



Full wwPDB EM Validation Report ⓘ

Nov 15, 2021 – 12:19 pm GMT

PDB ID : 7PEQ
EMDB ID : EMD-12814
Title : Model of the outer rings of the human nuclear pore complex
Authors : Schuller, A.P.; Wojtynek, M.; Mankus, D.; Tatli, M.; Kronenberg-Tenga, R.;
Regmi, S.G.; Dasso, M.; Weis, K.; Medalia, O.; Schwartz, T.U.
Deposited on : 2021-08-11
Resolution : 35.00 Å(reported)
Based on initial model : 5A9Q

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

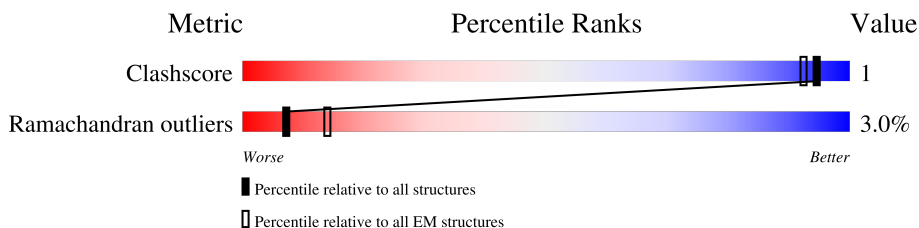
EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 35.00 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.



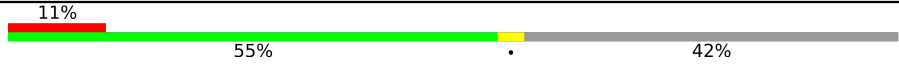
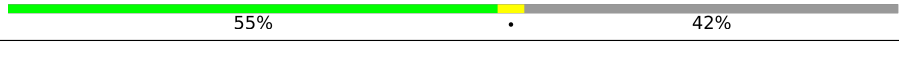
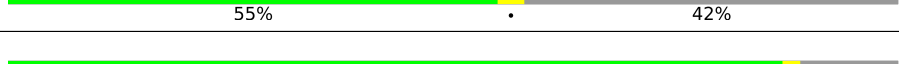
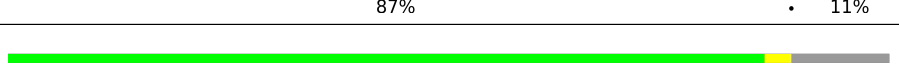
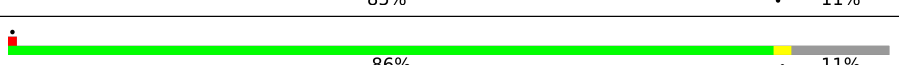


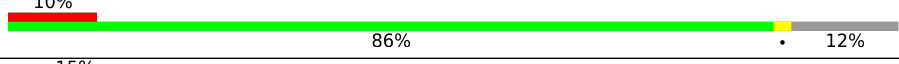
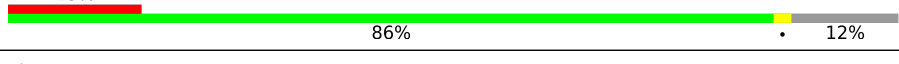

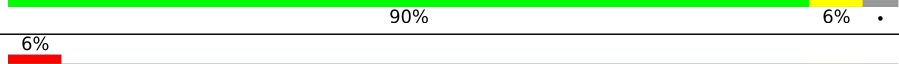
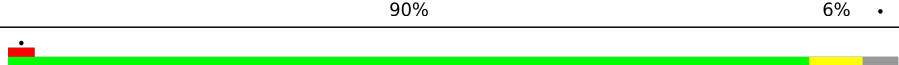
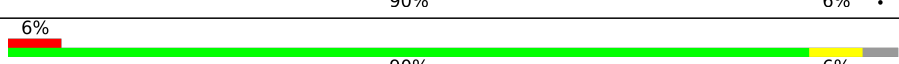
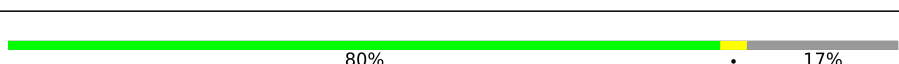
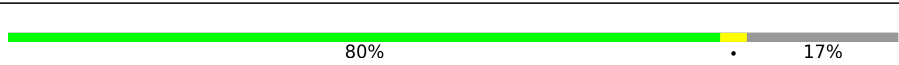

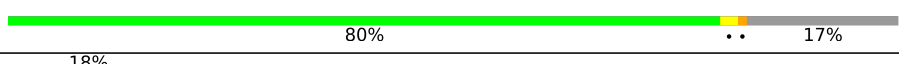



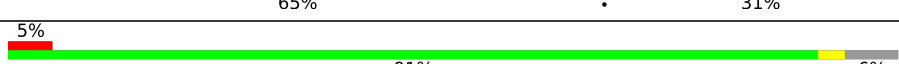
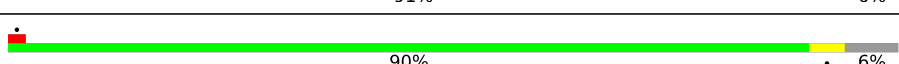



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	AC	1156	45% 54%
1	BC	1156	45% 54%
1	CC	1156	6% 45% 54%
1	DC	1156	45% 54%
2	AD	925	70% 27%
2	BD	925	72% 27%
2	CD	925	72% 27%
2	DD	925	72% 27%
3	AE	937	54% 42%

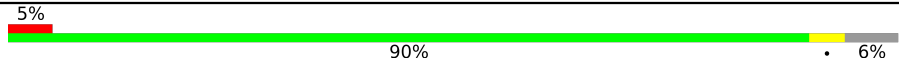
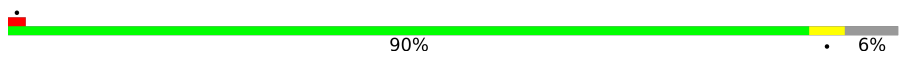
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Mol	Chain	Length	Quality of chain
3	BE	937	
3	CE	937	
3	DE	937	
4	AF	322	
4	BF	322	
4	CF	322	
4	DF	322	
5	AG	360	
5	BG	360	
5	CG	360	
5	DG	360	
6	AH	656	
6	BH	656	
6	CH	656	
6	DH	656	
7	AI	380	
7	BI	380	
7	CI	380	
7	DI	380	
8	AJ	1436	
8	BJ	1436	
8	CJ	1436	
8	DJ	1436	
9	AK	326	
9	BK	326	

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Mol	Chain	Length	Quality of chain
9	CK	326	 <p>5% 90% 6%</p>
9	DK	326	 <p>5% 90% 6%</p>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 91352 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 Nuclear pore complex protein Nup133.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	AC	528	2629	1573	528	528	0	0
1	BC	528	2629	1573	528	528	0	0
1	CC	528	2629	1573	528	528	0	0
1	DC	528	2629	1573	528	528	0	0

- Molecule 2 is a protein called Nuclear pore complex protein Nup107.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	AD	678	3367	2011	678	678	0	0
2	BD	678	3367	2011	678	678	0	0
2	CD	678	3367	2011	678	678	0	0
2	DD	678	3367	2011	678	678	0	0

- Molecule 3 is a protein called Nuclear pore complex protein Nup96.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	AE	543	2700	1614	543	543	0	0
3	BE	543	2700	1614	543	543	0	0
3	CE	543	2700	1614	543	543	0	0
3	DE	543	2700	1614	543	543	0	0

- Molecule 4 is a protein called Protein SEC13 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	AF	285	Total	C	N	O	0	0
			1402	832	285	285		
4	BF	285	Total	C	N	O	0	0
			1402	832	285	285		
4	CF	285	Total	C	N	O	0	0
			1402	832	285	285		
4	DF	285	Total	C	N	O	0	0
			1402	832	285	285		

- Molecule 5 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AG	316	Total	C	N	O	0	0
			1564	932	316	316		
5	BG	316	Total	C	N	O	0	0
			1564	932	316	316		
5	CG	316	Total	C	N	O	0	0
			1564	932	316	316		
5	DG	316	Total	C	N	O	0	0
			1564	932	316	316		

- Molecule 6 is a protein called Nuclear pore complex protein Nup85.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	AH	632	Total	C	N	O	0	0
			3134	1870	632	632		
6	BH	632	Total	C	N	O	0	0
			3134	1870	632	632		
6	CH	632	Total	C	N	O	0	0
			3134	1870	632	632		
6	DH	632	Total	C	N	O	0	0
			3134	1870	632	632		

- Molecule 7 is a protein called Nucleoporin Nup43.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AI	316	Total	C	N	O	22	0
			1599	963	318	318		
7	BI	316	Total	C	N	O	22	0
			1599	963	318	318		
7	CI	316	Total	C	N	O	18	0
			1599	963	318	318		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	DI	316	1599	963	318	318	18	0

- Molecule 8 is a protein called Nuclear pore complex protein Nup160.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	AJ	996	4932	2940	996	996	0	0
8	BJ	996	4932	2940	996	996	0	0
8	CJ	996	4932	2940	996	996	0	0
8	DJ	996	4932	2940	996	996	0	0

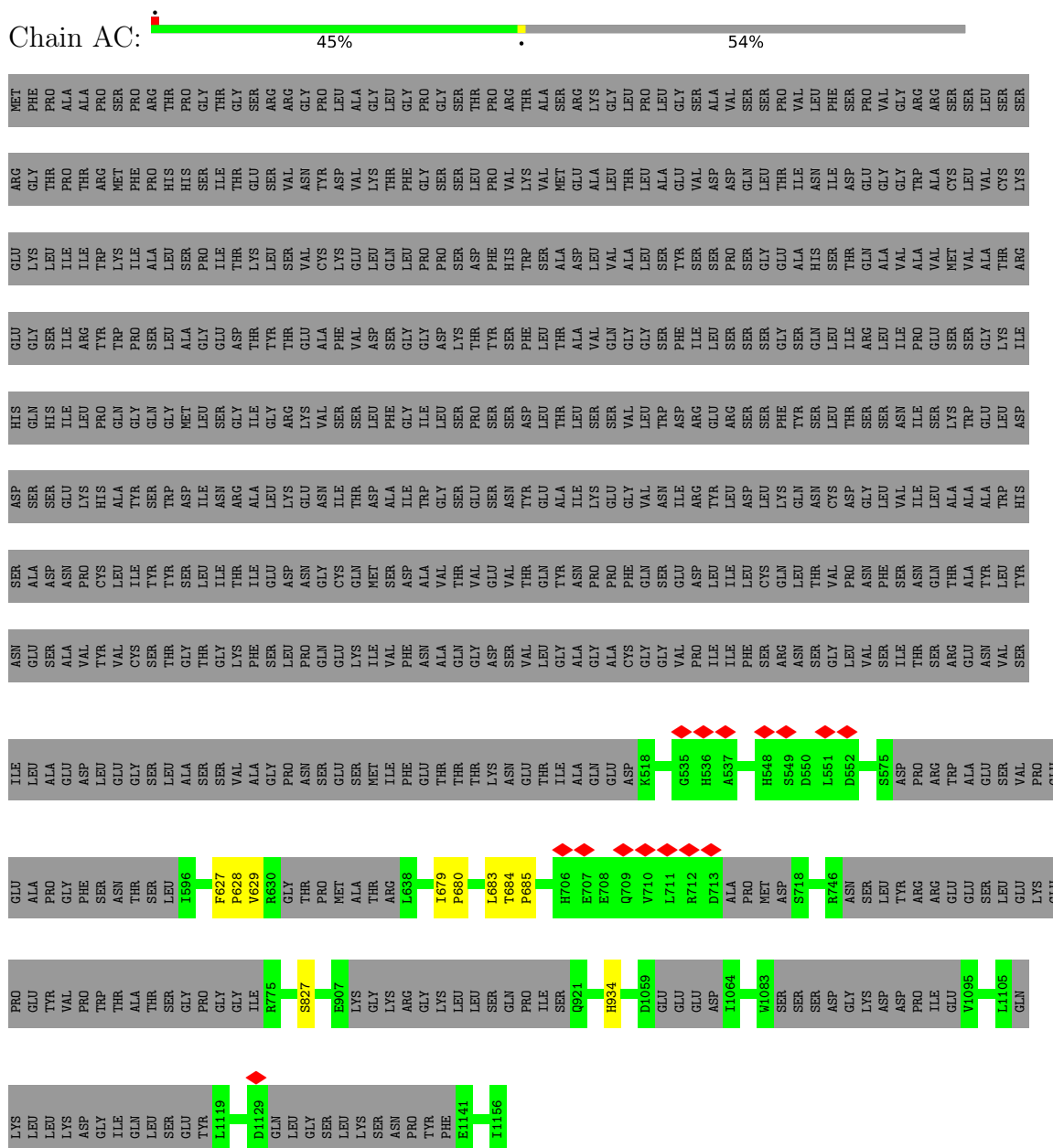
- Molecule 9 is a protein called Nucleoporin Nup37.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	AK	307	1511	897	307	307	0	0
9	BK	307	1511	897	307	307	0	0
9	CK	307	1511	897	307	307	0	0
9	DK	307	1511	897	307	307	0	0

