



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:34 PM UTC

PDB ID : 8X2U / pdb_00008x2u
EMDB ID : EMD-38020
Title : Radial spoke head-neck dimer
Authors : Meng, X.; Cong, Y.
Deposited on : 2023-11-10
Resolution : 3.57 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:

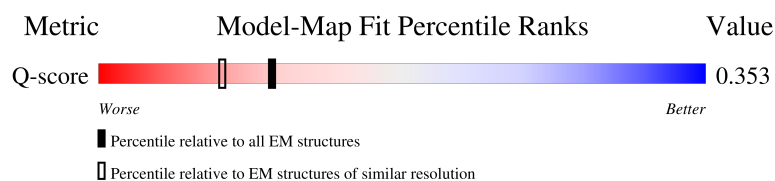
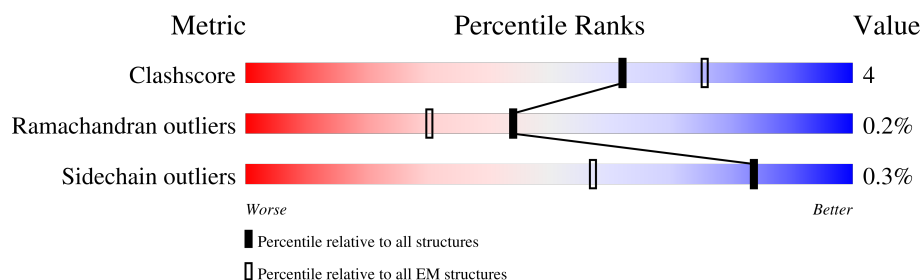
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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

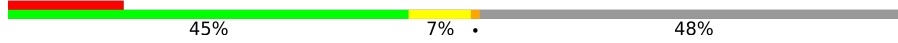
The reported resolution of this entry is 3.57 Å.

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.



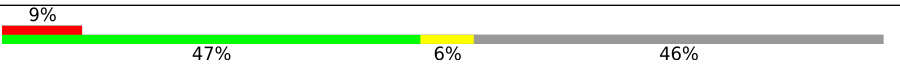
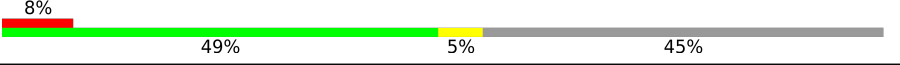
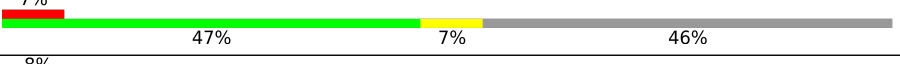
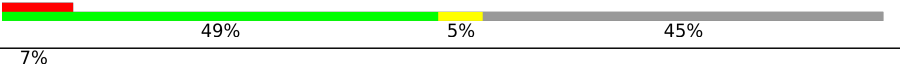
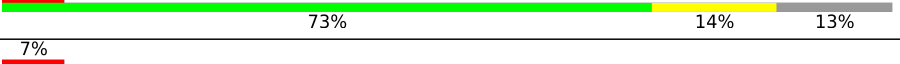
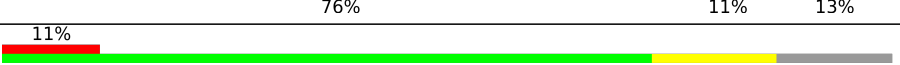
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12682 (3.07 - 4.07)

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	159	 29% 71%
1	C	159	 27% 71%
2	B	349	 13% 45% 7% 48%
2	K	349	 13% 47% 48%

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Mol	Chain	Length	Quality of chain
3	D	389	
3	L	389	
4	E	225	
4	M	225	
5	F	313	
5	I	313	
5	N	313	
5	Q	313	
6	G	716	
6	J	716	
6	O	716	
6	R	716	
7	H	276	
7	P	276	
7	c	276	
7	d	276	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33922 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 DPY30 domain containing 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	46	Total	C	N	O	S	0	0
			369	238	63	66	2		
1	C	46	Total	C	N	O	S	0	0
			369	238	63	66	2		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9D3X8
A	-18	TYR	-	expression tag	UNP Q9D3X8
A	-17	PRO	-	expression tag	UNP Q9D3X8
A	-16	TYR	-	expression tag	UNP Q9D3X8
A	-15	ASP	-	expression tag	UNP Q9D3X8
A	-14	VAL	-	expression tag	UNP Q9D3X8
A	-13	PRO	-	expression tag	UNP Q9D3X8
A	-12	ASP	-	expression tag	UNP Q9D3X8
A	-11	TYR	-	expression tag	UNP Q9D3X8
A	-10	ALA	-	expression tag	UNP Q9D3X8
A	-9	GLU	-	expression tag	UNP Q9D3X8
A	-8	ASN	-	expression tag	UNP Q9D3X8
A	-7	LEU	-	expression tag	UNP Q9D3X8
A	-6	TYR	-	expression tag	UNP Q9D3X8
A	-5	PHE	-	expression tag	UNP Q9D3X8
A	-4	GLN	-	expression tag	UNP Q9D3X8
A	-3	GLY	-	expression tag	UNP Q9D3X8
A	-2	ALA	-	expression tag	UNP Q9D3X8
A	-1	ALA	-	expression tag	UNP Q9D3X8
A	0	ALA	-	expression tag	UNP Q9D3X8
C	-19	MET	-	initiating methionine	UNP Q9D3X8
C	-18	TYR	-	expression tag	UNP Q9D3X8
C	-17	PRO	-	expression tag	UNP Q9D3X8
C	-16	TYR	-	expression tag	UNP Q9D3X8
C	-15	ASP	-	expression tag	UNP Q9D3X8
C	-14	VAL	-	expression tag	UNP Q9D3X8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	PRO	-	expression tag	UNP Q9D3X8
C	-12	ASP	-	expression tag	UNP Q9D3X8
C	-11	TYR	-	expression tag	UNP Q9D3X8
C	-10	ALA	-	expression tag	UNP Q9D3X8
C	-9	GLU	-	expression tag	UNP Q9D3X8
C	-8	ASN	-	expression tag	UNP Q9D3X8
C	-7	LEU	-	expression tag	UNP Q9D3X8
C	-6	TYR	-	expression tag	UNP Q9D3X8
C	-5	PHE	-	expression tag	UNP Q9D3X8
C	-4	GLN	-	expression tag	UNP Q9D3X8
C	-3	GLY	-	expression tag	UNP Q9D3X8
C	-2	ALA	-	expression tag	UNP Q9D3X8
C	-1	ALA	-	expression tag	UNP Q9D3X8
C	0	ALA	-	expression tag	UNP Q9D3X8

- Molecule 2 is a protein called DnaJ homolog subfamily B member 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	181	Total	C	N	O	S	0	0
			1489	965	256	263	5		
2	K	181	Total	C	N	O	S	0	0
			1489	965	256	263	5		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-32	MET	-	initiating methionine	UNP Q80Y75
B	-31	ASP	-	expression tag	UNP Q80Y75
B	-30	TYR	-	expression tag	UNP Q80Y75
B	-29	LYS	-	expression tag	UNP Q80Y75
B	-28	ASP	-	expression tag	UNP Q80Y75
B	-27	HIS	-	expression tag	UNP Q80Y75
B	-26	ASP	-	expression tag	UNP Q80Y75
B	-25	GLY	-	expression tag	UNP Q80Y75
B	-24	ASP	-	expression tag	UNP Q80Y75
B	-23	TYR	-	expression tag	UNP Q80Y75
B	-22	LYS	-	expression tag	UNP Q80Y75
B	-21	ASP	-	expression tag	UNP Q80Y75
B	-20	HIS	-	expression tag	UNP Q80Y75
B	-19	ASP	-	expression tag	UNP Q80Y75
B	-18	ILE	-	expression tag	UNP Q80Y75
B	-17	ASP	-	expression tag	UNP Q80Y75

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	TYR	-	expression tag	UNP Q80Y75
B	-15	LYS	-	expression tag	UNP Q80Y75
B	-14	ASP	-	expression tag	UNP Q80Y75
B	-13	ASP	-	expression tag	UNP Q80Y75
B	-12	ASP	-	expression tag	UNP Q80Y75
B	-11	ASP	-	expression tag	UNP Q80Y75
B	-10	LYS	-	expression tag	UNP Q80Y75
B	-9	GLU	-	expression tag	UNP Q80Y75
B	-8	ASN	-	expression tag	UNP Q80Y75
B	-7	LEU	-	expression tag	UNP Q80Y75
B	-6	TYR	-	expression tag	UNP Q80Y75
B	-5	PHE	-	expression tag	UNP Q80Y75
B	-4	GLN	-	expression tag	UNP Q80Y75
B	-3	GLY	-	expression tag	UNP Q80Y75
B	-2	ALA	-	expression tag	UNP Q80Y75
B	-1	ALA	-	expression tag	UNP Q80Y75
B	0	ALA	-	expression tag	UNP Q80Y75
K	-32	MET	-	initiating methionine	UNP Q80Y75
K	-31	ASP	-	expression tag	UNP Q80Y75
K	-30	TYR	-	expression tag	UNP Q80Y75
K	-29	LYS	-	expression tag	UNP Q80Y75
K	-28	ASP	-	expression tag	UNP Q80Y75
K	-27	HIS	-	expression tag	UNP Q80Y75
K	-26	ASP	-	expression tag	UNP Q80Y75
K	-25	GLY	-	expression tag	UNP Q80Y75
K	-24	ASP	-	expression tag	UNP Q80Y75
K	-23	TYR	-	expression tag	UNP Q80Y75
K	-22	LYS	-	expression tag	UNP Q80Y75
K	-21	ASP	-	expression tag	UNP Q80Y75
K	-20	HIS	-	expression tag	UNP Q80Y75
K	-19	ASP	-	expression tag	UNP Q80Y75
K	-18	ILE	-	expression tag	UNP Q80Y75
K	-17	ASP	-	expression tag	UNP Q80Y75
K	-16	TYR	-	expression tag	UNP Q80Y75
K	-15	LYS	-	expression tag	UNP Q80Y75
K	-14	ASP	-	expression tag	UNP Q80Y75
K	-13	ASP	-	expression tag	UNP Q80Y75
K	-12	ASP	-	expression tag	UNP Q80Y75
K	-11	ASP	-	expression tag	UNP Q80Y75
K	-10	LYS	-	expression tag	UNP Q80Y75
K	-9	GLU	-	expression tag	UNP Q80Y75
K	-8	ASN	-	expression tag	UNP Q80Y75

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-7	LEU	-	expression tag	UNP Q80Y75
K	-6	TYR	-	expression tag	UNP Q80Y75
K	-5	PHE	-	expression tag	UNP Q80Y75
K	-4	GLN	-	expression tag	UNP Q80Y75
K	-3	GLY	-	expression tag	UNP Q80Y75
K	-2	ALA	-	expression tag	UNP Q80Y75
K	-1	ALA	-	expression tag	UNP Q80Y75
K	0	ALA	-	expression tag	UNP Q80Y75

- Molecule 3 is a protein called Radial spoke head protein 3 homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	46	Total	C	N	O	S	0	0
			387	242	69	72	4		
3	L	46	Total	C	N	O	S	0	0
			387	242	69	72	4		

- Molecule 4 is a protein called Nucleoside diphosphate kinase homolog 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	201	Total	C	N	O	S	0	0
			1612	1047	266	289	10		
4	M	201	Total	C	N	O	S	0	0
			1612	1047	266	289	10		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	MET	-	initiating methionine	UNP Q99MH5
E	-12	GLU	-	expression tag	UNP Q99MH5
E	-11	GLN	-	expression tag	UNP Q99MH5
E	-10	LYS	-	expression tag	UNP Q99MH5
E	-9	LEU	-	expression tag	UNP Q99MH5
E	-8	ILE	-	expression tag	UNP Q99MH5
E	-7	SER	-	expression tag	UNP Q99MH5
E	-6	GLU	-	expression tag	UNP Q99MH5
E	-5	GLU	-	expression tag	UNP Q99MH5
E	-4	ASP	-	expression tag	UNP Q99MH5
E	-3	LEU	-	expression tag	UNP Q99MH5
E	-2	GLY	-	expression tag	UNP Q99MH5
E	-1	SER	-	expression tag	UNP Q99MH5
E	0	GLY	-	expression tag	UNP Q99MH5

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-13	MET	-	initiating methionine	UNP Q99MH5
M	-12	GLU	-	expression tag	UNP Q99MH5
M	-11	GLN	-	expression tag	UNP Q99MH5
M	-10	LYS	-	expression tag	UNP Q99MH5
M	-9	LEU	-	expression tag	UNP Q99MH5
M	-8	ILE	-	expression tag	UNP Q99MH5
M	-7	SER	-	expression tag	UNP Q99MH5
M	-6	GLU	-	expression tag	UNP Q99MH5
M	-5	GLU	-	expression tag	UNP Q99MH5
M	-4	ASP	-	expression tag	UNP Q99MH5
M	-3	LEU	-	expression tag	UNP Q99MH5
M	-2	GLY	-	expression tag	UNP Q99MH5
M	-1	SER	-	expression tag	UNP Q99MH5
M	0	GLY	-	expression tag	UNP Q99MH5

