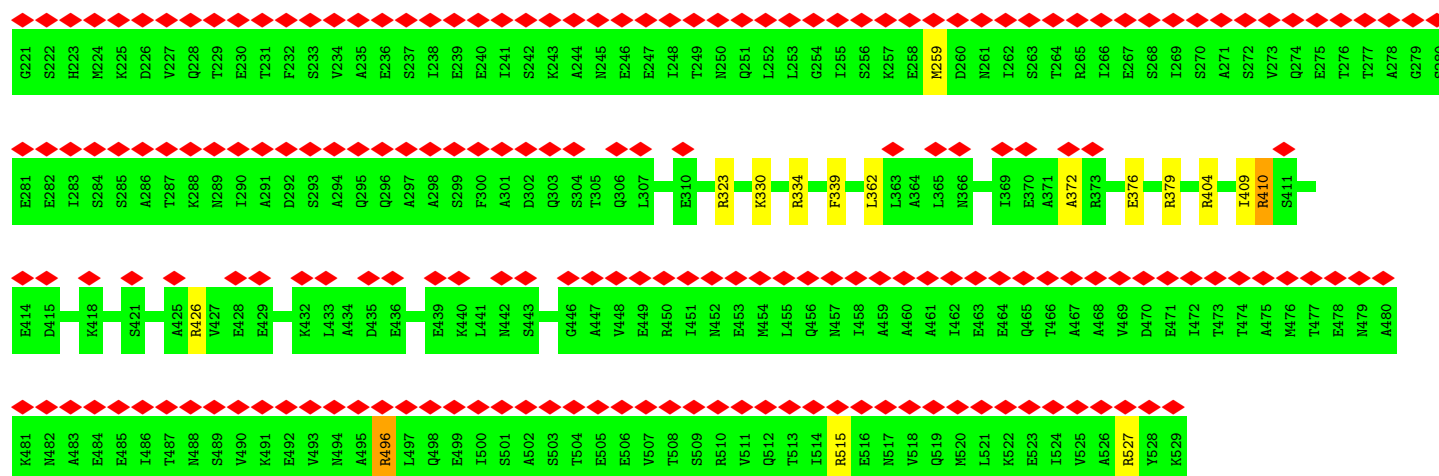
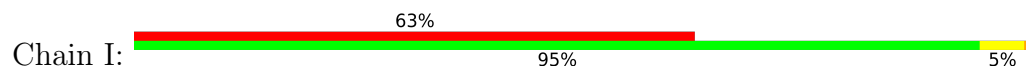