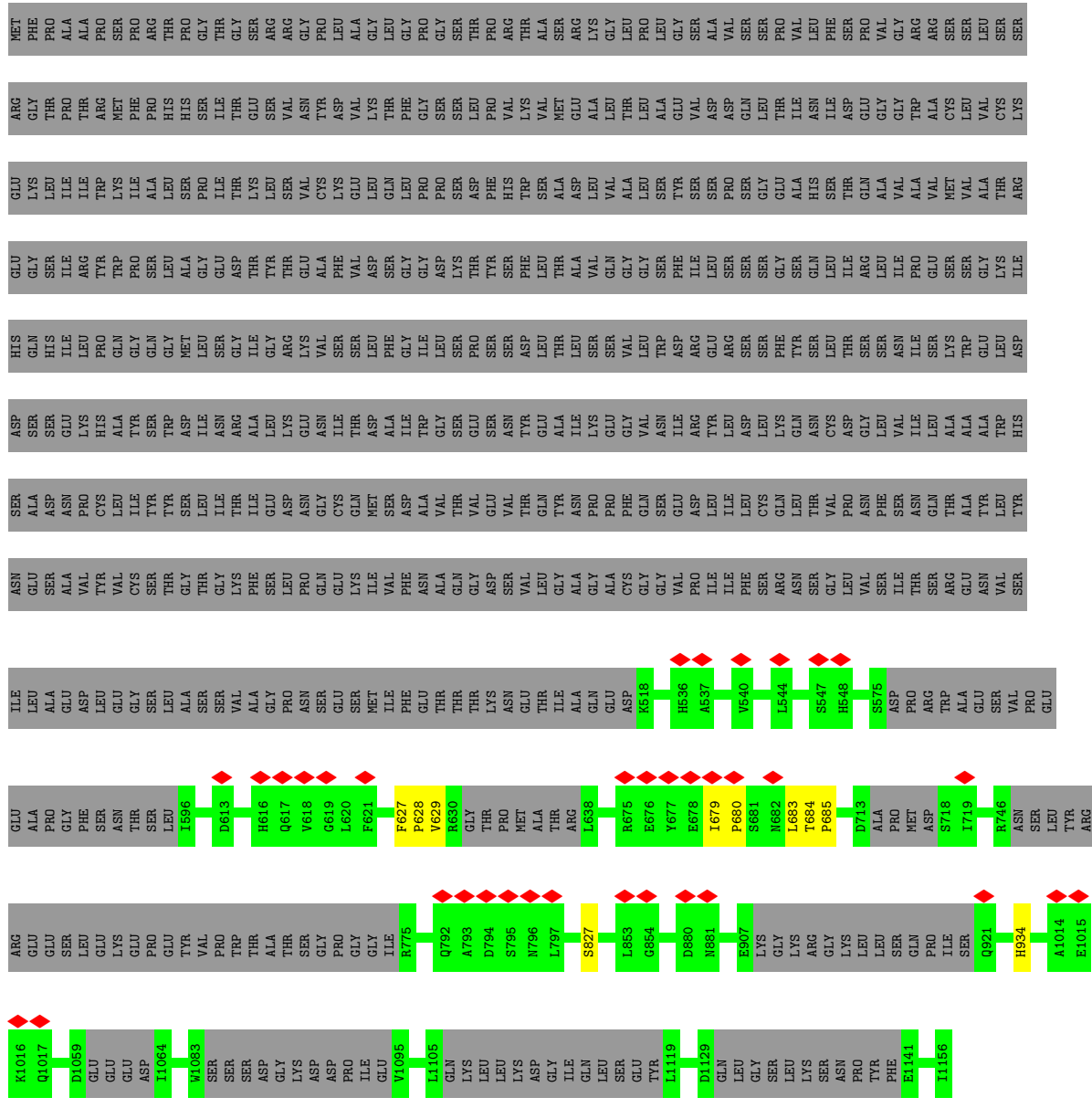
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

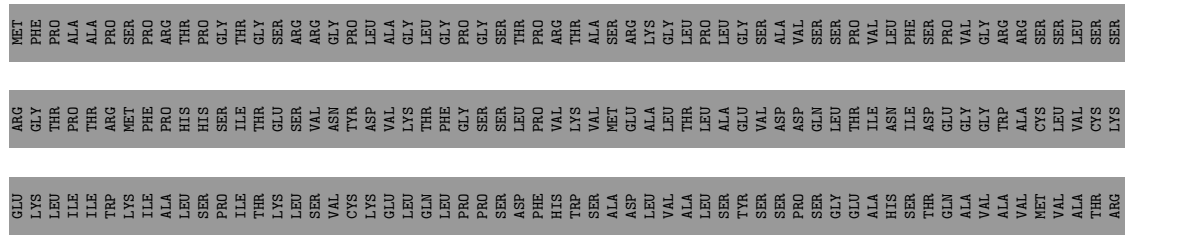
- Molecule 1: Nuclear pore complex protein Nup133

