



Full wwPDB EM Validation Report (i)

Jan 31, 2024 – 02:36 PM JST

PDB ID : 8X2U
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 (i) 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 \(i\)](#)) were used in the production of this report:

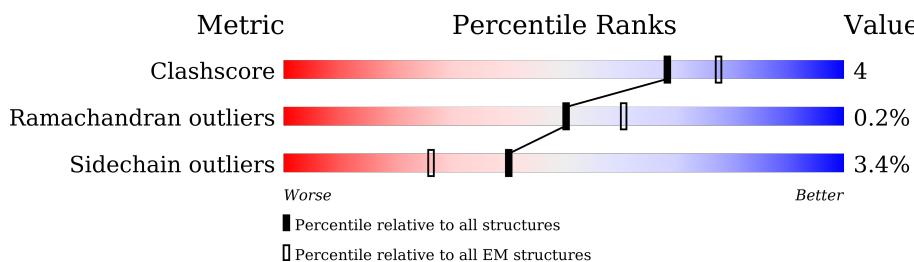
EMDB validation analysis : 0.0.1.dev70
MolProbit : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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)
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 <=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.



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Mol	Chain	Length	Quality of chain			
5	F	313	15%	51%	7%	41%
5	I	313	22%	53%	6%	41%
5	N	313	14%	51%	8%	41%
5	Q	313	22%	51%	8%	41%
6	G	716	9%	47%	7%	46%
6	J	716	8%	49%	6%	45%
6	O	716	7%	46%	7%	46%
6	R	716	8%	49%	6%	45%
7	H	276	7%	72%	13%	13%
7	P	276	7%	75%	11%	13%
7	c	276	11%	83%	•	13%
7	d	276	11%	83%	5%	13%

2 Entry composition (i)

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
			Total	C	N	O	S		
1	A	46	369	238	63	66	2	0	0
1	C	46	369	238	63	66	2	0	0

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		

Mol	Chain	Residues	Atoms					AltConf	Trace
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		

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

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		

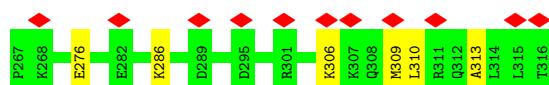
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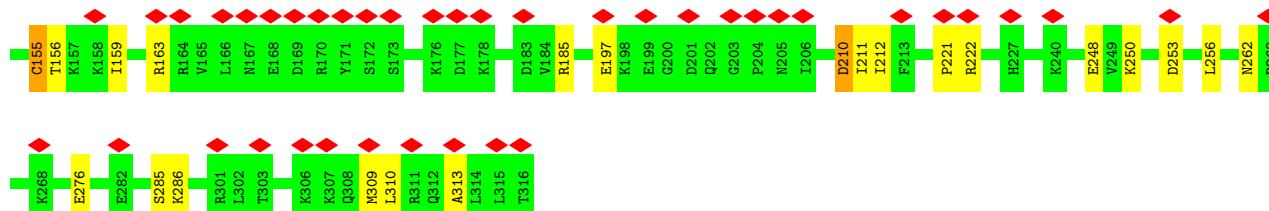
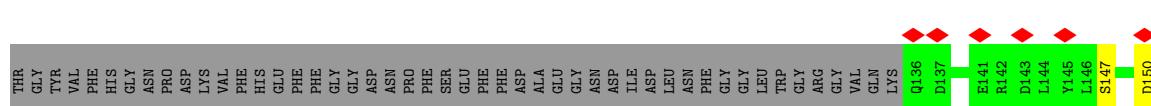
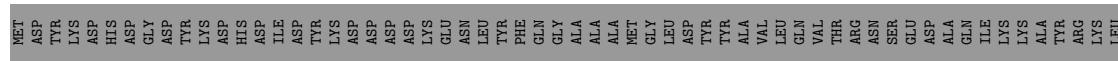
Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	392	Total	C	N	O	S		
			3139	2021	515	592	11	0	0
6	O	387	Total	C	N	O	S		
			3099	1997	506	586	10	0	0
6	R	392	Total	C	N	O	S		
			3139	2021	515	592	11	0	0

- 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		
			1912	1228	324	351	9	0	0
7	c	241	Total	C	N	O	S		
			1926	1238	326	353	9	0	0
7	P	239	Total	C	N	O	S		
			1912	1228	324	351	9	0	0
7	d	241	Total	C	N	O	S		
			1926	1238	326	353	9	0	0



- Molecule 2: DnaJ homolog subfamily B member 13

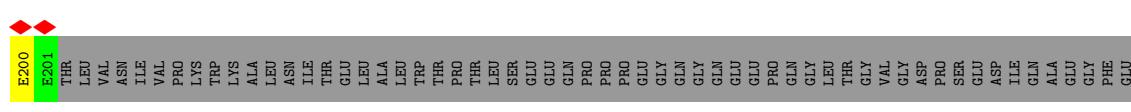
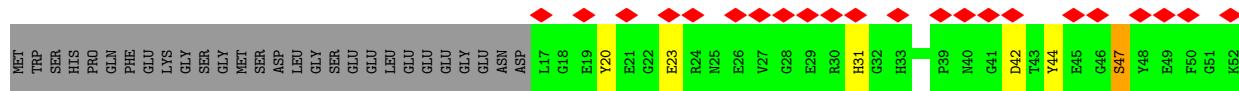


- Molecule 3: Radial spoke head protein 3 homolog B

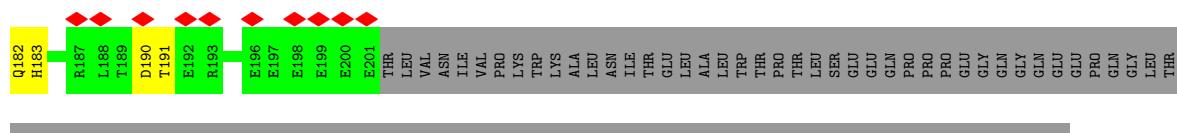




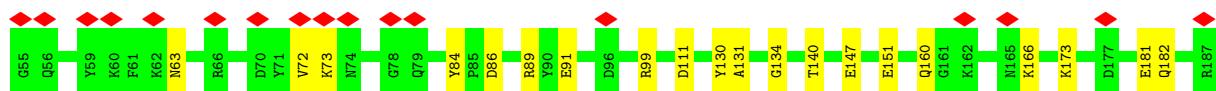
- Molecule 5: Radial spoke head 1 homolog



- Molecule 5: Radial spoke head 1 homolog

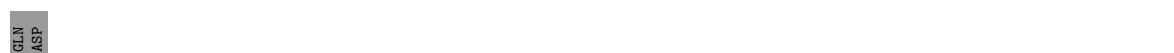
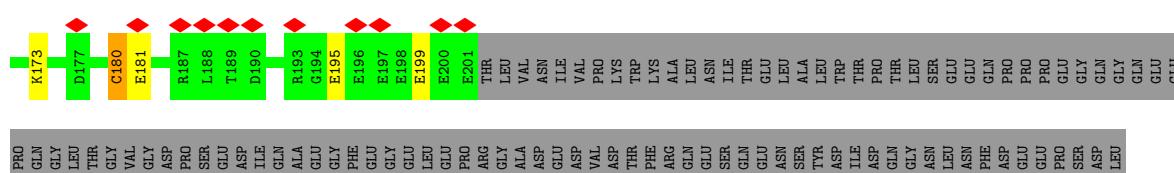
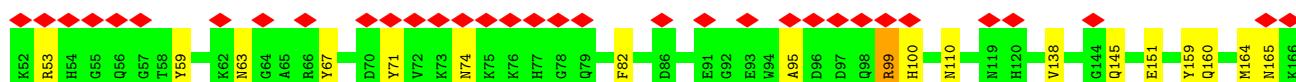