• Molecule 3: Methyl-accepting chemotaxis protein 2

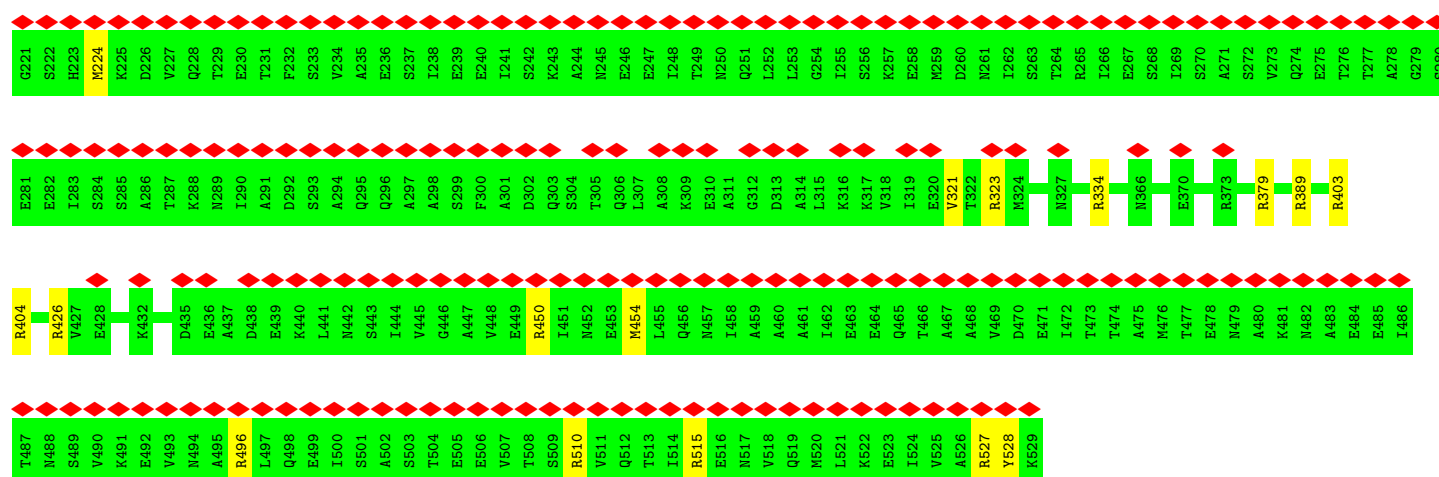




• Molecule 3: Methyl-accepting chemotaxis protein 2

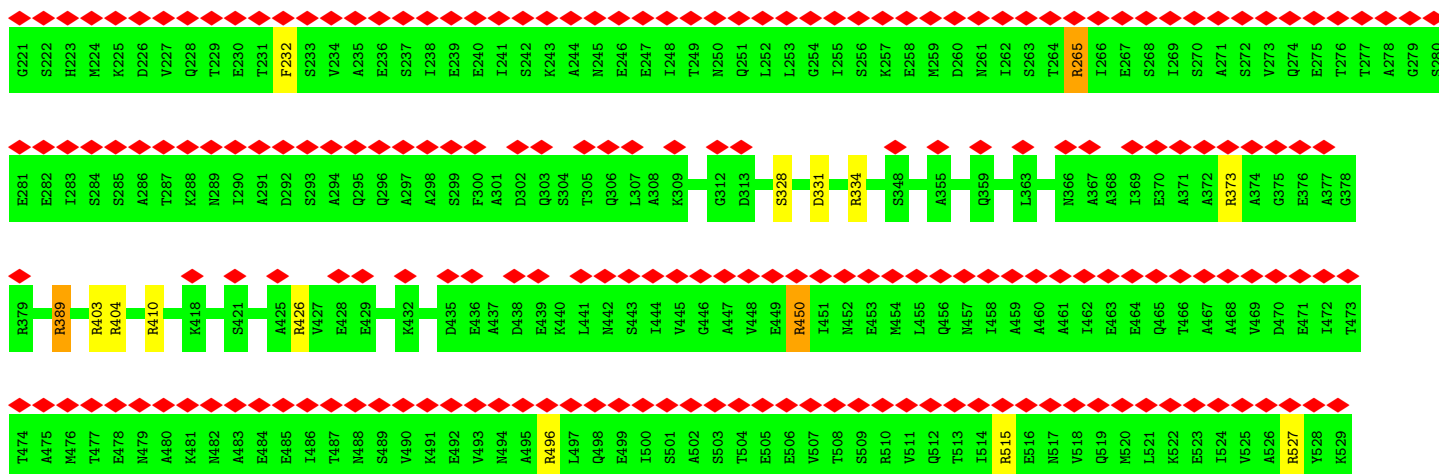


• Molecule 3: Methyl-accepting chemotaxis protein 2

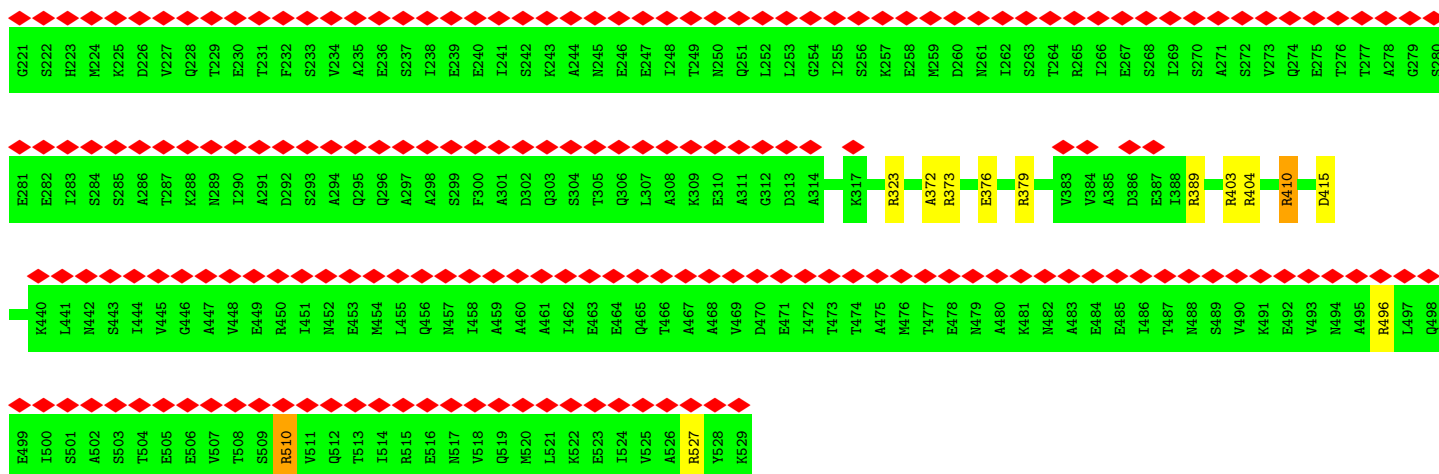


• Molecule 3: Methyl-accepting chemotaxis protein 2

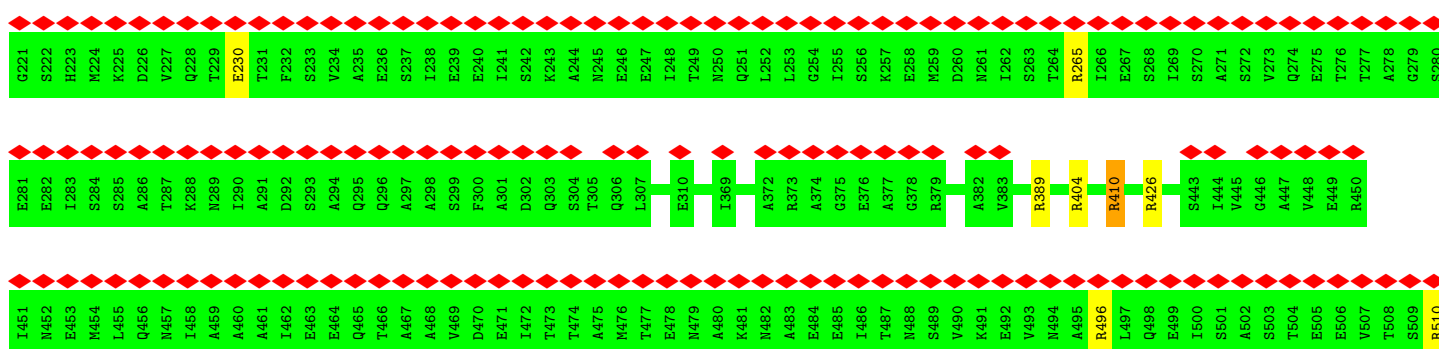


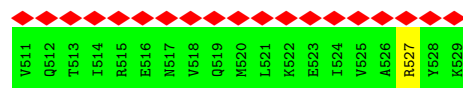