- Molecule 5 is a protein called Radial spoke head 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	185	Total	C	N	O	S	0	0
			1514	939	274	299	2		
5	I	185	Total	C	N	O	S	0	0
			1514	939	274	299	2		
5	N	185	Total	C	N	O	S	0	0
			1514	939	274	299	2		
5	Q	185	Total	C	N	O	S	0	0
			1514	939	274	299	2		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	MET	-	initiating methionine	UNP Q8VIG3
F	-10	TRP	-	expression tag	UNP Q8VIG3
F	-9	SER	-	expression tag	UNP Q8VIG3
F	-8	HIS	-	expression tag	UNP Q8VIG3
F	-7	PRO	-	expression tag	UNP Q8VIG3
F	-6	GLN	-	expression tag	UNP Q8VIG3
F	-5	PHE	-	expression tag	UNP Q8VIG3
F	-4	GLU	-	expression tag	UNP Q8VIG3
F	-3	LYS	-	expression tag	UNP Q8VIG3
F	-2	GLY	-	expression tag	UNP Q8VIG3
F	-1	SER	-	expression tag	UNP Q8VIG3
F	0	GLY	-	expression tag	UNP Q8VIG3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	MET	-	initiating methionine	UNP Q8VIG3
I	-10	TRP	-	expression tag	UNP Q8VIG3
I	-9	SER	-	expression tag	UNP Q8VIG3
I	-8	HIS	-	expression tag	UNP Q8VIG3
I	-7	PRO	-	expression tag	UNP Q8VIG3
I	-6	GLN	-	expression tag	UNP Q8VIG3
I	-5	PHE	-	expression tag	UNP Q8VIG3
I	-4	GLU	-	expression tag	UNP Q8VIG3
I	-3	LYS	-	expression tag	UNP Q8VIG3
I	-2	GLY	-	expression tag	UNP Q8VIG3
I	-1	SER	-	expression tag	UNP Q8VIG3
I	0	GLY	-	expression tag	UNP Q8VIG3
N	-11	MET	-	initiating methionine	UNP Q8VIG3
N	-10	TRP	-	expression tag	UNP Q8VIG3
N	-9	SER	-	expression tag	UNP Q8VIG3
N	-8	HIS	-	expression tag	UNP Q8VIG3
N	-7	PRO	-	expression tag	UNP Q8VIG3
N	-6	GLN	-	expression tag	UNP Q8VIG3
N	-5	PHE	-	expression tag	UNP Q8VIG3
N	-4	GLU	-	expression tag	UNP Q8VIG3
N	-3	LYS	-	expression tag	UNP Q8VIG3
N	-2	GLY	-	expression tag	UNP Q8VIG3
N	-1	SER	-	expression tag	UNP Q8VIG3
N	0	GLY	-	expression tag	UNP Q8VIG3
Q	-11	MET	-	initiating methionine	UNP Q8VIG3
Q	-10	TRP	-	expression tag	UNP Q8VIG3
Q	-9	SER	-	expression tag	UNP Q8VIG3
Q	-8	HIS	-	expression tag	UNP Q8VIG3
Q	-7	PRO	-	expression tag	UNP Q8VIG3
Q	-6	GLN	-	expression tag	UNP Q8VIG3
Q	-5	PHE	-	expression tag	UNP Q8VIG3
Q	-4	GLU	-	expression tag	UNP Q8VIG3
Q	-3	LYS	-	expression tag	UNP Q8VIG3
Q	-2	GLY	-	expression tag	UNP Q8VIG3
Q	-1	SER	-	expression tag	UNP Q8VIG3
Q	0	GLY	-	expression tag	UNP Q8VIG3

- Molecule 6 is a protein called Radial spoke head protein 4 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	387	Total	C	N	O	S	0	0
			3099	1997	506	586	10		

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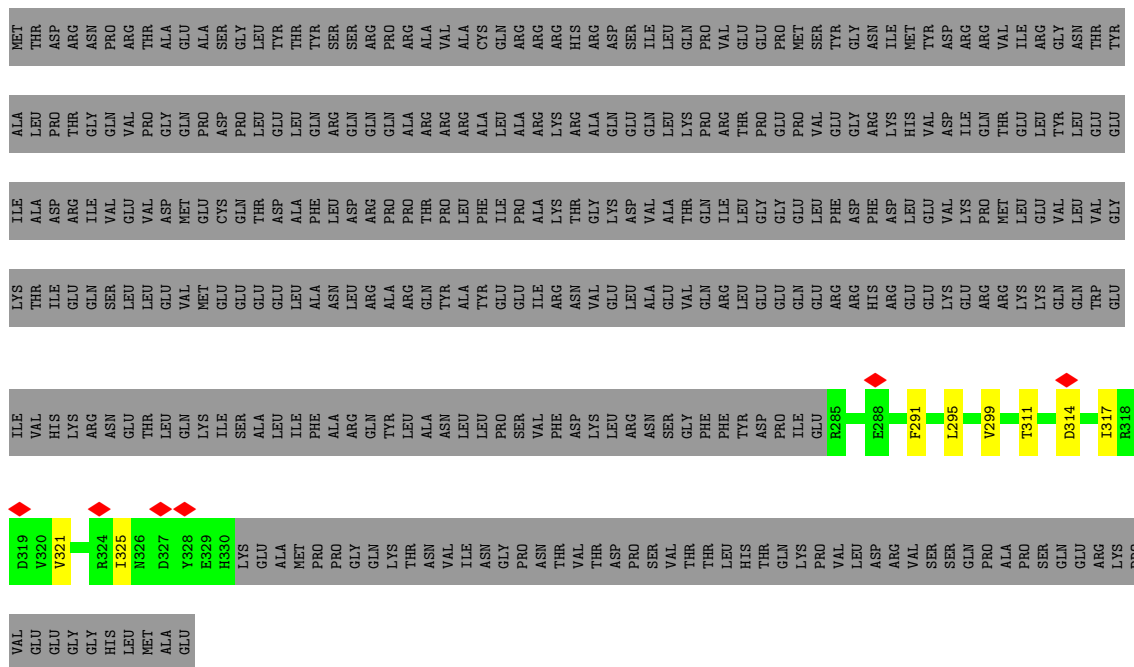
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Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	392	Total	C	N	O	S	0	0
			3139	2021	515	592	11		
6	O	387	Total	C	N	O	S	0	0
			3099	1997	506	586	10		
6	R	392	Total	C	N	O	S	0	0
			3139	2021	515	592	11		

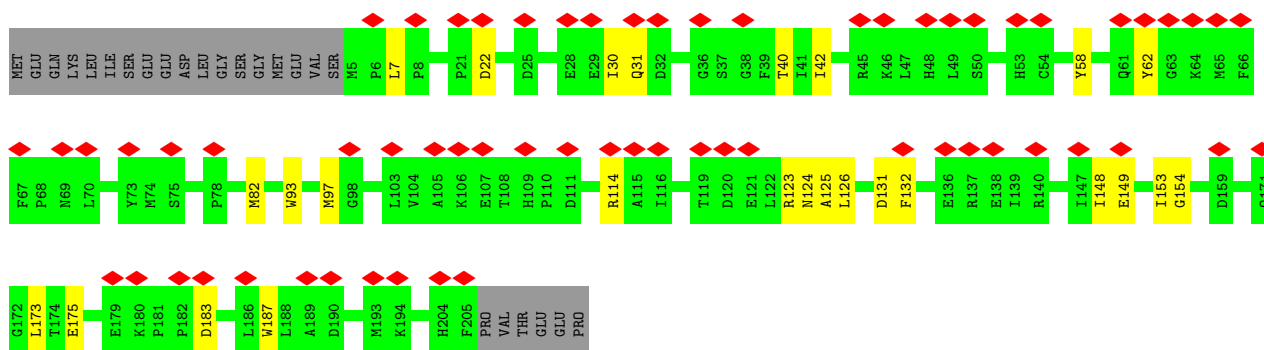
- Molecule 7 is a protein called Radial spoke head protein 9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	239	Total	C	N	O	S	0	0
			1912	1228	324	351	9		
7	c	241	Total	C	N	O	S	0	0
			1926	1238	326	353	9		
7	P	239	Total	C	N	O	S	0	0
			1912	1228	324	351	9		
7	d	241	Total	C	N	O	S	0	0
			1926	1238	326	353	9		

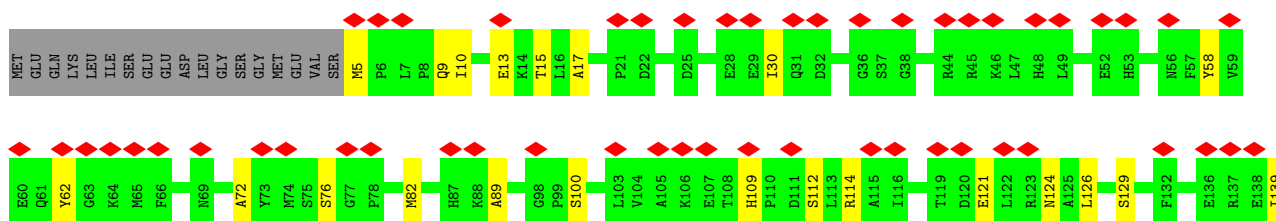
Chain L: 10% 88%

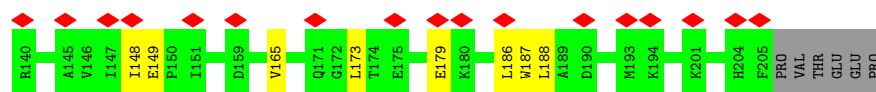


Chain E:

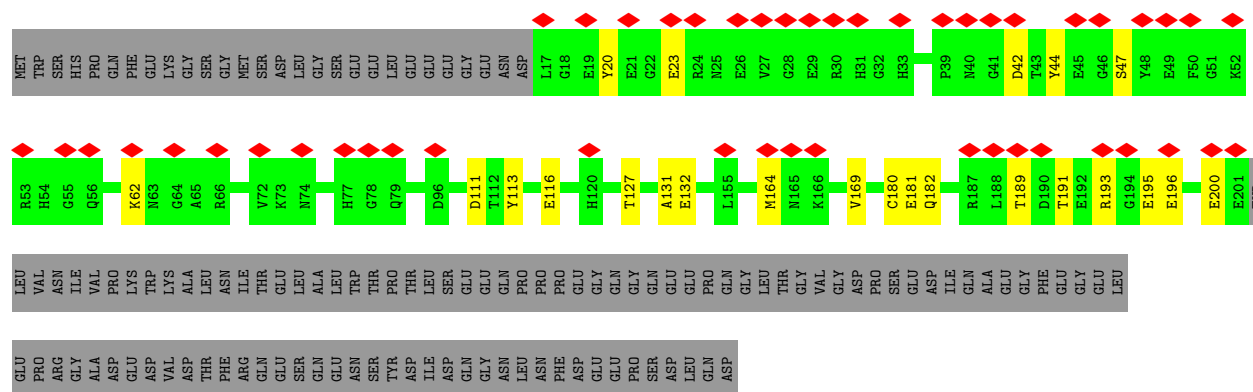


Chain M: 31% 76% 13% 11%

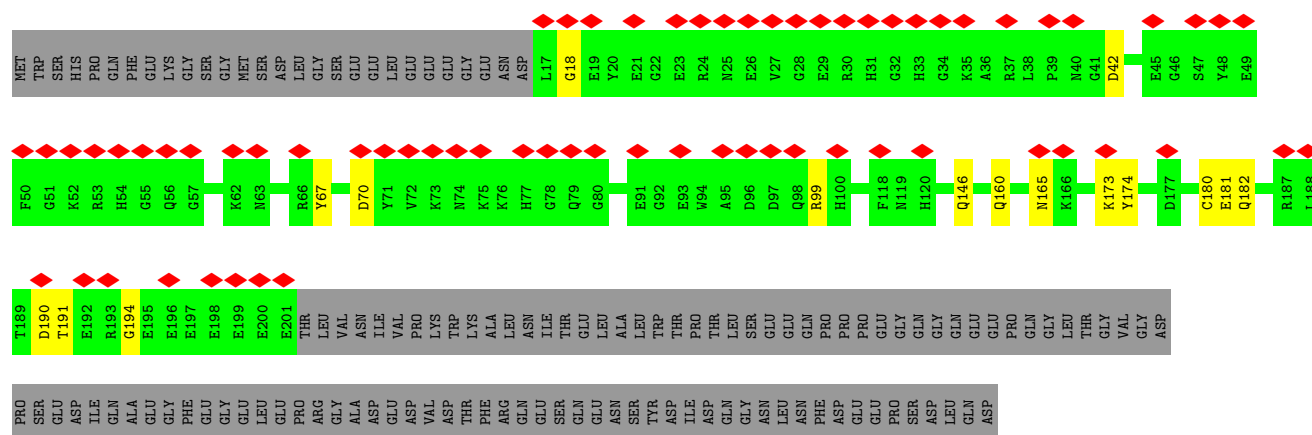




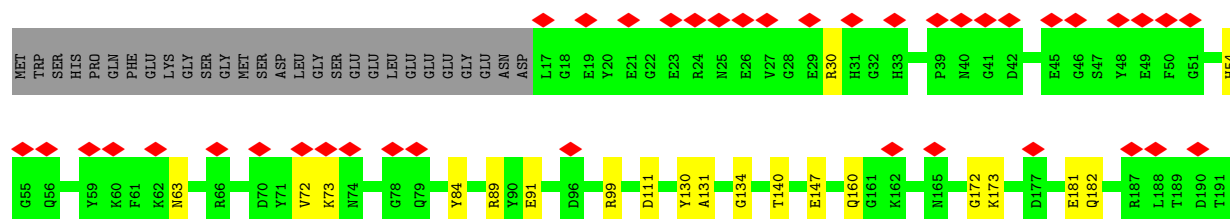
• Molecule 5: Radial spoke head 1 homolog