- Molecule 5: Radial spoke head 1 homolog

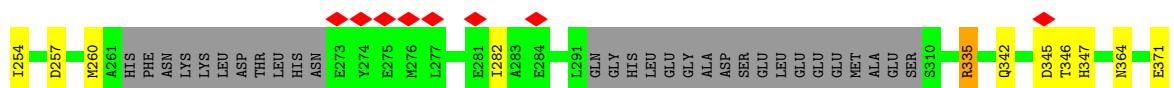
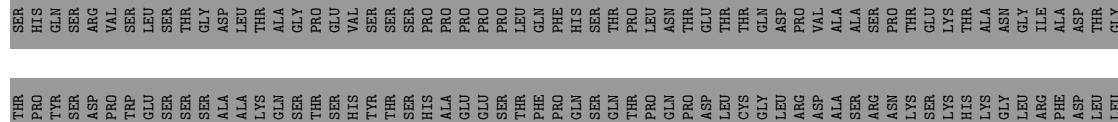


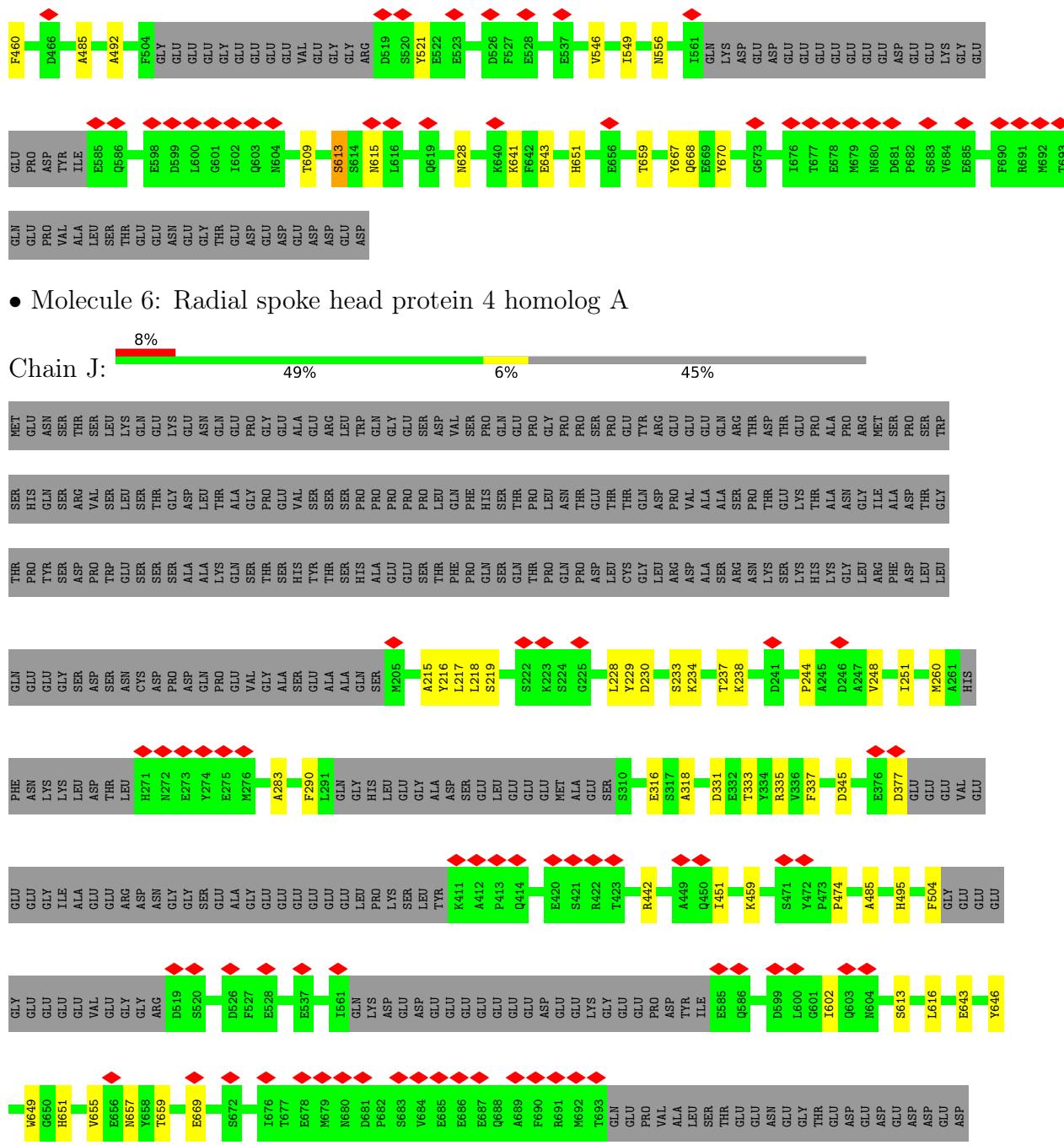


- Molecule 5: Radial spoke head 1 homolog

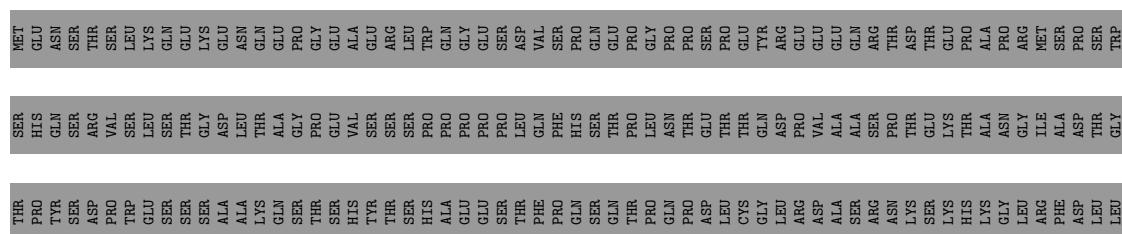
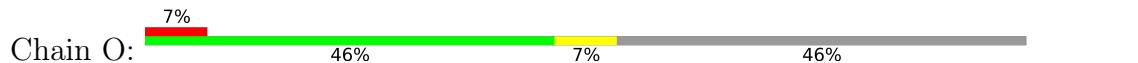


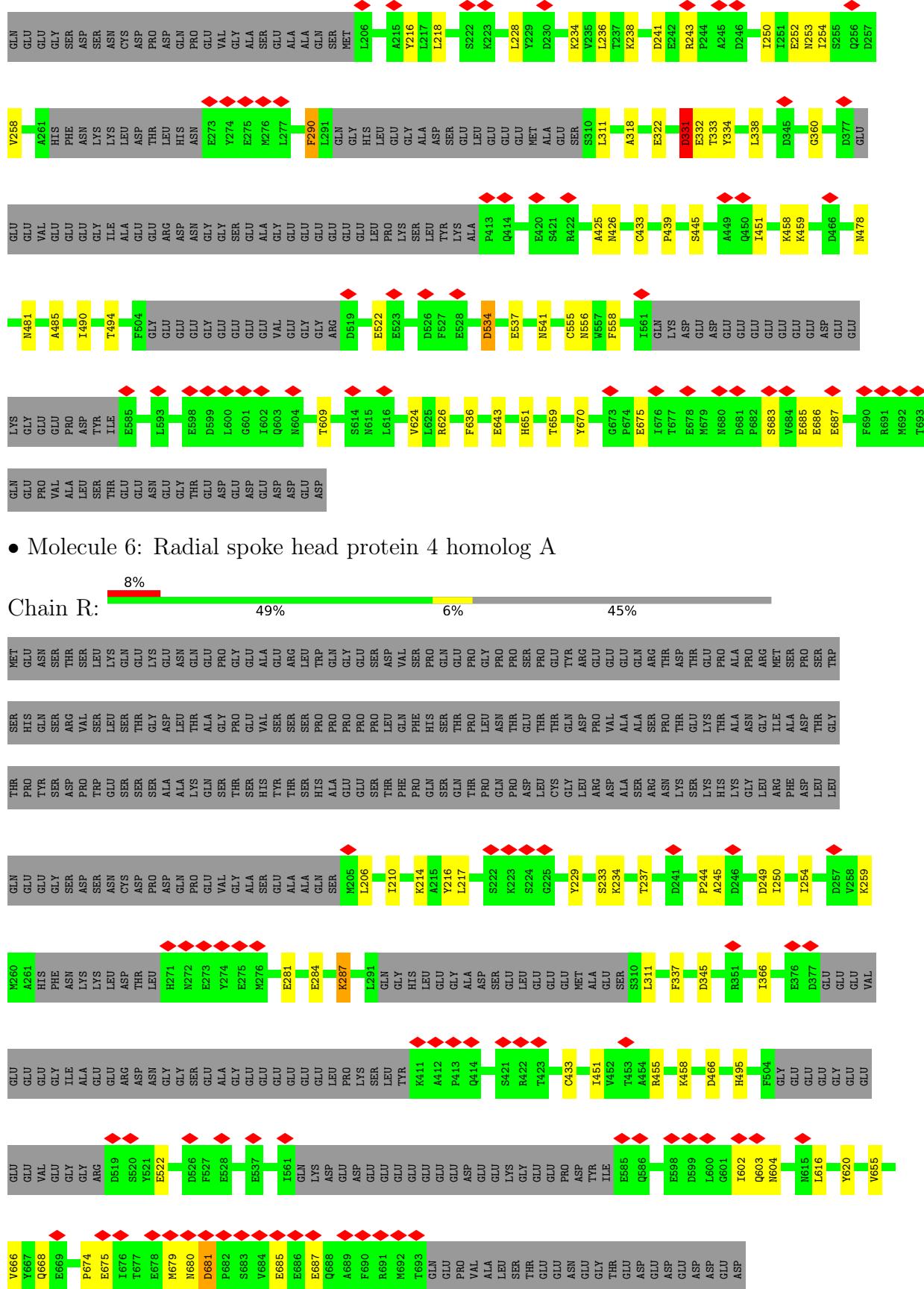
- Molecule 6: Radial spoke head protein 4 homolog A