• Molecule 3: Methyl-accepting chemotaxis protein 2

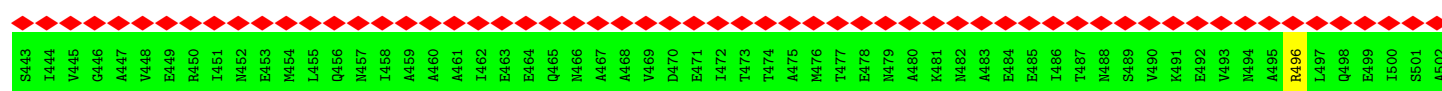
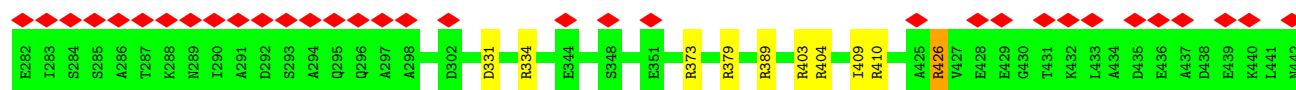
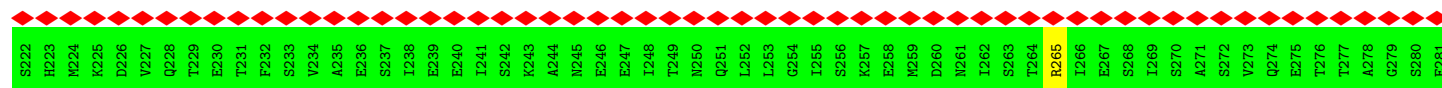


• Molecule 3: Methyl-accepting chemotaxis protein 2

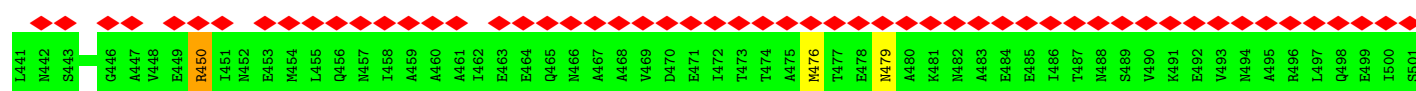
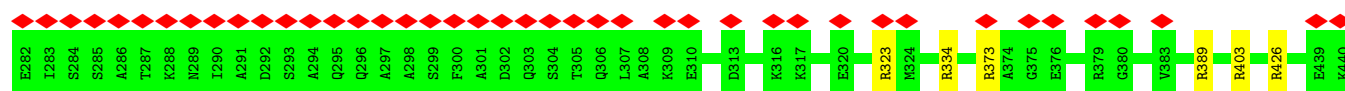
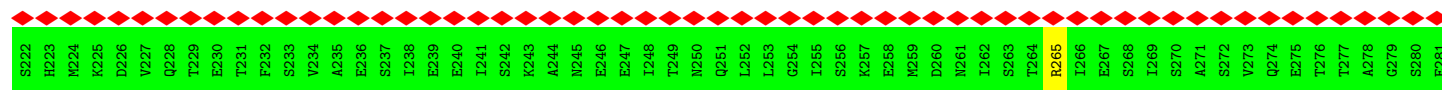




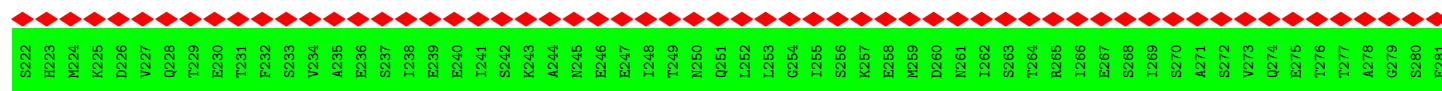
• Molecule 4: Methyl-accepting chemotaxis protein 2

