Full wwPDB EM Validation Report ⓘ

Dec 13, 2022 – 12:26 pm GMT

PDB ID	:	8BBG
EMDB ID	:	EMD-4304
Title	:	Structure of the IFT-A complex; anterograde IFT-A train model
Authors	:	Hesketh, S.J.; Mukhopadhyay, A.G.; Nakamura, D.; Toropova, K.; Roberts, A.J.
Deposited on	:	2022-10-12
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

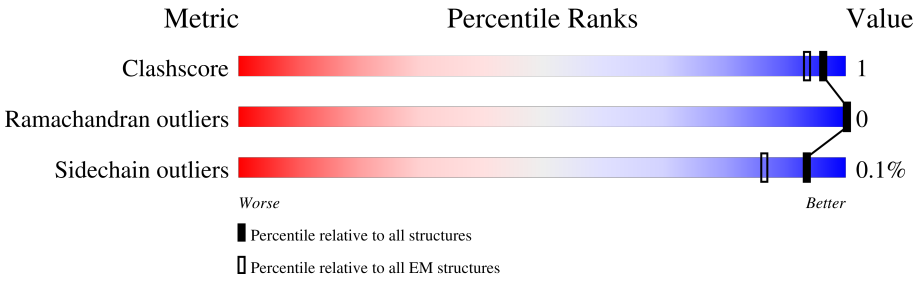
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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.

Mol	Chain	Length	Quality of chain
1	A	1357	27% 96%
2	B	1477	25% 90% 6%
3	C	1241	6% 91% 5%
4	D	1500	16% 84% 12%
5	E	1184	8% 90% 6%
6	F	209	26% 73%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 51335 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 WD repeat-containing protein 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1342	10643	6768	1809	1991	75	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1343	GLU	-	expression tag	UNP Q8NEZ3
A	1344	ASN	-	expression tag	UNP Q8NEZ3
A	1345	LEU	-	expression tag	UNP Q8NEZ3
A	1346	TYR	-	expression tag	UNP Q8NEZ3
A	1347	PHE	-	expression tag	UNP Q8NEZ3
A	1348	GLN	-	expression tag	UNP Q8NEZ3
A	1349	SER	-	expression tag	UNP Q8NEZ3
A	1350	ASP	-	expression tag	UNP Q8NEZ3
A	1351	TYR	-	expression tag	UNP Q8NEZ3
A	1352	LYS	-	expression tag	UNP Q8NEZ3
A	1353	ASP	-	expression tag	UNP Q8NEZ3
A	1354	ASP	-	expression tag	UNP Q8NEZ3
A	1355	ASP	-	expression tag	UNP Q8NEZ3
A	1356	ASP	-	expression tag	UNP Q8NEZ3
A	1357	LYS	-	expression tag	UNP Q8NEZ3

- Molecule 2 is a protein called Intraflagellar transport protein 140 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1426	11319	7136	1980	2131	72	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1463	GLU	-	expression tag	UNP Q96RY7
B	1464	ASN	-	expression tag	UNP Q96RY7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1465	LEU	-	expression tag	UNP Q96RY7
B	1466	TYR	-	expression tag	UNP Q96RY7
B	1467	PHE	-	expression tag	UNP Q96RY7
B	1468	GLN	-	expression tag	UNP Q96RY7
B	1469	SER	-	expression tag	UNP Q96RY7
B	1470	TRP	-	expression tag	UNP Q96RY7
B	1471	SER	-	expression tag	UNP Q96RY7
B	1472	HIS	-	expression tag	UNP Q96RY7
B	1473	PRO	-	expression tag	UNP Q96RY7
B	1474	GLN	-	expression tag	UNP Q96RY7
B	1475	PHE	-	expression tag	UNP Q96RY7
B	1476	GLU	-	expression tag	UNP Q96RY7
B	1477	LYS	-	expression tag	UNP Q96RY7

- Molecule 3 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1174	Total	C	N	O	S	0	0
			9447	6032	1613	1743	59		

- Molecule 4 is a protein called SNAP-tag,Tetratricopeptide repeat protein 21B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1316	Total	C	N	O	S	0	0
			10593	6714	1831	1978	70		

- Molecule 5 is a protein called WD repeat-containing protein 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1112	Total	C	N	O	S	0	0
			8863	5657	1497	1650	59		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	PHE	-	expression tag	UNP Q9P2L0
E	-1	GLN	-	expression tag	UNP Q9P2L0
E	0	GLY	-	expression tag	UNP Q9P2L0

- Molecule 6 is a protein called Intraflagellar transport protein 43 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	57	Total	C	N	O	S	0	0
			470	296	74	98	2		

There is a discrepancy between the modelled and reference sequences:

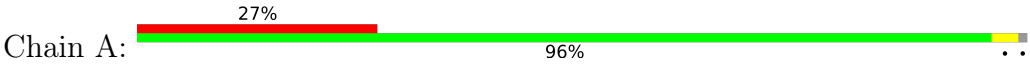
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	expression tag	UNP Q96FT9

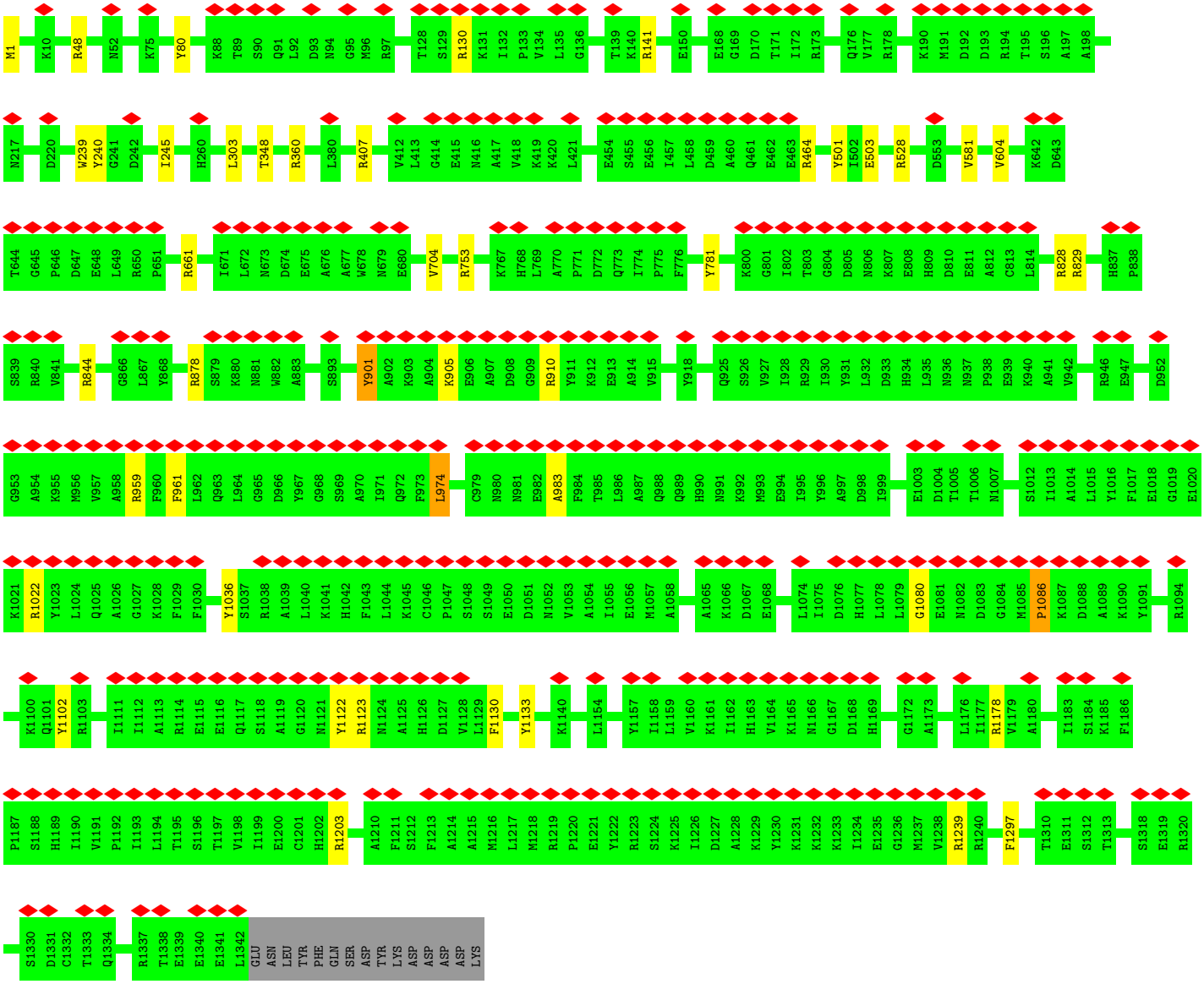
3 Residue-property plots (i)