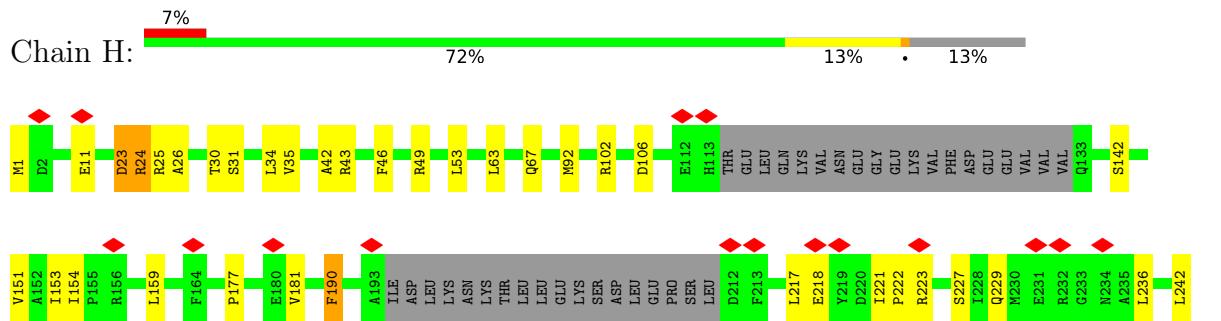


- Molecule 6: Radial spoke head protein 4 homolog A





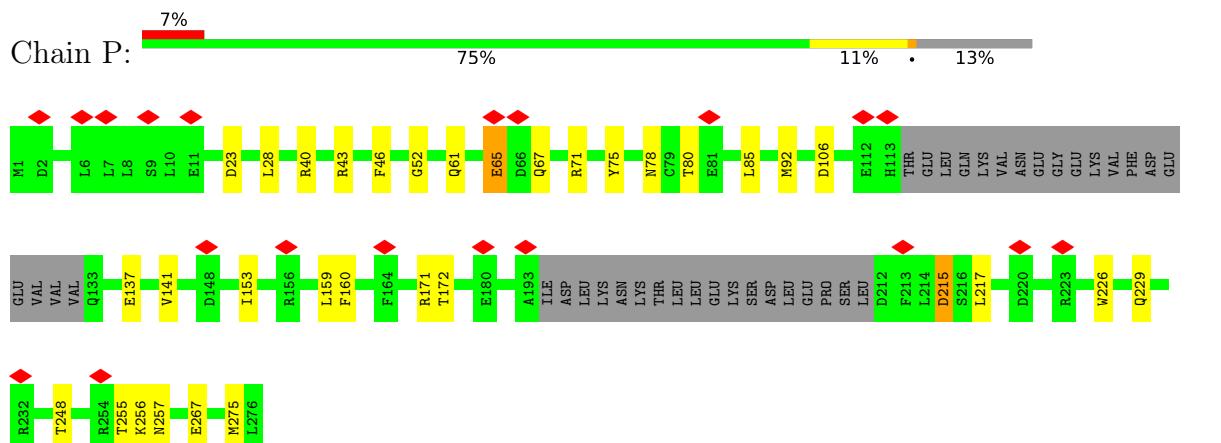
- Molecule 7: Radial spoke head protein 9 homolog



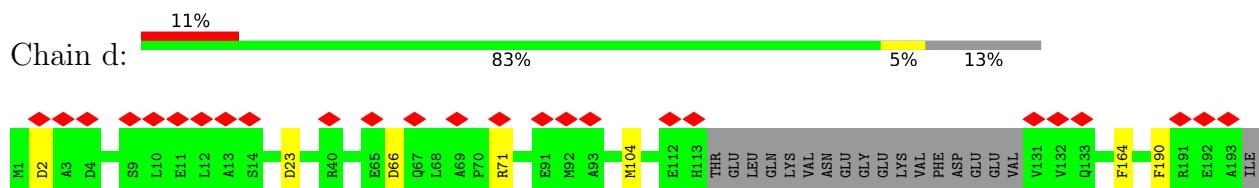
- Molecule 7: Radial spoke head protein 9 homolog



- Molecule 7: Radial spoke head protein 9 homolog



- Molecule 7: Radial spoke head protein 9 homolog





4 Experimental information (i)

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 i

5.1 Standard geometry i

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	0.35	0/379	0.77	1/517 (0.2%)
1	C	0.39	0/379	0.76	0/517
2	B	0.32	0/1525	0.75	3/2061 (0.1%)
2	K	0.34	0/1525	0.76	3/2061 (0.1%)
3	D	0.49	0/393	0.99	0/528
3	L	0.41	0/393	0.93	0/528
4	E	0.39	0/1657	0.80	3/2251 (0.1%)
4	M	0.36	0/1657	0.73	3/2251 (0.1%)
5	F	0.37	0/1558	0.75	1/2096 (0.0%)
5	I	0.38	0/1558	0.75	0/2096
5	N	0.34	0/1558	0.72	1/2096 (0.0%)
5	Q	0.35	0/1558	0.76	2/2096 (0.1%)
6	G	0.37	0/3183	0.71	1/4335 (0.0%)
6	J	0.37	0/3224	0.75	4/4390 (0.1%)
6	O	0.36	0/3183	0.68	1/4335 (0.0%)
6	R	0.37	0/3224	0.76	7/4390 (0.2%)
7	H	0.38	0/1956	0.80	2/2645 (0.1%)
7	P	0.34	0/1956	0.78	2/2645 (0.1%)
7	c	0.37	0/1970	0.86	3/2665 (0.1%)
7	d	0.37	0/1970	0.86	3/2665 (0.1%)
All	All	0.37	0/34806	0.76	40/47168 (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 (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	245	ALA	C-N-CA	10.59	148.16	121.70
6	R	345	ASP	CB-CG-OD1	9.38	126.75	118.30
7	P	23	ASP	CB-CG-OD2	9.38	126.74	118.30
7	c	23	ASP	CB-CG-OD1	9.33	126.70	118.30
6	J	345	ASP	CB-CG-OD1	9.16	126.55	118.30
7	d	66	ASP	CB-CG-OD1	9.13	126.52	118.30
7	c	2	ASP	CB-CG-OD1	8.92	126.33	118.30
7	d	2	ASP	CB-CG-OD1	8.91	126.32	118.30
7	P	65	GLU	C-N-CA	8.54	143.05	121.70
4	E	183	ASP	CB-CG-OD1	8.29	125.76	118.30
6	O	331	ASP	CB-CG-OD1	8.19	125.67	118.30
6	R	674	PRO	CA-N-CD	-7.98	100.33	111.50
6	J	616	LEU	C-N-CA	7.92	141.50	121.70
5	N	86	ASP	CB-CG-OD1	7.92	125.43	118.30
5	F	86	ASP	CB-CG-OD1	7.86	125.37	118.30
2	K	309	MET	CB-CG-SD	7.63	135.29	112.40
7	c	270	MET	CG-SD-CE	7.50	112.19	100.20
7	d	220	ASP	CB-CG-OD1	7.48	125.03	118.30
5	Q	159	TYR	C-N-CA	7.37	140.12	121.70
7	H	106	ASP	CB-CG-OD1	7.33	124.89	118.30
6	R	249	ASP	CB-CG-OD1	7.32	124.89	118.30
2	K	309	MET	CA-CB-CG	6.66	124.62	113.30
1	A	6	LEU	CA-CB-CG	6.47	130.18	115.30
6	R	466	ASP	CB-CG-OD1	6.37	124.03	118.30
5	Q	99	ARG	C-N-CA	6.34	137.54	121.70
2	B	309	MET	CA-CB-CG	6.33	124.06	113.30
4	M	186	LEU	CA-CB-CG	6.16	129.46	115.30
6	J	331	ASP	CB-CG-OD1	6.13	123.82	118.30
4	E	122	LEU	CA-CB-CG	6.12	129.38	115.30
2	K	210	ASP	CB-CG-OD1	6.12	123.80	118.30
4	E	186	LEU	CA-CB-CG	6.05	129.22	115.30
2	B	253	ASP	CB-CG-OD1	5.80	123.52	118.30
4	M	183	ASP	CB-CG-OD1	5.53	123.28	118.30
7	H	151	VAL	CG1-CB-CG2	-5.52	102.06	110.90
4	M	74	MET	CA-CB-CG	5.50	122.66	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	309	MET	CB-CG-SD	5.47	128.81	112.40
6	R	458	LYS	CA-CB-CG	5.27	125.00	113.40
6	G	219	SER	C-N-CA	5.16	134.60	121.70
6	R	206	LEU	CA-CB-CG	5.13	127.09	115.30
6	J	474	PRO	C-N-CA	5.06	134.35	121.70