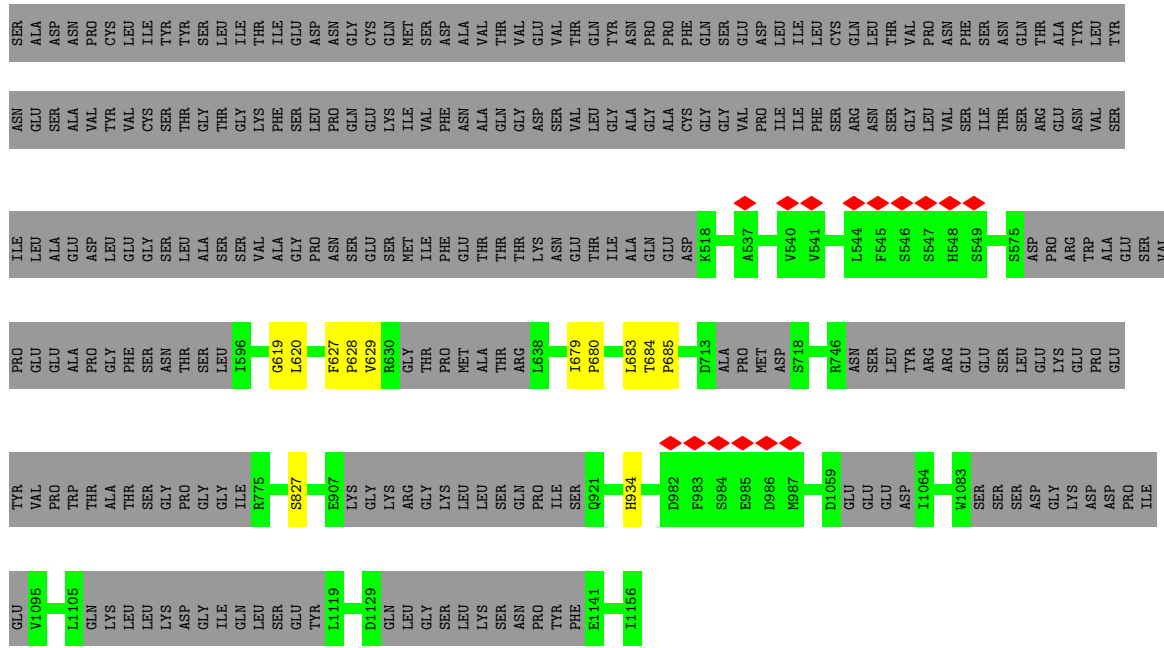


● Molecule 1: Nuclear pore complex protein Nup133

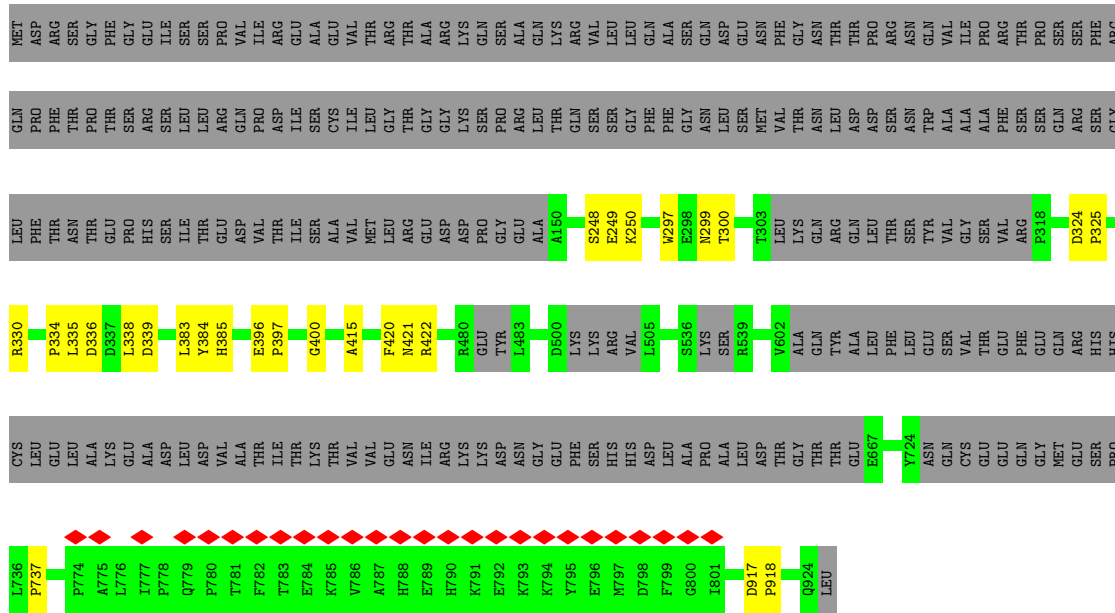


● Molecule 1: Nuclear pore complex protein Nup133

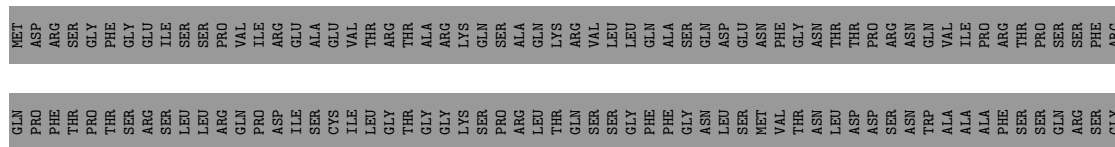


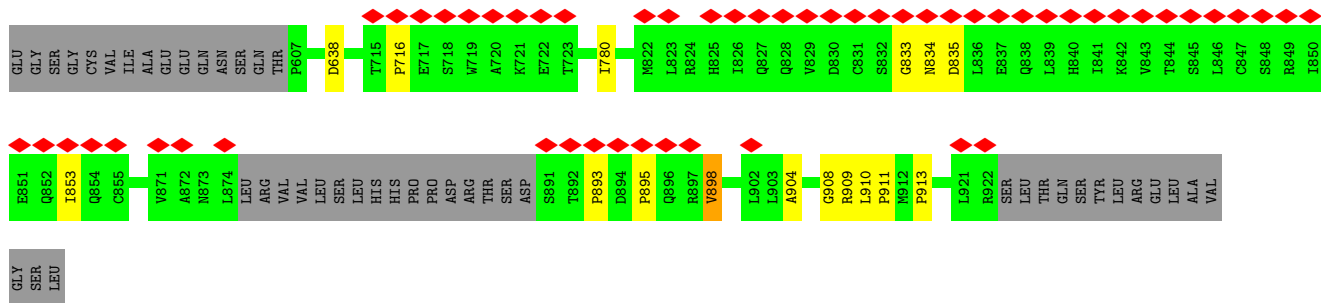


• Molecule 2: Nuclear pore complex protein Nup107

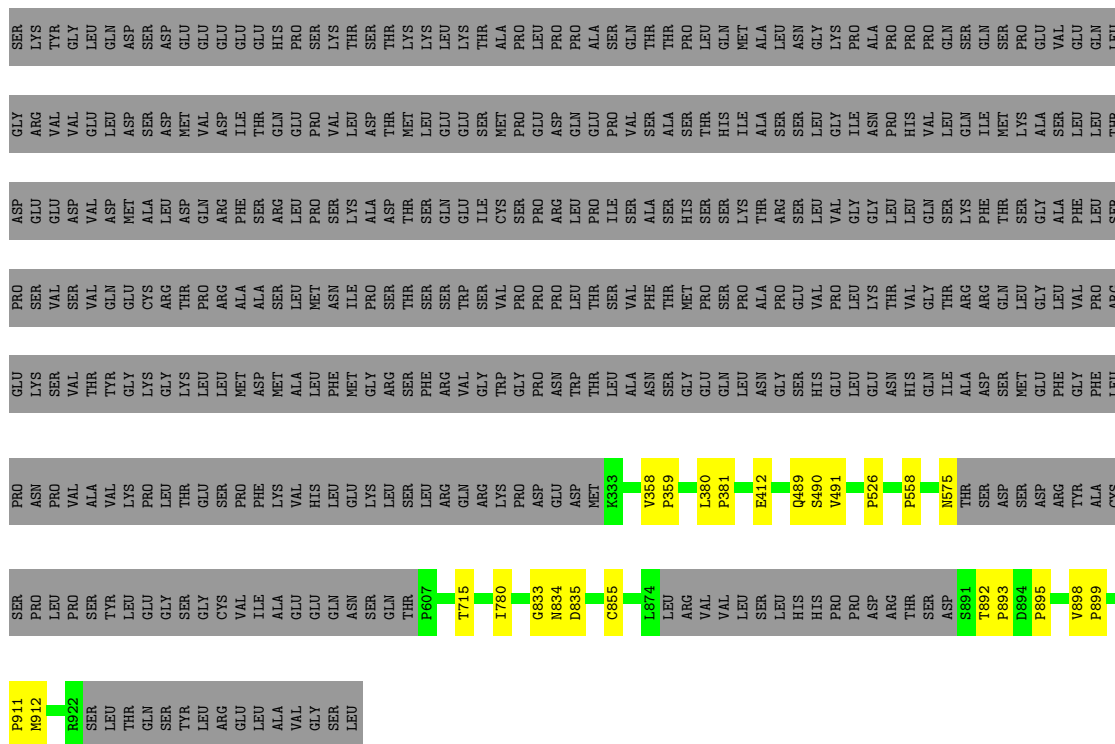


• Molecule 2: Nuclear pore complex protein Nup107

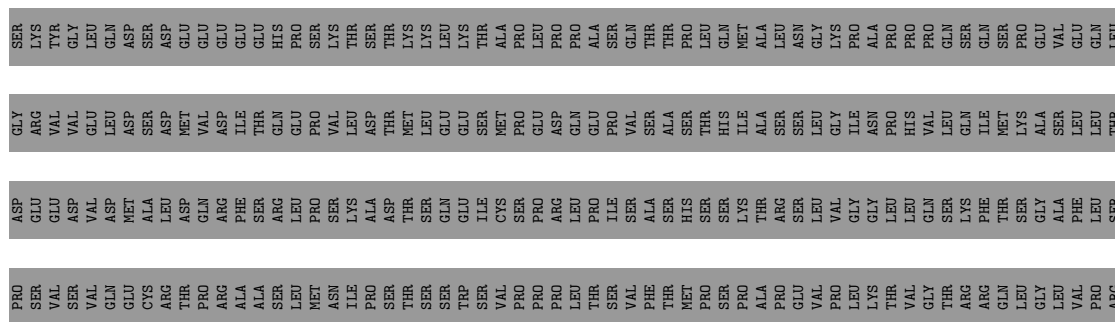


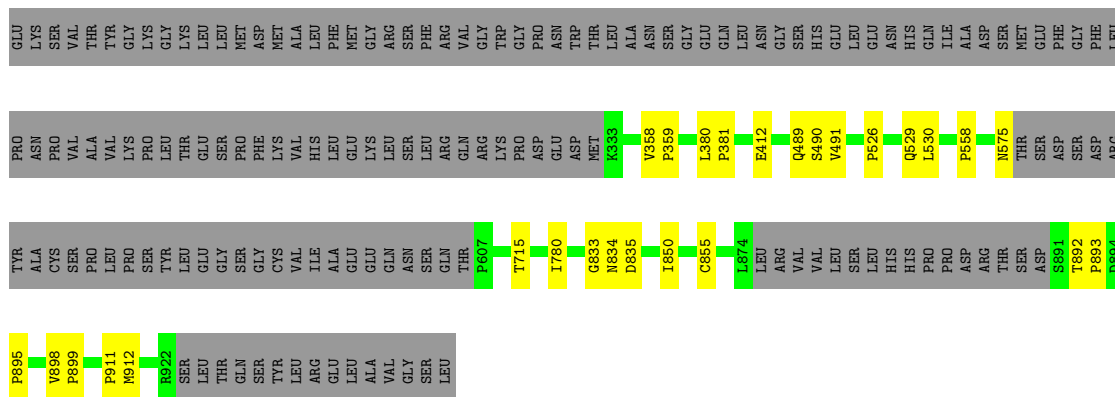


• Molecule 3: Nuclear pore complex protein Nup96

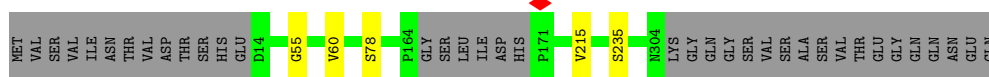
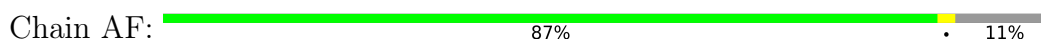


• Molecule 3: Nuclear pore complex protein Nup96

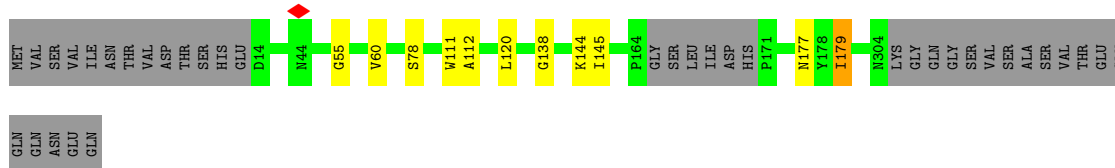
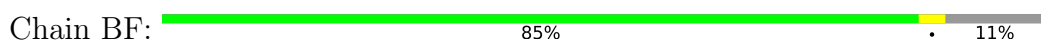




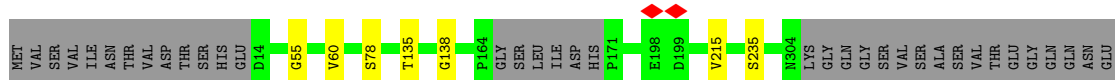
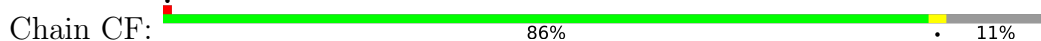
• Molecule 4: Protein SEC13 homolog



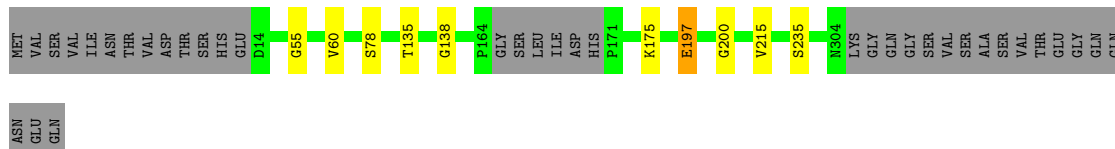
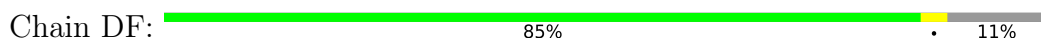
• Molecule 4: Protein SEC13 homolog



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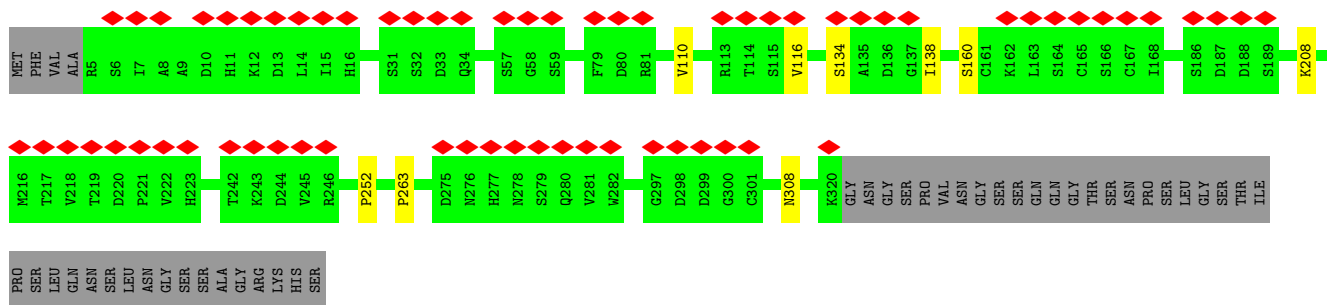


• Molecule 4: Protein SEC13 homolog

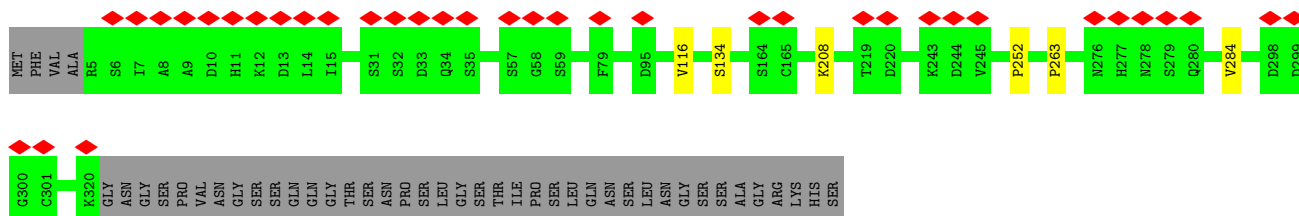
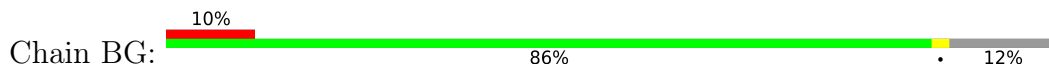


• Molecule 5: Nucleoporin SEH1

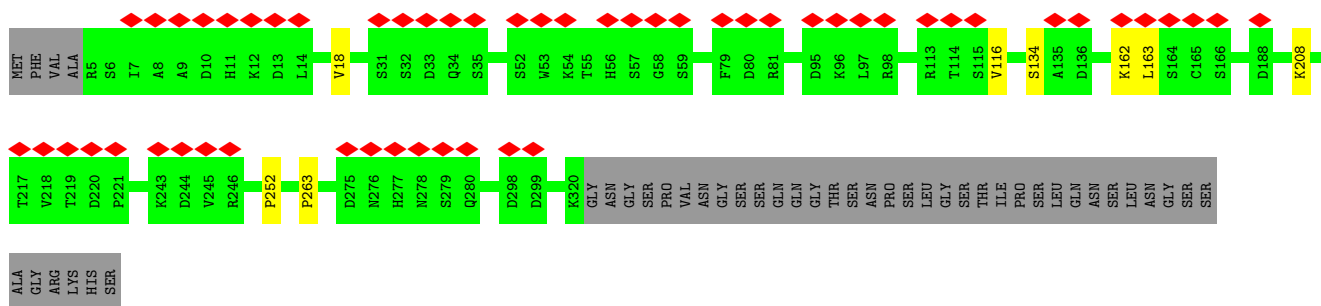
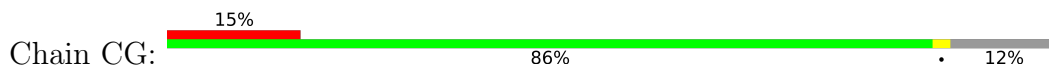




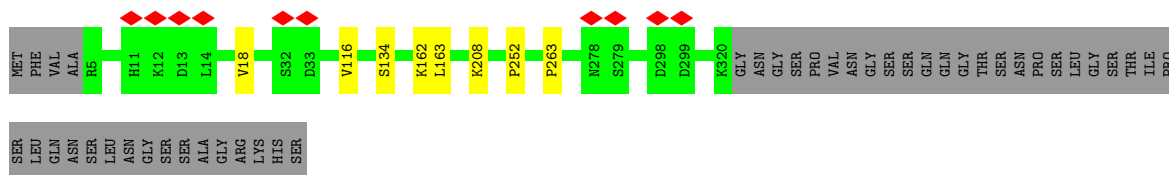
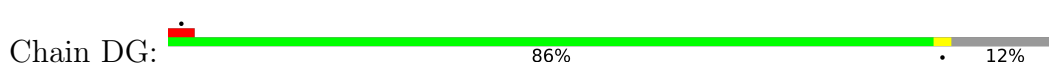
• Molecule 5: Nucleoporin SEH1



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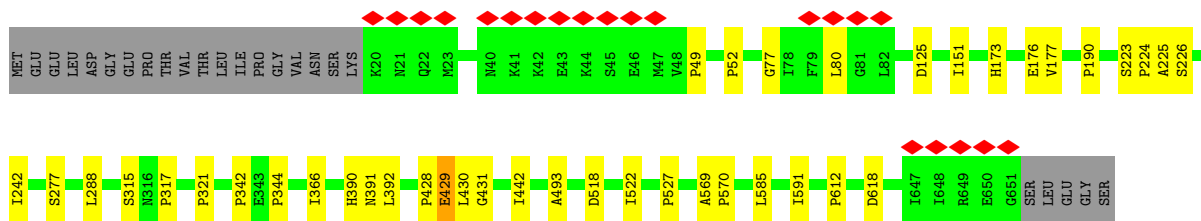