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: WD repeat-containing protein 19

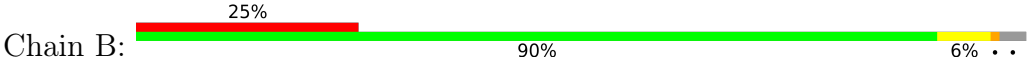
Chain A:

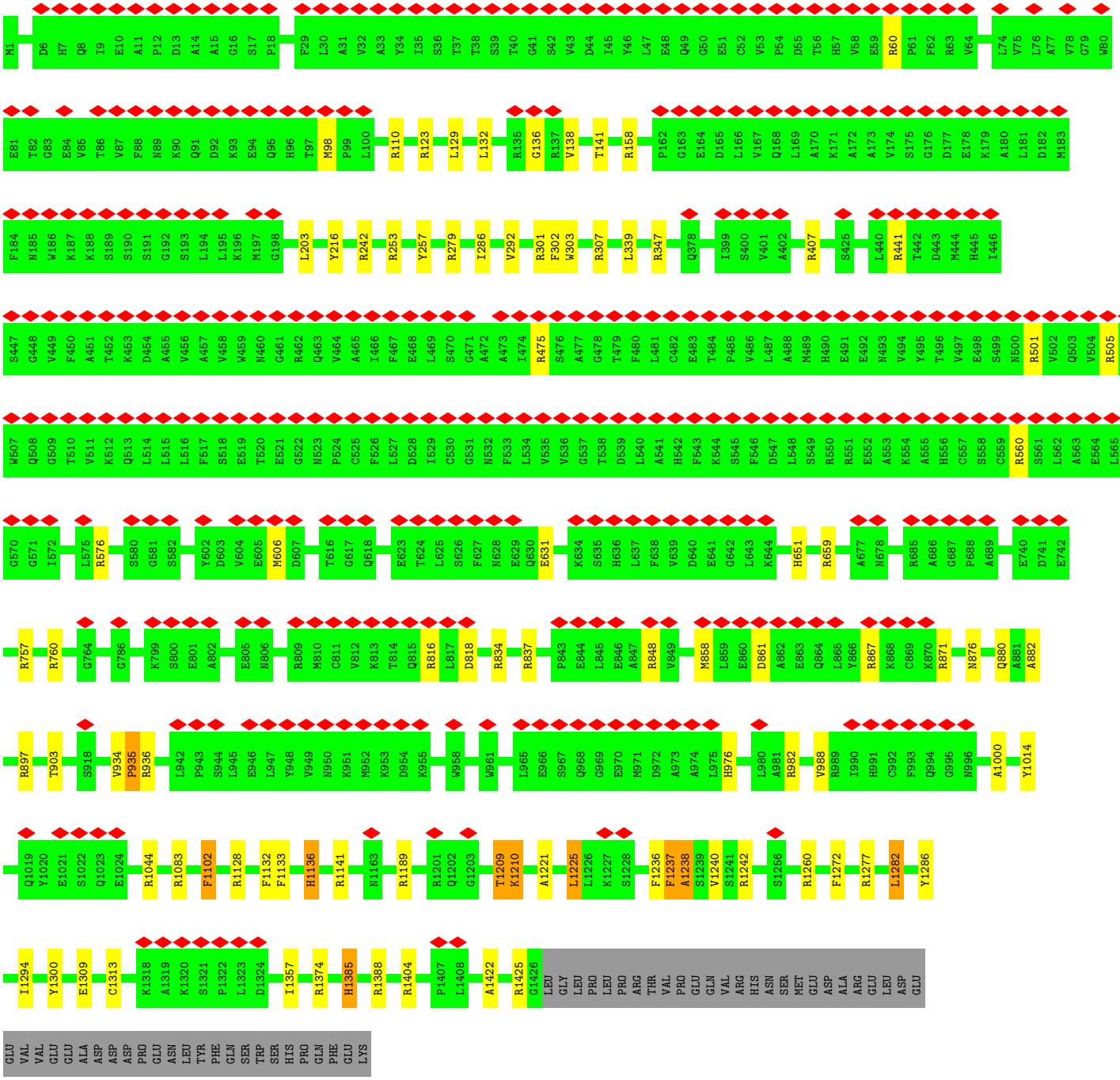




• Molecule 2: Intraflagellar transport protein 140 homolog

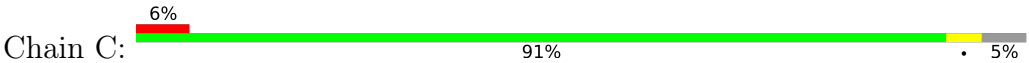
Chain B:

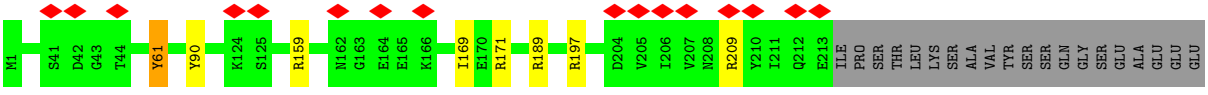


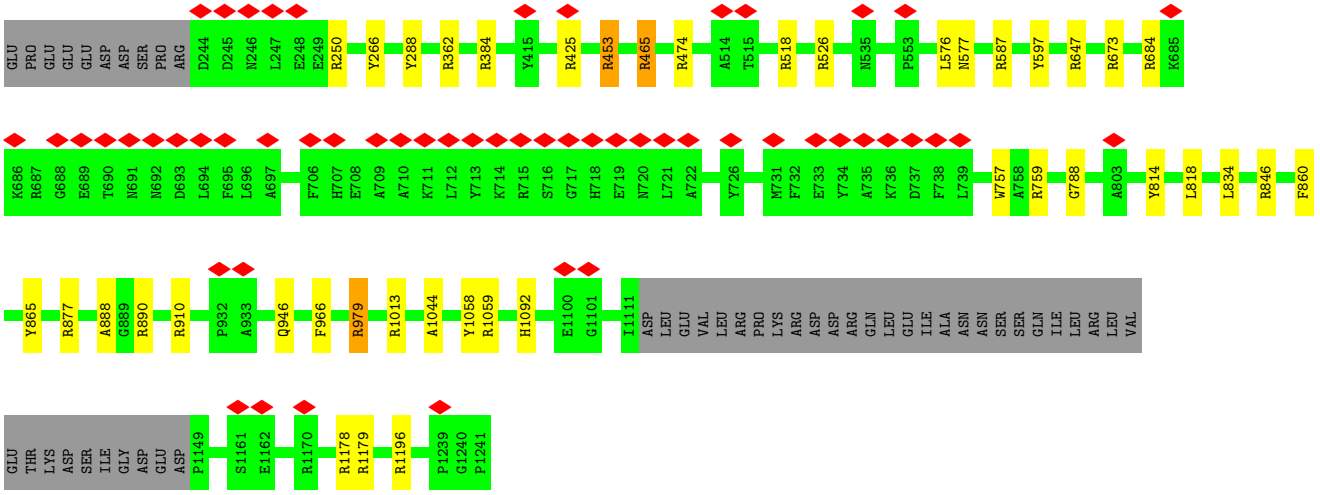


• Molecule 3: Intraflagellar transport protein 122 homolog

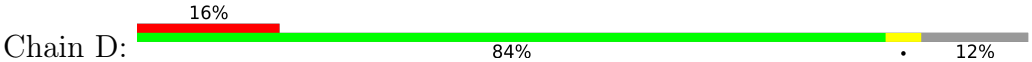
Chain C:

