



Full wwPDB EM Validation Report ⓘ

Aug 6, 2025 – 05:12 PM JST

PDB ID : 9LVJ / pdb_00009lvj
EMDB ID : EMD-63421
Title : Cryo-EM structure of Sestrin2 bound human GATOR2 complex
Authors : Su, M.-Y.
Deposited on : 2025-02-12
Resolution : 3.82 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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

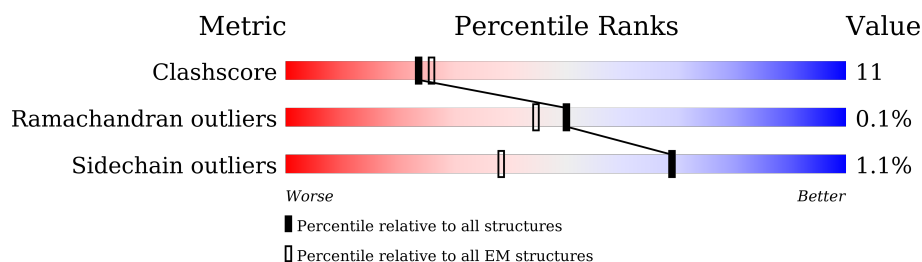
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.82 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	875	
1	B	875	
1	K	875	
1	L	875	
2	C	790	
2	M	790	
3	D	974	
3	N	974	

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Mol	Chain	Length	Quality of chain
4	E	421	
4	F	421	
4	G	421	
4	O	421	
4	P	421	
4	Q	421	
5	H	368	
5	R	368	
6	U	480	
6	V	480	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 47837 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 GATOR2 complex protein MIOS.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	744	Total	C	N	O	S	0	0
			4468	2761	854	833	20		
1	B	724	Total	C	N	O		0	0
			3726	2253	742	731			
1	K	737	Total	C	N	O	S	0	0
			4204	2597	814	774	19		
1	L	730	Total	C	N	O		0	0
			3665	2193	742	730			

- Molecule 2 is a protein called GATOR2 complex protein WDR24.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	573	Total	C	N	O	S	0	0
			4210	2667	769	736	38		
2	M	572	Total	C	N	O	S	0	0
			4115	2613	768	702	32		

- Molecule 3 is a protein called GATOR2 complex protein WDR59.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	273	Total	C	N	O	S	0	0
			1843	1169	340	316	18		
3	N	269	Total	C	N	O	S	0	0
			1788	1125	333	311	19		

- Molecule 4 is a protein called Isoform B of Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	302	Total	C	N	O	S	0	0
			2099	1347	378	361	13		
4	F	301	Total	C	N	O		0	0
			1490	888	301	301			

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	303	Total	C	N	O	S	0	0
			2299	1456	411	417	15		
4	O	302	Total	C	N	O	S	0	0
			2057	1326	383	340	8		
4	P	307	Total	C	N	O		0	0
			1519	905	307	307			
4	Q	304	Total	C	N	O	S	0	0
			2293	1455	415	407	16		

- Molecule 5 is a protein called Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	284	Total	C	N	O	S	0	0
			1802	1142	331	321	8		
5	R	285	Total	C	N	O	S	0	0
			1616	1010	311	294	1		

- Molecule 6 is a protein called Sestrin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	313	Total	C	N	O	S	0	0
			2350	1530	404	407	9		
6	V	307	Total	C	N	O	S	0	0
			2261	1467	395	390	9		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	4	Total	Zn	0
			4	4	
7	B	4	Total	Zn	0
			4	4	
7	C	4	Total	Zn	0
			4	4	
7	D	4	Total	Zn	0
			4	4	
7	K	4	Total	Zn	0
			4	4	
7	L	4	Total	Zn	0
			4	4	