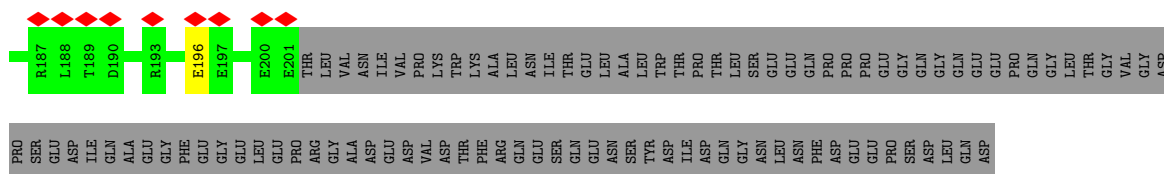
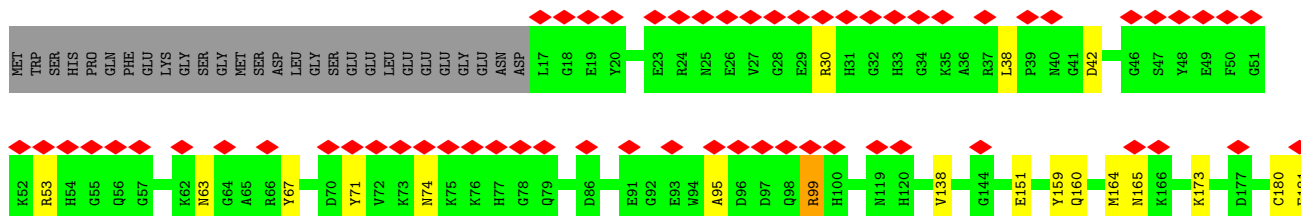
• Molecule 5: Radial spoke head 1 homolog



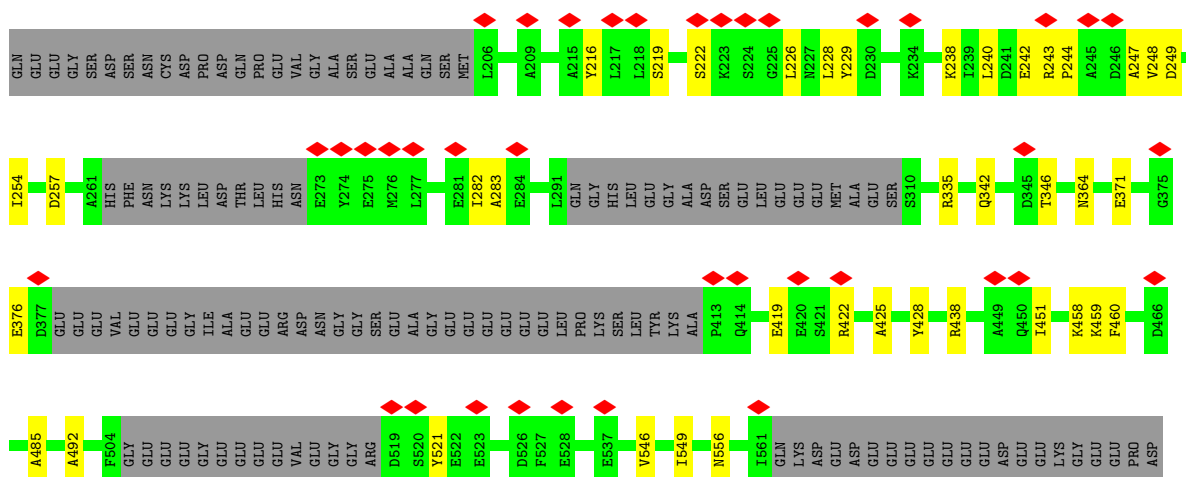
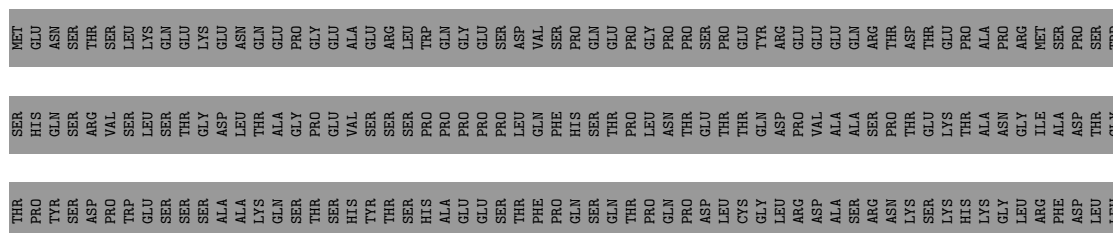
• Molecule 5: Radial spoke head 1 homolog

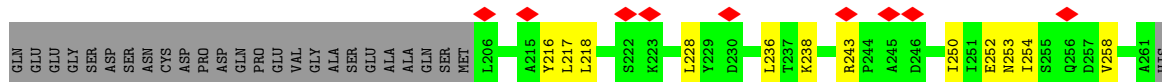
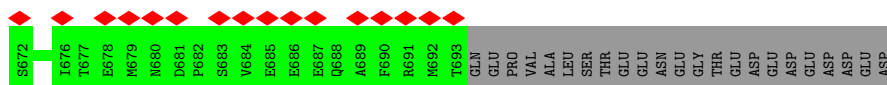


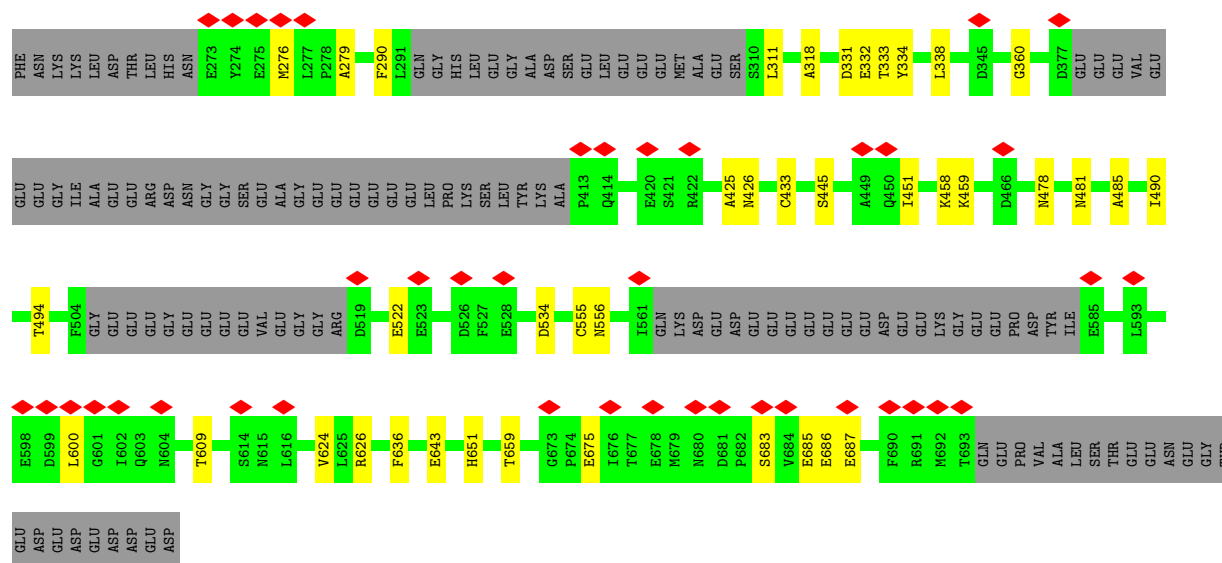
- Molecule 5: Radial spoke head 1 homolog



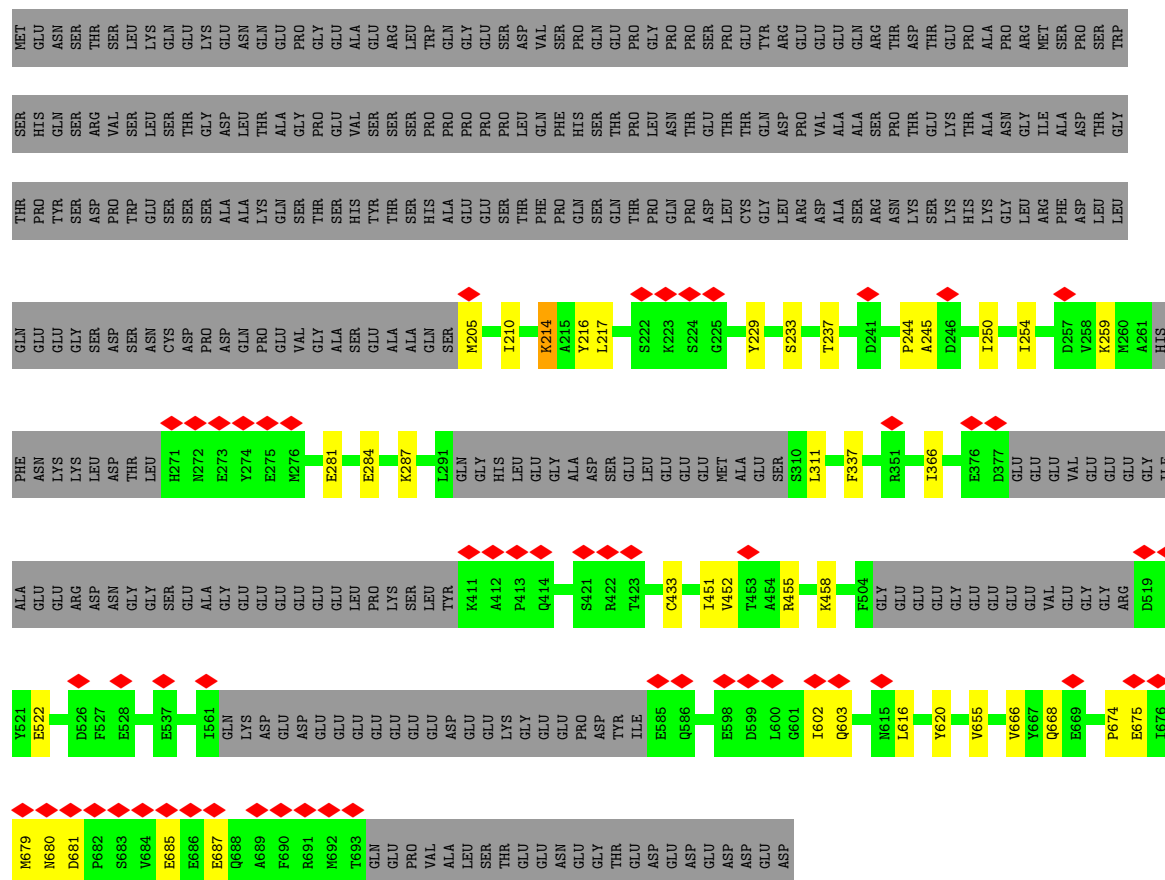
- Molecule 6: Radial spoke head protein 4 homolog A