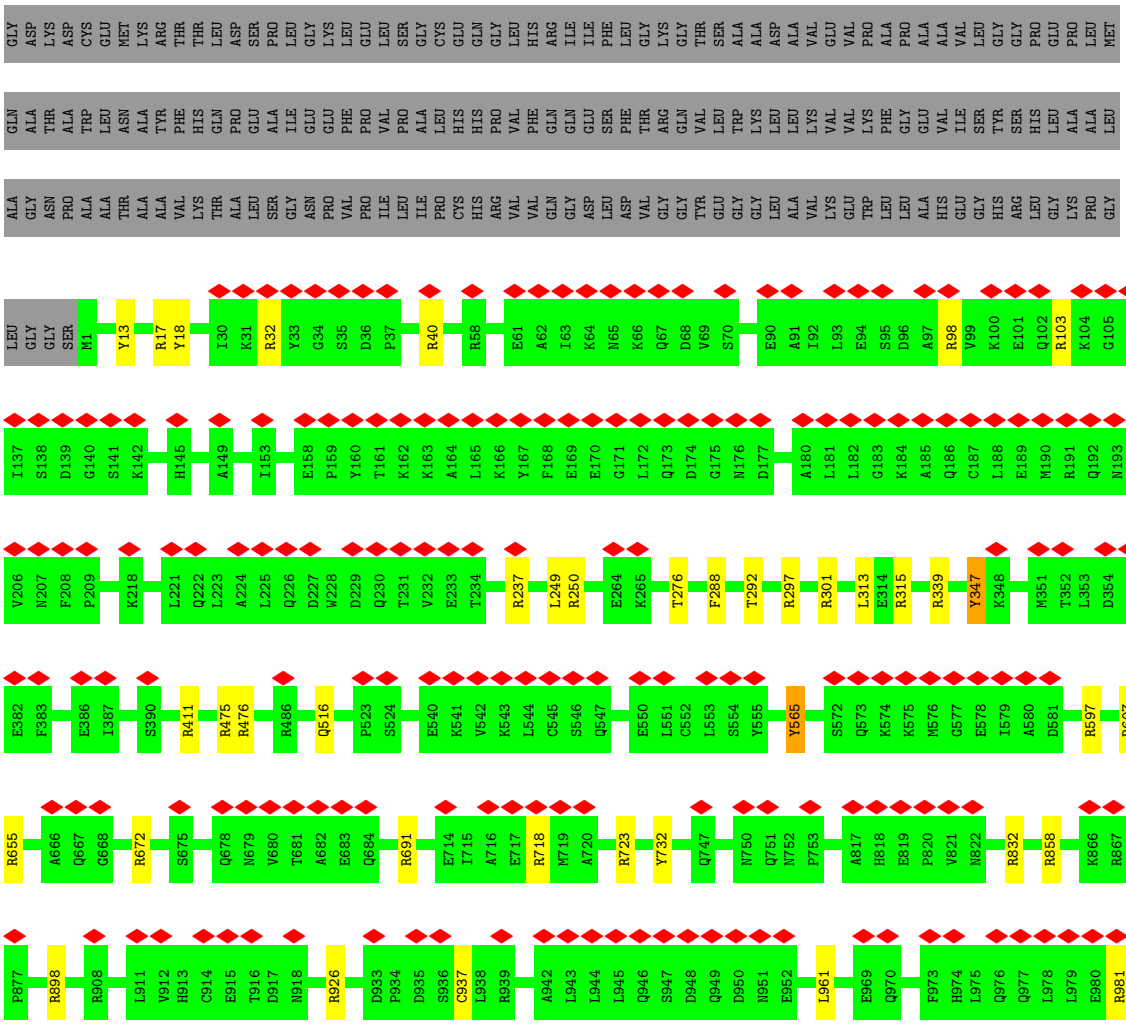


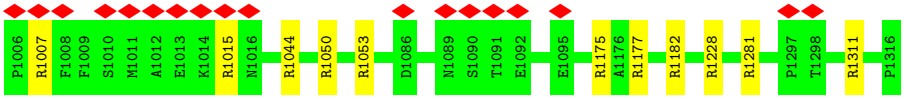




• Molecule 4: SNAP-tag,Tetratricopeptide repeat protein 21B

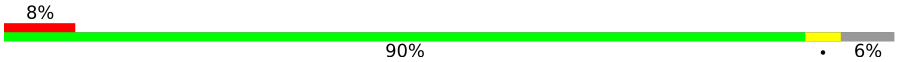


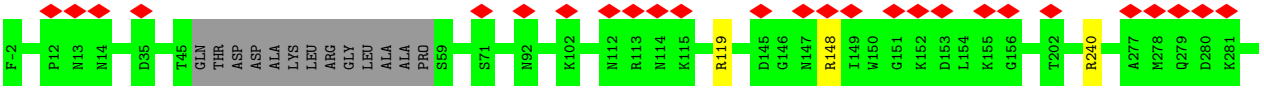


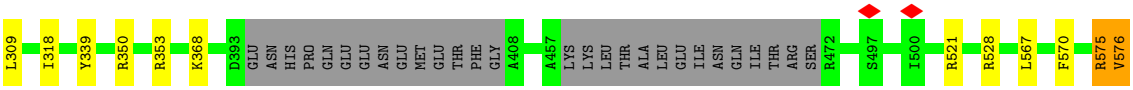


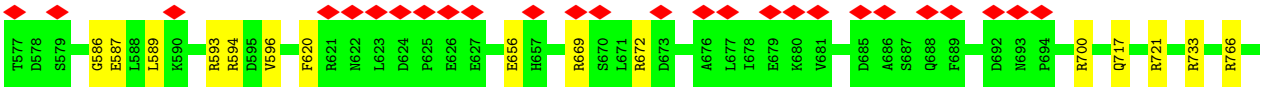
• Molecule 5: WD repeat-containing protein 35

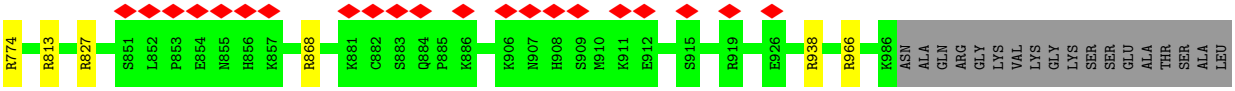
Chain E:

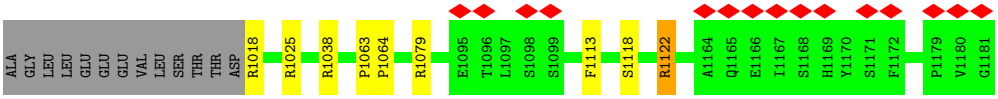






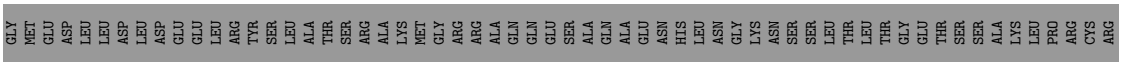


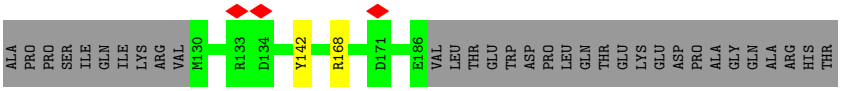




• Molecule 6: Intraflagellar transport protein 43 homolog

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242645	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.829	Depositor
Minimum map value	-2.661	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.532	Depositor
Recommended contour level	0.512	Depositor
Map size (Å)	310.86002, 240.21, 466.29	wwPDB
Map dimensions	22, 17, 33	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	14.130001, 14.13, 14.13	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.68	0/10866	0.96	26/14701 (0.2%)
2	B	0.69	1/11561 (0.0%)	1.01	49/15630 (0.3%)
3	C	0.68	0/9661	1.01	32/13051 (0.2%)
4	D	0.67	0/10784	0.96	44/14540 (0.3%)
5	E	0.66	0/9049	1.02	29/12229 (0.2%)
6	F	0.68	0/479	1.03	2/650 (0.3%)
All	All	0.68	1/52400 (0.0%)	0.99	182/70801 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	7
3	C	0	8
4	D	0	4
5	E	0	4
All	All	0	29

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	935	PRO	N-CD	8.15	1.59	1.47