• Molecule 5: Nucleoporin SEH1

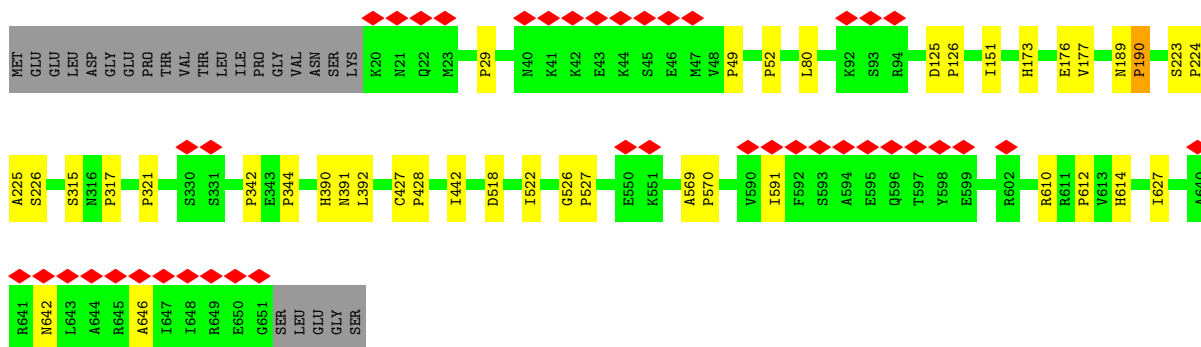


• Molecule 6: Nuclear pore complex protein Nup85

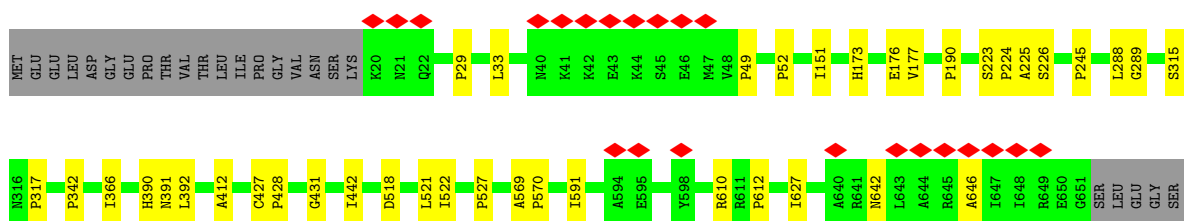




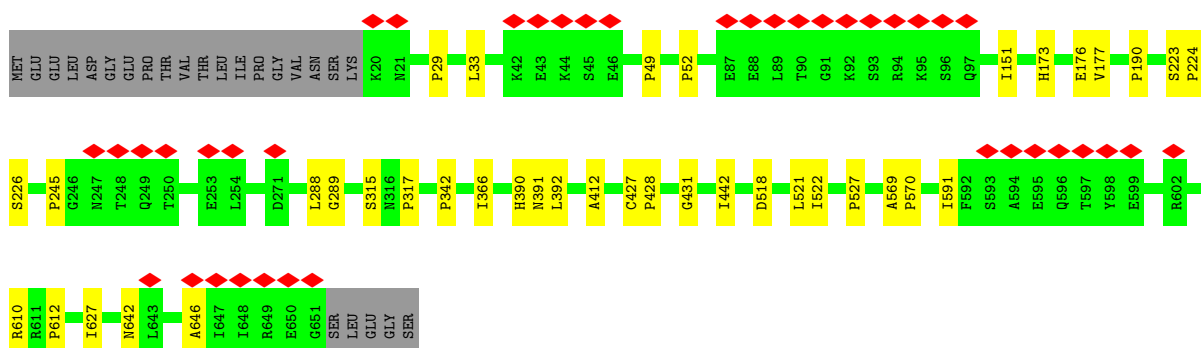
• Molecule 6: Nuclear pore complex protein Nup85



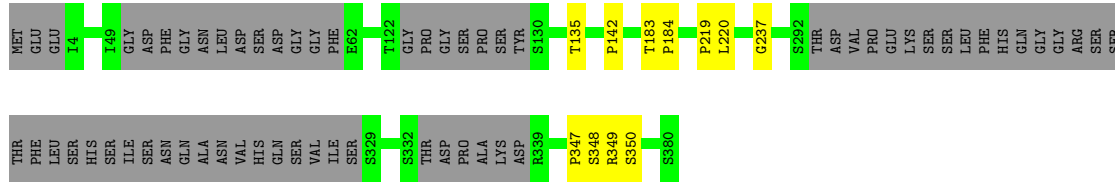
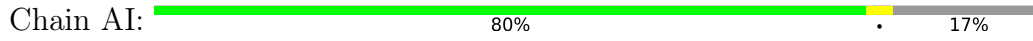
• Molecule 6: Nuclear pore complex protein Nup85



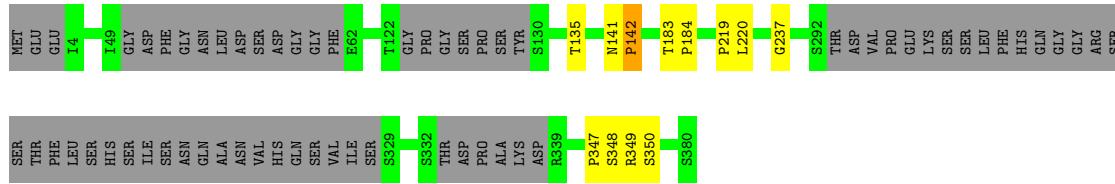
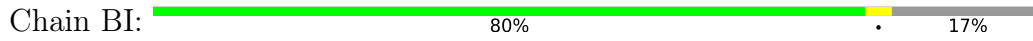
• Molecule 6: Nuclear pore complex protein Nup85



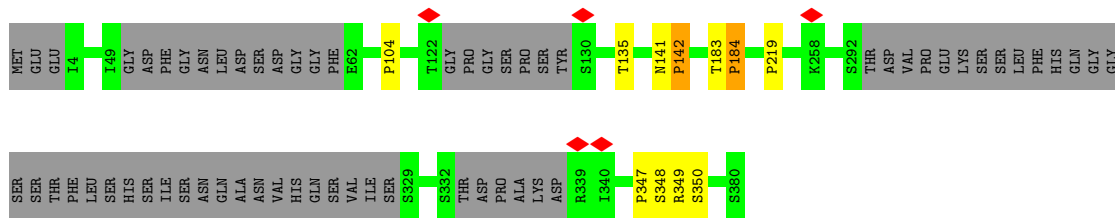
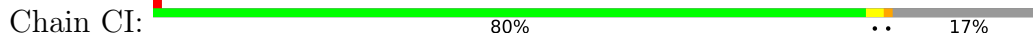
• Molecule 7: Nucleoporin Nup43



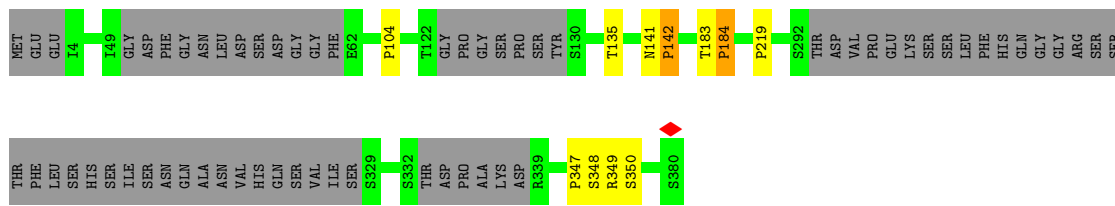
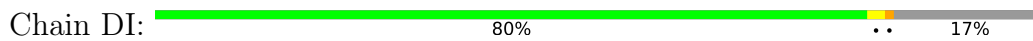
• Molecule 7: Nucleoporin Nup43



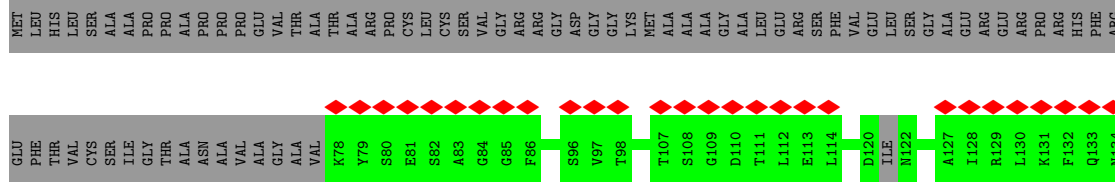
• Molecule 7: Nucleoporin Nup43



• Molecule 7: Nucleoporin Nup43



• Molecule 8: Nuclear pore complex protein Nup160



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of subtomograms used	1252	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.4	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.000	Depositor
Minimum map value	0.000	Depositor
Average map value	0.351	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.44	Depositor
Map size (\AA)	2188.8, 2188.8, 2188.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	6.84, 6.84, 6.84	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	AC	0.22	0/2619	0.37	0/3644
1	BC	0.22	0/2619	0.37	0/3644
1	CC	0.22	0/2619	0.37	0/3644
1	DC	0.22	0/2619	0.37	0/3644
2	AD	0.26	0/3362	0.44	0/4685
2	BD	0.26	0/3362	0.44	0/4685
2	CD	0.26	0/3362	0.44	0/4685
2	DD	0.26	0/3362	0.44	0/4685
3	AE	0.23	0/2699	0.38	0/3768
3	BE	0.23	0/2699	0.39	0/3768
3	CE	0.23	0/2698	0.38	0/3765
3	DE	0.23	0/2698	0.38	0/3765
4	AF	0.25	0/1400	0.45	0/1943
4	BF	0.25	0/1400	0.45	0/1943
4	CF	0.25	0/1400	0.45	0/1943
4	DF	0.25	0/1400	0.46	0/1943
5	AG	0.24	0/1563	0.46	0/2177
5	BG	0.24	0/1563	0.46	0/2177
5	CG	0.24	0/1563	0.46	0/2177
5	DG	0.24	0/1563	0.46	0/2177
6	AH	0.23	0/3133	0.39	0/4369
6	BH	0.23	0/3133	0.38	0/4369
6	CH	0.23	0/3130	0.38	0/4360
6	DH	0.23	0/3130	0.38	0/4360
7	AI	0.24	0/1647	0.44	0/2287
7	BI	0.24	0/1647	0.44	0/2287
7	CI	0.24	0/1647	0.45	0/2287
7	DI	0.24	0/1647	0.45	0/2287
8	AJ	0.23	0/4925	0.40	0/6855
8	BJ	0.23	0/4925	0.40	0/6855
8	CJ	0.23	0/4925	0.40	0/6855
8	DJ	0.23	0/4925	0.40	0/6855
9	AK	0.26	0/1510	0.49	0/2098
9	BK	0.26	0/1510	0.49	0/2098

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	CK	0.25	0/1509	0.48	0/2095
9	DK	0.25	0/1509	0.48	0/2095
All	All	0.24	0/91422	0.42	0/127274