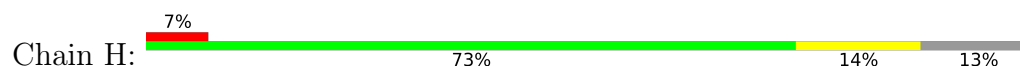


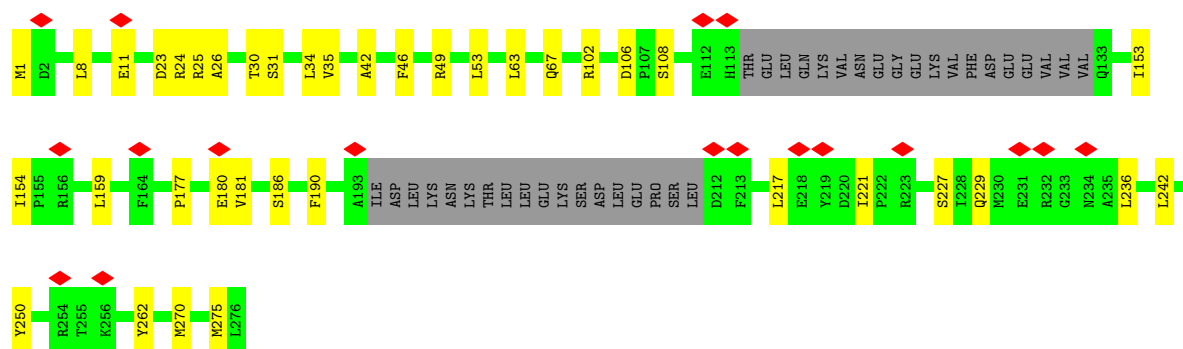


• Molecule 6: Radial spoke head protein 4 homolog A

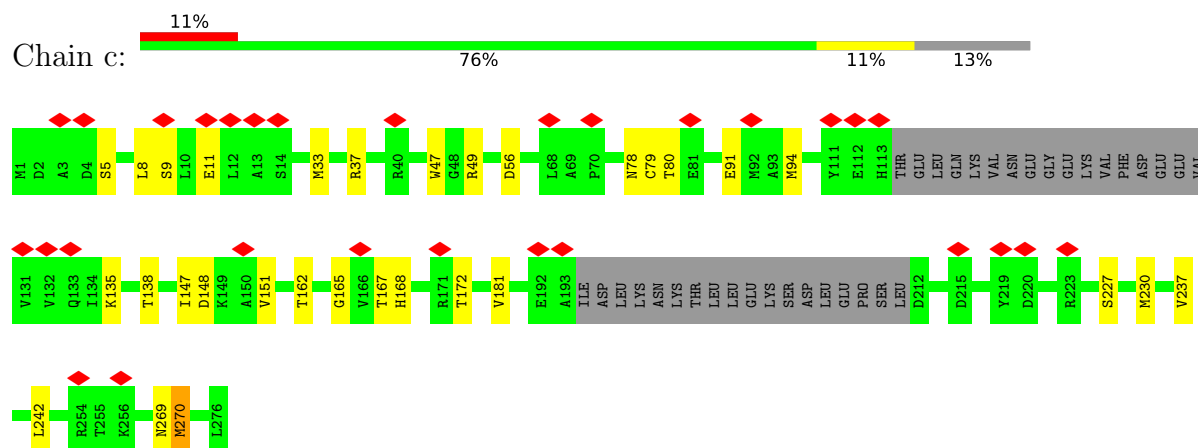


• Molecule 7: Radial spoke head protein 9 homolog

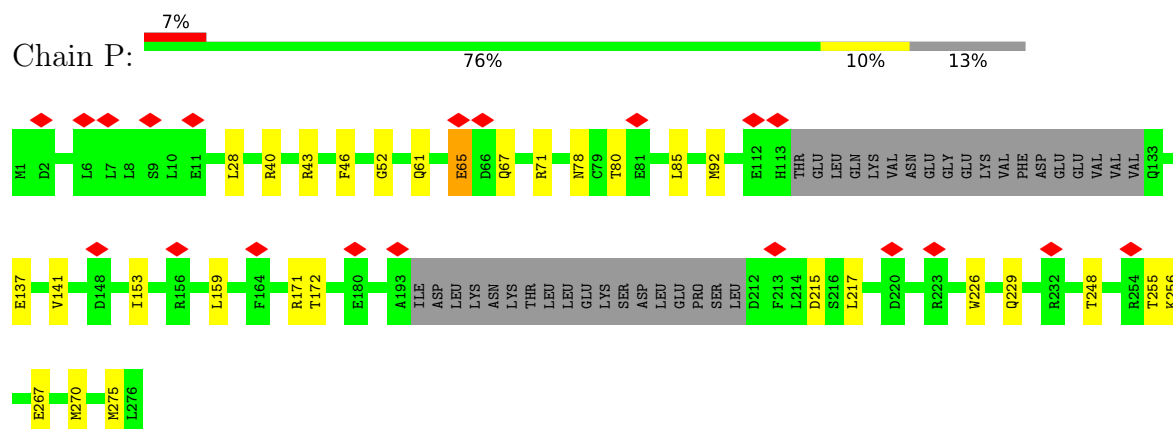




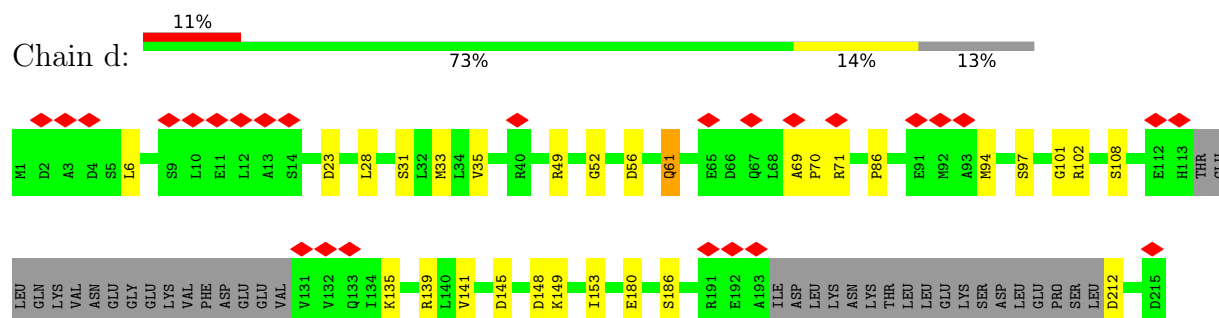
• Molecule 7: Radial spoke head protein 9 homolog

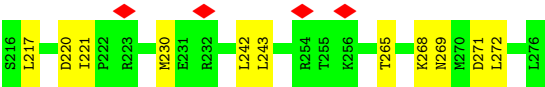


• Molecule 7: Radial spoke head protein 9 homolog



• Molecule 7: Radial spoke head protein 9 homolog





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	338084	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.164	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	478.24, 478.24, 478.24	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.854, 0.854, 0.854	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	0.31	0/379	0.67	0/517
1	C	0.35	0/379	0.66	0/517
2	B	0.28	0/1525	0.67	6/2061 (0.3%)
2	K	0.29	0/1525	0.68	6/2061 (0.3%)
3	D	0.45	0/393	0.93	1/528 (0.2%)
3	L	0.38	0/393	0.78	0/528
4	E	0.34	0/1657	0.69	0/2251
4	M	0.33	0/1657	0.64	0/2251
5	F	0.30	0/1558	0.63	0/2096
5	I	0.31	0/1558	0.69	2/2096 (0.1%)
5	N	0.27	0/1558	0.58	2/2096 (0.1%)
5	Q	0.28	0/1558	0.74	4/2096 (0.2%)
6	G	0.30	0/3183	0.66	4/4335 (0.1%)
6	J	0.30	0/3224	0.68	6/4390 (0.1%)
6	O	0.29	0/3183	0.62	4/4335 (0.1%)
6	R	0.30	0/3224	0.74	8/4390 (0.2%)
7	H	0.31	0/1956	0.65	0/2645
7	P	0.29	0/1956	0.69	2/2645 (0.1%)
7	c	0.33	0/1970	0.70	1/2665 (0.0%)
7	d	0.32	0/1970	0.71	6/2665 (0.2%)
All	All	0.31	0/34806	0.68	52/47168 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
4	E	0	2
5	I	0	1
6	G	0	2
7	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	c	0	1
All	All	0	8

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	245	ALA	CA-C-N	14.70	148.16	121.70
6	R	245	ALA	C-N-CA	14.70	148.16	121.70
7	P	65	GLU	CA-C-N	11.86	143.05	121.70
7	P	65	GLU	C-N-CA	11.86	143.05	121.70
6	J	616	LEU	CA-C-N	11.00	141.50	121.70
6	J	616	LEU	C-N-CA	11.00	141.50	121.70
5	Q	159	TYR	CA-C-N	10.23	140.12	121.70
5	Q	159	TYR	C-N-CA	10.23	140.12	121.70
5	Q	99	ARG	CA-C-N	8.80	137.54	121.70
5	Q	99	ARG	C-N-CA	8.80	137.54	121.70
6	R	674	PRO	CA-N-CD	-8.34	100.33	112.00
2	K	309	MET	CB-CG-SD	7.53	135.29	112.70
6	G	219	SER	CA-C-N	7.17	134.60	121.70
6	G	219	SER	C-N-CA	7.17	134.60	121.70
6	J	474	PRO	CA-C-N	7.03	134.35	121.70
6	J	474	PRO	C-N-CA	7.03	134.35	121.70
6	G	613	SER	CA-C-N	6.82	133.97	121.70
6	G	613	SER	C-N-CA	6.82	133.97	121.70
2	K	212	ILE	CA-C-N	6.54	133.47	121.70
2	K	212	ILE	C-N-CA	6.54	133.47	121.70
2	B	161	ILE	CA-C-N	6.53	133.45	121.70
2	B	161	ILE	C-N-CA	6.53	133.45	121.70
6	R	452	VAL	CA-C-N	6.34	133.11	121.70
6	R	452	VAL	C-N-CA	6.34	133.11	121.70
7	d	70	PRO	CA-C-N	6.30	133.04	121.70
7	d	70	PRO	C-N-CA	6.30	133.04	121.70
5	N	172	GLY	CA-C-N	6.19	132.84	121.70
5	N	172	GLY	C-N-CA	6.19	132.84	121.70
2	K	221	PRO	CA-C-N	6.14	132.75	121.70
2	K	221	PRO	C-N-CA	6.14	132.75	121.70
5	I	18	GLY	CA-C-N	5.96	132.44	121.70
5	I	18	GLY	C-N-CA	5.96	132.44	121.70
2	B	170	ARG	CA-C-N	5.95	132.42	121.70
2	B	170	ARG	C-N-CA	5.95	132.42	121.70
7	d	61	GLN	CA-C-N	5.94	132.39	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	d	61	GLN	C-N-CA	5.94	132.39	121.70
6	O	217	LEU	CA-C-N	5.85	132.23	121.70
6	O	217	LEU	C-N-CA	5.85	132.23	121.70
6	R	214	LYS	N-CA-CB	5.79	118.46	110.07
6	R	458	LYS	CB-CA-C	5.66	118.44	111.43
6	J	600	LEU	CA-C-N	5.47	131.54	121.70
6	J	600	LEU	C-N-CA	5.47	131.54	121.70
6	R	458	LYS	CA-CB-CG	5.45	125.00	114.10
2	B	309	MET	CB-CG-SD	5.37	128.81	112.70
6	O	600	LEU	CA-C-N	5.34	131.31	121.70
6	O	600	LEU	C-N-CA	5.34	131.31	121.70
2	K	309	MET	CA-CB-CG	5.26	124.62	114.10
7	d	149	LYS	CA-C-N	5.24	131.14	121.70
7	d	149	LYS	C-N-CA	5.24	131.14	121.70
3	D	294	TRP	N-CA-C	-5.19	105.52	111.07
2	B	284	PRO	CA-N-CD	-5.14	104.80	112.00
7	c	270	MET	CG-SD-CE	5.13	112.19	100.90

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	216	LYS	Peptide
4	E	148	ILE	Peptide
4	E	183	ASP	Peptide
6	G	335	ARG	Sidechain
6	G	613	SER	Peptide
5	I	191	THR	Peptide
7	P	65	GLU	Peptide
7	c	37	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	369	0	363	0	0
1	C	369	0	363	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1489	0	1538	13	0
2	K	1489	0	1538	12	0
3	D	387	0	380	8	0
3	L	387	0	380	9	0
4	E	1612	0	1623	15	0
4	M	1612	0	1623	21	0
5	F	1514	0	1346	13	0
5	I	1514	0	1346	10	0
5	N	1514	0	1346	13	0
5	Q	1514	0	1346	13	0
6	G	3099	0	3009	39	0
6	J	3139	0	3048	27	0
6	O	3099	0	3009	38	0
6	R	3139	0	3048	30	0
7	H	1912	0	1907	28	0
7	P	1912	0	1907	21	0
7	c	1926	0	1925	20	0
7	d	1926	0	1925	22	0
All	All	33922	0	32970	284	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 4.