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	61	TYR	CB-CG-CD2	-10.23	114.86	121.00
1	A	1086	PRO	CA-N-CD	-9.75	97.85	111.50
5	E	669	ARG	NE-CZ-NH2	9.39	124.99	120.30
4	D	18	TYR	CB-CG-CD2	-9.25	115.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	347	ARG	NE-CZ-NH2	9.17	124.89	120.30
1	A	528	ARG	NE-CZ-NH2	8.63	124.61	120.30
5	E	938	ARG	NE-CZ-NH2	8.60	124.60	120.30
4	D	997	ARG	NE-CZ-NH2	8.49	124.55	120.30
5	E	576	VAL	CA-CB-CG2	8.41	123.52	110.90
5	E	1122	ARG	NE-CZ-NH2	8.40	124.50	120.30
3	C	910	ARG	NE-CZ-NH2	8.34	124.47	120.30
3	C	189	ARG	NE-CZ-NH2	8.26	124.43	120.30
2	B	158	ARG	NE-CZ-NH2	8.11	124.35	120.30
2	B	1225	LEU	CB-CG-CD1	-8.10	97.23	111.00
2	B	307	ARG	NE-CZ-NH2	8.02	124.31	120.30
4	D	1044	ARG	NE-CZ-NH2	7.98	124.29	120.30
4	D	672	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	A	959	ARG	NE-CZ-NH2	7.71	124.16	120.30
1	A	829	ARG	NE-CZ-NH2	7.65	124.12	120.30
4	D	1007	ARG	NE-CZ-NH2	7.64	124.12	120.30
3	C	250	ARG	NE-CZ-NH2	7.64	124.12	120.30
5	E	521	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	A	753	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	B	60	ARG	NE-CZ-NH2	7.39	123.99	120.30
6	F	168	ARG	NE-CZ-NH2	7.35	123.97	120.30
3	C	684	ARG	NE-CZ-NH2	7.32	123.96	120.30
2	B	1404	ARG	NE-CZ-NH2	7.31	123.95	120.30
4	D	607	ARG	NE-CZ-NH2	7.20	123.90	120.30
4	D	981	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	A	1178	ARG	NE-CZ-NH2	7.17	123.89	120.30
5	E	593	ARG	NE-CZ-NH2	7.14	123.87	120.30
2	B	1128	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	1123	ARG	NE-CZ-NH2	7.11	123.86	120.30
5	E	1038	ARG	NE-CZ-NH2	7.09	123.85	120.30
3	C	647	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	A	878	ARG	NE-CZ-NH2	7.03	123.82	120.30
1	A	1239	ARG	NE-CZ-NH2	7.02	123.81	120.30
5	E	1079	ARG	NE-CZ-NH2	7.01	123.80	120.30
4	D	1228	ARG	NE-CZ-NH2	6.98	123.79	120.30
3	C	159	ARG	NE-CZ-NH2	6.97	123.78	120.30
2	B	1083	ARG	NE-CZ-NH2	6.96	123.78	120.30
4	D	1175	ARG	NE-CZ-NH2	6.90	123.75	120.30
3	C	453	ARG	NE-CZ-NH2	6.87	123.74	120.30
3	C	1179	ARG	NE-CZ-NH2	6.87	123.74	120.30
2	B	242	ARG	NE-CZ-NH2	6.82	123.71	120.30
2	B	871	ARG	NE-CZ-NH2	6.82	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	575	ARG	NE-CZ-NH2	6.79	123.69	120.30
4	D	103	ARG	NE-CZ-NH2	6.78	123.69	120.30
2	B	301	ARG	NE-CZ-NH2	6.78	123.69	120.30
5	E	669	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	141	ARG	NE-CZ-NH2	6.75	123.67	120.30
4	D	628	ARG	NE-CZ-NH2	6.69	123.64	120.30
2	B	936	ARG	NE-CZ-NH2	6.64	123.62	120.30
4	D	339	ARG	NE-CZ-NH2	6.62	123.61	120.30
4	D	301	ARG	NE-CZ-NH2	6.61	123.61	120.30
2	B	123	ARG	NE-CZ-NH2	6.54	123.57	120.30
3	C	171	ARG	NE-CZ-NH2	6.54	123.57	120.30
4	D	1050	ARG	NE-CZ-NH2	6.54	123.57	120.30
4	D	832	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	A	130	ARG	NE-CZ-NH2	6.52	123.56	120.30
5	E	353	ARG	NE-CZ-NH2	6.50	123.55	120.30
3	C	587	ARG	NE-CZ-NH2	6.49	123.54	120.30
2	B	816	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	A	1203	ARG	NE-CZ-NH2	6.39	123.49	120.30
3	C	877	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	B	560	ARG	NE-CZ-NH2	6.32	123.46	120.30
3	C	384	ARG	NE-CZ-NH2	6.29	123.44	120.30
4	D	616	ARG	NE-CZ-NH2	6.29	123.44	120.30
4	D	237	ARG	NE-CZ-NH2	6.27	123.44	120.30
2	B	1388	ARG	NE-CZ-NH2	6.23	123.41	120.30
4	D	128	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A	661	ARG	NE-CZ-NH2	6.21	123.41	120.30
3	C	1013	ARG	NE-CZ-NH2	6.20	123.40	120.30
2	B	1374	ARG	NE-CZ-NH2	6.18	123.39	120.30
5	E	350	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	A	48	ARG	NE-CZ-NH2	6.12	123.36	120.30
4	D	597	ARG	NE-CZ-NH2	6.12	123.36	120.30
3	C	890	ARG	NE-CZ-NH2	6.11	123.36	120.30
5	E	721	ARG	NE-CZ-NH2	6.09	123.35	120.30
2	B	1044	ARG	NE-CZ-NH2	6.07	123.33	120.30
2	B	757	ARG	NE-CZ-NH2	6.07	123.33	120.30
2	B	837	ARG	NE-CZ-NH2	6.04	123.32	120.30
5	E	700	ARG	NE-CZ-NH2	6.04	123.32	120.30
4	D	98	ARG	NE-CZ-NH2	6.03	123.32	120.30
5	E	240	ARG	NE-CZ-NH2	6.02	123.31	120.30
3	C	1059	ARG	NE-CZ-NH2	6.00	123.30	120.30
3	C	209	ARG	NE-CZ-NH2	6.00	123.30	120.30
5	E	868	ARG	NE-CZ-NH2	5.99	123.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1022	ARG	NE-CZ-NH2	5.98	123.29	120.30
4	D	476	ARG	NE-CZ-NH2	5.97	123.29	120.30
5	E	672	ARG	NE-CZ-NH2	5.97	123.29	120.30
2	B	141	THR	CA-CB-CG2	5.95	120.73	112.40
4	D	411	ARG	NE-CZ-NH2	5.94	123.27	120.30
3	C	1044	ALA	N-CA-CB	-5.94	101.79	110.10
4	D	32	ARG	NE-CZ-NH2	5.92	123.26	120.30
2	B	407	ARG	NE-CZ-NH2	5.91	123.26	120.30
3	C	759	ARG	NE-CZ-NH2	5.86	123.23	120.30
3	C	846	ARG	NE-CZ-NH2	5.82	123.21	120.30
2	B	279	ARG	NE-CZ-NH2	5.81	123.21	120.30
2	B	1277	ARG	NE-CZ-NH2	5.81	123.21	120.30
2	B	501	ARG	NE-CZ-NH2	5.80	123.20	120.30
2	B	1102	PHE	CB-CG-CD2	-5.80	116.74	120.80
5	E	1025	ARG	NE-CZ-NH2	5.78	123.19	120.30
5	E	119	ARG	NE-CZ-NH2	5.78	123.19	120.30
4	D	898	ARG	NE-CZ-NH2	5.77	123.19	120.30
2	B	505	ARG	NE-CZ-NH2	5.75	123.18	120.30
3	C	1178	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	A	464	ARG	NE-CZ-NH2	5.74	123.17	120.30
3	C	518	ARG	NE-CZ-NH2	5.74	123.17	120.30
5	E	966	ARG	NE-CZ-NH2	5.74	123.17	120.30
3	C	474	ARG	NE-CZ-NH2	5.74	123.17	120.30
4	D	1281	ARG	NE-CZ-NH2	5.73	123.16	120.30
5	E	594	ARG	NE-CZ-NH2	5.73	123.16	120.30
4	D	1015	ARG	NE-CZ-NH2	5.73	123.16	120.30
1	A	1036	TYR	CB-CG-CD1	-5.72	117.57	121.00
2	B	110	ARG	NE-CZ-NH2	5.71	123.15	120.30
2	B	347	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	B	982	ARG	NE-CZ-NH2	5.70	123.15	120.30
2	B	834	ARG	NE-CZ-NH2	5.69	123.15	120.30
4	D	691	ARG	NE-CZ-NH2	5.69	123.14	120.30
2	B	441	ARG	NE-CZ-NH2	5.67	123.14	120.30
2	B	897	ARG	NE-CZ-NH2	5.67	123.14	120.30
4	D	133	ARG	NE-CZ-NH2	5.65	123.13	120.30
4	D	723	ARG	NE-CZ-NH2	5.65	123.12	120.30
3	C	465	ARG	NE-CZ-NH2	5.62	123.11	120.30
2	B	1282	LEU	CB-CG-CD2	-5.62	101.45	111.00
2	B	1014	TYR	CB-CG-CD2	-5.61	117.63	121.00
2	B	1209	THR	CA-CB-CG2	-5.61	104.54	112.40
4	D	40	ARG	NE-CZ-NH2	5.59	123.09	120.30
5	E	528	ARG	NE-CZ-NH2	5.57	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	425	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	974	LEU	CB-CG-CD1	5.57	120.47	111.00
5	E	774	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	A	407	ARG	NE-CZ-NH2	5.55	123.07	120.30
2	B	1189	ARG	NE-CZ-NH2	5.54	123.07	120.30
2	B	1313	CYS	CA-CB-SG	-5.53	104.04	114.00
3	C	1196	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	A	828	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	1123	ARG	NE-CZ-NH1	-5.52	117.54	120.30
2	B	1260	ARG	NE-CZ-NH2	5.52	123.06	120.30
3	C	197	ARG	NE-CZ-NH2	5.51	123.05	120.30
2	B	475	ARG	NE-CZ-NH2	5.51	123.05	120.30
5	E	813	ARG	NE-CZ-NH2	5.51	123.05	120.30
2	B	1242	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	360	ARG	NE-CZ-NH2	5.49	123.05	120.30
3	C	979	ARG	NE-CZ-NH2	5.49	123.04	120.30
5	E	766	ARG	NE-CZ-NH2	5.46	123.03	120.30
4	D	655	ARG	NE-CZ-NH2	5.45	123.02	120.30
4	D	17	ARG	NE-CZ-NH2	5.40	123.00	120.30
2	B	253	ARG	NE-CZ-NH2	5.39	123.00	120.30
4	D	565	TYR	CB-CG-CD2	-5.39	117.77	121.00
6	F	142	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	1130	PHE	CB-CG-CD2	-5.33	117.07	120.80
4	D	1053	ARG	NE-CZ-NH2	5.32	122.96	120.30
2	B	867	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	910	ARG	NE-CZ-NH2	5.31	122.96	120.30
5	E	1018	ARG	NE-CZ-NH2	5.31	122.95	120.30
3	C	673	ARG	NE-CZ-NH2	5.29	122.95	120.30
5	E	148	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	A	844	ARG	NE-CZ-NH2	5.28	122.94	120.30
2	B	1210	LYS	CA-CB-CG	5.26	124.97	113.40
4	D	858	ARG	NE-CZ-NH2	5.24	122.92	120.30
4	D	475	ARG	NE-CZ-NH2	5.24	122.92	120.30
4	D	1177	ARG	NE-CZ-NH2	5.23	122.91	120.30
2	B	1238	ALA	CB-CA-C	5.21	117.92	110.10
4	D	718	ARG	NE-CZ-NH2	5.21	122.90	120.30
3	C	362	ARG	NE-CZ-NH2	5.19	122.89	120.30
3	C	526	ARG	NE-CZ-NH2	5.18	122.89	120.30
4	D	926	ARG	NE-CZ-NH2	5.17	122.89	120.30
2	B	848	ARG	NE-CZ-NH2	5.17	122.88	120.30
3	C	61	TYR	CA-CB-CG	5.17	123.22	113.40
2	B	576	ARG	NE-CZ-NH2	5.16	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	315	ARG	NE-CZ-NH2	5.13	122.86	120.30
2	B	1141	ARG	NE-CZ-NH2	5.11	122.86	120.30
4	D	1182	ARG	NE-CZ-NH2	5.11	122.86	120.30
4	D	1311	ARG	NE-CZ-NH2	5.10	122.85	120.30
2	B	760	ARG	NE-CZ-NH2	5.09	122.85	120.30
4	D	297	ARG	NE-CZ-NH2	5.05	122.83	120.30
4	D	250	ARG	NE-CZ-NH2	5.05	122.83	120.30
5	E	620	PHE	CB-CG-CD2	-5.04	117.27	120.80
5	E	827	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	A	1086	PRO	N-CD-CG	5.02	110.73	103.20