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AC	2629	0	1167	2	0
1	BC	2629	0	1167	2	0
1	CC	2629	0	1167	3	0
1	DC	2629	0	1167	3	0
2	AD	3367	0	1489	15	0
2	BD	3367	0	1489	4	0
2	CD	3367	0	1489	4	0
2	DD	3367	0	1489	2	0
3	AE	2700	0	1200	6	0
3	BE	2700	0	1200	4	0
3	CE	2700	0	1199	3	0
3	DE	2700	0	1199	5	0
4	AF	1402	0	648	2	0
4	BF	1402	0	648	6	0
4	CF	1402	0	648	3	0
4	DF	1402	0	648	4	0
5	AG	1564	0	712	2	0
5	BG	1564	0	712	1	0
5	CG	1564	0	712	2	0
5	DG	1564	0	712	3	0
6	AH	3134	0	1393	5	0
6	BH	3134	0	1393	6	0
6	CH	3134	0	1390	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	DH	3134	0	1390	6	0
7	AI	1599	0	706	4	0
7	BI	1599	0	706	5	0
7	CI	1599	0	707	4	0
7	DI	1599	0	707	4	0
8	AJ	4932	0	2159	5	0
8	BJ	4932	0	2159	6	0
8	CJ	4932	0	2158	9	0
8	DJ	4932	0	2158	9	0
9	AK	1511	0	674	0	0
9	BK	1511	0	674	1	0
9	CK	1511	0	673	2	0
9	DK	1511	0	673	2	0
All	All	91352	0	40582	140	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 1.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:297:TRP:CB	2:AD:339:ASP:CB	2.28	1.12
2:AD:297:TRP:HA	2:AD:339:ASP:CB	2.00	0.92
2:AD:297:TRP:CA	2:AD:339:ASP:CB	2.51	0.88
2:AD:300:THR:CB	2:AD:336:ASP:N	2.43	0.80
2:DD:297:TRP:CB	2:DD:339:ASP:CB	2.64	0.75
1:DC:683:LEU:H	1:DC:684:THR:HA	1.51	0.75
1:CC:683:LEU:H	1:CC:684:THR:HA	1.51	0.74
1:AC:683:LEU:H	1:AC:684:THR:HA	1.53	0.72
1:BC:683:LEU:H	1:BC:684:THR:HA	1.53	0.72
2:CD:418:GLU:HA	4:DF:197:GLU:H	1.59	0.68
8:DJ:425:GLU:H	8:DJ:426:HIS:HA	1.59	0.67
8:CJ:425:GLU:H	8:CJ:426:HIS:HA	1.59	0.67
6:CH:390:HIS:H	6:CH:391:ASN:HA	1.60	0.66
2:DD:249:GLU:CB	2:DD:383:LEU:CB	2.73	0.66
2:AD:249:GLU:CB	2:AD:383:LEU:CB	2.74	0.66
6:BH:390:HIS:H	6:BH:391:ASN:HA	1.62	0.65
6:AH:390:HIS:H	6:AH:391:ASN:HA	1.62	0.64
6:DH:390:HIS:H	6:DH:391:ASN:HA	1.60	0.64
5:DG:162:LYS:H	5:DG:163:LEU:HA	1.63	0.64
5:CG:162:LYS:H	5:CG:163:LEU:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:250:LYS:CB	2:AD:385:HIS:CB	2.79	0.61
7:CI:348[A]:SER:O	7:CI:350[A]:SER:N	2.35	0.60
2:AD:299:ASN:CB	2:AD:338:LEU:CB	2.81	0.59
7:AI:348[A]:SER:O	7:AI:350[A]:SER:N	2.35	0.59
7:DI:348[A]:SER:O	7:DI:350[A]:SER:N	2.35	0.58
7:BI:348[A]:SER:O	7:BI:350[A]:SER:N	2.35	0.58
2:CD:297:TRP:CB	2:CD:339:ASP:CB	2.81	0.58
3:DE:855:CYS:HA	4:DF:138:GLY:H	1.68	0.58
3:CE:855:CYS:HA	4:CF:138:GLY:H	1.69	0.58
2:BD:250:LYS:CB	2:BD:385:HIS:CB	2.81	0.57
3:AE:897:ARG:H	8:AJ:1138:GLU:H	1.52	0.57
7:DI:348[B]:SER:O	7:DI:350[B]:SER:N	2.38	0.56
2:BD:249:GLU:CB	2:BD:383:LEU:CB	2.84	0.56
6:DH:642:ASN:O	6:DH:646:ALA:HB3	2.06	0.56
6:CH:642:ASN:O	6:CH:646:ALA:HB3	2.06	0.55
7:AI:348[B]:SER:O	7:AI:350[B]:SER:N	2.38	0.55
8:DJ:425:GLU:N	8:DJ:426:HIS:HA	2.21	0.55
6:BH:390:HIS:N	6:BH:391:ASN:HA	2.22	0.55
7:BI:348[B]:SER:O	7:BI:350[B]:SER:N	2.38	0.54
6:DH:390:HIS:N	6:DH:391:ASN:HA	2.22	0.54
2:AD:330:ARG:HA	4:BF:144:LYS:HA	1.89	0.53
3:BE:833:GLY:O	3:BE:835:ASP:N	2.41	0.53
7:CI:348[B]:SER:O	7:CI:350[B]:SER:N	2.38	0.53
6:BH:642:ASN:O	6:BH:646:ALA:HB3	2.09	0.52
6:AH:390:HIS:N	6:AH:391:ASN:HA	2.22	0.51
2:CD:249:GLU:CB	2:CD:383:LEU:CB	2.88	0.51
6:AH:224:PRO:O	6:AH:226:SER:N	2.43	0.51
6:CH:33:LEU:H	6:CH:412:ALA:HA	1.74	0.51
6:BH:224:PRO:O	6:BH:226:SER:N	2.43	0.51
6:CH:390:HIS:N	6:CH:391:ASN:HA	2.22	0.51
6:DH:33:LEU:H	6:DH:412:ALA:HA	1.74	0.51
6:AH:429:GLU:O	6:AH:431:GLY:N	2.43	0.51
6:DH:224:PRO:O	6:DH:226:SER:N	2.43	0.51
2:AD:421:ASN:N	4:BF:179:ILE:O	2.44	0.50
6:CH:224:PRO:O	6:CH:226:SER:N	2.43	0.50
5:CG:116:VAL:HA	5:CG:134:SER:HA	1.94	0.50
8:CJ:425:GLU:N	8:CJ:426:HIS:HA	2.21	0.50
2:AD:415:ALA:HB1	4:BF:177:ASN:HA	1.93	0.50
8:BJ:856:GLU:HA	8:BJ:860:ALA:HB3	1.92	0.49
9:DK:168:GLY:HA2	9:DK:185:GLU:HA	1.94	0.49
8:CJ:1090:TYR:O	8:CJ:1095:ARG:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CK:168:GLY:HA2	9:CK:185:GLU:HA	1.94	0.49
3:DE:529:GLN:HA	3:DE:530:LEU:HA	1.55	0.49
2:AD:422:ARG:HA	4:BF:179:ILE:HA	1.95	0.48
3:DE:489:GLN:O	3:DE:491:VAL:N	2.47	0.48
3:BE:489:GLN:O	3:BE:491:VAL:N	2.47	0.48
3:CE:489:GLN:O	3:CE:491:VAL:N	2.47	0.48
6:CH:176:GLU:HA	6:CH:177:VAL:HA	1.58	0.48
3:DE:833:GLY:O	3:DE:835:ASP:N	2.47	0.48
5:DG:116:VAL:HA	5:DG:134:SER:HA	1.94	0.47
2:AD:248:SER:CB	2:AD:385:HIS:HA	2.44	0.47
3:AE:833:GLY:O	3:AE:835:ASP:N	2.47	0.47
3:CE:833:GLY:O	3:CE:835:ASP:N	2.47	0.47
3:AE:489:GLN:O	3:AE:491:VAL:N	2.47	0.47
7:DI:141:ASN:HA	7:DI:142:PRO:HA	1.72	0.47
8:BJ:150:ARG:HA	8:BJ:151:VAL:HA	1.53	0.47
8:DJ:480:CYS:HA	8:DJ:481:ARG:HA	1.49	0.47
4:BF:111:TRP:HA	4:BF:120:LEU:HA	1.97	0.47
8:DJ:237:GLY:HA2	8:DJ:277:GLY:HA2	1.97	0.47
5:AG:116:VAL:HA	5:AG:134:SER:HA	1.98	0.46
8:CJ:237:GLY:HA2	8:CJ:277:GLY:HA2	1.97	0.46
2:BD:297:TRP:CB	2:BD:339:ASP:CB	2.93	0.46
8:CJ:150:ARG:HA	8:CJ:151:VAL:HA	1.53	0.46
8:DJ:150:ARG:HA	8:DJ:151:VAL:HA	1.53	0.45
3:AE:529:GLN:HA	3:AE:530:LEU:HA	1.55	0.45
1:BC:683:LEU:N	1:BC:684:THR:HA	2.21	0.45
4:AF:215:VAL:HA	4:AF:235:SER:HA	1.99	0.45
6:BH:189:ASN:HA	6:BH:190:PRO:HA	1.73	0.45
6:BH:176:GLU:HA	6:BH:177:VAL:HA	1.58	0.45
7:BI:141:ASN:HA	7:BI:142:PRO:HA	1.72	0.45
1:CC:683:LEU:N	1:CC:684:THR:HA	2.20	0.45
8:CJ:858:ILE:HA	8:CJ:859:THR:HA	1.48	0.45
1:DC:683:LEU:N	1:DC:684:THR:HA	2.20	0.45
4:DF:215:VAL:HA	4:DF:235:SER:HA	1.99	0.45
8:AJ:858:ILE:HA	8:AJ:859:THR:HA	1.53	0.45
5:AG:138:ILE:HA	5:AG:160:SER:HA	1.98	0.44
7:AI:183:THR:HA	7:AI:184:PRO:HA	1.71	0.44
8:DJ:1090:TYR:O	8:DJ:1095:ARG:N	2.39	0.44
8:AJ:239:PHE:HA	8:AJ:258:LYS:HA	1.98	0.44
3:AE:900:LEU:N	8:AJ:1135:ILE:O	2.46	0.44
7:BI:220:LEU:HA	7:BI:237:GLY:HA2	2.00	0.44
8:CJ:168:HIS:HA	8:CJ:169:PRO:HA	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:176:GLU:HA	6:AH:177:VAL:HA	1.59	0.44
5:BG:116:VAL:HA	5:BG:134:SER:HA	1.99	0.43
8:CJ:480:CYS:HA	8:CJ:481:ARG:HA	1.50	0.43
7:BI:183:THR:HA	7:BI:184:PRO:HA	1.72	0.43
4:CF:215:VAL:HA	4:CF:235:SER:HA	2.00	0.43
1:AC:683:LEU:N	1:AC:684:THR:HA	2.21	0.43
8:CJ:488:ASP:O	8:CJ:490:SER:N	2.52	0.43
3:AE:850:ILE:HA	3:AE:855:CYS:H	1.84	0.42
7:CI:141:ASN:HA	7:CI:142:PRO:HA	1.72	0.42
3:BE:908:GLY:O	3:BE:910:LEU:N	2.52	0.42
8:DJ:488:ASP:O	8:DJ:490:SER:N	2.52	0.42
2:BD:248:SER:CB	2:BD:385:HIS:HA	2.50	0.42
8:BJ:237:GLY:HA2	8:BJ:277:GLY:HA2	2.00	0.42
4:CF:60:VAL:HA	4:CF:78:SER:HA	2.02	0.42
6:DH:176:GLU:HA	6:DH:177:VAL:HA	1.58	0.42
2:AD:297:TRP:HA	2:AD:339:ASP:CA	2.48	0.42
4:DF:60:VAL:HA	4:DF:78:SER:HA	2.01	0.42
5:DG:162:LYS:N	5:DG:163:LEU:HA	2.28	0.42
8:BJ:168:HIS:HA	8:BJ:169:PRO:HA	1.73	0.42
2:AD:300:THR:CB	2:AD:335:LEU:C	2.87	0.42
8:AJ:150:ARG:HA	8:AJ:151:VAL:HA	1.51	0.42
1:CC:619:GLY:HA2	1:CC:620:LEU:C	2.40	0.42
8:DJ:858:ILE:HA	8:DJ:859:THR:HA	1.49	0.41
3:BE:898:VAL:HA	8:BJ:1138:GLU:HA	2.02	0.41
8:BJ:488:ASP:O	8:BJ:490:SER:N	2.53	0.41
4:BF:60:VAL:HA	4:BF:78:SER:HA	2.02	0.41
9:BK:168:GLY:HA2	9:BK:185:GLU:HA	2.02	0.41
7:CI:183:THR:HA	7:CI:184:PRO:HA	1.72	0.41
2:CD:297:TRP:HA	2:CD:339:ASP:CB	2.51	0.41
9:DK:193:TYR:HA	9:DK:199:GLN:HA	2.03	0.41
8:DJ:168:HIS:HA	8:DJ:169:PRO:HA	1.75	0.41
9:CK:193:TYR:HA	9:CK:199:GLN:HA	2.03	0.41
2:AD:384:TYR:HA	2:AD:400:GLY:HA3	2.01	0.41
4:AF:60:VAL:HA	4:AF:78:SER:HA	2.02	0.40
7:DI:183:THR:HA	7:DI:184:PRO:HA	1.72	0.40
3:DE:850:ILE:HA	3:DE:855:CYS:H	1.87	0.40
7:AI:220:LEU:HA	7:AI:237:GLY:HA2	2.03	0.40
1:DC:619:GLY:HA2	1:DC:620:LEU:C	2.40	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	AC	508/1156 (44%)	465 (92%)	35 (7%)	8 (2%)	9	44
1	BC	508/1156 (44%)	465 (92%)	35 (7%)	8 (2%)	9	44
1	CC	508/1156 (44%)	466 (92%)	34 (7%)	8 (2%)	9	44
1	DC	508/1156 (44%)	466 (92%)	34 (7%)	8 (2%)	9	44
2	AD	668/925 (72%)	618 (92%)	41 (6%)	9 (1%)	12	48
2	BD	668/925 (72%)	627 (94%)	34 (5%)	7 (1%)	15	55
2	CD	668/925 (72%)	622 (93%)	41 (6%)	5 (1%)	22	63
2	DD	668/925 (72%)	625 (94%)	39 (6%)	4 (1%)	25	66
3	AE	541/937 (58%)	451 (83%)	67 (12%)	23 (4%)	2	22
3	BE	541/937 (58%)	453 (84%)	67 (12%)	21 (4%)	3	23
3	CE	539/937 (58%)	453 (84%)	67 (12%)	19 (4%)	3	25
3	DE	539/937 (58%)	453 (84%)	67 (12%)	19 (4%)	3	25
4	AF	281/322 (87%)	245 (87%)	35 (12%)	1 (0%)	34	72
4	BF	281/322 (87%)	217 (77%)	59 (21%)	5 (2%)	8	40
4	CF	281/322 (87%)	246 (88%)	33 (12%)	2 (1%)	22	63
4	DF	281/322 (87%)	239 (85%)	37 (13%)	5 (2%)	8	40
5	AG	314/360 (87%)	266 (85%)	43 (14%)	5 (2%)	9	44
5	BG	314/360 (87%)	266 (85%)	44 (14%)	4 (1%)	12	48
5	CG	314/360 (87%)	272 (87%)	38 (12%)	4 (1%)	12	48
5	DG	314/360 (87%)	272 (87%)	38 (12%)	4 (1%)	12	48
6	AH	630/656 (96%)	516 (82%)	80 (13%)	34 (5%)	2	19
6	BH	630/656 (96%)	518 (82%)	81 (13%)	31 (5%)	2	20
6	CH	624/656 (95%)	518 (83%)	76 (12%)	30 (5%)	2	21
6	DH	624/656 (95%)	518 (83%)	76 (12%)	30 (5%)	2	21
7	AI	324/380 (85%)	274 (85%)	44 (14%)	6 (2%)	8	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BI	324/380 (85%)	273 (84%)	45 (14%)	6 (2%)	8	38
7	CI	324/380 (85%)	282 (87%)	34 (10%)	8 (2%)	5	32
7	DI	324/380 (85%)	282 (87%)	34 (10%)	8 (2%)	5	32
8	AJ	983/1436 (68%)	804 (82%)	135 (14%)	44 (4%)	2	22
8	BJ	983/1436 (68%)	806 (82%)	130 (13%)	47 (5%)	2	21
8	CJ	982/1436 (68%)	809 (82%)	130 (13%)	43 (4%)	2	22
8	DJ	982/1436 (68%)	812 (83%)	127 (13%)	43 (4%)	2	22
9	AK	305/326 (94%)	246 (81%)	49 (16%)	10 (3%)	4	26
9	BK	305/326 (94%)	247 (81%)	47 (15%)	11 (4%)	3	25
9	CK	303/326 (93%)	249 (82%)	44 (14%)	10 (3%)	4	26
9	DK	303/326 (93%)	249 (82%)	44 (14%)	10 (3%)	4	26
All	All	18194/25992 (70%)	15590 (86%)	2064 (11%)	540 (3%)	7	28