All (284) 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)
4:M:10:ILE:HD13	6:R:210:ILE:HD12	1.46	0.93
6:J:216:TYR:O	6:J:219:SER:OG	2.04	0.76
5:Q:160:GLN:OE1	5:Q:173:LYS:NZ	2.21	0.74
6:G:458:LYS:NZ	7:H:275:MET:SD	2.61	0.74
6:G:216:TYR:OH	6:J:244:PRO:O	2.05	0.74
2:B:147:SER:OG	2:B:150:ASP:OD2	2.07	0.73
6:O:458:LYS:NZ	7:P:275:MET:SD	2.60	0.73
6:R:284:GLU:OE1	6:R:287:LYS:NZ	2.23	0.72
4:E:114:ARG:NE	4:E:124:ASN:OD1	2.23	0.71
7:P:43:ARG:NH1	7:P:67:GLN:OE1	2.24	0.71
5:F:182:GLN:NE2	7:H:270:MET:O	2.25	0.70
2:K:147:SER:OG	2:K:150:ASP:OD2	2.08	0.70
3:D:319:ASP:OD2	6:G:229:TYR:OH	2.10	0.69
3:D:318:ARG:NH2	4:E:7:LEU:O	2.24	0.69
7:c:49:ARG:NH2	7:c:56:ASP:OD1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:426:ASN:OD1	6:O:445:SER:OG	2.07	0.69
3:D:314:ASP:OD1	6:J:229:TYR:OH	2.11	0.68
6:G:238:LYS:NZ	6:G:257:ASP:OD2	2.26	0.68
4:E:22:ASP:OD2	4:E:123:ARG:NH1	2.27	0.68
6:G:428:TYR:OH	6:G:521:TYR:OH	2.13	0.67
6:J:318:ALA:HB2	6:J:333:THR:HG21	1.77	0.67
3:L:314:ASP:OD1	6:R:229:TYR:OH	2.12	0.67
5:I:99:ARG:NH2	6:J:669:GLU:OE1	2.28	0.66
6:J:459:LYS:O	6:J:651:HIS:NE2	2.27	0.66
6:O:490:ILE:O	6:O:494:THR:OG1	2.10	0.66
5:F:44:TYR:OH	5:F:47:SER:O	2.11	0.66
7:H:11:GLU:OE2	7:H:25:ARG:NH1	2.29	0.66
6:R:522:GLU:OE2	6:R:522:GLU:N	2.28	0.66
7:d:49:ARG:NH1	7:d:56:ASP:OD1	2.29	0.66
6:O:318:ALA:HB2	6:O:333:THR:HG21	1.77	0.65
4:M:58:TYR:O	4:M:62:TYR:N	2.29	0.65
4:E:58:TYR:O	4:E:62:TYR:N	2.29	0.65
1:C:41:ARG:NH1	4:M:186:LEU:HD22	2.12	0.65
5:N:89:ARG:NH2	5:N:91:GLU:OE2	2.29	0.64
7:P:153:ILE:HD12	7:P:217:LEU:HD11	1.79	0.64
6:O:252:GLU:OE1	6:R:259:LYS:NZ	2.31	0.64
6:G:376:GLU:N	6:G:376:GLU:OE2	2.32	0.63
6:J:646:TYR:OH	6:J:649:TRP:O	2.15	0.62
6:R:233:SER:O	6:R:237:THR:OG1	2.15	0.62
4:M:121:GLU:O	4:M:124:ASN:ND2	2.33	0.62
5:N:182:GLN:NE2	5:N:196:GLU:O	2.32	0.62
7:d:52:GLY:O	7:d:102:ARG:NH2	2.34	0.61
6:G:609:THR:OG1	7:H:53:LEU:O	2.11	0.61
2:B:209:ALA:HB1	2:B:211:ILE:HD11	1.80	0.61
2:K:248:GLU:HG2	2:K:256:LEU:HD11	1.81	0.61
7:H:34:LEU:HD21	6:J:283:ALA:HB3	1.81	0.61
7:d:102:ARG:NH1	7:d:265:THR:OG1	2.34	0.61
7:H:23:ASP:OD2	7:H:24:ARG:NH1	2.34	0.60
5:F:193:ARG:NH2	5:F:196:GLU:OE1	2.34	0.60
5:I:180:CYS:SG	5:I:181:GLU:N	2.75	0.60
6:G:342:GLN:O	6:G:346:THR:OG1	2.16	0.59
6:R:666:VAL:O	6:R:668:GLN:NE2	2.36	0.59
6:G:613:SER:O	7:H:24:ARG:NH2	2.36	0.59
6:G:643:GLU:N	6:G:643:GLU:OE2	2.35	0.59
6:O:243:ARG:N	6:R:216:TYR:OH	2.36	0.59
6:O:522:GLU:OE2	6:O:522:GLU:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:54:HIS:ND1	5:N:72:VAL:O	2.36	0.59
4:M:100:SER:O	4:M:114:ARG:NH2	2.36	0.58
2:K:262:ASN:ND2	7:P:137:GLU:OE1	2.35	0.58
5:I:182:GLN:OE1	7:c:270:MET:HE2	2.04	0.58
6:G:459:LYS:O	6:G:651:HIS:NE2	2.36	0.58
2:K:197:GLU:N	2:K:197:GLU:OE1	2.35	0.58
6:G:242:GLU:OE1	7:c:172:THR:OG1	2.19	0.58
6:O:236:LEU:HD11	6:R:217:LEU:HD11	1.85	0.57
4:M:30:ILE:HD13	4:M:126:LEU:HD21	1.85	0.57
6:O:643:GLU:N	6:O:643:GLU:OE2	2.38	0.57
3:L:291:PHE:CZ	3:L:295:LEU:HD12	2.39	0.57
6:O:243:ARG:N	6:R:216:TYR:HH	2.03	0.56
6:R:214:LYS:O	6:R:217:LEU:N	2.38	0.56
7:d:220:ASP:OD1	7:d:221:ILE:N	2.38	0.56
2:B:190:GLN:NE2	2:B:217:GLU:OE1	2.38	0.56
5:F:20:TYR:OH	5:F:23:GLU:O	2.23	0.56
7:P:267:GLU:N	7:P:267:GLU:OE2	2.39	0.56
5:Q:30:ARG:NH2	6:R:687:GLU:OE2	2.38	0.56
2:B:309:MET:HE1	2:K:309:MET:HE3	1.87	0.56
3:L:295:LEU:O	3:L:299:VAL:HG23	2.06	0.56
6:O:250:ILE:HD11	7:P:171:ARG:HE	1.71	0.55
5:N:63:ASN:ND2	6:O:675:GLU:O	2.39	0.55
6:O:290:PHE:HB3	6:R:616:LEU:HD13	1.88	0.55
7:P:153:ILE:HD11	7:P:226:TRP:CH2	2.42	0.55
6:O:459:LYS:O	6:O:651:HIS:NE2	2.38	0.55
7:d:108:SER:O	7:d:135:LYS:NZ	2.35	0.55
5:F:191:THR:HA	6:G:659:THR:HG21	1.87	0.55
1:C:18:LEU:HD22	4:M:165:VAL:HG11	1.88	0.55
4:M:114:ARG:NH1	4:M:126:LEU:O	2.40	0.55
7:d:33:MET:HA	7:d:33:MET:HE2	1.88	0.54
6:O:624:VAL:HG13	6:O:636:PHE:CE2	2.43	0.54
5:I:174:TYR:N	5:I:182:GLN:O	2.40	0.54
6:G:556:ASN:N	6:G:556:ASN:OD1	2.41	0.54
2:K:253:ASP:O	7:P:40:ARG:NH2	2.41	0.53
3:D:291:PHE:CZ	3:D:295:LEU:HD22	2.43	0.53
6:O:451:ILE:HG22	6:O:485:ALA:HB2	1.90	0.53
6:J:377:ASP:OD2	6:J:442:ARG:NH1	2.41	0.53
5:I:194:GLY:HA3	7:c:270:MET:HE3	1.91	0.53
5:I:190:ASP:O	6:J:659:THR:OG1	2.26	0.53
6:J:602:ILE:HG12	6:J:655:VAL:HG12	1.90	0.53
6:O:686:GLU:OE2	6:O:686:GLU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:228:LEU:HD11	6:J:251:ILE:HD11	1.91	0.53
4:E:131:ASP:OD1	4:E:132:PHE:N	2.41	0.53
2:K:155:CYS:SG	2:K:156:THR:N	2.82	0.53
6:G:247:ALA:HB1	6:J:228:LEU:HD22	1.91	0.52
6:O:331:ASP:OD1	6:O:332:GLU:N	2.43	0.52
4:E:31:GLN:CG	4:E:82:MET:HE1	2.39	0.52
6:R:205:MET:HA	6:R:205:MET:HE3	1.91	0.52
6:G:460:PHE:CZ	7:H:242:LEU:HD22	2.43	0.52
4:M:179:GLU:OE1	4:M:187:TRP:NE1	2.42	0.52
3:D:291:PHE:HE2	4:E:173:LEU:HD13	1.74	0.52
6:G:364:ASN:ND2	7:H:229:GLN:OE1	2.42	0.52
5:I:146:GLN:N	5:I:146:GLN:OE1	2.42	0.52
6:O:624:VAL:HG13	6:O:636:PHE:HE2	1.73	0.52
6:G:451:ILE:CG2	6:G:485:ALA:HB2	2.40	0.52
7:c:11:GLU:N	7:c:11:GLU:OE1	2.42	0.52
6:O:216:TYR:OH	6:R:244:PRO:O	2.28	0.52
7:d:180:GLU:O	7:d:186:SER:OG	2.24	0.52
4:M:15:THR:OG1	4:M:129:SER:OG	2.23	0.52
7:d:153:ILE:HD12	7:d:217:LEU:HD11	1.92	0.52
7:H:227:SER:OG	7:H:242:LEU:HD21	2.09	0.52
5:N:84:TYR:OH	5:N:99:ARG:NH1	2.43	0.52
3:D:307:MET:HE2	3:D:307:MET:HA	1.92	0.51
6:O:218:LEU:HD22	6:O:228:LEU:HD23	1.91	0.51
7:P:85:LEU:HG	7:P:141:VAL:HG22	1.92	0.51
6:G:419:GLU:OE2	6:G:425:ALA:N	2.42	0.51
7:c:230:MET:HE3	7:c:230:MET:HA	1.92	0.51
6:O:683:SER:OG	6:O:685:GLU:OE2	2.28	0.51
5:N:111:ASP:OD1	5:N:131:ALA:N	2.44	0.51
7:H:153:ILE:HD13	7:H:217:LEU:HD11	1.93	0.51
7:c:242:LEU:O	7:c:269:ASN:ND2	2.43	0.51
5:Q:164:MET:O	5:Q:164:MET:HE3	2.11	0.51
6:J:205:MET:HE3	6:J:205:MET:HA	1.92	0.50
6:G:238:LYS:HE3	6:G:254:ILE:HD12	1.93	0.50
6:O:238:LYS:CE	6:O:254:ILE:HG23	2.42	0.50
6:O:478:ASN:OD1	6:O:481:ASN:ND2	2.45	0.50
7:P:92:MET:HE1	7:P:141:VAL:HG11	1.94	0.50
3:L:291:PHE:HE2	4:M:173:LEU:HD23	1.77	0.50
5:Q:196:GLU:OE1	7:d:268:LYS:NZ	2.40	0.50
6:G:283:ALA:CB	7:c:33:MET:HE1	2.42	0.50
3:L:311:THR:OG1	4:M:9:GLN:NE2	2.45	0.50
4:M:109:HIS:O	4:M:112:SER:OG	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:283:ALA:HB2	7:c:33:MET:HE1	1.94	0.50
5:Q:138:VAL:O	5:Q:151:GLU:N	2.45	0.50
7:H:1:MET:N	7:H:46:PHE:O	2.45	0.49
7:P:78:ASN:O	7:P:80:THR:N	2.42	0.49
5:Q:63:ASN:ND2	6:R:675:GLU:OE1	2.44	0.49
5:Q:95:ALA:N	5:Q:99:ARG:O	2.46	0.49
4:E:93:TRP:NE1	4:E:97:MET:HE3	2.28	0.49
5:F:180:CYS:SG	5:F:181:GLU:N	2.85	0.49
7:c:78:ASN:O	7:c:80:THR:N	2.45	0.49
5:N:130:TYR:O	5:N:134:GLY:N	2.43	0.49
6:J:361:LEU:O	7:c:227:SER:OG	2.14	0.49
6:G:371:GLU:OE1	6:G:422:ARG:NH1	2.45	0.49
7:c:91:GLU:O	7:c:94:MET:HE3	2.13	0.49
2:B:313:ALA:HB1	2:K:310:LEU:HD12	1.95	0.49
7:c:47:TRP:NE1	7:c:148:ASP:OD1	2.44	0.49
5:N:181:GLU:N	5:N:181:GLU:OE2	2.46	0.48
6:O:556:ASN:OD1	6:O:556:ASN:N	2.44	0.48
6:G:240:LEU:O	6:G:243:ARG:NH1	2.47	0.48
7:d:69:ALA:HB1	7:d:71:ARG:HB3	1.93	0.48
6:G:249:ASP:OD2	6:G:249:ASP:N	2.46	0.48
4:E:125:ALA:O	4:E:126:LEU:HD23	2.13	0.48
7:d:101:GLY:O	7:d:139:ARG:NH2	2.46	0.48
4:M:139:ILE:HG21	4:M:148:ILE:HG21	1.96	0.48
7:d:212:ASP:OD2	7:d:212:ASP:N	2.46	0.48
7:c:147:ILE:O	7:c:151:VAL:HG22	2.13	0.48
6:R:451:ILE:O	6:R:455:ARG:N	2.47	0.48
7:c:162:THR:OG1	7:c:165:GLY:O	2.11	0.48
7:d:94:MET:O	7:d:97:SER:OG	2.33	0.47
6:G:628:ASN:OD1	7:H:102:ARG:NH1	2.46	0.47
4:M:17:ALA:HB3	4:M:82:MET:HG3	1.95	0.47
7:P:137:GLU:O	7:P:141:VAL:HG23	2.14	0.47
6:G:492:ALA:HA	6:G:546:VAL:HG11	1.96	0.47
7:H:270:MET:HE3	7:H:270:MET:HA	1.96	0.47
3:L:321:VAL:O	3:L:325:ILE:HD12	2.15	0.47
7:P:270:MET:HE3	7:P:270:MET:HA	1.96	0.47
6:O:626:ARG:NH2	7:P:52:GLY:O	2.48	0.47
5:Q:180:CYS:SG	5:Q:181:GLU:N	2.88	0.47
7:d:86:PRO:O	7:d:141:VAL:HG21	2.15	0.47
6:G:222:SER:OG	6:J:246:ASP:OD1	2.29	0.47
5:F:195:GLU:N	5:F:195:GLU:OE1	2.48	0.46
5:N:30:ARG:NH2	6:O:687:GLU:OE2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:243:LEU:O	7:d:269:ASN:N	2.46	0.46
5:Q:38:LEU:HD12	5:Q:42:ASP:OD1	2.16	0.46
6:R:685:GLU:OE2	6:R:685:GLU:N	2.47	0.46
5:I:67:TYR:OH	5:I:70:ASP:O	2.17	0.46
5:N:160:GLN:O	5:N:173:LYS:N	2.48	0.46
7:H:236:LEU:HD21	7:H:250:TYR:HB2	1.97	0.46
7:c:5:SER:O	7:c:9:SER:N	2.43	0.46
6:O:334:TYR:CE2	6:O:338:LEU:HD11	2.51	0.46
1:C:1:MET:SD	1:C:1:MET:N	2.80	0.46
2:B:253:ASP:OD2	2:B:255:ARG:NE	2.49	0.46
2:B:310:LEU:HD22	2:K:313:ALA:HB1	1.98	0.46
3:D:304:GLU:OE1	4:E:153:ILE:HD11	2.16	0.46
6:G:242:GLU:HB3	6:G:244:PRO:HD3	1.97	0.46
5:Q:53:ARG:HH12	6:R:679:MET:HE2	1.81	0.45
6:R:281:GLU:OE2	6:R:281:GLU:N	2.43	0.45
6:R:250:ILE:O	6:R:254:ILE:HG22	2.16	0.45
7:d:61:GLN:NE2	7:d:148:ASP:OD2	2.48	0.45
6:J:318:ALA:CB	6:J:333:THR:HG21	2.44	0.45
6:O:318:ALA:CB	6:O:333:THR:HG21	2.44	0.45
2:B:158:LYS:C	2:B:159:ILE:HD13	2.41	0.45
5:F:111:ASP:OD1	5:F:131:ALA:N	2.48	0.45
3:L:317:ILE:HD13	6:R:217:LEU:HD12	1.99	0.45
7:c:167:THR:OG1	7:c:168:HIS:N	2.44	0.45
7:d:6:LEU:HD13	7:d:28:LEU:HD23	1.99	0.45
2:B:222:ARG:NH1	2:B:250:LYS:O	2.51	0.44
5:F:113:TYR:OH	5:F:116:GLU:O	2.33	0.44
4:M:5:MET:HE2	4:M:5:MET:N	2.33	0.44
6:G:615:ASN:OD1	7:H:24:ARG:NH1	2.48	0.44
7:H:8:LEU:HD22	7:c:8:LEU:HA	1.99	0.44
2:K:159:ILE:HD13	2:K:212:ILE:HG21	1.99	0.44
2:K:210:ASP:OD1	2:K:211:ILE:N	2.50	0.44
7:d:230:MET:HE3	7:d:230:MET:HA	2.00	0.44
3:D:287:ILE:HD12	3:D:287:ILE:H	1.81	0.44
5:N:72:VAL:HG23	5:N:73:LYS:H	1.83	0.44
6:R:679:MET:SD	6:R:681:ASP:N	2.91	0.44
4:E:30:ILE:HD12	4:E:30:ILE:H	1.81	0.44
5:F:42:ASP:OD1	5:F:62:LYS:N	2.50	0.44
5:F:164:MET:HE3	5:F:169:VAL:HB	1.99	0.44
7:P:61:GLN:OE1	7:P:71:ARG:NE	2.50	0.44
6:R:366:ILE:N	6:R:433:CYS:O	2.49	0.44
6:R:602:ILE:CG2	6:R:655:VAL:HG22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:LEU:HD13	2:B:184:VAL:HG11	1.99	0.44
6:J:451:ILE:CG2	6:J:485:ALA:HB2	2.47	0.44
6:O:254:ILE:O	6:O:258:VAL:HG23	2.18	0.43
2:B:309:MET:CE	2:K:309:MET:HE3	2.48	0.43
4:M:72:ALA:O	4:M:76:SER:N	2.50	0.43
6:O:276:MET:HE2	6:O:279:ALA:HB3	2.01	0.43
7:P:215:ASP:N	7:P:215:ASP:OD1	2.50	0.43
4:E:153:ILE:HD12	4:E:154:GLY:H	1.84	0.43
7:H:67:GLN:CB	7:H:159:LEU:HD11	2.49	0.43
5:I:160:GLN:O	5:I:173:LYS:N	2.48	0.43
7:c:181:VAL:HG13	7:c:237:VAL:HG11	2.00	0.43
5:N:192:GLU:HB2	6:O:659:THR:HG22	2.01	0.43
6:G:226:LEU:HB2	6:J:248:VAL:HG21	2.01	0.42
6:G:492:ALA:HB2	6:G:549:ILE:HD12	2.01	0.42
7:H:177:PRO:O	7:H:181:VAL:HG23	2.19	0.42
4:E:175:GLU:OE1	4:E:187:TRP:NE1	2.52	0.42
5:F:132:GLU:OE2	6:G:667:TYR:OH	2.32	0.42
7:H:31:SER:O	7:H:35:VAL:HG23	2.19	0.42
6:J:217:LEU:HD23	6:J:228:LEU:HD23	2.01	0.42
7:P:28:LEU:HD21	7:P:46:PHE:CG	2.54	0.42
6:G:238:LYS:HE2	6:G:254:ILE:HG23	2.01	0.42
7:H:26:ALA:HB1	6:J:335:ARG:NH1	2.35	0.42
2:B:306:LYS:O	2:B:310:LEU:HD23	2.18	0.42
5:Q:53:ARG:N	5:Q:74:ASN:OD1	2.49	0.42
6:R:311:LEU:HD13	6:R:337:PHE:CE1	2.55	0.42
6:G:248:VAL:O	6:J:259:LYS:NZ	2.37	0.42
6:G:282:ILE:HG22	6:G:438:ARG:NH2	2.34	0.42
5:F:200:GLU:CB	7:H:221:ILE:HG21	2.50	0.42
6:G:247:ALA:CB	6:J:228:LEU:HD22	2.50	0.42
4:M:173:LEU:HD12	4:M:188:LEU:HD13	2.00	0.42
6:O:311:LEU:O	6:R:620:TYR:OH	2.23	0.42
1:C:18:LEU:HD12	3:L:295:LEU:HD22	2.01	0.42
4:M:10:ILE:O	6:R:214:LYS:NZ	2.49	0.42
7:H:180:GLU:O	7:H:186:SER:OG	2.36	0.42
5:N:140:THR:OG1	5:N:147:GLU:O	2.37	0.41
7:d:242:LEU:HB3	7:d:272:LEU:HD13	2.03	0.41
7:H:154:ILE:HD11	7:H:190:PHE:CZ	2.54	0.41
6:O:425:ALA:N	6:O:555:CYS:SG	2.93	0.41
6:O:253:ASN:ND2	7:P:172:THR:OG1	2.53	0.41
4:M:13:GLU:OE1	4:M:89:ALA:N	2.52	0.41
4:M:149:GLU:OE2	4:M:149:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:255:THR:OG1	7:P:256:LYS:N	2.52	0.41
7:H:106:ASP:OD1	7:H:108:SER:OG	2.27	0.41
6:G:451:ILE:HG23	6:G:485:ALA:HB2	2.02	0.41
3:L:321:VAL:HG11	6:R:210:ILE:HG22	2.01	0.41
6:O:534:ASP:N	6:O:534:ASP:OD1	2.53	0.41
7:d:145:ASP:OD1	7:d:145:ASP:N	2.54	0.41
4:E:40:THR:OG1	6:J:215:ALA:HB1	2.20	0.41
4:E:42:ILE:HG23	6:J:218:LEU:O	2.20	0.41
5:I:42:ASP:OD2	5:I:42:ASP:N	2.53	0.41
7:P:67:GLN:NE2	7:P:159:LEU:HD22	2.36	0.41
6:O:609:THR:N	6:O:626:ARG:O	2.54	0.41
7:H:30:THR:HG21	6:J:290:PHE:HE2	1.86	0.40
7:d:31:SER:O	7:d:35:VAL:HG23	2.21	0.40
6:J:646:TYR:HH	6:J:649:TRP:C	2.23	0.40
5:Q:164:MET:HE3	5:Q:164:MET:C	2.46	0.40
7:H:49:ARG:N	7:H:262:TYR:O	2.46	0.40
6:O:360:GLY:O	7:P:229:GLN:NE2	2.54	0.40
7:c:135:LYS:O	7:c:138:THR:OG1	2.38	0.40
5:Q:67:TYR:O	5:Q:71:TYR:OH	2.39	0.40
2:B:165:VAL:HG22	2:B:200:GLY:O	2.22	0.40
7:H:42:ALA:N	7:H:63:LEU:O	2.55	0.40
6:R:679:MET:SD	6:R:680:ASN:N	2.95	0.40
7:d:271:ASP:N	7:d:271:ASP:OD1	2.54	0.40