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1102	TYR	Sidechain
1	A	1122	TYR	Sidechain
1	A	781	TYR	Sidechain
1	A	80	TYR	Sidechain
1	A	901	TYR	Sidechain
1	A	961	PHE	Sidechain
2	B	1133	PHE	Sidechain
2	B	1136	HIS	Sidechain
2	B	1237	PHE	Sidechain
2	B	1385	HIS	Sidechain
2	B	216	TYR	Sidechain
2	B	257	TYR	Sidechain
2	B	976	HIS	Sidechain
3	C	288	TYR	Sidechain
3	C	453	ARG	Sidechain
3	C	465	ARG	Sidechain
3	C	61	TYR	Sidechain
3	C	814	TYR	Sidechain
3	C	90	TYR	Sidechain
3	C	966	PHE	Sidechain
3	C	979	ARG	Sidechain
4	D	13	TYR	Sidechain
4	D	347	TYR	Sidechain
4	D	565	TYR	Sidechain
4	D	732	TYR	Sidechain
5	E	1122	ARG	Sidechain
5	E	339	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	E	575	ARG	Sidechain
5	E	733	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	10643	0	10570	16	0
2	B	11319	0	11127	38	0
3	C	9447	0	9382	9	0
4	D	10593	0	10665	6	0
5	E	8863	0	8810	14	0
6	F	470	0	441	0	0
All	All	51335	0	50995	80	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 (80) 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)
1:A:974:LEU:CB	1:A:983:ALA:HB2	2.15	0.76
1:A:974:LEU:HB2	1:A:983:ALA:HB2	1.73	0.71
2:B:1209:THR:HG23	2:B:1221:ALA:HB1	1.74	0.70
2:B:132:LEU:HD23	2:B:136:GLY:O	1.93	0.68
2:B:1238:ALA:HB3	2:B:1272:PHE:CZ	2.33	0.64
3:C:865:TYR:HB2	3:C:888:ALA:HB2	1.80	0.63
2:B:1209:THR:HG22	2:B:1237:PHE:CZ	2.36	0.60
2:B:1225:LEU:CD1	2:B:1237:PHE:CZ	2.85	0.60
2:B:1225:LEU:HD11	2:B:1237:PHE:CZ	2.37	0.59
2:B:858:MET:HE1	2:B:861:ASP:OD2	2.02	0.59
2:B:1209:THR:HG22	2:B:1237:PHE:CE2	2.37	0.59
2:B:934:VAL:HB	2:B:935:PRO:HD3	1.86	0.58
2:B:858:MET:CE	2:B:861:ASP:OD2	2.52	0.57
5:E:576:VAL:HG22	5:E:587:GLU:CG	2.34	0.57
2:B:880:GLN:NE2	2:B:903:THR:HG22	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1210:LYS:HE2	2:B:1236:PHE:CG	2.41	0.56
2:B:1225:LEU:HD11	2:B:1237:PHE:CE1	2.42	0.55
4:D:288:PHE:O	4:D:292:THR:HG23	2.08	0.53
5:E:576:VAL:HG22	5:E:587:GLU:HA	1.89	0.53
1:A:974:LEU:HB3	1:A:983:ALA:HB2	1.91	0.53
2:B:876:ASN:HD21	2:B:903:THR:HG21	1.74	0.53
2:B:1422:ALA:HA	2:B:1425:ARG:HD2	1.91	0.53
1:A:704:VAL:HG22	2:B:882:ALA:HA	1.91	0.52
1:A:901:TYR:CZ	1:A:905:LYS:HE3	2.45	0.52
2:B:1210:LYS:HE2	2:B:1236:PHE:CD2	2.45	0.52
2:B:1357:ILE:HD11	2:B:1385:HIS:CE1	2.44	0.52
1:A:1133:TYR:CD1	1:A:1297:PHE:CZ	2.99	0.51
2:B:1237:PHE:HA	2:B:1240:VAL:H	1.74	0.51
5:E:567:LEU:HB2	5:E:596:VAL:HG21	1.93	0.51
3:C:865:TYR:CB	3:C:888:ALA:HB2	2.40	0.50
2:B:631:GLU:H	2:B:631:GLU:CD	2.14	0.50
5:E:587:GLU:CD	5:E:589:LEU:HD23	2.32	0.50
5:E:576:VAL:HG22	5:E:587:GLU:HG3	1.94	0.49
2:B:988:VAL:HG13	2:B:1000:ALA:HB1	1.94	0.49
2:B:1294:ILE:HG23	2:B:1300:TYR:CZ	2.48	0.49
1:A:1080:GLY:HA3	1:A:1086:PRO:HD3	1.95	0.48
3:C:757:TRP:CD1	5:E:717:GLN:HG2	2.49	0.48
3:C:757:TRP:CG	5:E:717:GLN:HG2	2.48	0.48
2:B:129:LEU:HD21	2:B:203:LEU:HD22	1.95	0.48
2:B:1102:PHE:HB3	2:B:1132:PHE:CE1	2.49	0.47
1:A:974:LEU:HD13	1:A:983:ALA:HA	1.96	0.47
5:E:309:LEU:HD11	5:E:318:ILE:HD11	1.97	0.47
5:E:570:PHE:CE1	5:E:586:GLY:C	2.88	0.47
1:A:581:VAL:HG23	1:A:604:VAL:CG2	2.46	0.46
1:A:239:TRP:CZ2	1:A:245:ILE:HD11	2.50	0.46
1:A:581:VAL:HG23	1:A:604:VAL:HG21	1.97	0.46
5:E:576:VAL:CG2	5:E:587:GLU:HA	2.46	0.46
2:B:1209:THR:HG23	2:B:1221:ALA:CB	2.45	0.46
2:B:1209:THR:CG2	2:B:1237:PHE:CZ	2.99	0.46
2:B:1210:LYS:HG2	2:B:1237:PHE:CD1	2.51	0.45
2:B:1102:PHE:CD1	2:B:1132:PHE:CG	3.05	0.45
5:E:1113:PHE:CG	5:E:1118:SER:HB3	2.53	0.44
2:B:1132:PHE:CZ	2:B:1136:HIS:CE1	3.05	0.44
3:C:834:LEU:HB3	3:C:860:PHE:CE2	2.52	0.44
2:B:1209:THR:CG2	2:B:1237:PHE:HZ	2.31	0.44
3:C:169:ILE:HD13	3:C:266:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1102:PHE:HA	2:B:1132:PHE:CZ	2.53	0.43
5:E:570:PHE:HE1	5:E:586:GLY:O	2.01	0.43
2:B:1286:TYR:CZ	2:B:1309:GLU:HB3	2.53	0.43
4:D:937:CYS:SG	4:D:961:LEU:HD11	2.59	0.43
1:A:974:LEU:HD13	1:A:983:ALA:CA	2.49	0.43
2:B:292:VAL:HG22	2:B:302:PHE:CD2	2.54	0.42
5:E:368:LYS:HZ1	5:E:656:GLU:CD	2.23	0.42
3:C:576:LEU:C	3:C:577:ASN:HD22	2.23	0.42
4:D:249:LEU:CD1	4:D:276:THR:HG21	2.49	0.42
1:A:240:TYR:CD1	1:A:303:LEU:HD13	2.55	0.42
4:D:516:GLN:HB3	4:D:872:GLN:HA	2.02	0.41
1:A:1:MET:CE	1:A:348:THR:HG22	2.50	0.41
1:A:501:TYR:CZ	1:A:503:GLU:HB3	2.55	0.41
2:B:98:MET:SD	2:B:138:VAL:CG2	3.09	0.41
2:B:1282:LEU:HG	2:B:1286:TYR:CD2	2.55	0.41
3:C:1058:TYR:CG	3:C:1092:HIS:HA	2.56	0.41
2:B:286:ILE:HD11	2:B:339:LEU:HD13	2.02	0.41
2:B:818:ASP:N	2:B:818:ASP:OD1	2.53	0.41
4:D:292:THR:HG21	4:D:313:LEU:HB2	2.02	0.41
4:D:347:TYR:CZ	4:D:363:GLY:HA3	2.56	0.41
5:E:1063:PRO:HA	5:E:1064:PRO:HD3	1.99	0.41
1:A:240:TYR:CE1	1:A:303:LEU:HD13	2.57	0.40
3:C:788:GLY:HA2	3:C:818:LEU:HD22	2.03	0.40
2:B:1209:THR:HG23	2:B:1221:ALA:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1340/1357 (99%)	1305 (97%)	35 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1424/1477 (96%)	1373 (96%)	51 (4%)	0	100	100
3	C	1168/1241 (94%)	1128 (97%)	40 (3%)	0	100	100
4	D	1314/1500 (88%)	1277 (97%)	37 (3%)	0	100	100
5	E	1102/1184 (93%)	1052 (96%)	50 (4%)	0	100	100
6	F	55/209 (26%)	55 (100%)	0	0	100	100
All	All	6403/6968 (92%)	6190 (97%)	213 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1156/1171 (99%)	1156 (100%)	0	100	100
2	B	1213/1261 (96%)	1209 (100%)	4 (0%)	92	97
3	C	1029/1091 (94%)	1027 (100%)	2 (0%)	93	98
4	D	1137/1279 (89%)	1137 (100%)	0	100	100
5	E	961/1020 (94%)	961 (100%)	0	100	100
6	F	53/181 (29%)	53 (100%)	0	100	100
All	All	5549/6003 (92%)	5543 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	303	TRP
2	B	606	MET
2	B	651	HIS
2	B	659	ARG
3	C	597	TYR
3	C	946	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
2	B	532	ASN
2	B	1138	GLN
2	B	1385	HIS
5	E	1116	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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.