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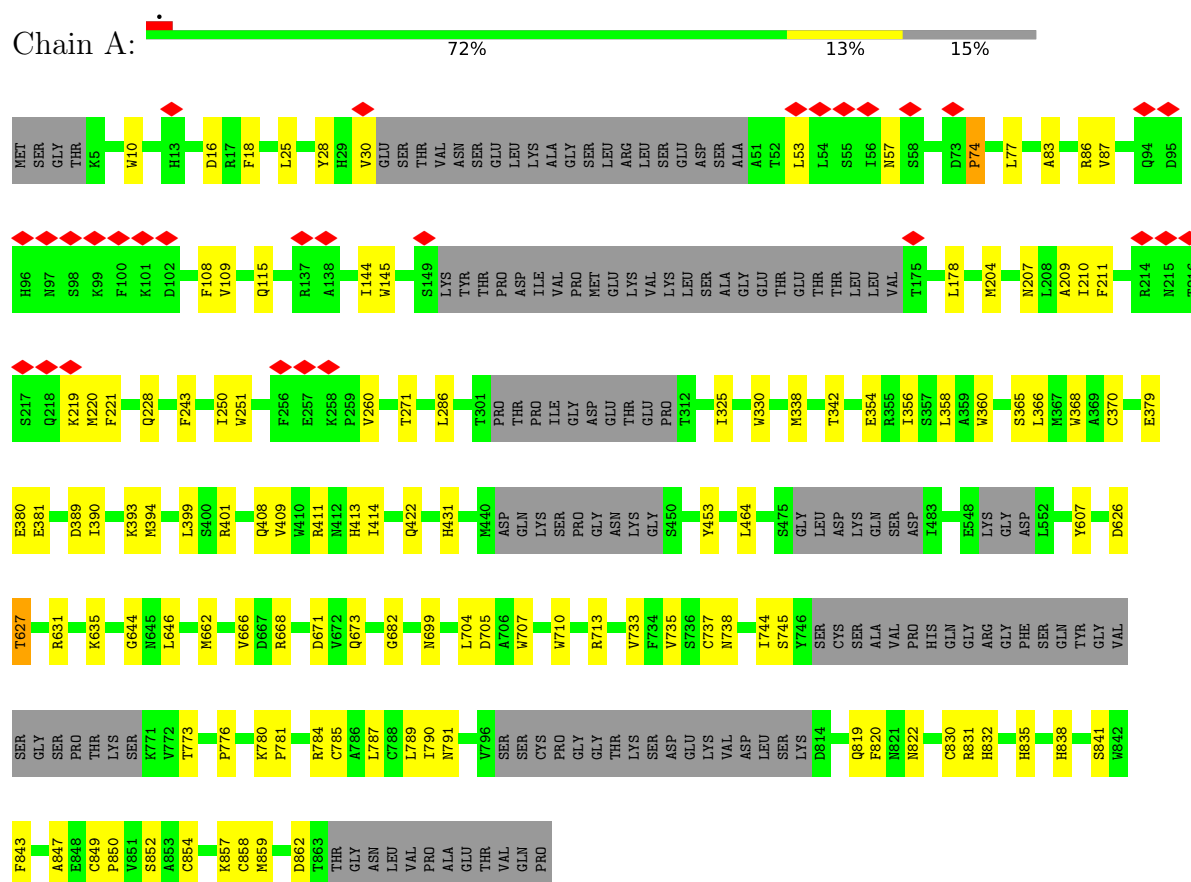
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Mol	Chain	Residues	Atoms		AltConf
7	M	4	Total 4	Zn 4	0
7	N	4	Total 4	Zn 4	0

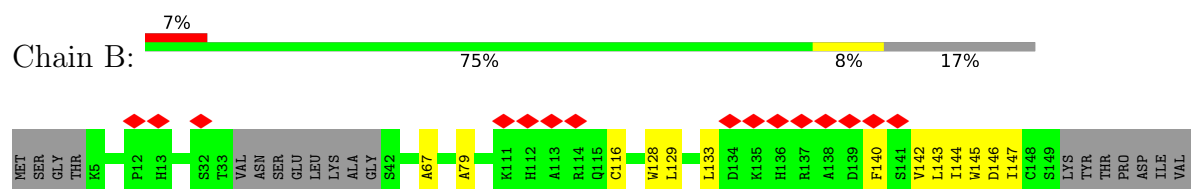
3 Residue-property plots

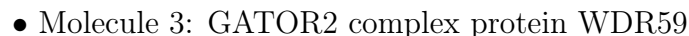
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