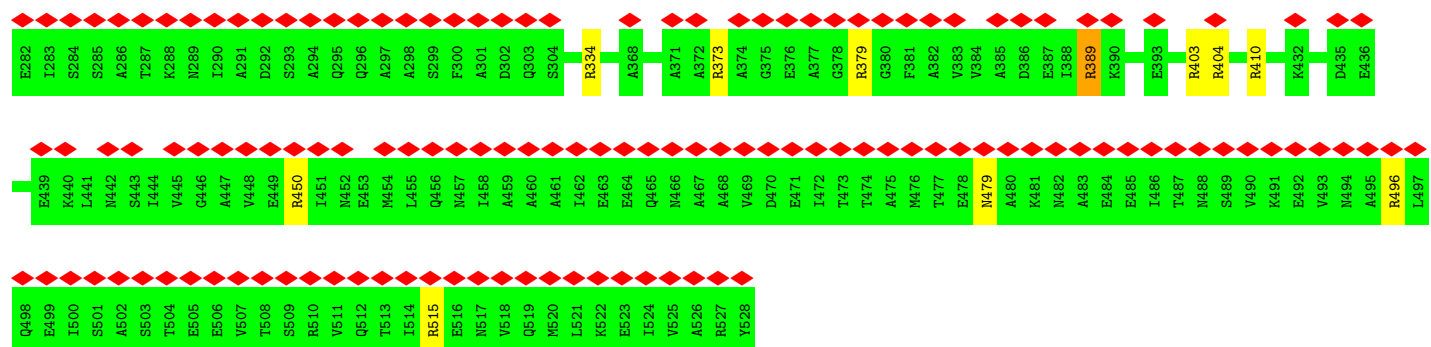


• Molecule 4: Methyl-accepting chemotaxis protein 2

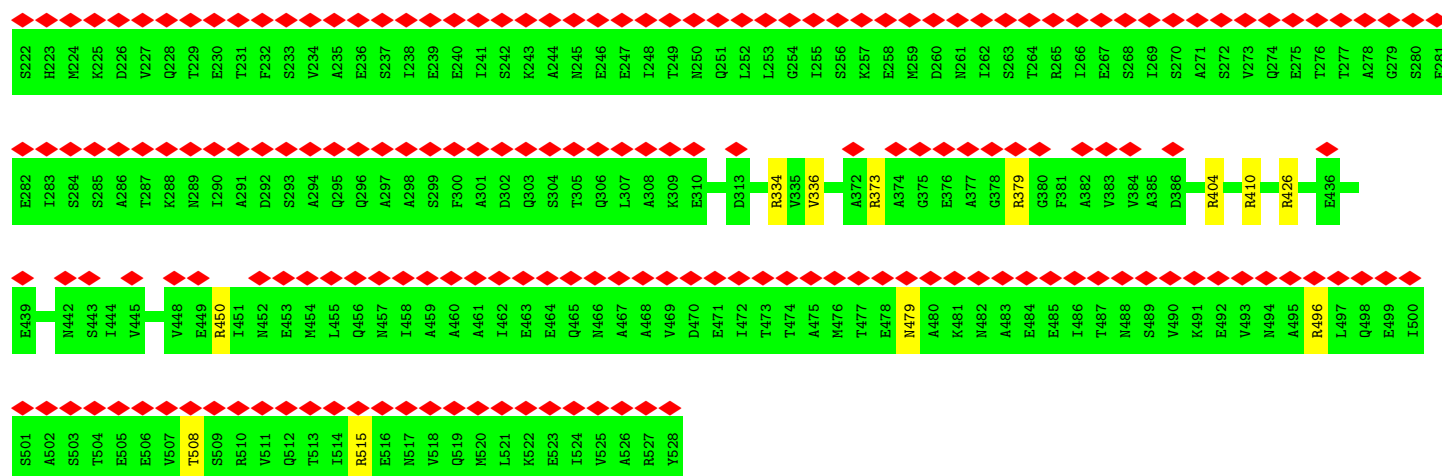


• Molecule 4: Methyl-accepting chemotaxis protein 2

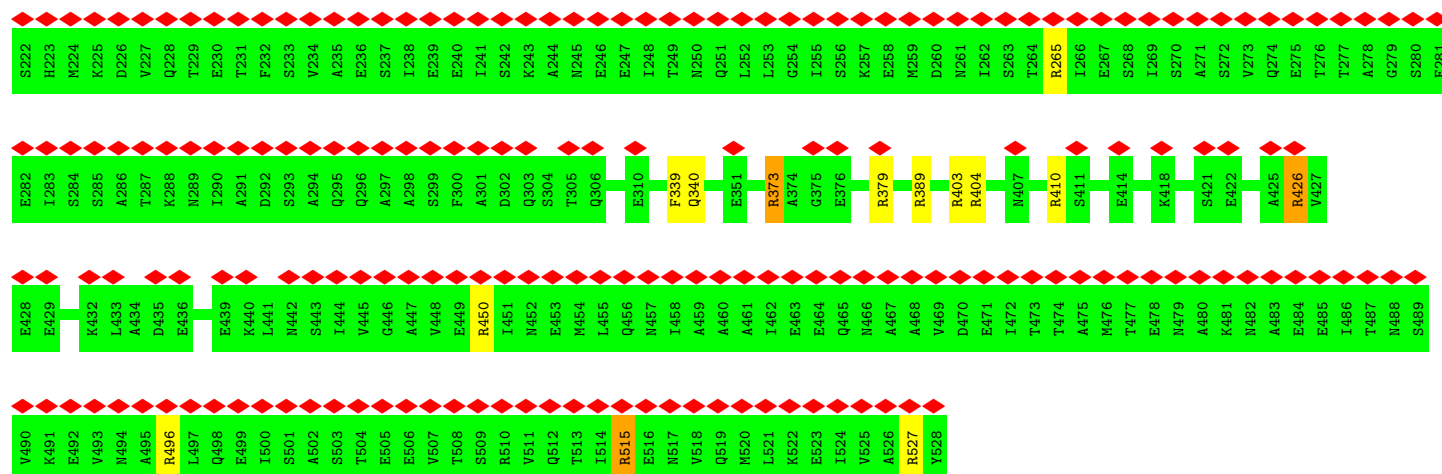




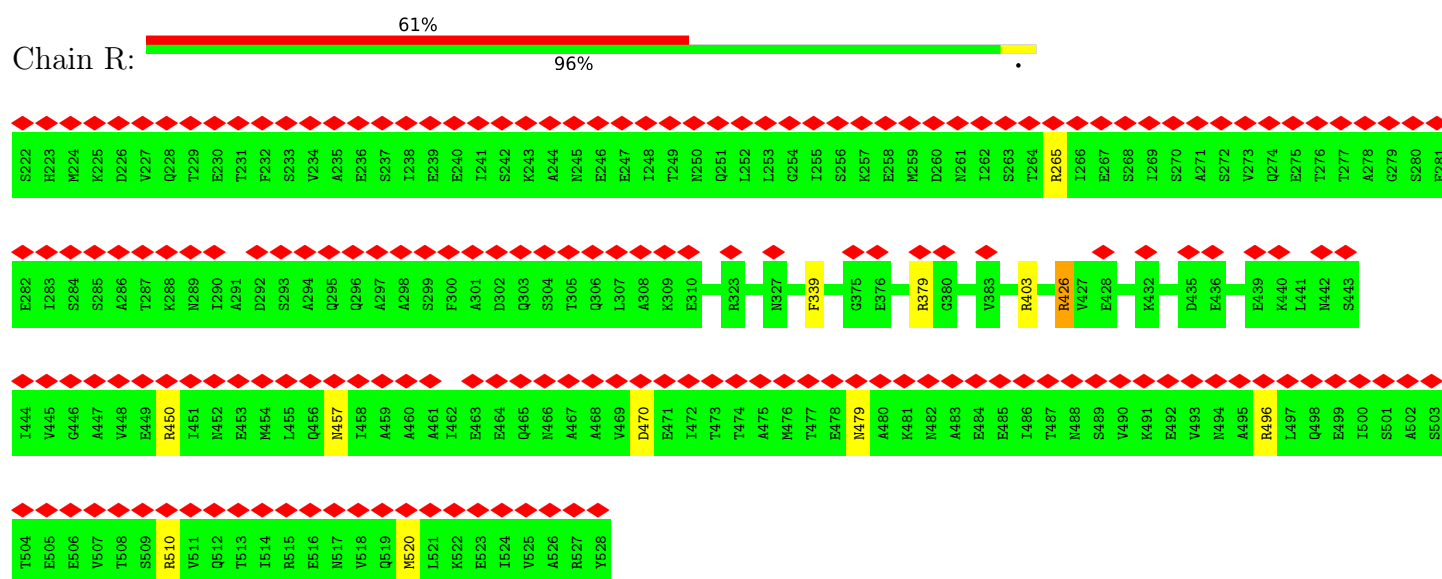
• Molecule 4: Methyl-accepting chemotaxis protein 2



• 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	0.67	0/1116	1.09	8/1501 (0.5%)
1	B	0.68	0/1116	1.05	7/1501 (0.5%)
1	D	0.67	0/1116	1.16	12/1501 (0.8%)
1	F	0.68	0/1116	1.08	6/1501 (0.4%)
2	C	0.66	0/3009	1.08	19/4051 (0.5%)
2	E	0.66	0/3009	1.09	24/4051 (0.6%)
3	G	0.67	0/2340	1.07	15/3153 (0.5%)
3	I	0.66	0/2340	1.05	13/3153 (0.4%)
3	K	0.66	0/2340	1.09	18/3153 (0.6%)
3	M	0.67	0/2340	1.06	16/3153 (0.5%)
3	O	0.67	0/2340	1.07	12/3153 (0.4%)
3	Q	0.68	0/2340	1.03	5/3153 (0.2%)
4	H	0.67	0/2328	1.09	15/3138 (0.5%)
4	J	0.66	0/2328	1.04	9/3138 (0.3%)
4	L	0.67	0/2328	1.03	10/3138 (0.3%)
4	N	0.67	0/2328	1.02	8/3138 (0.3%)
4	P	0.67	0/2328	1.04	14/3138 (0.4%)
4	R	0.66	0/2328	1.05	13/3138 (0.4%)
All	All	0.67	0/38490	1.06	224/51852 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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.

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	421	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	97	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	D	135	TYR	CB-CG-CD2	-8.52	115.89	121.00
4	R	403	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	D	103	ARG	NE-CZ-NH1	8.45	124.53	120.30

There are no chirality outliers.

5 of 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

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.

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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	0	0
1	F	1105	1169	1166	0	0
2	C	2979	3131	3128	2	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	2	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 (2) 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: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%)	4	29
1	B	137/139 (99%)	118 (86%)	17 (12%)	2 (2%)	10	46
1	D	137/139 (99%)	122 (89%)	14 (10%)	1 (1%)	22	63
1	F	137/139 (99%)	123 (90%)	13 (10%)	1 (1%)	22	63
2	C	377/379 (100%)	355 (94%)	19 (5%)	3 (1%)	19	60
2	E	377/379 (100%)	354 (94%)	19 (5%)	4 (1%)	14	52
3	G	307/309 (99%)	305 (99%)	2 (1%)	0	100	100
3	I	307/309 (99%)	301 (98%)	4 (1%)	2 (1%)	22	63
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%)	22	63
3	Q	307/309 (99%)	305 (99%)	2 (1%)	0	100	100
4	H	305/307 (99%)	301 (99%)	4 (1%)	0	100	100
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%)	38	72