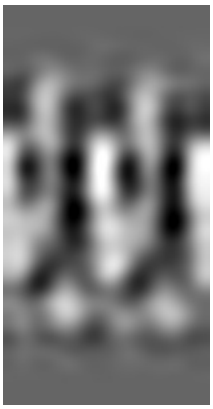
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4304. 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

6.1.1 Primary map



X

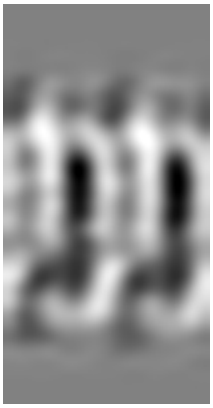
Y

Z

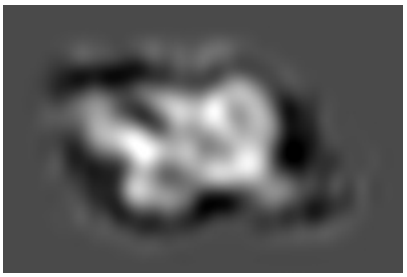
The images above show the map projected in three orthogonal directions.

6.2 Central slices

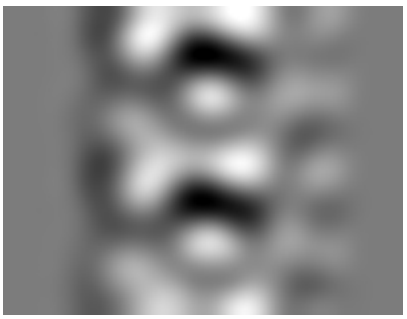
6.2.1 Primary map



X Index: 11



Y Index: 8

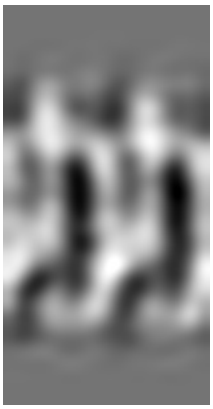


Z Index: 16

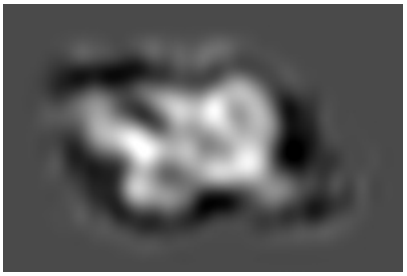
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 10



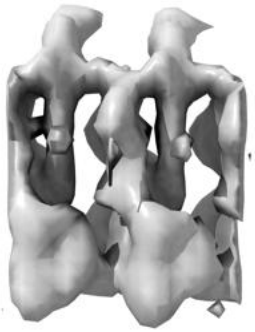
Y Index: 8

Z Index: 18

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 0.512. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