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	44/159 (28%)	43 (98%)	1 (2%)	0	100	100
1	C	44/159 (28%)	41 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	179/349 (51%)	162 (90%)	17 (10%)	0	100	100
2	K	179/349 (51%)	165 (92%)	13 (7%)	1 (1%)	21	54
3	D	44/389 (11%)	43 (98%)	1 (2%)	0	100	100
3	L	44/389 (11%)	44 (100%)	0	0	100	100
4	E	199/225 (88%)	184 (92%)	14 (7%)	1 (0%)	24	57
4	M	199/225 (88%)	187 (94%)	12 (6%)	0	100	100
5	F	183/313 (58%)	175 (96%)	7 (4%)	1 (0%)	24	57
5	I	183/313 (58%)	166 (91%)	16 (9%)	1 (0%)	24	57
5	N	183/313 (58%)	170 (93%)	13 (7%)	0	100	100
5	Q	183/313 (58%)	169 (92%)	13 (7%)	1 (0%)	24	57
6	G	375/716 (52%)	358 (96%)	17 (4%)	0	100	100
6	J	380/716 (53%)	358 (94%)	21 (6%)	1 (0%)	36	65
6	O	375/716 (52%)	350 (93%)	25 (7%)	0	100	100
6	R	380/716 (53%)	363 (96%)	16 (4%)	1 (0%)	36	65
7	H	233/276 (84%)	222 (95%)	11 (5%)	0	100	100
7	P	233/276 (84%)	227 (97%)	6 (3%)	0	100	100
7	c	235/276 (85%)	216 (92%)	18 (8%)	1 (0%)	30	60
7	d	235/276 (85%)	226 (96%)	9 (4%)	0	100	100
All	All	4110/7464 (55%)	3869 (94%)	233 (6%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	149	GLU
6	J	613	SER
5	F	189	THR
5	I	165	ASN
7	c	79	CYS
2	K	221	PRO
5	Q	165	ASN
6	R	603	GLN

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	38/137 (28%)	38 (100%)	0	100	100
1	C	38/137 (28%)	38 (100%)	0	100	100
2	B	169/307 (55%)	167 (99%)	2 (1%)	63	73
2	K	169/307 (55%)	168 (99%)	1 (1%)	78	79
3	D	44/349 (13%)	44 (100%)	0	100	100
3	L	44/349 (13%)	44 (100%)	0	100	100
4	E	177/199 (89%)	177 (100%)	0	100	100
4	M	177/199 (89%)	177 (100%)	0	100	100
5	F	148/259 (57%)	147 (99%)	1 (1%)	76	78
5	I	148/259 (57%)	148 (100%)	0	100	100
5	N	148/259 (57%)	148 (100%)	0	100	100
5	Q	148/259 (57%)	148 (100%)	0	100	100
6	G	334/625 (53%)	334 (100%)	0	100	100
6	J	343/625 (55%)	340 (99%)	3 (1%)	70	76
6	O	339/625 (54%)	338 (100%)	1 (0%)	86	83
6	R	343/625 (55%)	343 (100%)	0	100	100
7	H	207/243 (85%)	207 (100%)	0	100	100
7	P	207/243 (85%)	206 (100%)	1 (0%)	81	80
7	c	209/243 (86%)	209 (100%)	0	100	100
7	d	209/243 (86%)	208 (100%)	1 (0%)	81	80
All	All	3639/6492 (56%)	3629 (100%)	10 (0%)	84	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	250	LYS
2	B	286	LYS
5	F	127	THR

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Mol	Chain	Res	Type
6	J	238	LYS
6	J	647	ILE
6	J	657	ASN
2	K	155	CYS
6	O	433	CYS
7	P	248	THR
7	d	23	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	74	ASN
6	G	603	GLN
6	G	611	GLN
7	H	109	HIS
7	H	146	GLN
5	I	119	ASN
5	I	145	GLN
5	I	154	HIS
6	J	541	ASN
6	J	657	ASN
6	J	688	GLN
5	N	98	GLN
6	O	544	HIS
7	P	168	HIS
7	d	189	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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.

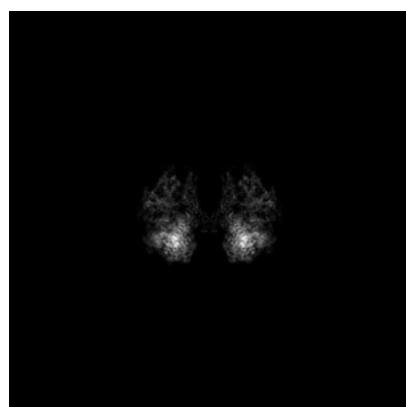
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38020. These allow visual inspection of the internal detail of the map and identification of artifacts.