All (540) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AC	627	PHE
1	AC	680	PRO
1	AC	685	PRO
2	AD	324	ASP
2	AD	325	PRO
2	AD	334	PRO
2	AD	737	PRO
2	AD	917	ASP
3	AE	381	PRO
3	AE	893	PRO
3	AE	898	VAL
3	AE	899	PRO
3	AE	911	PRO
5	AG	263	PRO
6	AH	52	PRO
6	AH	190	PRO
6	AH	223	SER
6	AH	428	PRO
6	AH	527	PRO
6	AH	569	ALA
6	AH	570	PRO
6	AH	612	PRO

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Mol	Chain	Res	Type
7	AI	219	PRO
8	AJ	168	HIS
8	AJ	169	PRO
8	AJ	208	PRO
8	AJ	211	SER
8	AJ	212	PRO
8	AJ	363	PRO
8	AJ	441	PRO
8	AJ	453	PRO
8	AJ	668	PRO
8	AJ	787	VAL
8	AJ	788	PRO
8	AJ	819	PRO
8	AJ	871	PRO
8	AJ	976	PRO
8	AJ	1137	PRO
9	AK	91	PRO
9	AK	134	PRO
9	AK	290	PRO
9	AK	309	PRO
1	BC	627	PHE
1	BC	680	PRO
1	BC	685	PRO
2	BD	334	PRO
2	BD	737	PRO
2	BD	917	ASP
3	BE	359	PRO
3	BE	716	PRO
3	BE	853	ILE
3	BE	893	PRO
3	BE	898	VAL
3	BE	911	PRO
3	BE	913	PRO
4	BF	112	ALA
5	BG	263	PRO
6	BH	29	PRO
6	BH	52	PRO
6	BH	427	CYS
6	BH	428	PRO
6	BH	527	PRO
6	BH	569	ALA
6	BH	570	PRO

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Mol	Chain	Res	Type
6	BH	612	PRO
7	BI	219	PRO
8	BJ	167	PRO
8	BJ	208	PRO
8	BJ	211	SER
8	BJ	212	PRO
8	BJ	363	PRO
8	BJ	441	PRO
8	BJ	453	PRO
8	BJ	668	PRO
8	BJ	787	VAL
8	BJ	788	PRO
8	BJ	871	PRO
8	BJ	976	PRO
8	BJ	1137	PRO
9	BK	91	PRO
9	BK	134	PRO
9	BK	290	PRO
9	BK	309	PRO
1	CC	627	PHE
1	CC	680	PRO
1	CC	685	PRO
3	CE	381	PRO
3	CE	892	THR
3	CE	893	PRO
3	CE	898	VAL
3	CE	899	PRO
3	CE	912	MET
5	CG	263	PRO
6	CH	29	PRO
6	CH	190	PRO
6	CH	223	SER
6	CH	245	PRO
6	CH	427	CYS
6	CH	428	PRO
6	CH	569	ALA
6	CH	570	PRO
7	CI	219	PRO
8	CJ	208	PRO
8	CJ	211	SER
8	CJ	212	PRO
8	CJ	363	PRO

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Mol	Chain	Res	Type
8	CJ	441	PRO
8	CJ	452	ASP
8	CJ	453	PRO
8	CJ	668	PRO
8	CJ	788	PRO
8	CJ	871	PRO
8	CJ	976	PRO
8	CJ	1135	ILE
8	CJ	1137	PRO
9	CK	91	PRO
9	CK	134	PRO
9	CK	290	PRO
9	CK	309	PRO
1	DC	627	PHE
1	DC	680	PRO
1	DC	685	PRO
3	DE	381	PRO
3	DE	892	THR
3	DE	893	PRO
3	DE	898	VAL
3	DE	912	MET
5	DG	263	PRO
6	DH	29	PRO
6	DH	190	PRO
6	DH	223	SER
6	DH	245	PRO
6	DH	427	CYS
6	DH	428	PRO
6	DH	569	ALA
6	DH	570	PRO
7	DI	219	PRO
8	DJ	208	PRO
8	DJ	211	SER
8	DJ	212	PRO
8	DJ	363	PRO
8	DJ	441	PRO
8	DJ	452	ASP
8	DJ	453	PRO
8	DJ	668	PRO
8	DJ	788	PRO
8	DJ	871	PRO
8	DJ	976	PRO

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Mol	Chain	Res	Type
8	DJ	1135	ILE
8	DJ	1137	PRO
9	DK	91	PRO
9	DK	134	PRO
9	DK	290	PRO
9	DK	309	PRO
1	AC	628	PRO
1	AC	629	VAL
3	AE	526	PRO
5	AG	110	VAL
6	AH	366	ILE
6	AH	442	ILE
8	AJ	138	LEU
8	AJ	232	PRO
8	AJ	452	ASP
8	AJ	783	LEU
8	AJ	955	VAL
1	BC	628	PRO
1	BC	629	VAL
3	BE	895	PRO
4	BF	145	ILE
4	BF	179	ILE
6	BH	190	PRO
6	BH	223	SER
6	BH	518	ASP
8	BJ	452	ASP
8	BJ	482	GLY
8	BJ	489	LEU
8	BJ	889	VAL
8	BJ	955	VAL
8	BJ	1136	ARG
9	BK	90	PRO
9	BK	243	PRO
1	CC	628	PRO
1	CC	629	VAL
2	CD	334	PRO
3	CE	526	PRO
3	CE	895	PRO
6	CH	52	PRO
6	CH	521	LEU
8	CJ	167	PRO
8	CJ	434	PRO

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Mol	Chain	Res	Type
8	CJ	489	LEU
8	CJ	819	PRO
8	CJ	955	VAL
8	CJ	1112	VAL
8	CJ	1142	ILE
8	CJ	1145	PRO
1	DC	628	PRO
1	DC	629	VAL
2	DD	334	PRO
3	DE	526	PRO
3	DE	895	PRO
3	DE	899	PRO
6	DH	52	PRO
6	DH	521	LEU
8	DJ	167	PRO
8	DJ	434	PRO
8	DJ	489	LEU
8	DJ	819	PRO
8	DJ	955	VAL
8	DJ	1112	VAL
8	DJ	1142	ILE
8	DJ	1145	PRO
2	AD	420	PHE
3	AE	490	SER
3	AE	575	ASN
3	AE	834	ASN
3	AE	892	THR
3	AE	895	PRO
5	AG	208	LYS
6	AH	80	LEU
6	AH	173	HIS
6	AH	225	ALA
6	AH	288	LEU
6	AH	315	SER
6	AH	429	GLU
6	AH	430	LEU
6	AH	518	ASP
7	AI	347	PRO
7	AI	349[A]	ARG
7	AI	349[B]	ARG
8	AJ	167	PRO
8	AJ	198	PRO

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Mol	Chain	Res	Type
8	AJ	350	PRO
8	AJ	403	SER
8	AJ	489	LEU
8	AJ	744	LEU
8	AJ	958	PRO
8	AJ	1013	HIS
9	AK	243	PRO
3	BE	490	SER
3	BE	505	LEU
3	BE	575	ASN
3	BE	909	ARG
6	BH	49	PRO
6	BH	173	HIS
6	BH	225	ALA
6	BH	321	PRO
6	BH	442	ILE
7	BI	347	PRO
7	BI	349[A]	ARG
7	BI	349[B]	ARG
8	BJ	350	PRO
8	BJ	434	PRO
8	BJ	708	GLY
8	BJ	1013	HIS
8	BJ	1177	ILE
9	BK	89	LEU
2	CD	420	PHE
2	CD	917	ASP
3	CE	490	SER
3	CE	575	ASN
3	CE	834	ASN
6	CH	225	ALA
6	CH	288	LEU
6	CH	315	SER
6	CH	442	ILE
6	CH	518	ASP
6	CH	612	PRO
7	CI	349[A]	ARG
7	CI	349[B]	ARG
8	CJ	350	PRO
8	CJ	796	LEU
8	CJ	958	PRO
8	CJ	1013	HIS

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Mol	Chain	Res	Type
8	CJ	1113	ARG
9	CK	119	VAL
9	CK	243	PRO
2	DD	917	ASP
3	DE	490	SER
3	DE	575	ASN
3	DE	834	ASN
4	DF	175	LYS
6	DH	225	ALA
6	DH	288	LEU
6	DH	315	SER
6	DH	442	ILE
6	DH	518	ASP
6	DH	612	PRO
7	DI	349[A]	ARG
7	DI	349[B]	ARG
8	DJ	350	PRO
8	DJ	796	LEU
8	DJ	1013	HIS
8	DJ	1113	ARG
9	DK	119	VAL
9	DK	243	PRO
1	AC	934	HIS
3	AE	891	SER
3	AE	912	MET
6	AH	342	PRO
6	AH	392	LEU
6	AH	618	ASP
7	AI	142	PRO
8	AJ	353	GLY
8	AJ	449	ASP
8	AJ	666	ARG
1	BC	934	HIS
2	BD	397	PRO
3	BE	834	ASN
5	BG	208	LYS
6	BH	315	SER
6	BH	342	PRO
6	BH	392	LEU
6	BH	610	ARG
7	BI	142	PRO
8	BJ	232	PRO

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Mol	Chain	Res	Type
8	BJ	353	GLY
8	BJ	403	SER
8	BJ	449	ASP
8	BJ	666	ARG
8	BJ	782	CYS
8	BJ	958	PRO
8	BJ	1112	VAL
9	BK	53	GLU
9	BK	111	LEU
1	CC	827	SER
1	CC	934	HIS
2	CD	397	PRO
5	CG	208	LYS
6	CH	49	PRO
6	CH	366	ILE
6	CH	610	ARG
7	CI	135	THR
7	CI	142	PRO
7	CI	347	PRO
8	CJ	403	SER
8	CJ	449	ASP
8	CJ	666	ARG
9	CK	53	GLU
9	CK	111	LEU
1	DC	827	SER
1	DC	934	HIS
2	DD	397	PRO
3	DE	911	PRO
4	DF	197	GLU
5	DG	208	LYS
6	DH	366	ILE
6	DH	610	ARG
7	DI	135	THR
7	DI	142	PRO
7	DI	347	PRO
8	DJ	403	SER
8	DJ	449	ASP
8	DJ	666	ARG
9	DK	53	GLU
9	DK	111	LEU
1	AC	679	ILE
1	AC	827	SER

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Mol	Chain	Res	Type
2	AD	396	GLU
3	AE	359	PRO
3	AE	380	LEU
4	AF	55	GLY
5	AG	308	ASN
6	AH	49	PRO
6	AH	344	PRO
6	AH	493	ALA
6	AH	585	LEU
7	AI	135	THR
8	AJ	447	ILE
8	AJ	464	PRO
9	AK	43	TYR
9	AK	53	GLU
1	BC	679	ILE
1	BC	827	SER
2	BD	396	GLU
3	BE	380	LEU
4	BF	55	GLY
4	BF	138	GLY
6	BH	80	LEU
6	BH	126	PRO
6	BH	614	HIS
7	BI	135	THR
8	BJ	198	PRO
8	BJ	464	PRO
8	BJ	1095	ARG
9	BK	43	TYR
1	CC	679	ILE
2	CD	396	GLU
3	CE	359	PRO
3	CE	911	PRO
4	CF	55	GLY
6	CH	173	HIS
6	CH	342	PRO
6	CH	392	LEU
7	CI	104	PRO
8	CJ	198	PRO
8	CJ	232	PRO
8	CJ	353	GLY
8	CJ	464	PRO
9	CK	43	TYR

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Mol	Chain	Res	Type
1	DC	679	ILE
2	DD	396	GLU
3	DE	359	PRO
4	DF	55	GLY
6	DH	49	PRO
6	DH	173	HIS
6	DH	342	PRO
6	DH	392	LEU
7	DI	104	PRO
8	DJ	198	PRO
8	DJ	232	PRO
8	DJ	353	GLY
8	DJ	464	PRO
8	DJ	958	PRO
9	DK	43	TYR
2	AD	918	PRO
3	AE	358	VAL
3	AE	413	PRO
3	AE	558	PRO
5	AG	252	PRO
8	AJ	204	ILE
8	AJ	370	ILE
9	AK	111	LEU
2	BD	332	LYS
2	BD	918	PRO
3	BE	381	PRO
3	BE	556	LEU
3	BE	558	PRO
3	BE	780	ILE
5	BG	252	PRO
6	BH	125	ASP
6	BH	344	PRO
6	BH	522	ILE
8	BJ	803	GLU
8	BJ	1141	TRP
3	CE	358	VAL
3	CE	380	LEU
3	CE	558	PRO
3	CE	780	ILE
4	CF	135	THR
8	CJ	803	GLU
3	DE	358	VAL