5 of 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

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%)	124 (98%)	3 (2%)	49	69
1	B	127/127 (100%)	125 (98%)	2 (2%)	62	79
1	D	127/127 (100%)	126 (99%)	1 (1%)	81	89
1	F	127/127 (100%)	125 (98%)	2 (2%)	62	79
2	C	337/337 (100%)	335 (99%)	2 (1%)	86	92
2	E	337/337 (100%)	332 (98%)	5 (2%)	65	80
3	G	253/253 (100%)	251 (99%)	2 (1%)	81	89
3	I	253/253 (100%)	250 (99%)	3 (1%)	71	83
3	K	253/253 (100%)	250 (99%)	3 (1%)	71	83
3	M	253/253 (100%)	251 (99%)	2 (1%)	81	89
3	O	253/253 (100%)	252 (100%)	1 (0%)	91	94
3	Q	253/253 (100%)	250 (99%)	3 (1%)	71	83
4	H	252/252 (100%)	249 (99%)	3 (1%)	71	83
4	J	252/252 (100%)	247 (98%)	5 (2%)	55	74
4	L	252/252 (100%)	251 (100%)	1 (0%)	91	94
4	N	252/252 (100%)	248 (98%)	4 (2%)	62	79
4	P	252/252 (100%)	249 (99%)	3 (1%)	71	83
4	R	252/252 (100%)	248 (98%)	4 (2%)	62	79
All	All	4212/4212 (100%)	4163 (99%)	49 (1%)	72	83

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	224	MET
4	N	426	ARG
3	K	321	VAL
3	M	328	SER
4	N	508	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	578	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	409	ASN
2	E	413	HIS
3	M	223	HIS
4	P	465	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

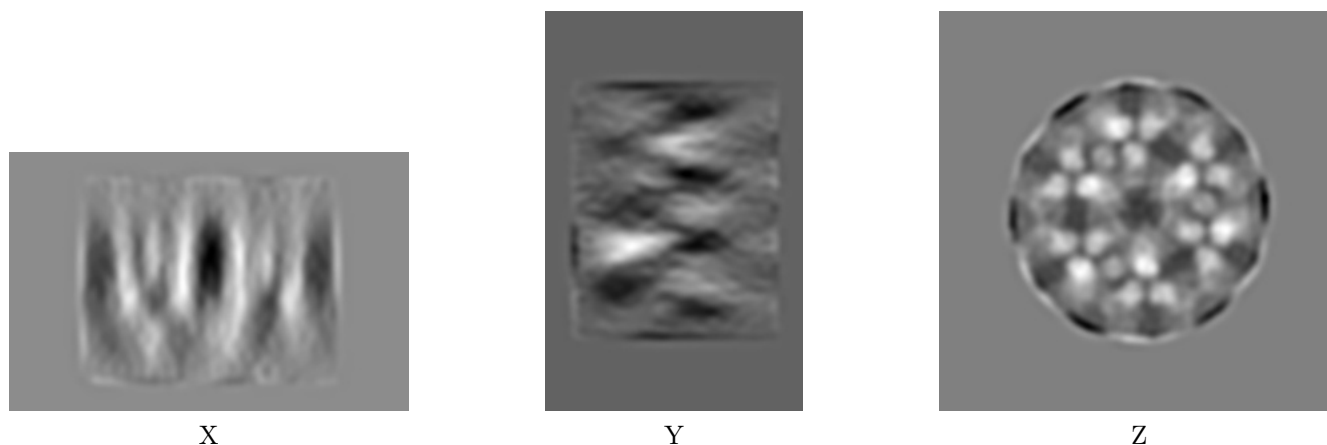
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

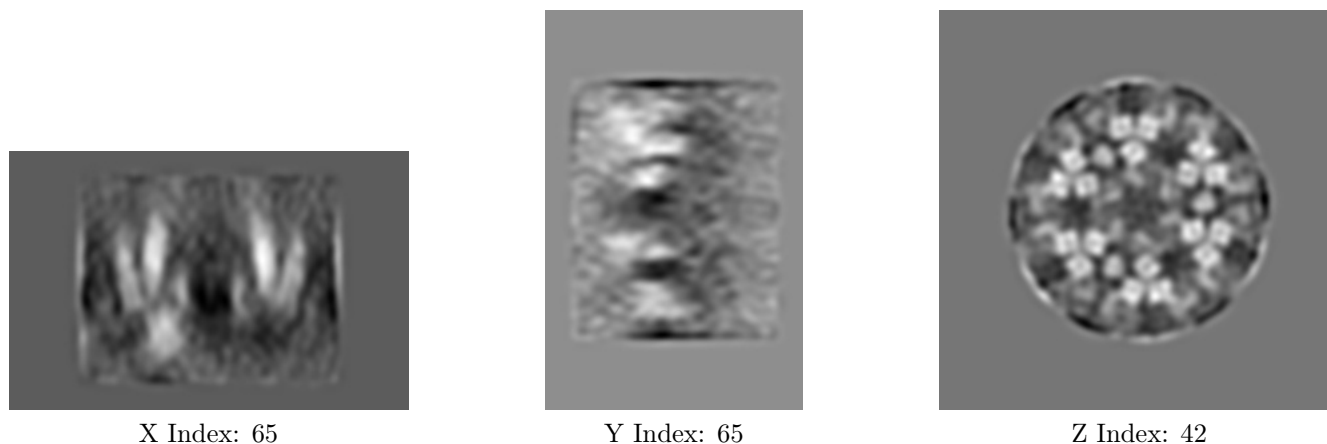
This section contains visualisations of the EMDB entry EMD-6319. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



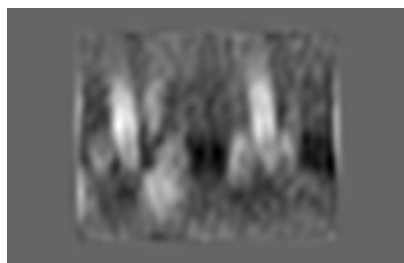
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)

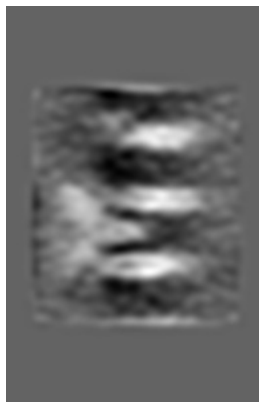


The images above show central slices of the tomogram in three orthogonal directions.