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 [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	369	0	363	0	0
1	C	369	0	363	4	0
2	B	1489	0	1538	11	0
2	K	1489	0	1538	10	0
3	D	387	0	380	7	0
3	L	387	0	380	9	0
4	E	1612	0	1623	13	0
4	M	1612	0	1623	19	0
5	F	1514	0	1346	11	0
5	I	1514	0	1346	8	0
5	N	1514	0	1346	13	0
5	Q	1514	0	1346	9	0
6	G	3099	0	3009	34	0
6	J	3139	0	3048	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	3099	0	3009	37	0
6	R	3139	0	3048	28	0
7	H	1912	0	1907	24	0
7	P	1912	0	1907	19	0
7	c	1926	0	1925	0	0
7	d	1926	0	1925	0	0
All	All	33922	0	32970	220	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 (220) 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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:646:TYR:OH	6:J:649:TRP:O	2.15	0.63
6:G:376:GLU:N	6:G:376:GLU:OE2	2.32	0.63
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
3:L:314:ASP:OD1	6:R:229:TYR:OH	2.12	0.62
5:N:182:GLN:NE2	5:N:196:GLU:O	2.32	0.62
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: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
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
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: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:R:214:LYS:O	6:R:217:LEU: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
6:O:243:ARG:N	6:R:216:TYR:HH	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:I:67:TYR:OH	5:I:70:ASP:O	2.17	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
6:J:602:ILE:HG12	6:J:655:VAL:HG12	1.90	0.53
6:O:490:ILE:O	6:O:494:THR:OG1	2.10	0.53
6:O:686:GLU:OE2	6:O:686:GLU:N	2.42	0.53
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
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
6:O:216:TYR:OH	6:R:244:PRO:O	2.28	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:478:ASN:OD1	6:O:481:ASN:ND2	2.45	0.50
3:L:291:PHE:HE2	4:M:173:LEU:HD23	1.77	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
5:Q:138:VAL:O	5:Q:151:GLU:N	2.45	0.50
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
5:F:180:CYS:SG	5:F:181:GLU:N	2.85	0.49
5:N:130:TYR:O	5:N:134:GLY:N	2.43	0.49
6:G:371:GLU:OE1	6:G:422:ARG:NH1	2.45	0.49
2:B:313:ALA:HB1	2:K:310:LEU:HD12	1.95	0.49
5:I:190:ASP:O	6:J:659:THR:OG1	2.26	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
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
4:M:139:ILE:HG21	4:M:148:ILE:HG21	1.96	0.48
6:R:451:ILE:O	6:R:455:ARG:N	2.47	0.48
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
3:L:321:VAL:O	3:L:325:ILE:HD12	2.15	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
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
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:318:ALA:CB	6:J:333:THR:HG21	2.44	0.45
7:H:1:MET:N	7:H:46:PHE:O	2.45	0.45
6:O:318:ALA:CB	6:O:333:THR:HG21	2.44	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
2:B:222:ARG:NH1	2:B:250:LYS:O	2.51	0.44
6:G:615:ASN:OD1	7:H:24:ARG:NH1	2.48	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:P:215:ASP:N	7:P:215:ASP:OD1	2.50	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
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
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
4:M:72:ALA:O	4:M:76:SER:N	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
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
6:J:233:SER:O	6:J:237:THR:OG1	2.35	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:282:ILE:HG22	6:G:438:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:N:140:THR:OG1	5:N:147:GLU:O	2.37	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
7:P:255:THR:OG1	7:P:256:LYS:N	2.52	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
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
2:B:158:LYS:C	2:B:159:ILE:HD13	2.41	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: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
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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	44/159 (28%)	43 (98%)	1 (2%)	0	100 100
1	C	44/159 (28%)	41 (93%)	3 (7%)	0	100 100
2	B	179/349 (51%)	162 (90%)	17 (10%)	0	100 100
2	K	179/349 (51%)	165 (92%)	13 (7%)	1 (1%)	25 64
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%)	29 67
4	M	199/225 (88%)	187 (94%)	12 (6%)	0	100 100
5	F	183/313 (58%)	175 (96%)	7 (4%)	1 (0%)	29 67
5	I	183/313 (58%)	166 (91%)	16 (9%)	1 (0%)	29 67
5	N	183/313 (58%)	170 (93%)	13 (7%)	0	100 100
5	Q	183/313 (58%)	169 (92%)	13 (7%)	1 (0%)	29 67
6	G	375/716 (52%)	358 (96%)	17 (4%)	0	100 100
6	J	380/716 (53%)	358 (94%)	21 (6%)	1 (0%)	41 74
6	O	375/716 (52%)	350 (93%)	25 (7%)	0	100 100
6	R	380/716 (53%)	363 (96%)	16 (4%)	1 (0%)	41 74
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%)	34 71
7	d	235/276 (85%)	226 (96%)	9 (4%)	0	100 100
All	All	4110/7464 (55%)	3869 (94%)	233 (6%)	8 (0%)	50 80

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 [\(i\)](#)

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%)	37 (97%)	1 (3%)	46 74
2	B	169/307 (55%)	165 (98%)	4 (2%)	49 76
2	K	169/307 (55%)	161 (95%)	8 (5%)	26 61
3	D	44/349 (13%)	42 (96%)	2 (4%)	27 62
3	L	44/349 (13%)	42 (96%)	2 (4%)	27 62
4	E	177/199 (89%)	174 (98%)	3 (2%)	60 83
4	M	177/199 (89%)	171 (97%)	6 (3%)	37 69
5	F	148/259 (57%)	140 (95%)	8 (5%)	22 57
5	I	148/259 (57%)	142 (96%)	6 (4%)	30 64
5	N	148/259 (57%)	144 (97%)	4 (3%)	44 74
5	Q	148/259 (57%)	139 (94%)	9 (6%)	18 53
6	G	339/625 (54%)	329 (97%)	10 (3%)	42 72
6	J	343/625 (55%)	333 (97%)	10 (3%)	42 72
6	O	339/625 (54%)	327 (96%)	12 (4%)	36 68
6	R	343/625 (55%)	338 (98%)	5 (2%)	65 85
7	H	207/243 (85%)	197 (95%)	10 (5%)	25 60
7	P	207/243 (85%)	200 (97%)	7 (3%)	37 69
7	c	209/243 (86%)	202 (97%)	7 (3%)	38 69
7	d	209/243 (86%)	199 (95%)	10 (5%)	25 60
All	All	3644/6492 (56%)	3520 (97%)	124 (3%)	40 69