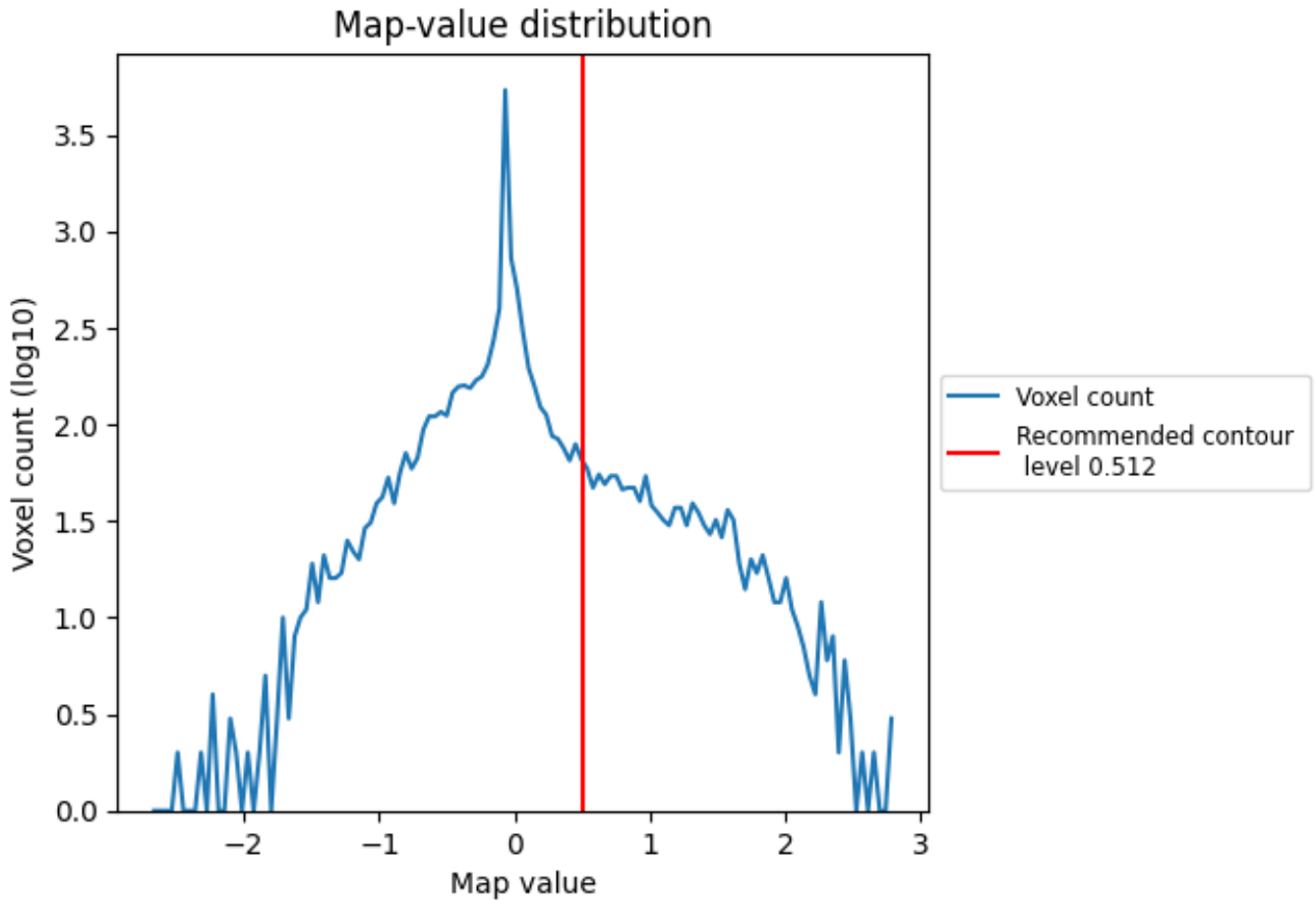
6.5 Mask visualisation (i)

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

7 Map analysis

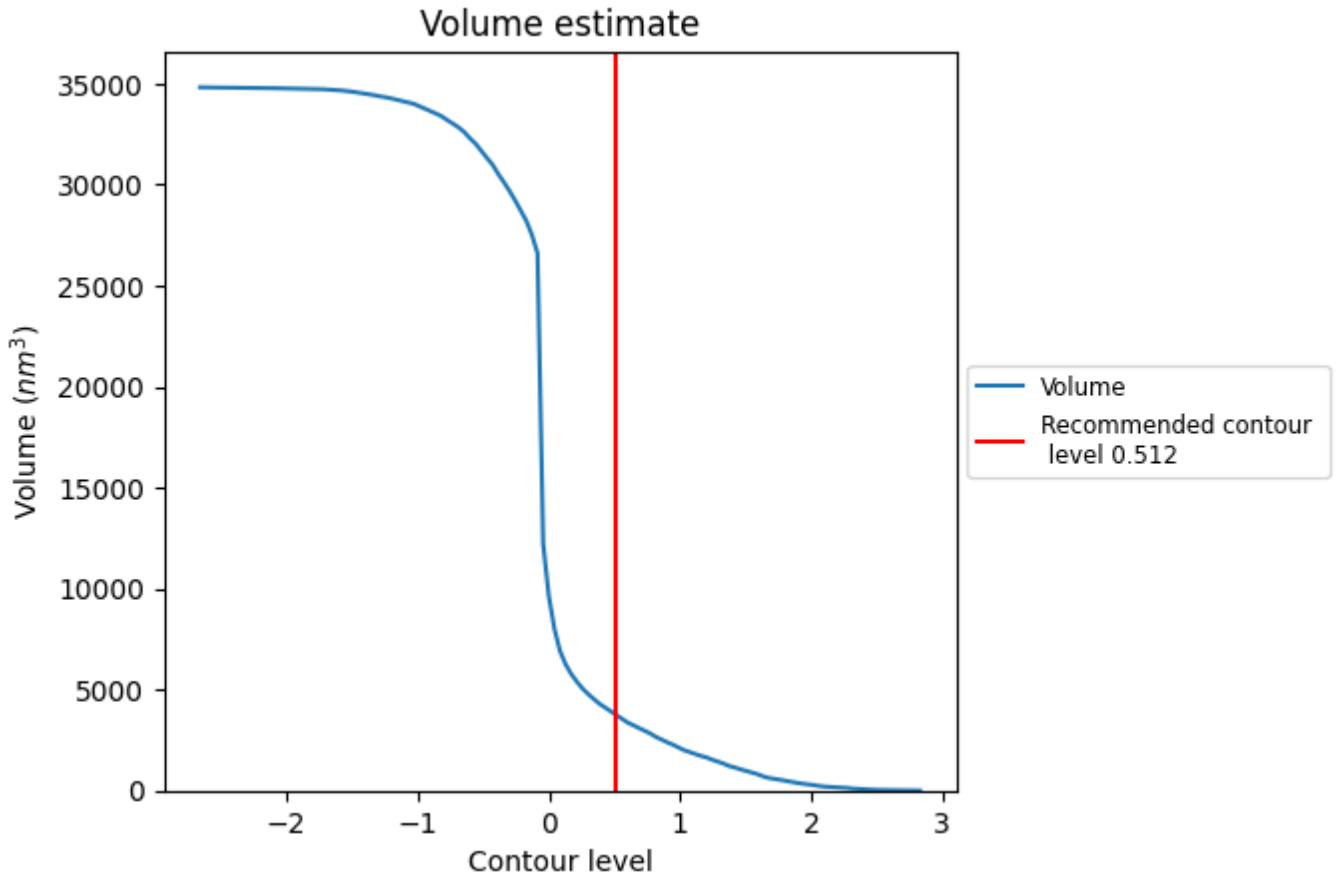
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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



The volume at the recommended contour level is 3741 nm^3; this corresponds to an approximate mass of 3380 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

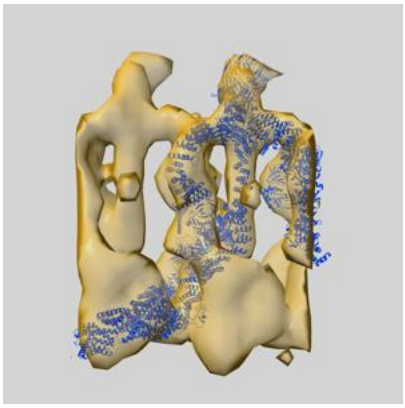
8 Fourier-Shell correlation (i)

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

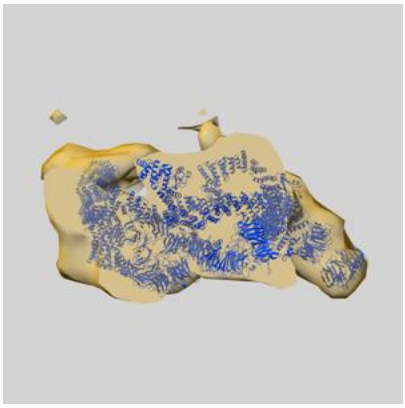
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4304 and PDB model 8BBG. Per-residue inclusion information can be found in section 3 on page 6.