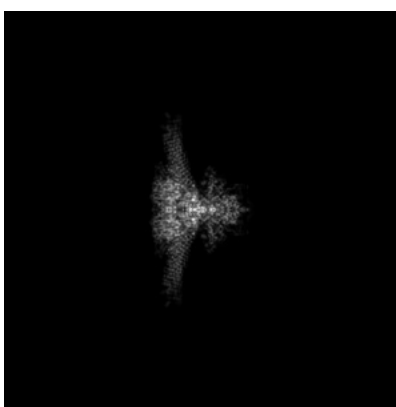
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

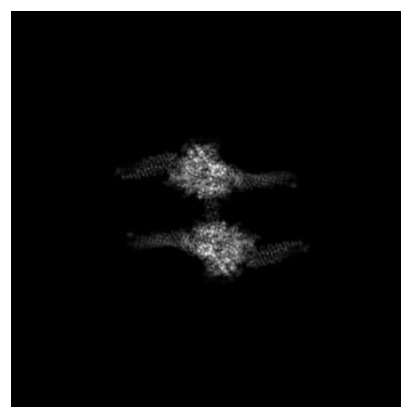
6.1.1 Primary map



X



Y

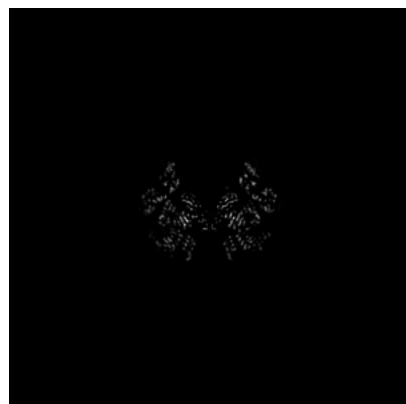


Z

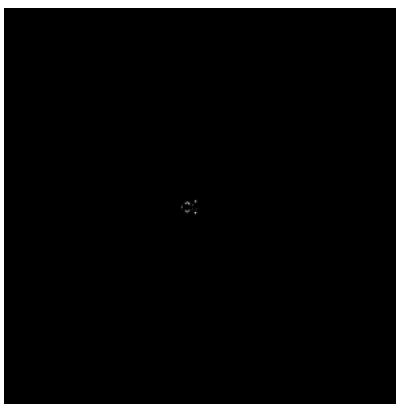
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

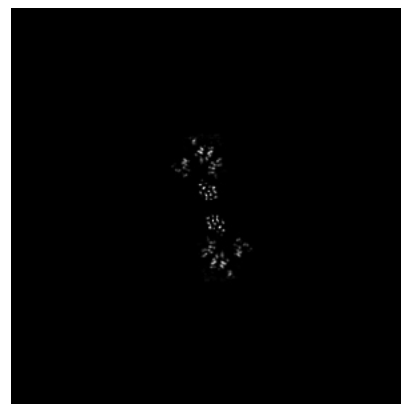
6.2.1 Primary map



X Index: 280



Y Index: 280

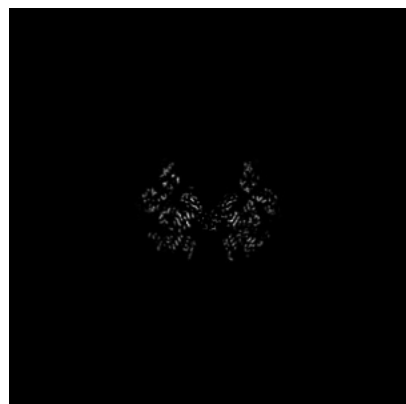


Z Index: 280

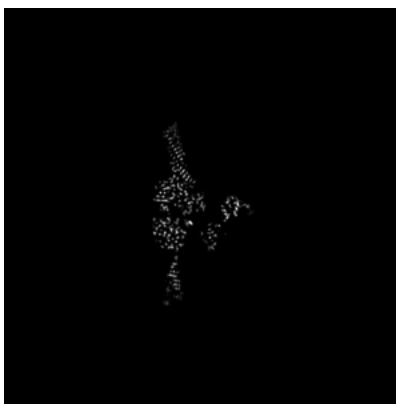
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 282



Y Index: 330



Z Index: 243

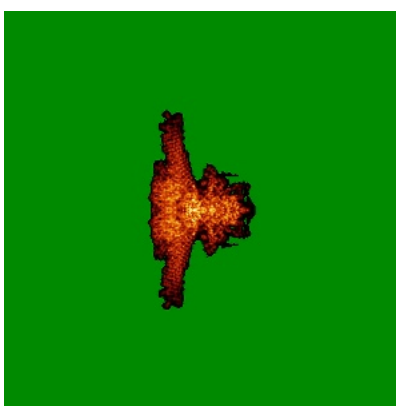
The images above show the largest variance slices of the map in three orthogonal directions.

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

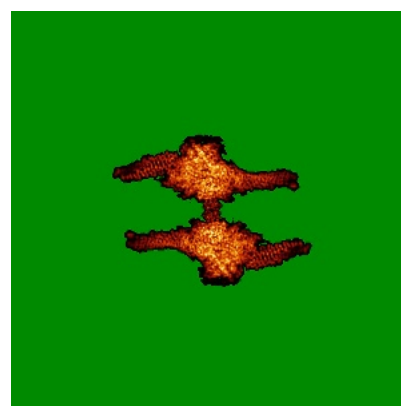
6.4.1 Primary map



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

This section was not generated.

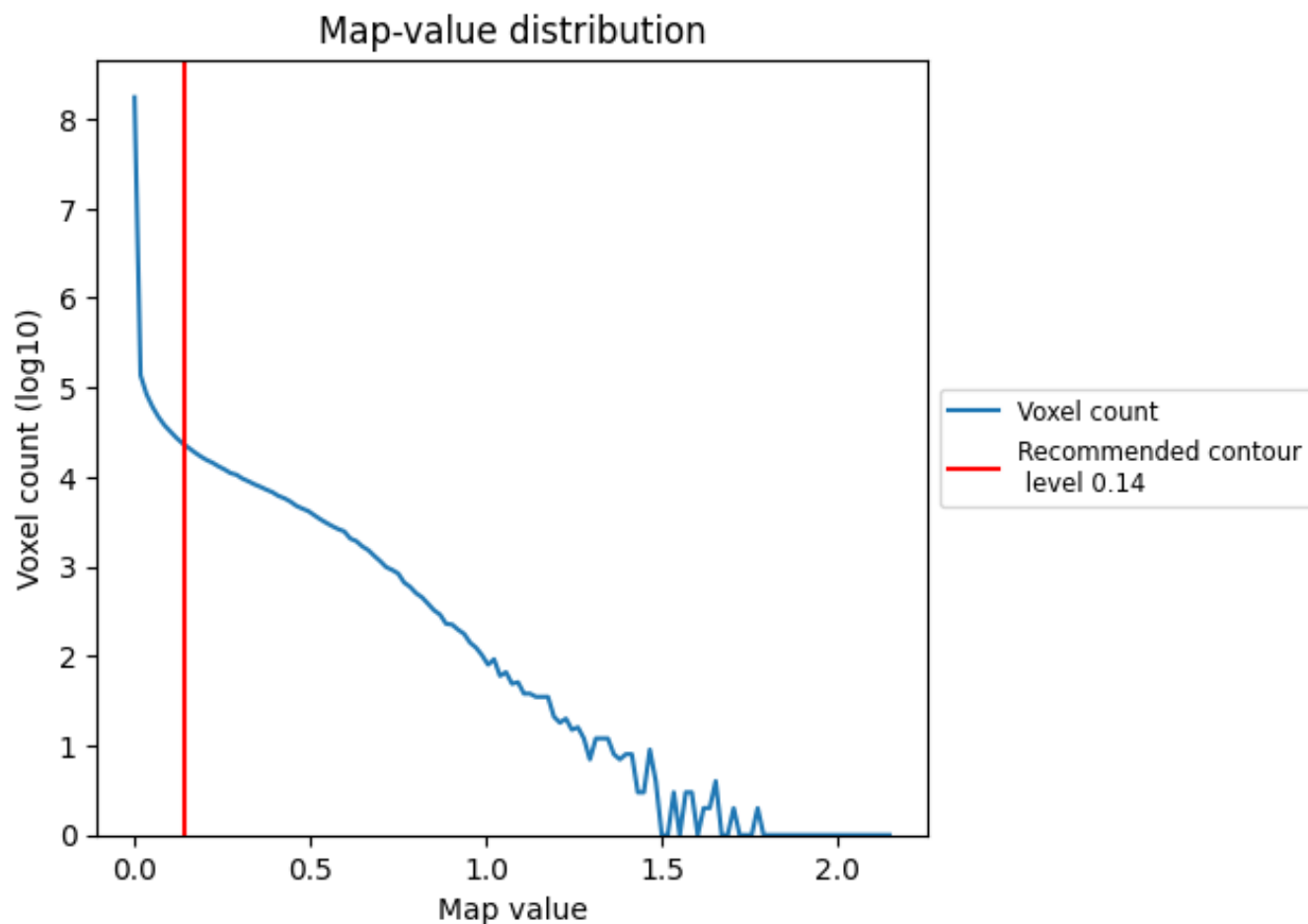
6.6 Mask visualisation

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

7 Map analysis [i](#)

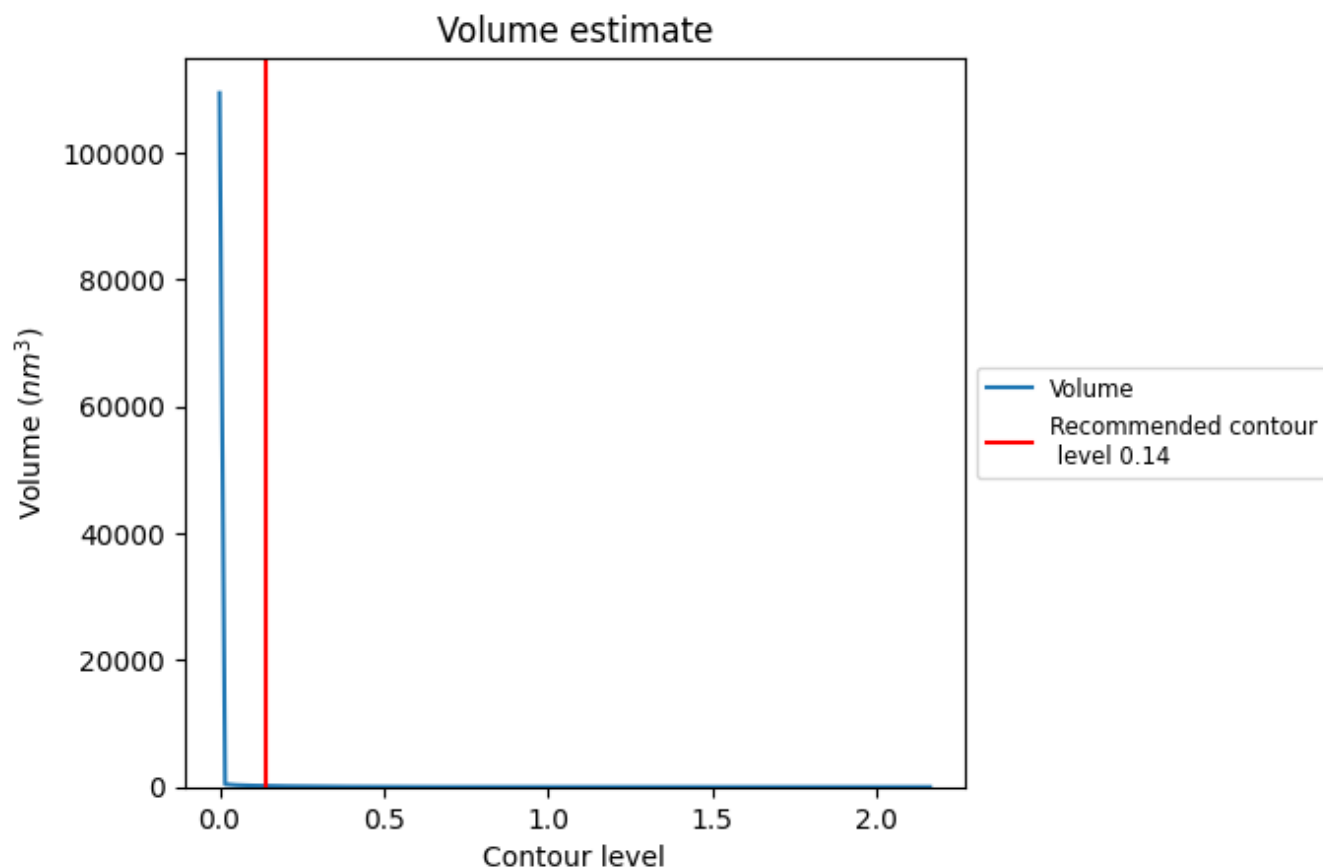
This section contains the results of statistical analysis of the map.

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.