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	155	CYS
2	B	254	ASP
2	B	276	GLU

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Mol	Chain	Res	Type
2	B	286	LYS
3	D	291	PHE
3	D	316	LEU
4	E	5	MET
4	E	65	MET
4	E	92	TYR
5	F	31	HIS
5	F	47	SER
5	F	61	PHE
5	F	86	ASP
5	F	90	TYR
5	F	102	GLN
5	F	118	PHE
5	F	145	GLN
6	G	216	TYR
6	G	229	TYR
6	G	260	MET
6	G	335	ARG
6	G	345	ASP
6	G	347	HIS
6	G	374	ASP
6	G	641	LYS
6	G	668	GLN
6	G	670	TYR
7	H	23	ASP
7	H	24	ARG
7	H	43	ARG
7	H	92	MET
7	H	142	SER
7	H	190	PHE
7	H	218	GLU
7	H	222	PRO
7	H	223	ARG
7	H	250	TYR
5	I	31	HIS
5	I	94	TRP
5	I	105	TYR
5	I	110	ASN
5	I	180	CYS
5	I	183	HIS
6	J	230	ASP
6	J	234	LYS

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Mol	Chain	Res	Type
6	J	238	LYS
6	J	260	MET
6	J	316	GLU
6	J	337	PHE
6	J	495	HIS
6	J	504	PHE
6	J	643	GLU
6	J	657	ASN
7	c	33	MET
7	c	92	MET
7	c	94	MET
7	c	160	PHE
7	c	164	PHE
7	c	190	PHE
7	c	213	PHE
1	C	5	TYR
2	K	155	CYS
2	K	163	ARG
2	K	185	ARG
2	K	222	ARG
2	K	250	LYS
2	K	276	GLU
2	K	285	SER
2	K	286	LYS
3	L	291	PHE
3	L	326	ASN
4	M	45	ARG
4	M	82	MET
4	M	86	ARG
4	M	92	TYR
4	M	114	ARG
4	M	195	ASN
5	N	25	ASN
5	N	54	HIS
5	N	151	GLU
5	N	166	LYS
6	O	234	LYS
6	O	241	ASP
6	O	290	PHE
6	O	322	GLU
6	O	331	ASP
6	O	433	CYS

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Mol	Chain	Res	Type
6	O	439	PRO
6	O	534	ASP
6	O	537	GLU
6	O	541	ASN
6	O	558	PHE
6	O	670	TYR
7	P	75	TYR
7	P	92	MET
7	P	106	ASP
7	P	160	PHE
7	P	215	ASP
7	P	248	THR
7	P	257	ASN
5	Q	59	TYR
5	Q	82	PHE
5	Q	100	HIS
5	Q	110	ASN
5	Q	145	GLN
5	Q	164	MET
5	Q	180	CYS
5	Q	195	GLU
5	Q	199	GLU
6	R	234	LYS
6	R	287	LYS
6	R	495	HIS
6	R	604	ASN
6	R	681	ASP
7	d	23	ASP
7	d	71	ARG
7	d	104	MET
7	d	164	PHE
7	d	190	PHE
7	d	213	PHE
7	d	218	GLU
7	d	231	GLU
7	d	250	TYR
7	d	267	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	54	HIS

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Mol	Chain	Res	Type
6	J	657	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 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.

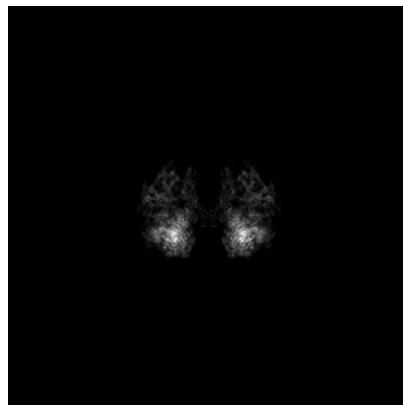
6 Map visualisation i

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.

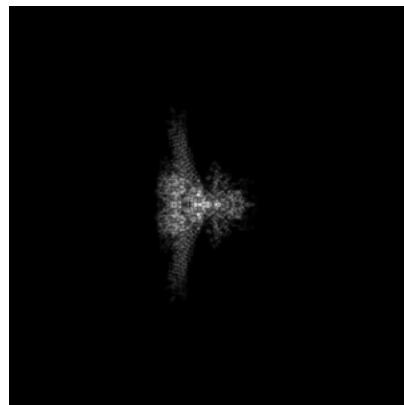
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections i

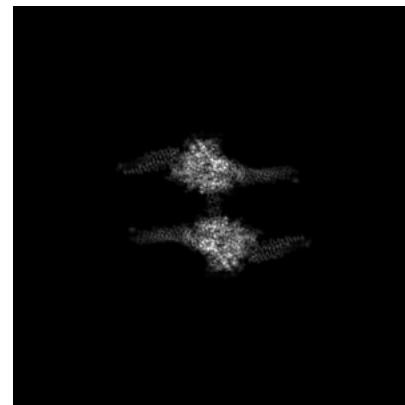
6.1.1 Primary map



X



Y

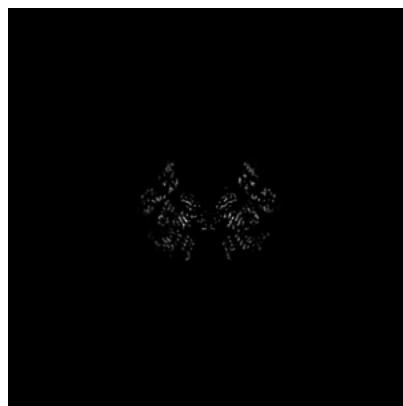


Z

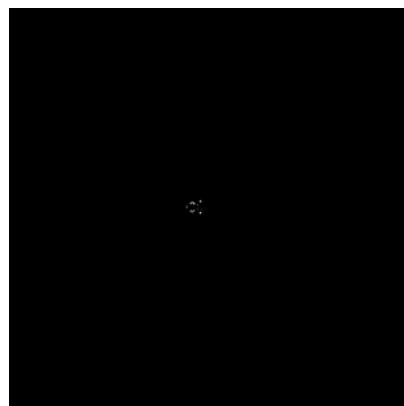
The images above show the map projected in three orthogonal directions.

6.2 Central slices i

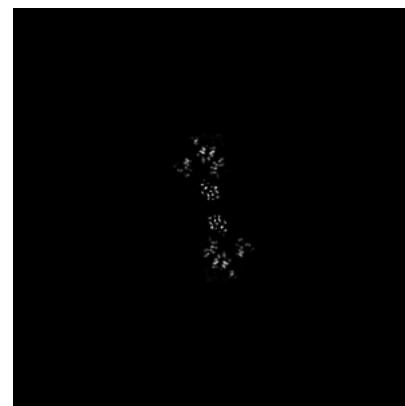
6.2.1 Primary map



X Index: 280



Y Index: 280



Z Index: 280

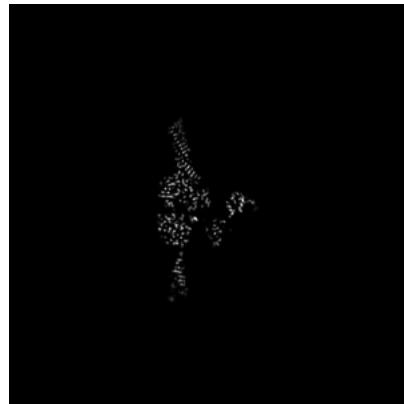
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

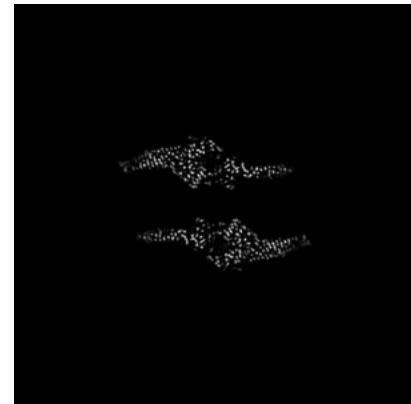
6.3.1 Primary map



X Index: 282



Y Index: 330



Z Index: 243

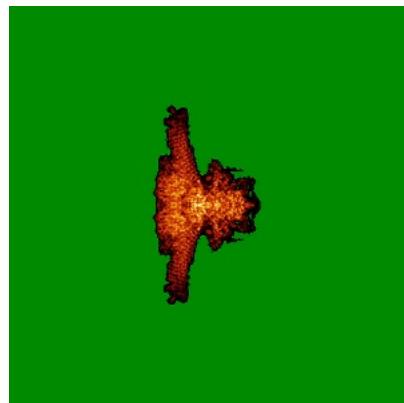
The images above show the largest variance slices of the map in three orthogonal directions.