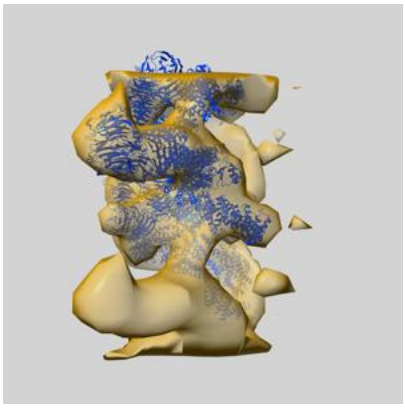
9.1 Map-model overlay



X



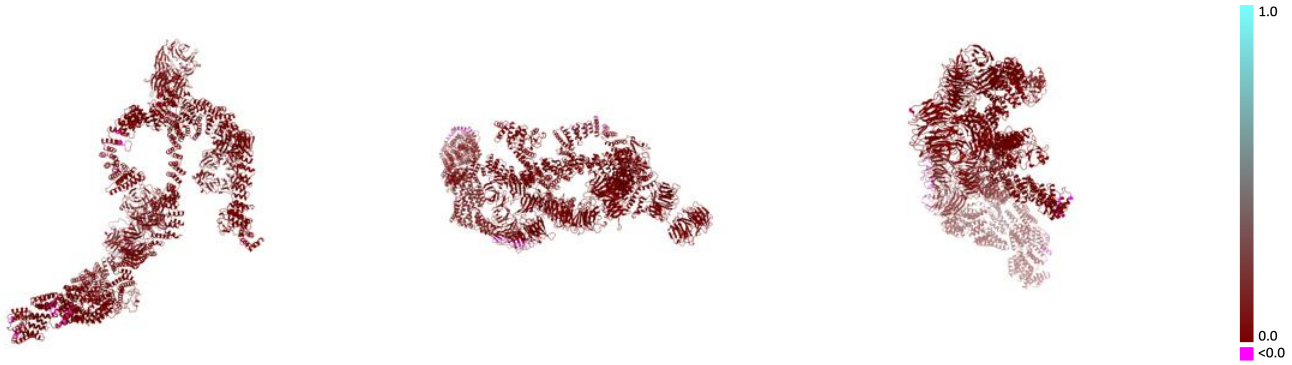
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.512 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.

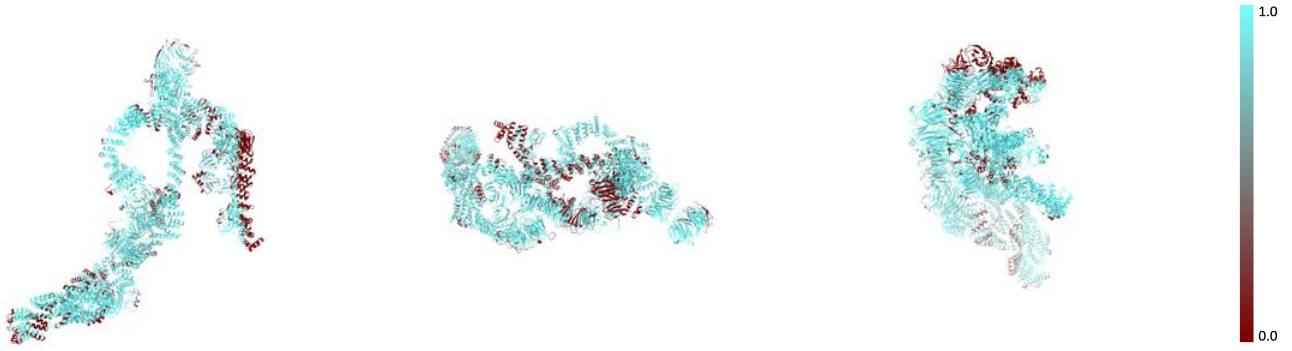
9.2 Q-score mapped to coordinate model



X Y Z

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.

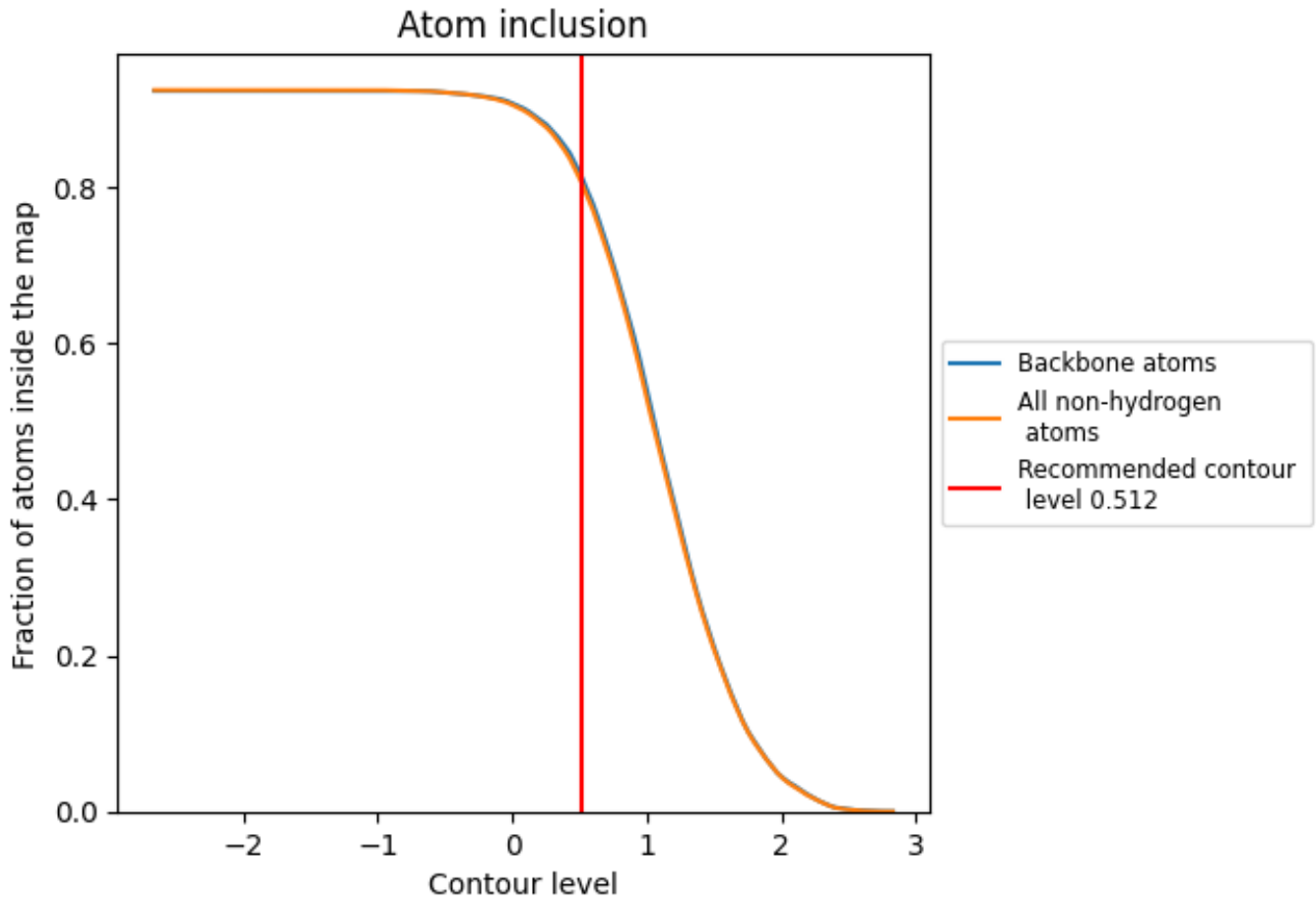
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.512).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.512) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8075	0.0010
A	0.7068	-0.0000
B	0.7284	0.0030
C	0.9295	0.0000
D	0.8006	0.0010
E	0.9011	0.0020
F	0.9286	0.0000