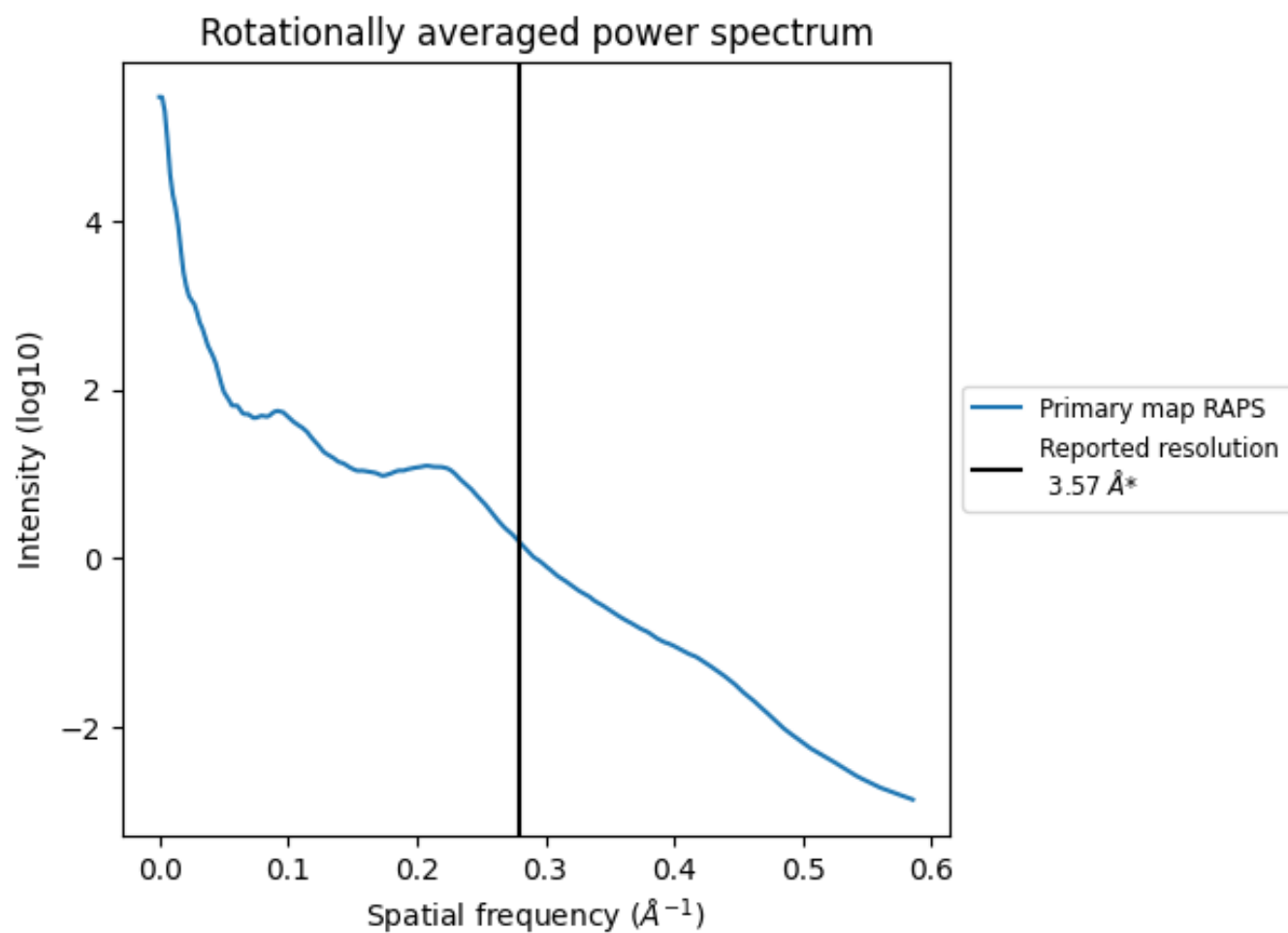
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm^3 ; this corresponds to an approximate mass of 151 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 0.280 Å⁻¹

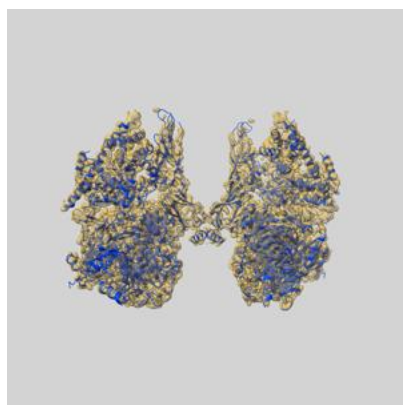
8 Fourier-Shell correlation ⓘ

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

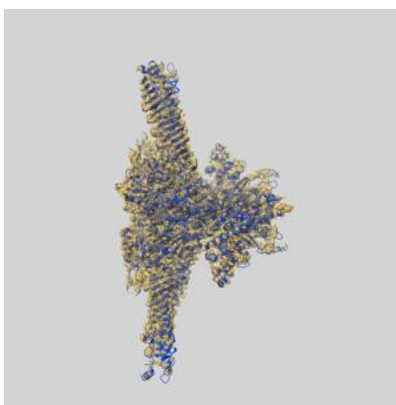
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38020 and PDB model 8X2U. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

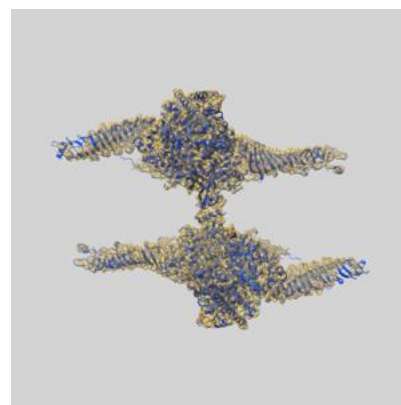
9.1 Map-model overlay [i](#)



X



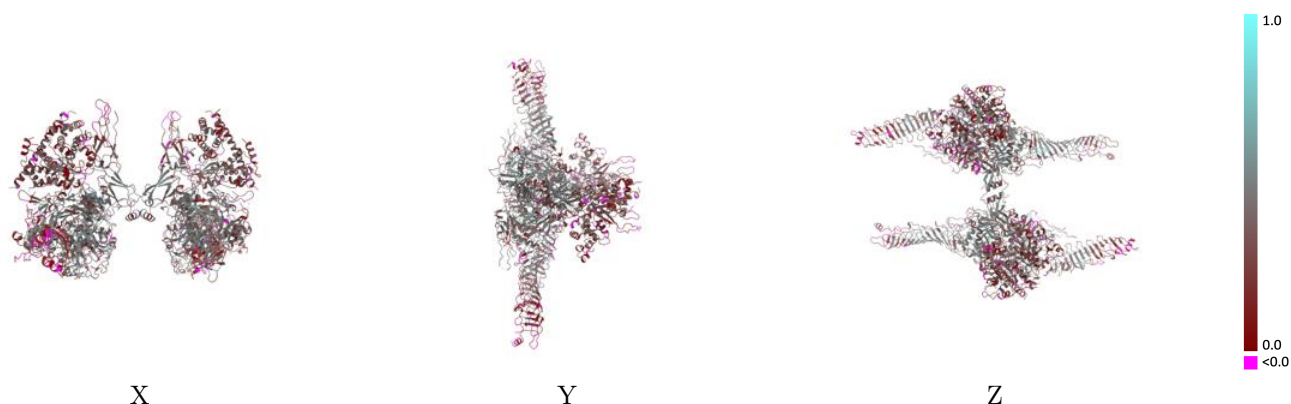
Y



Z

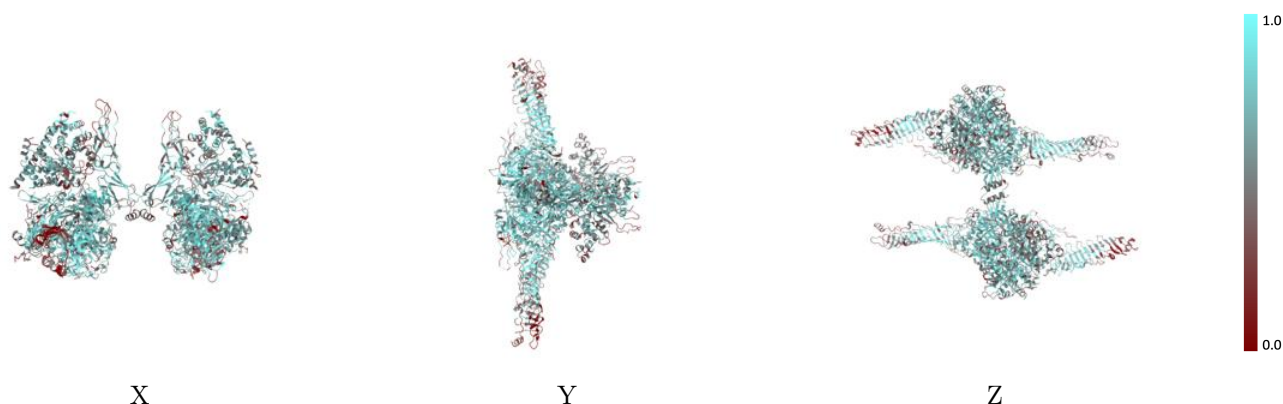
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



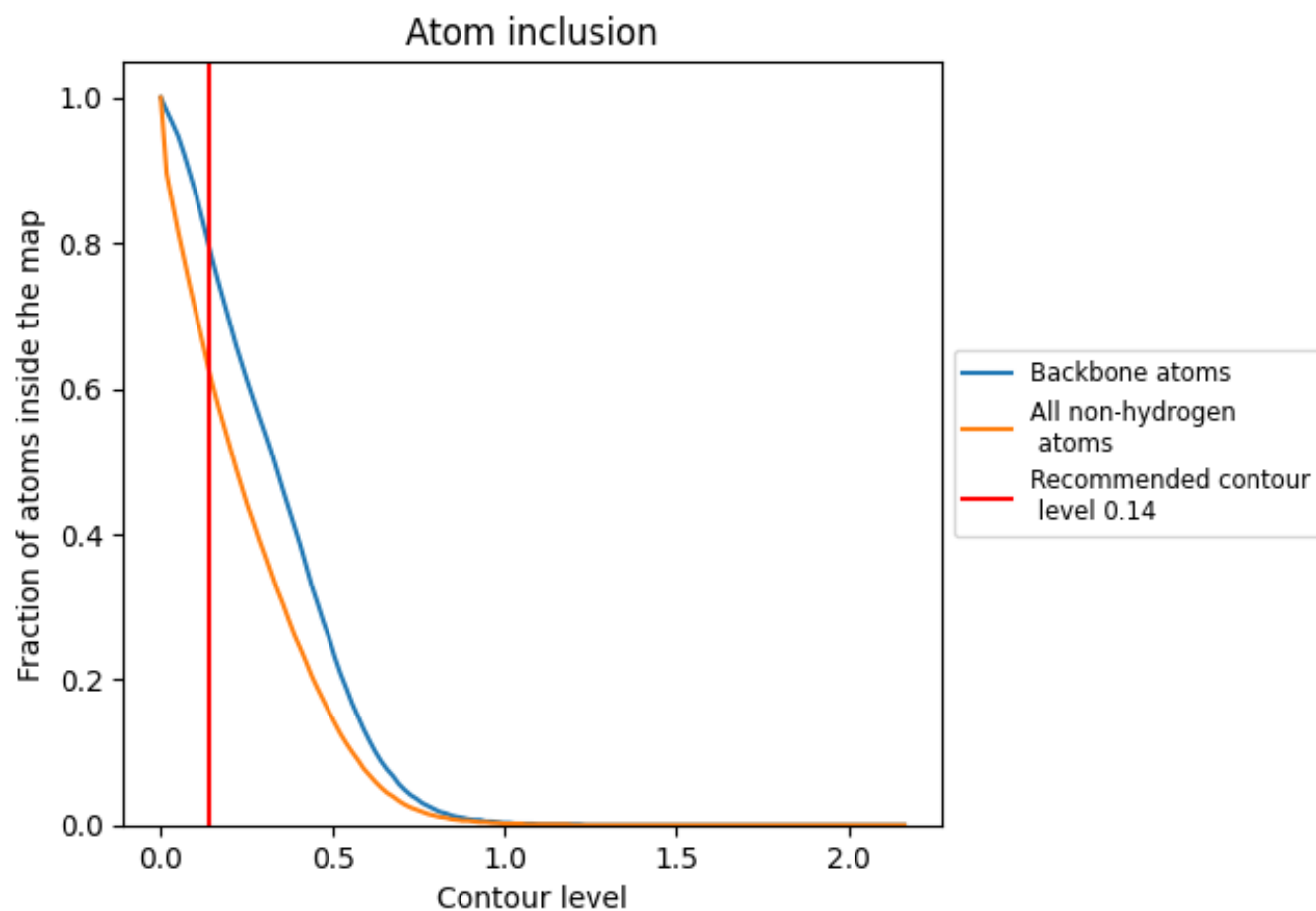
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 63% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6280	 0.3530
A	 0.6650	 0.3010
B	 0.5640	 0.3280
C	 0.6420	 0.3020
D	 0.6110	 0.2730
E	 0.5100	 0.2540
F	 0.5880	 0.3270
G	 0.6740	 0.3930
H	 0.7330	 0.4290
I	 0.4970	 0.2600
J	 0.6700	 0.3830
K	 0.5680	 0.3390
L	 0.6190	 0.2760
M	 0.5050	 0.2570
N	 0.5830	 0.3410
O	 0.6700	 0.3910
P	 0.7270	 0.4220
Q	 0.5040	 0.2680
R	 0.6760	 0.3910
c	 0.6630	 0.3610
d	 0.6650	 0.3720