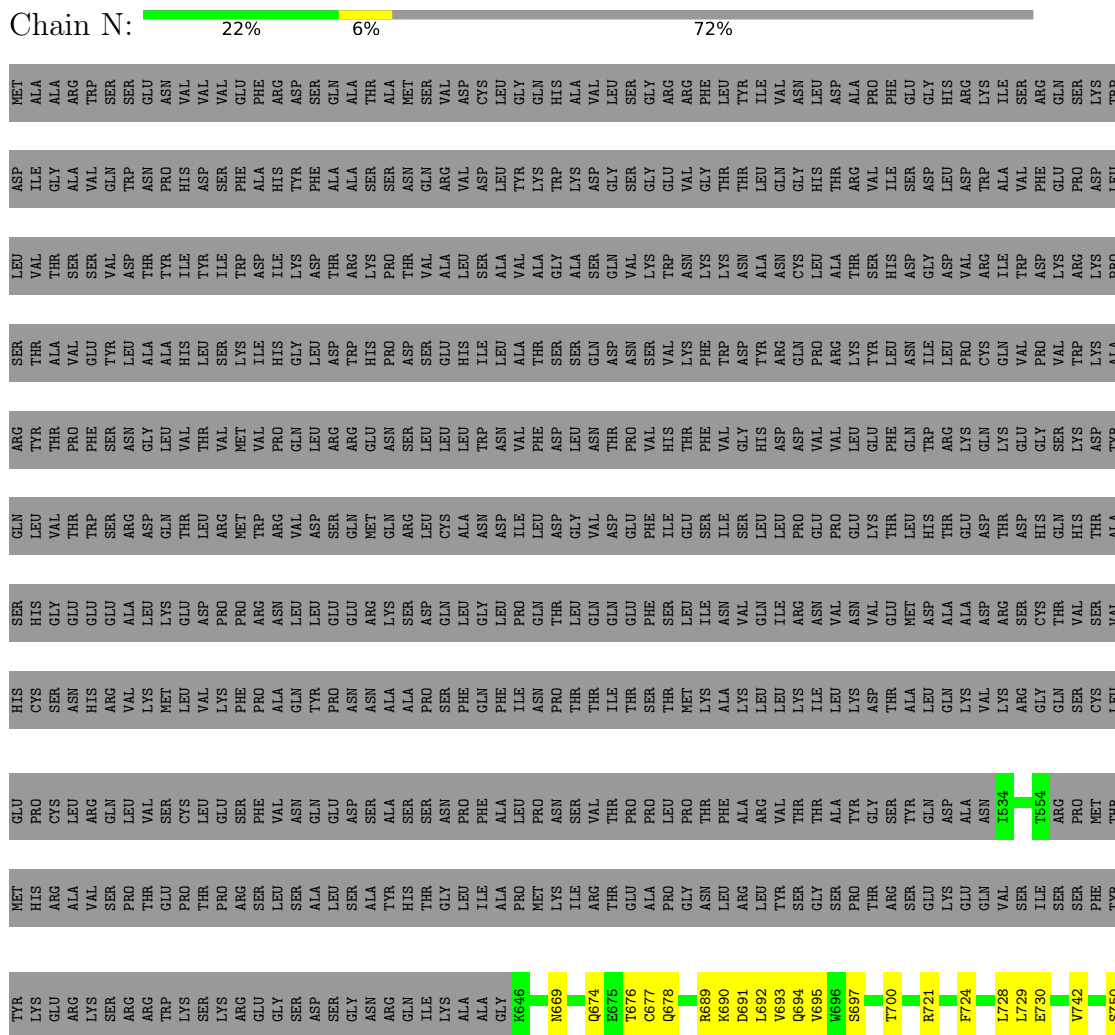
• Molecule 1: GATOR2 complex protein MIOS