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

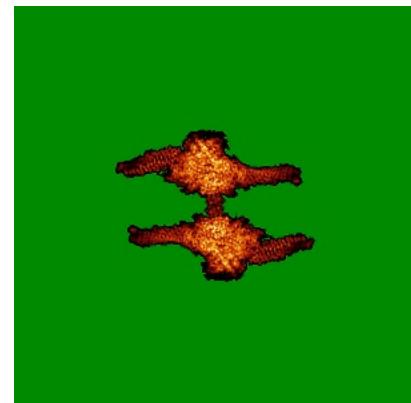
6.4.1 Primary map



X



Y

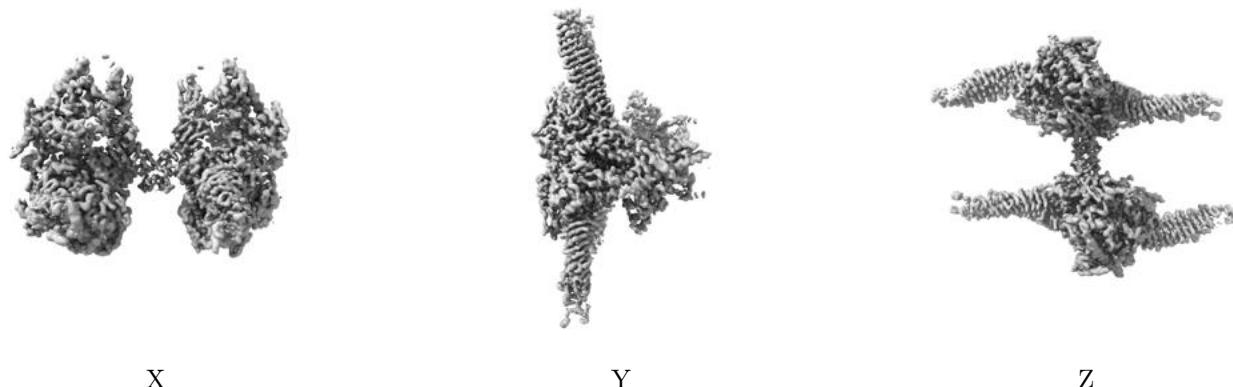


Z

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 [\(i\)](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

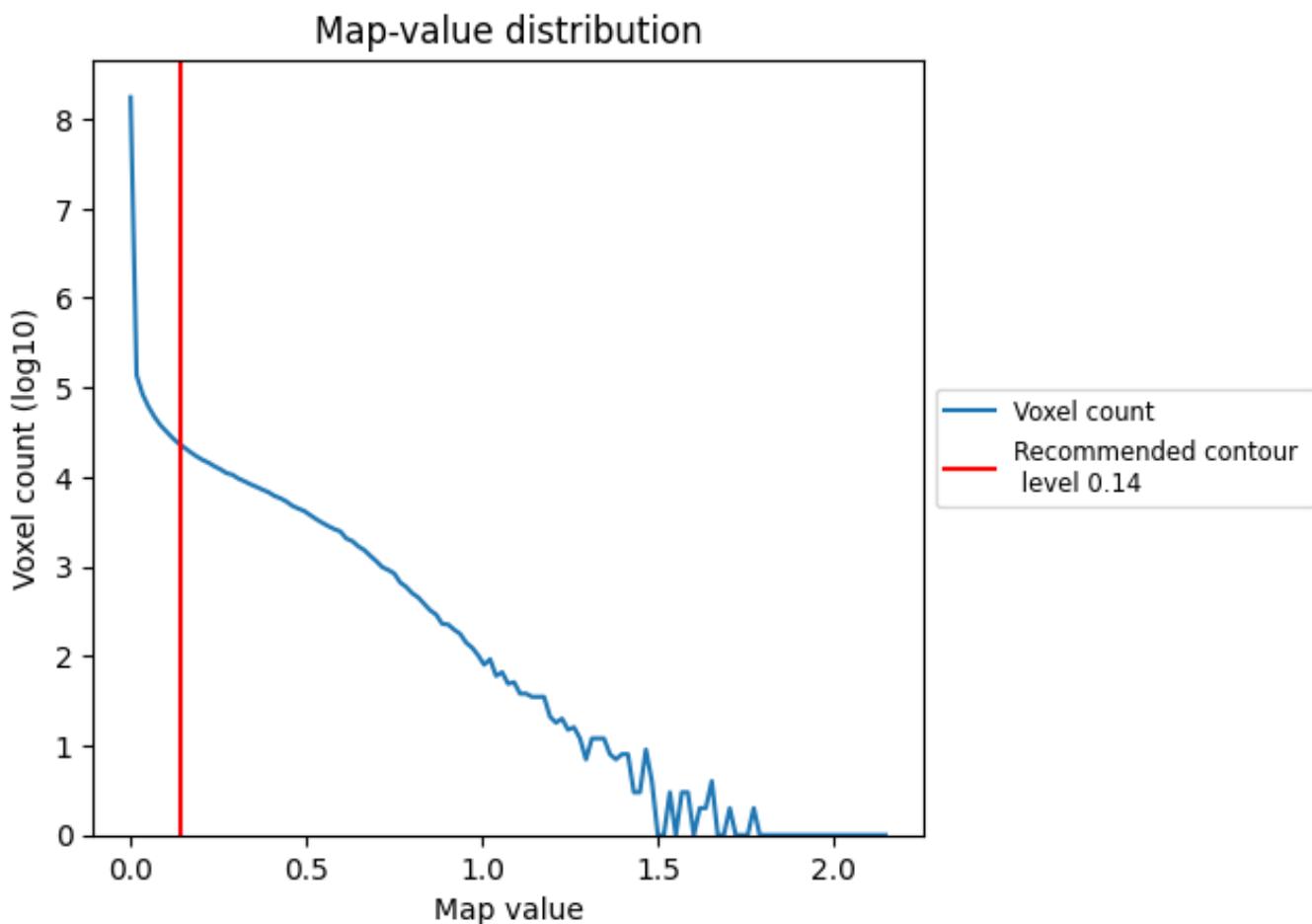
6.6 Mask visualisation [\(i\)](#)