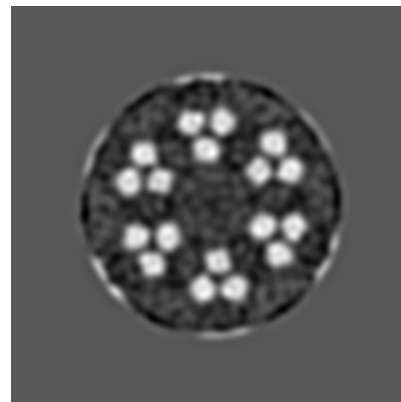
6.3 Largest variance slices [i](#)



X Index: 63



Y Index: 47



Z Index: 48

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

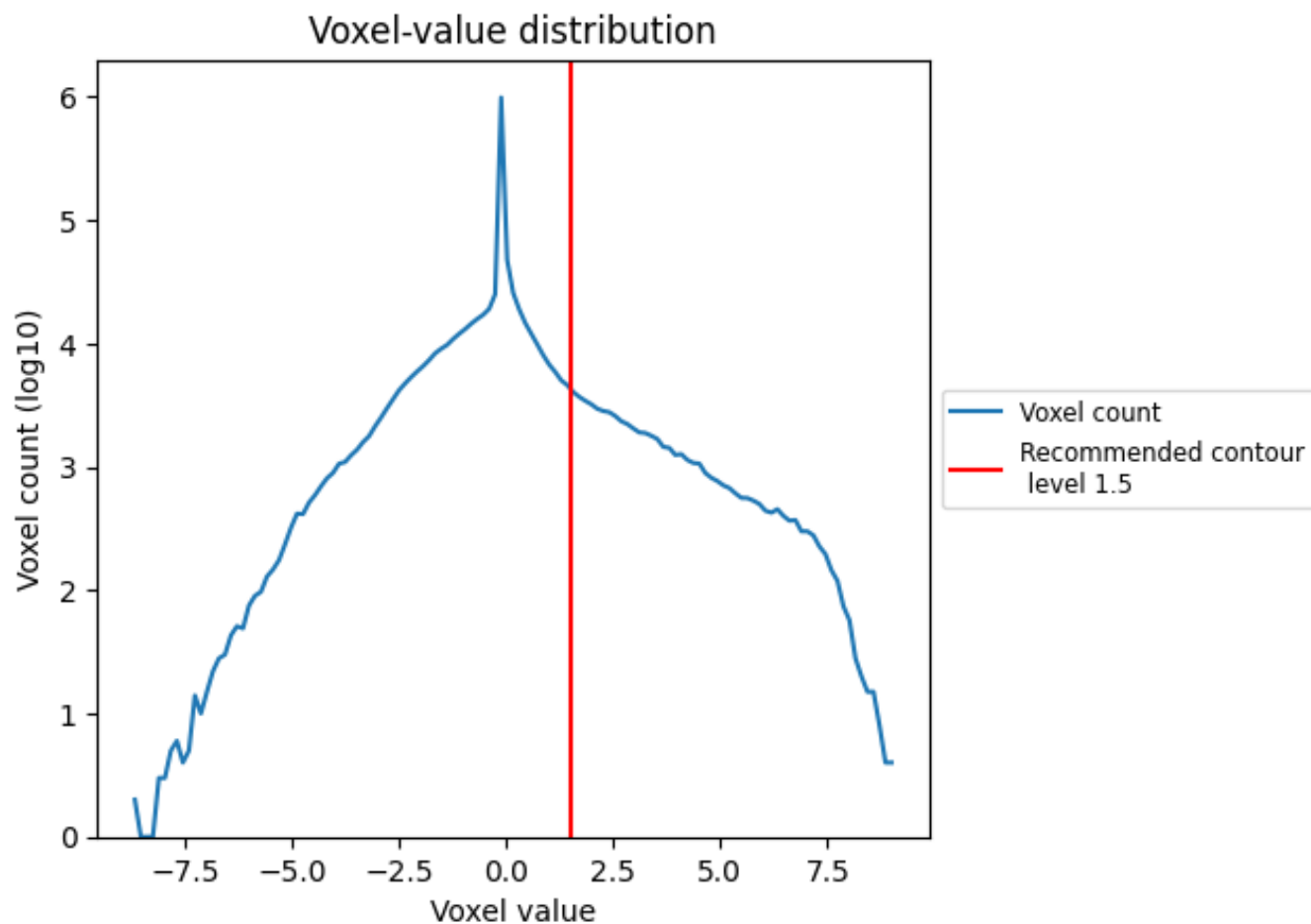
6.4 Mask visualisation [i](#)

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.