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Mol	Chain	Res	Type
3	DE	380	LEU
3	DE	558	PRO
3	DE	780	ILE
4	DF	135	THR
8	DJ	370	ILE
8	DJ	803	GLU
2	AD	397	PRO
3	AE	412	GLU
3	AE	556	LEU
3	AE	780	ILE
6	AH	522	ILE
3	BE	638	ASP
6	BH	151	ILE
6	BH	317	PRO
6	BH	591	ILE
8	BJ	819	PRO
8	BJ	823	VAL
8	BJ	858	ILE
6	CH	151	ILE
6	CH	627	ILE
8	CJ	370	ILE
8	CJ	787	VAL
6	DH	151	ILE
6	DH	627	ILE
8	DJ	787	VAL
3	AE	638	ASP
3	AE	908	GLY
6	AH	125	ASP
6	AH	321	PRO
8	AJ	140	GLY
8	AJ	142	VAL
8	AJ	446	VAL
8	AJ	482	GLY
8	AJ	708	GLY
8	AJ	822	ILE
8	AJ	1112	VAL
6	BH	526	GLY
8	BJ	370	ILE
8	BJ	447	ILE
6	CH	431	GLY
6	CH	591	ILE
8	CJ	446	VAL

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Mol	Chain	Res	Type
8	CJ	708	GLY
3	DE	715	THR
4	DF	200	GLY
6	DH	431	GLY
6	DH	591	ILE
8	DJ	446	VAL
8	DJ	708	GLY
6	AH	77	GLY
6	AH	317	PRO
6	AH	591	ILE
8	AJ	654	VAL
3	BE	412	GLU
5	BG	284	VAL
8	BJ	142	VAL
9	BK	137	GLY
3	CE	715	THR
6	CH	522	ILE
6	CH	527	PRO
8	CJ	142	VAL
8	CJ	144	VAL
8	CJ	654	VAL
6	DH	522	ILE
6	DH	527	PRO
8	DJ	142	VAL
8	DJ	144	VAL
8	DJ	654	VAL
6	AH	151	ILE
6	AH	277	SER
9	AK	137	GLY
3	BE	904	ALA
6	BH	627	ILE
8	BJ	801	VAL
5	CG	18	VAL
6	CH	289	GLY
8	CJ	447	ILE
5	DG	18	VAL
6	DH	289	GLY
8	DJ	447	ILE
6	AH	242	ILE
8	AJ	144	VAL
9	AK	288	PRO
8	BJ	446	VAL

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Mol	Chain	Res	Type
8	BJ	1142	ILE
3	CE	412	GLU
5	CG	252	PRO
6	CH	317	PRO
8	CJ	818	SER
9	CK	137	GLY
3	DE	412	GLU
5	DG	252	PRO
6	DH	317	PRO
8	DJ	818	SER
9	DK	137	GLY
8	BJ	169	PRO
7	CI	184	PRO
7	DI	184	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	CJ	3
8	DJ	3
6	CH	3
6	DH	3
9	CK	1
9	DK	1
3	CE	1
3	DE	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CJ	784:ALA	C	785:THR	N	25.54
1	DJ	784:ALA	C	785:THR	N	25.54
1	CH	613:VAL	C	614:HIS	N	24.84
1	DH	613:VAL	C	614:HIS	N	24.83
1	CH	525:LEU	C	526:GLY	N	22.68
1	DH	525:LEU	C	526:GLY	N	22.68
1	DJ	933:ALA	C	934:ALA	N	19.75
1	CK	117:TYR	C	118:LYS	N	11.44
1	DK	117:TYR	C	118:LYS	N	11.44
1	CJ	933:ALA	C	934:ALA	N	8.02
1	CJ	511:THR	C	512:GLU	N	6.04
1	DJ	511:THR	C	512:GLU	N	6.04
1	CH	411:PHE	C	412:ALA	N	4.67
1	DH	411:PHE	C	412:ALA	N	4.67
1	CE	732:PRO	C	733:ALA	N	3.61
1	DE	732:PRO	C	733:ALA	N	3.61

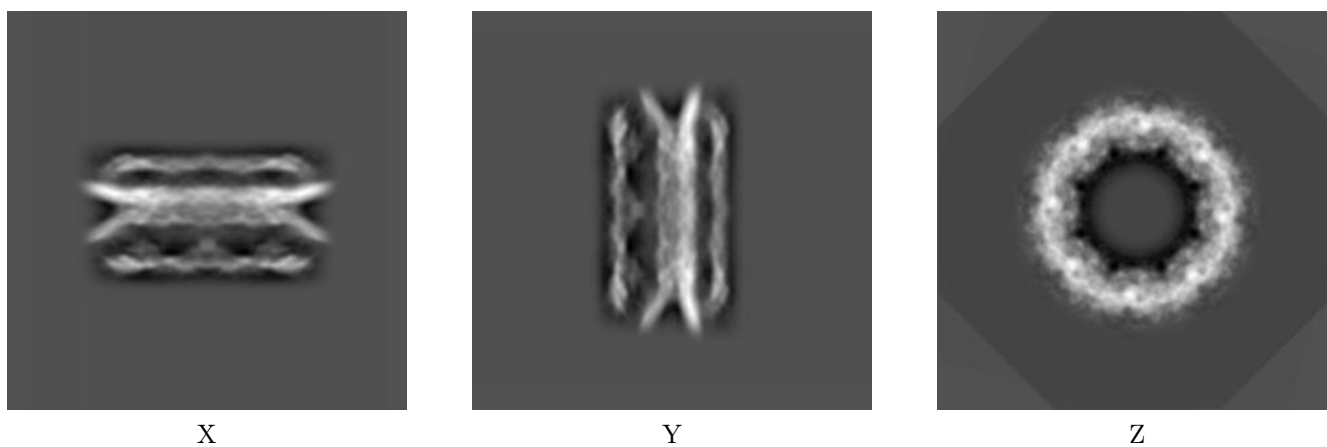
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12814. 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](#)

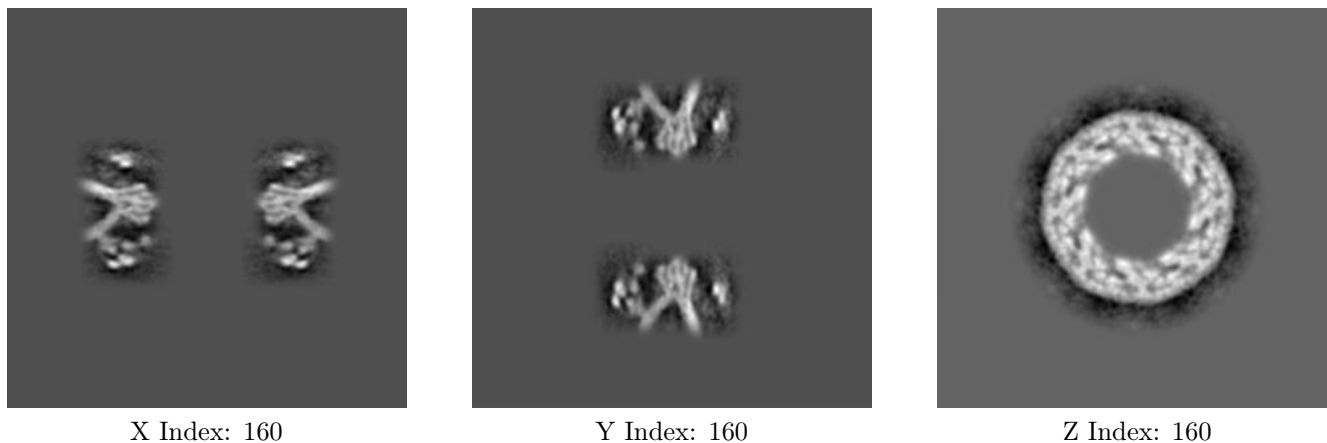
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