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

7 Map analysis (i)

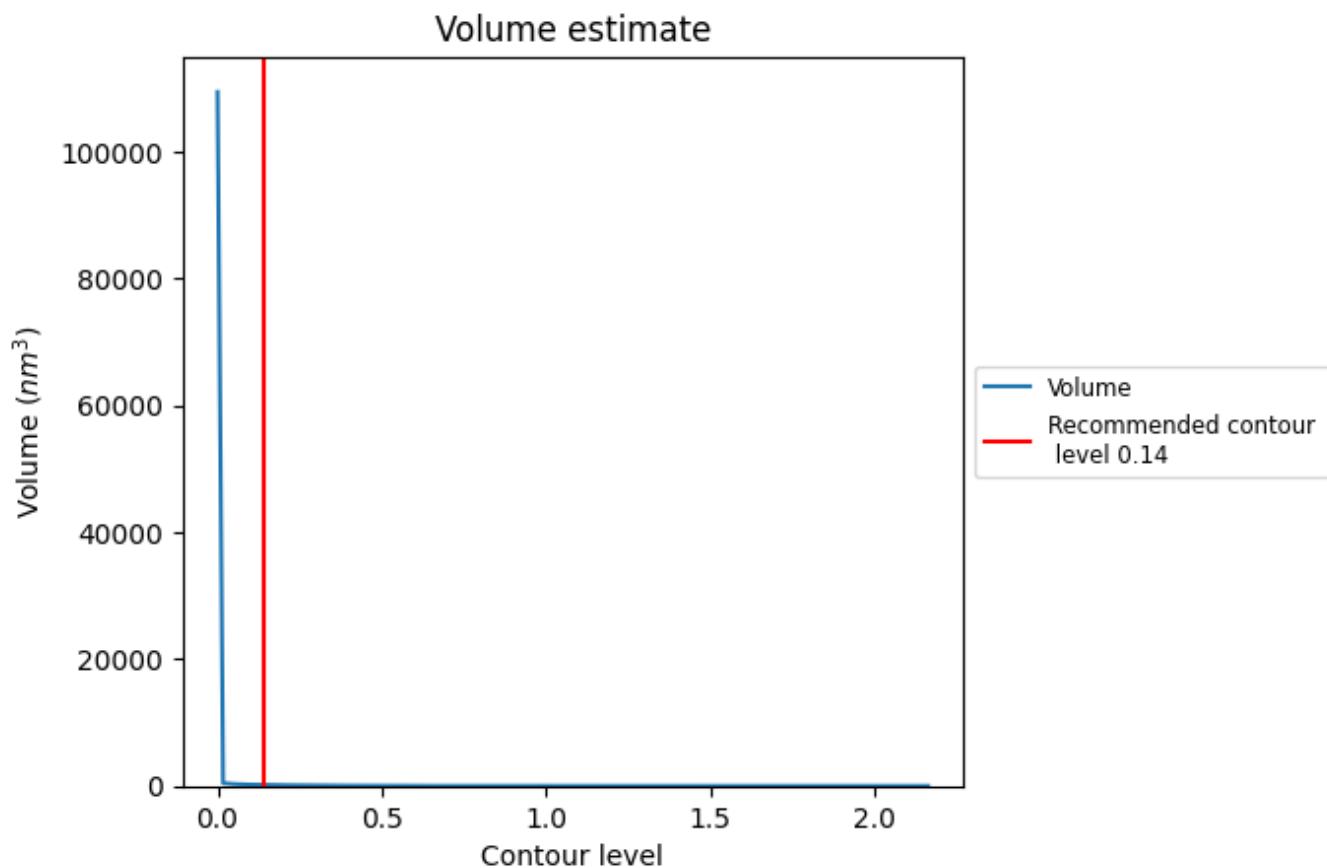
This section contains the results of statistical analysis of the map.

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.

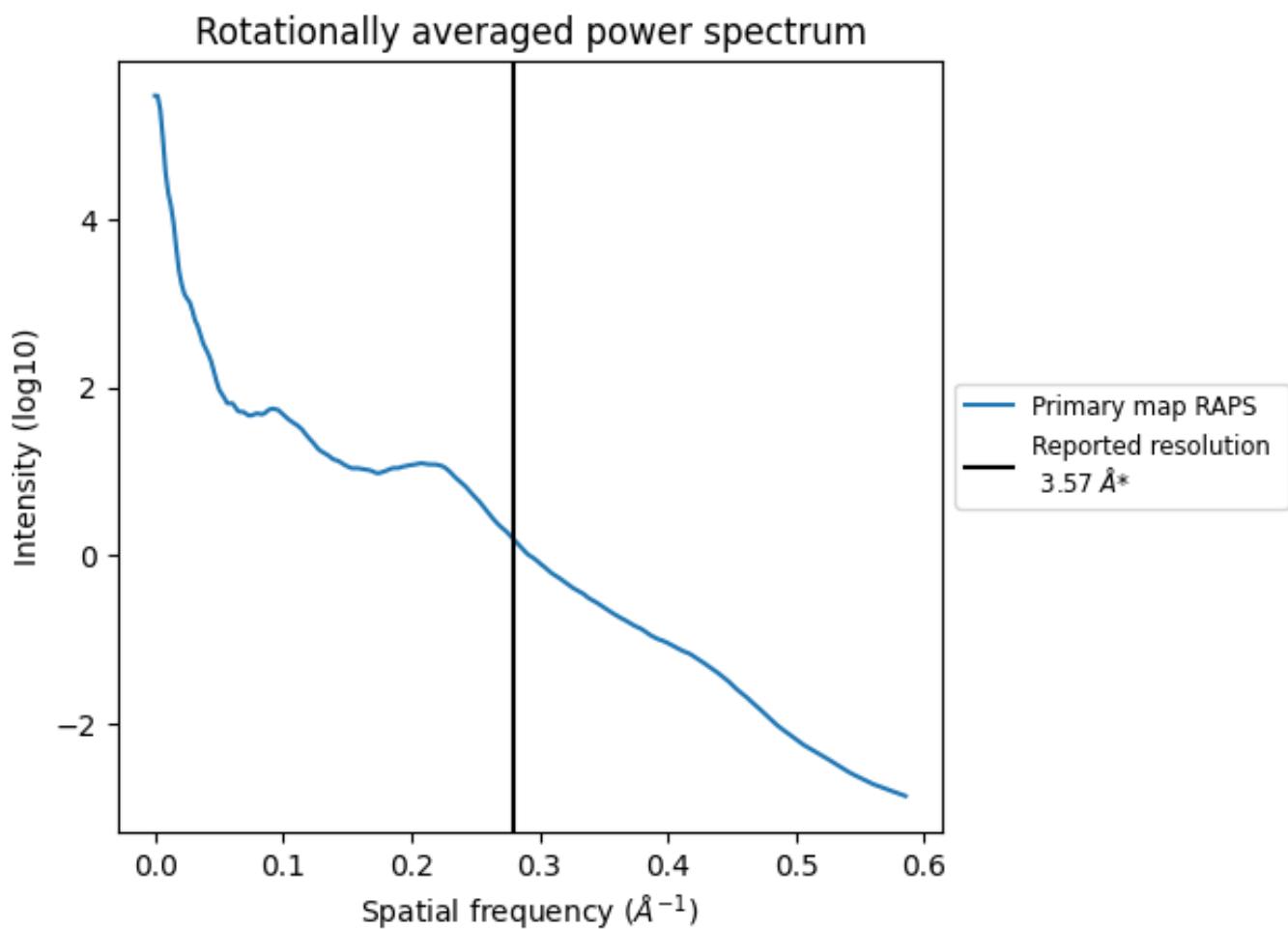
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 167 nm³; 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 [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.280 \AA^{-1}