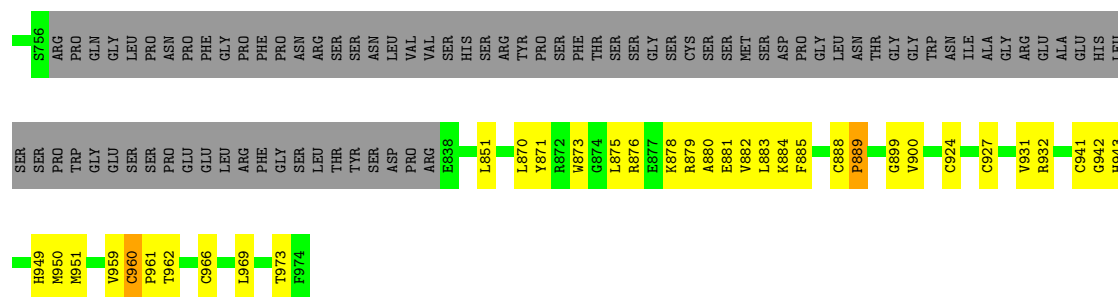


• Molecule 1: GATOR2 complex protein MIOS



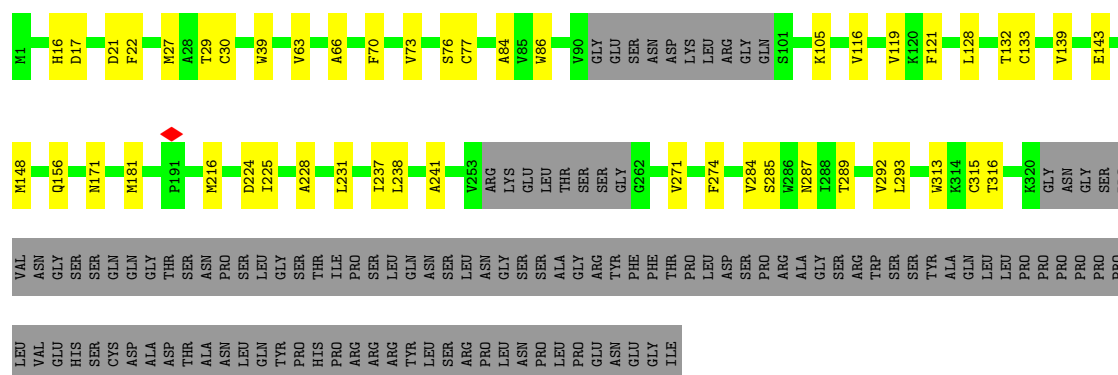
[illegible]





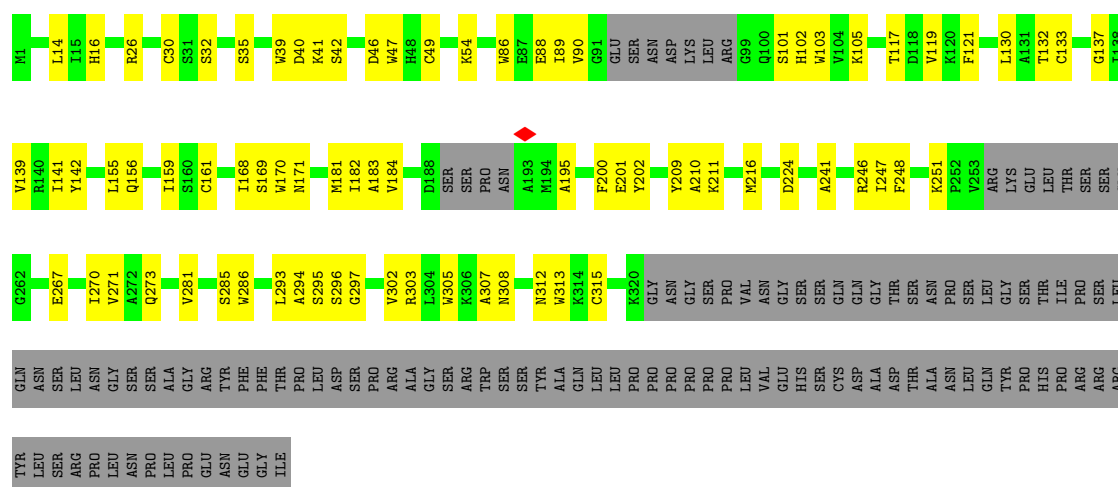
• Molecule 4: Isoform B of Nucleoporin SEH1

Chain E: 60% 11% 28%



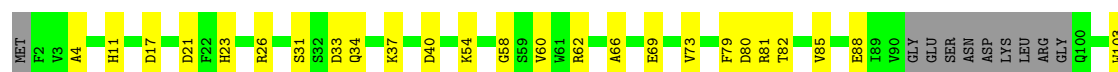
• Molecule 4: Isoform B of Nucleoporin SEH1