Y Index: 160

Z Index: 160

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

6.3 Largest variance slices [i](#)

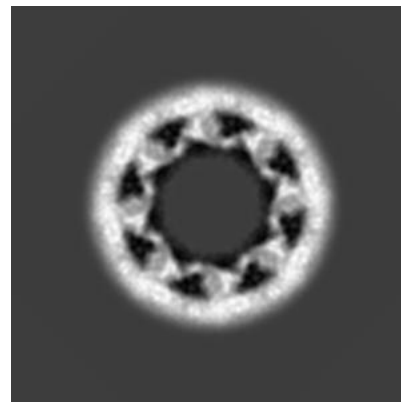
6.3.1 Primary map



X Index: 100



Y Index: 220



Z Index: 174

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

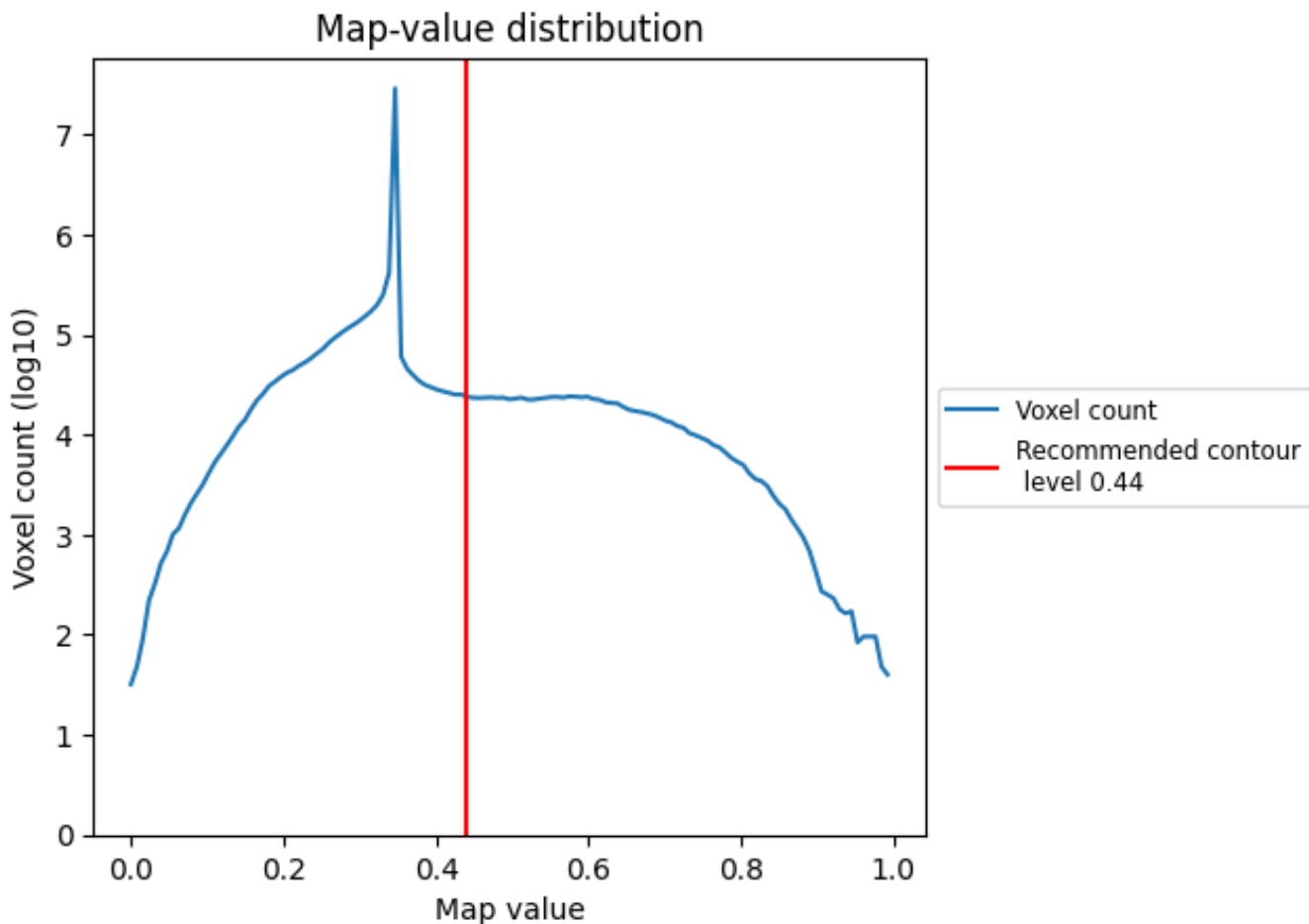
6.5 Mask visualisation

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

7 Map analysis [i](#)

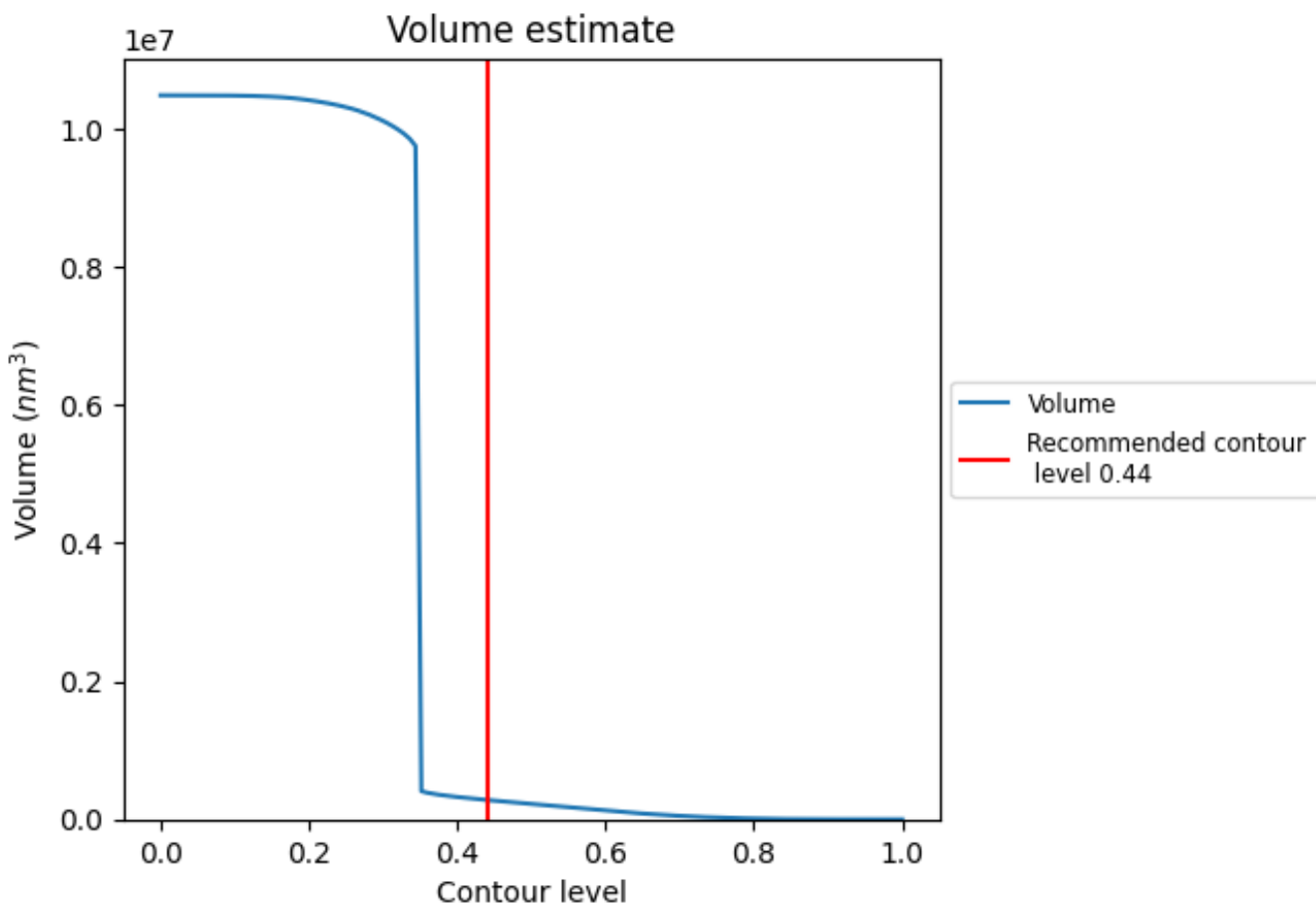
This section contains the results of statistical analysis of the map.

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.

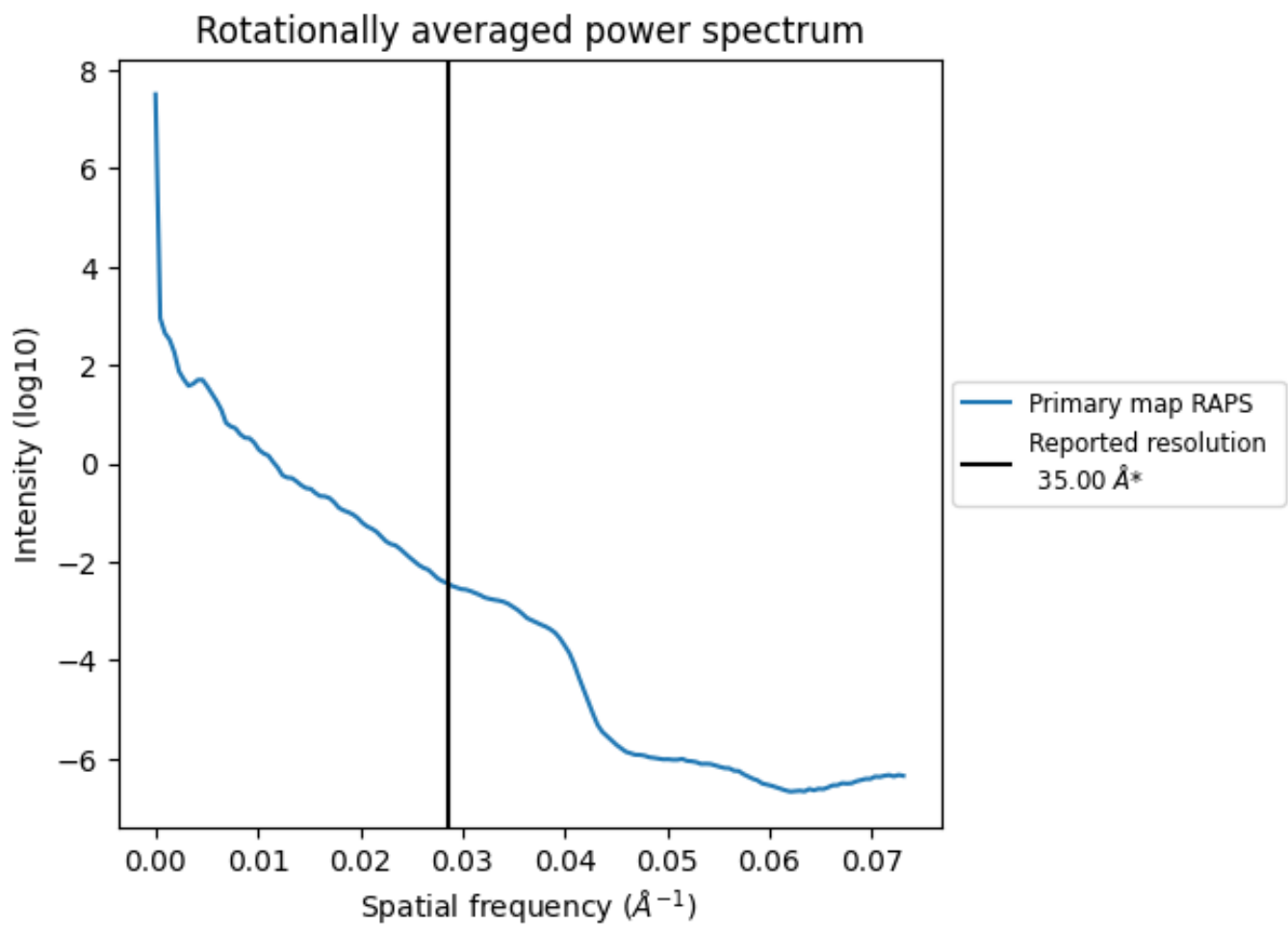
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 280168 nm^3 ; this corresponds to an approximate mass of 253083 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 0.029 Å⁻¹

8 Fourier-Shell correlation

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

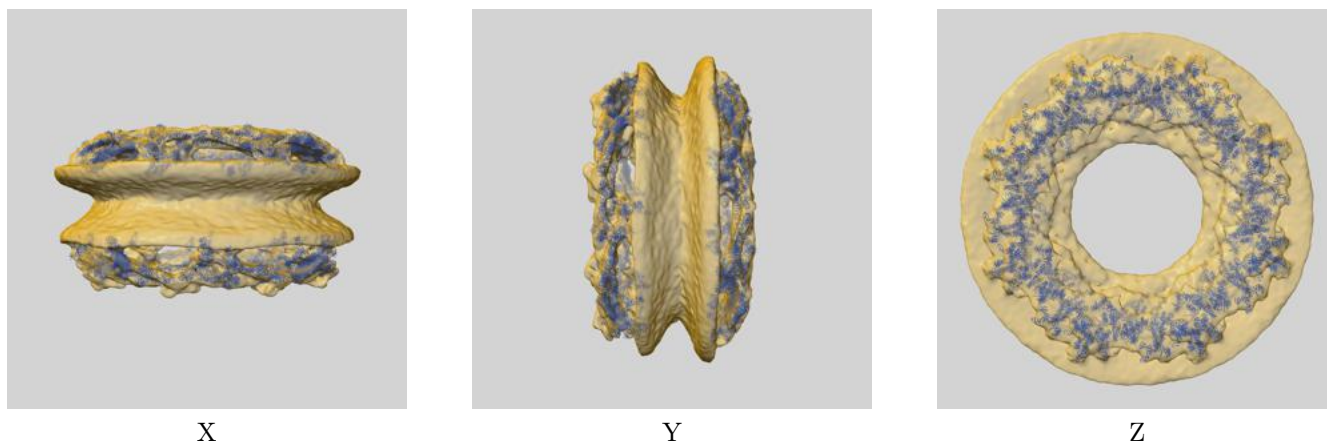
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12814 and PDB model 7PEQ. Per-residue inclusion information can be found in section 3 on page 8.

9.0.1 Map-model overlay [i](#)

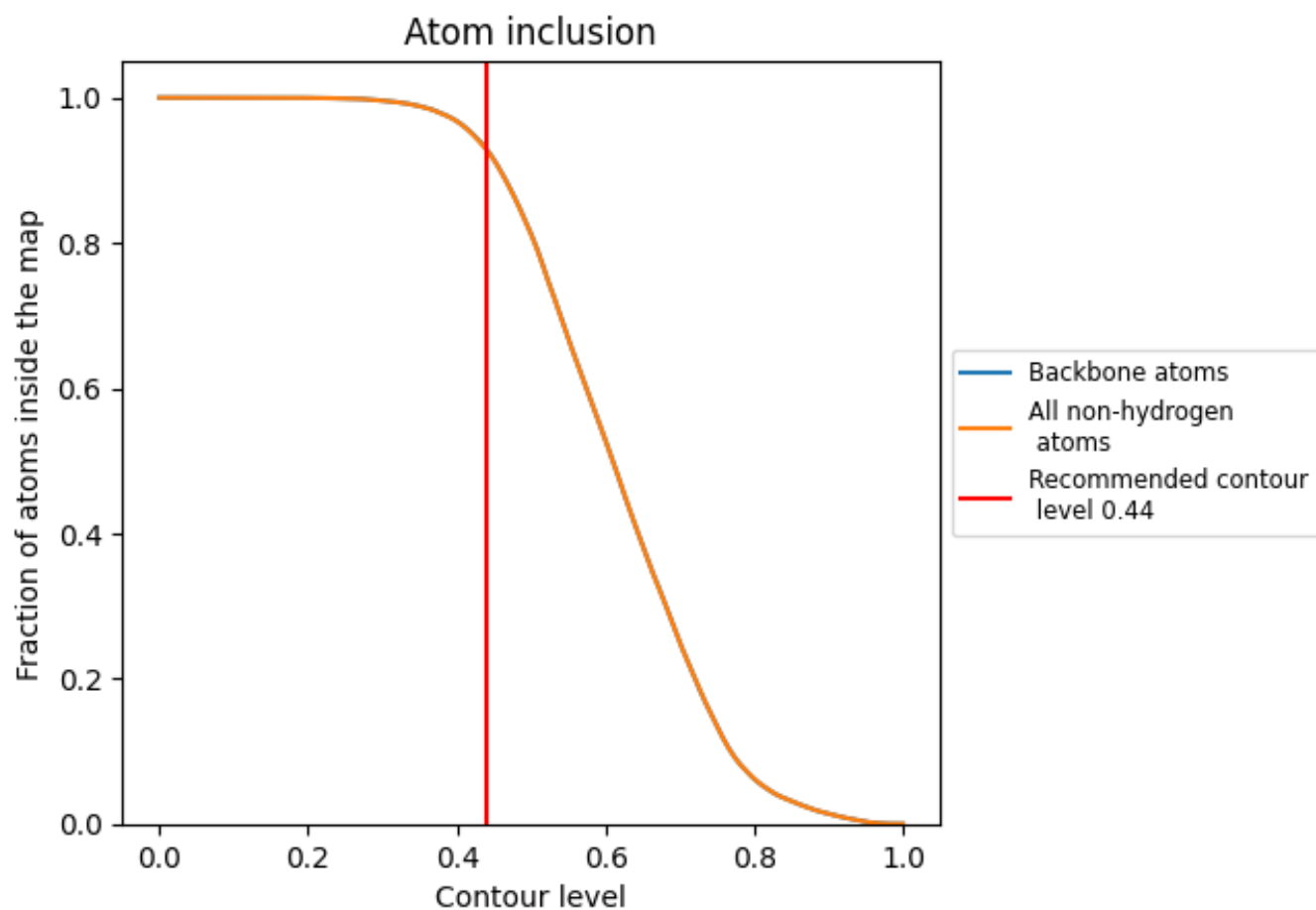


9.0.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.44 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.

9.1 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.