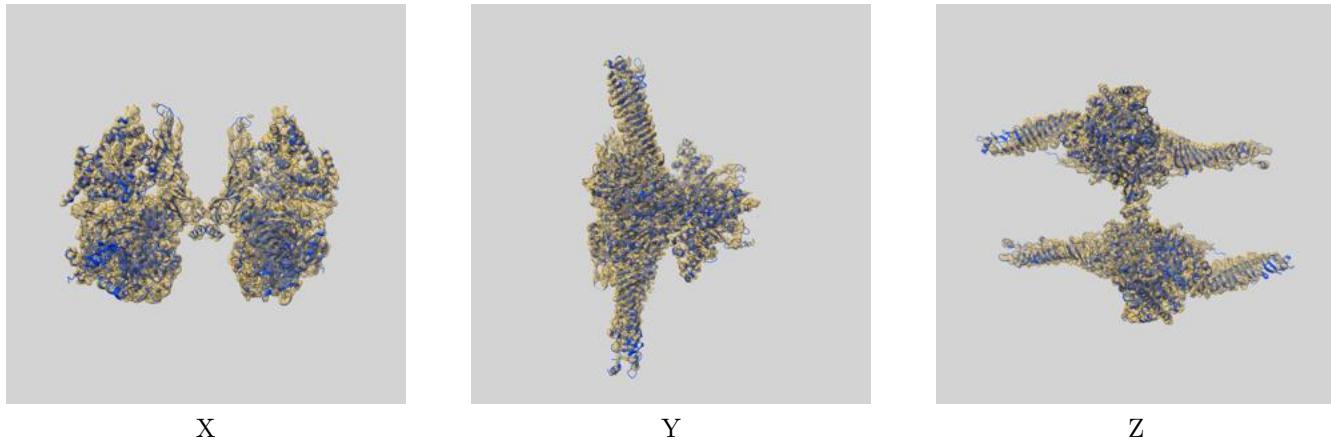
8 Fourier-Shell correlation

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

9 Map-model fit i

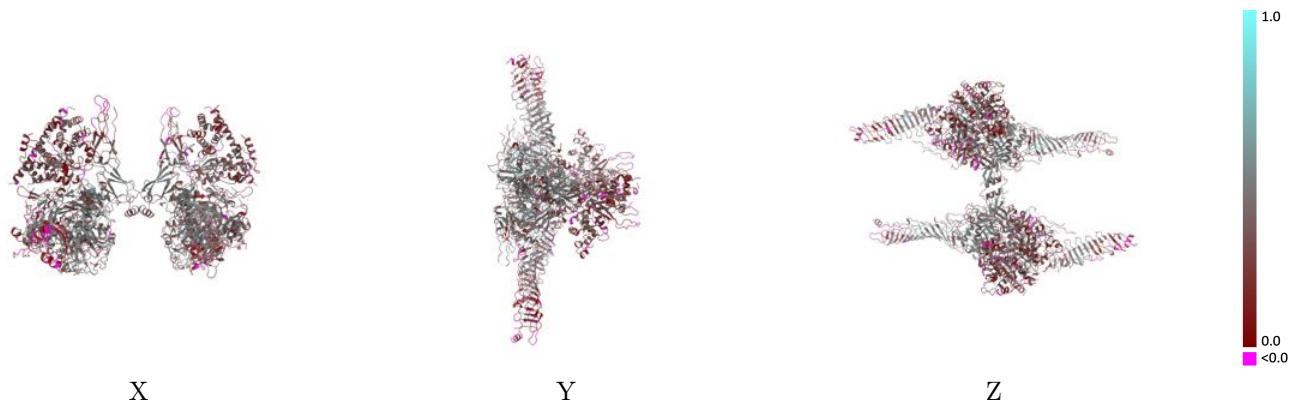
This section contains information regarding the fit between EMDB map EMD-38020 and PDB model 8X2U. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay i



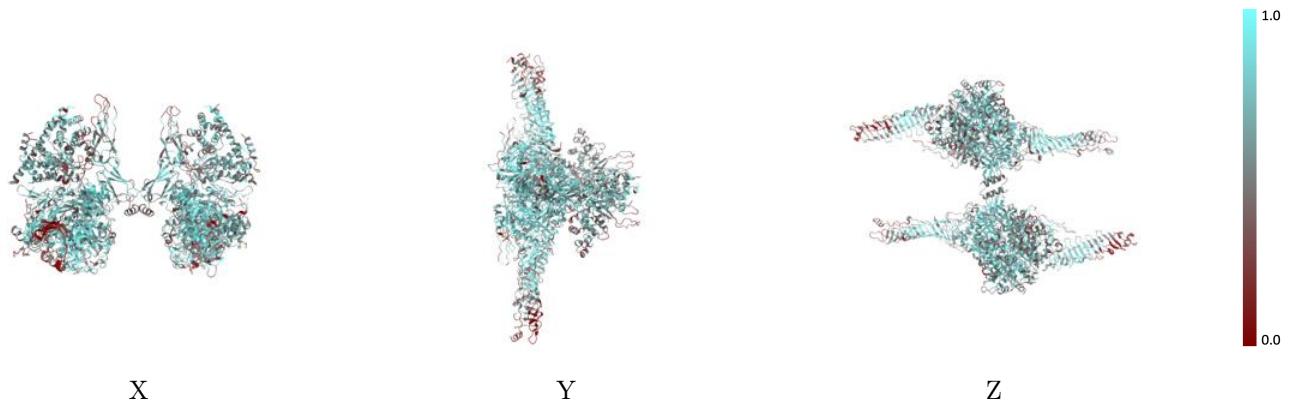
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



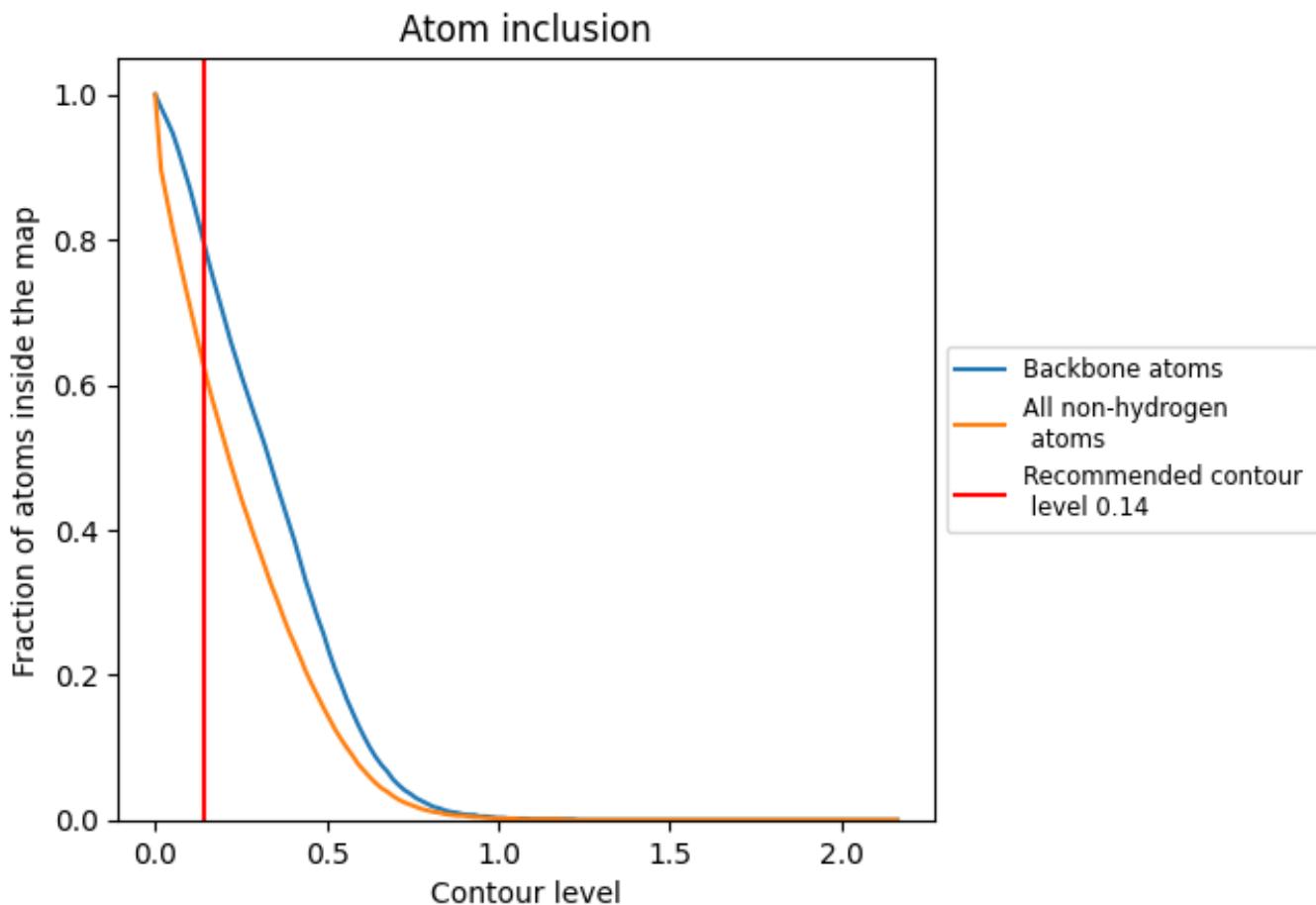
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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