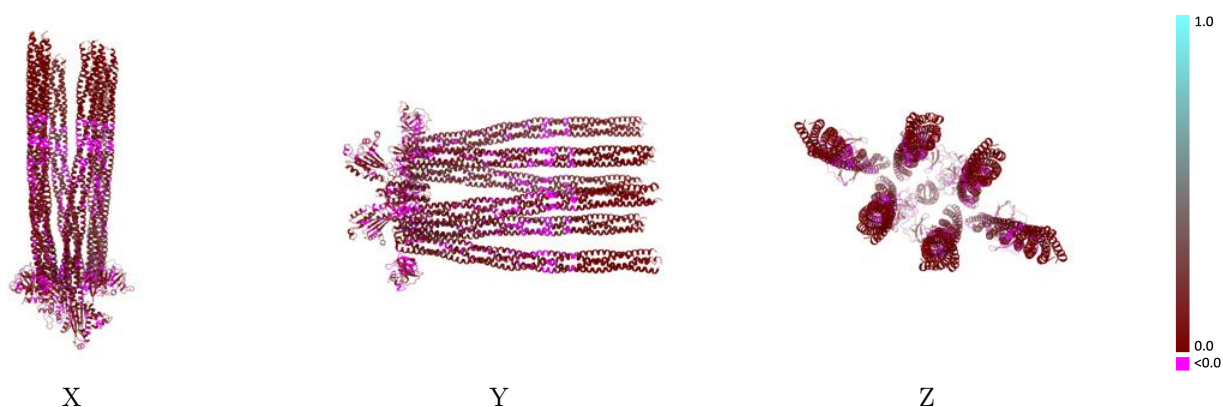
8 Map-model fit [i](#)

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](#)

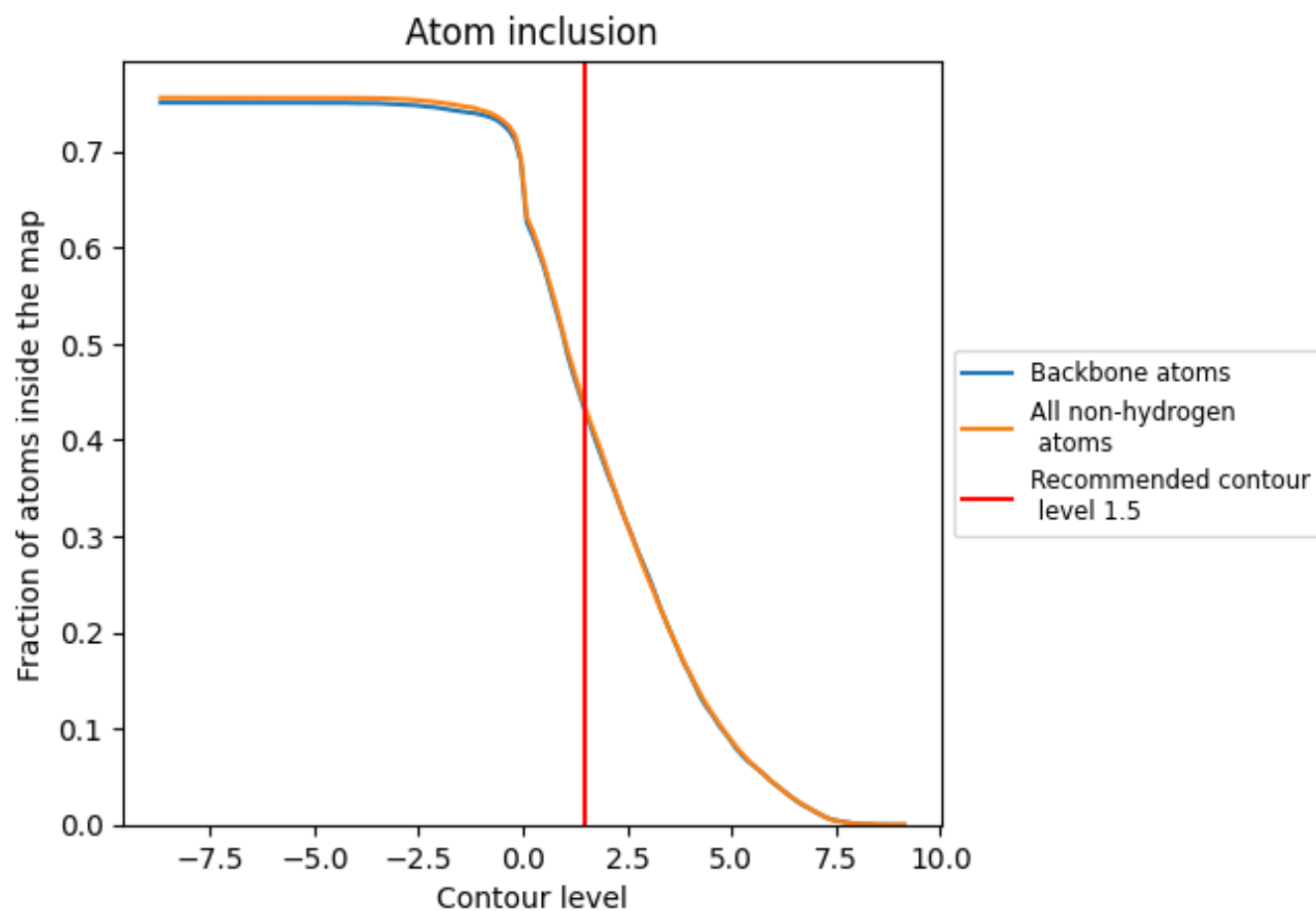


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.4323	 0.0420
A	 0.6284	 0.0630
B	 0.5101	 0.0390
C	 0.7746	 0.0580
D	 0.4147	 0.0440
E	 0.7852	 0.0550
F	 0.4835	 0.0470
G	 0.3769	 0.0410
H	 0.3693	 0.0410
I	 0.3265	 0.0300
J	 0.3811	 0.0560
K	 0.3343	 0.0290
L	 0.3418	 0.0420
M	 0.3144	 0.0320
N	 0.3671	 0.0470
O	 0.3634	 0.0390
P	 0.3317	 0.0310
Q	 0.3734	 0.0370
R	 0.3627	 0.0350