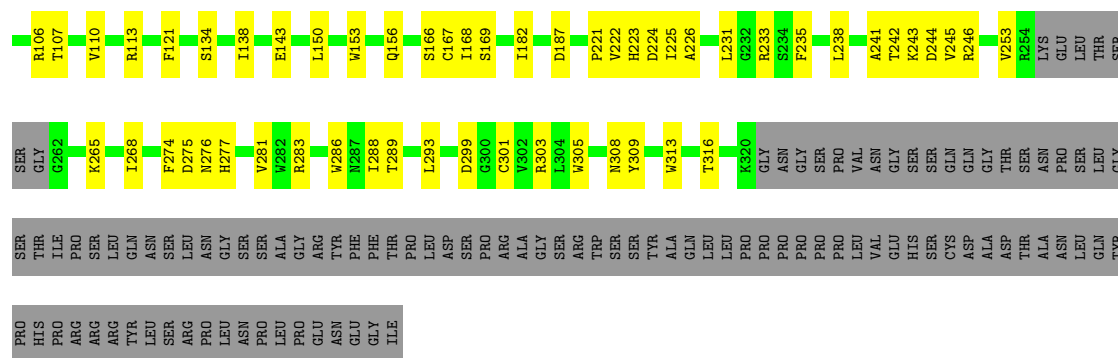
Chain F: 53% 19% 29%



• Molecule 4: Isoform B of Nucleoporin SEH1

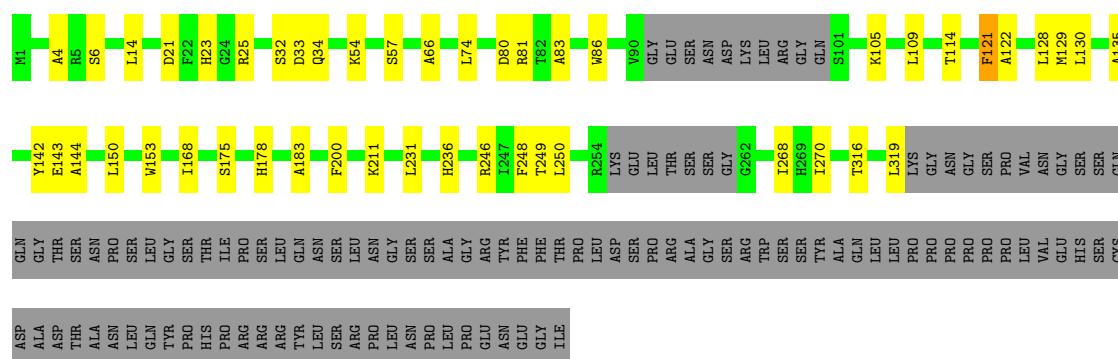
Chain G: 53% 19% 28%





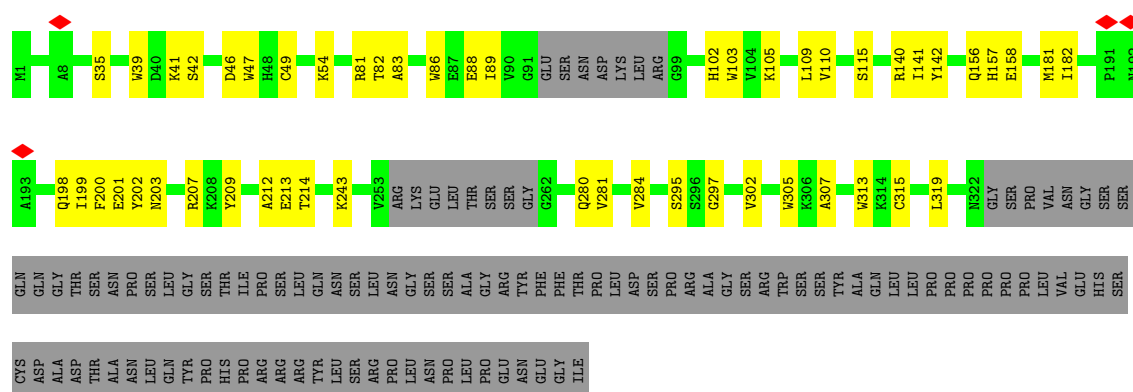
• Molecule 4: Isoform B of Nucleoporin SEH1

Chain O: 61% 11% 28%



• Molecule 4: Isoform B of Nucleoporin SEH1

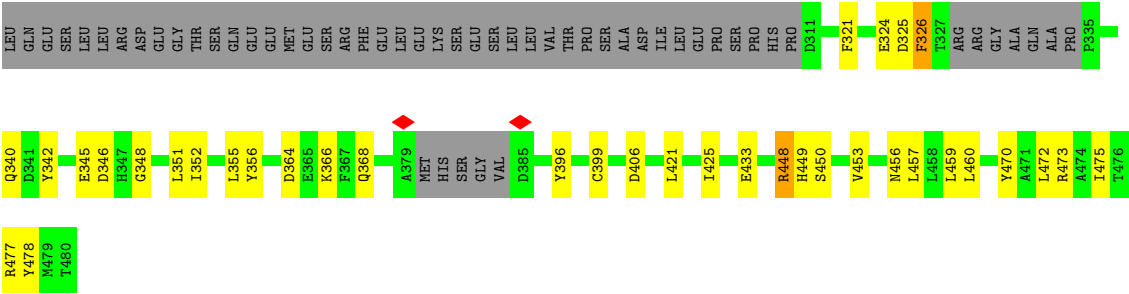
Chain P: 61% 12% 27%



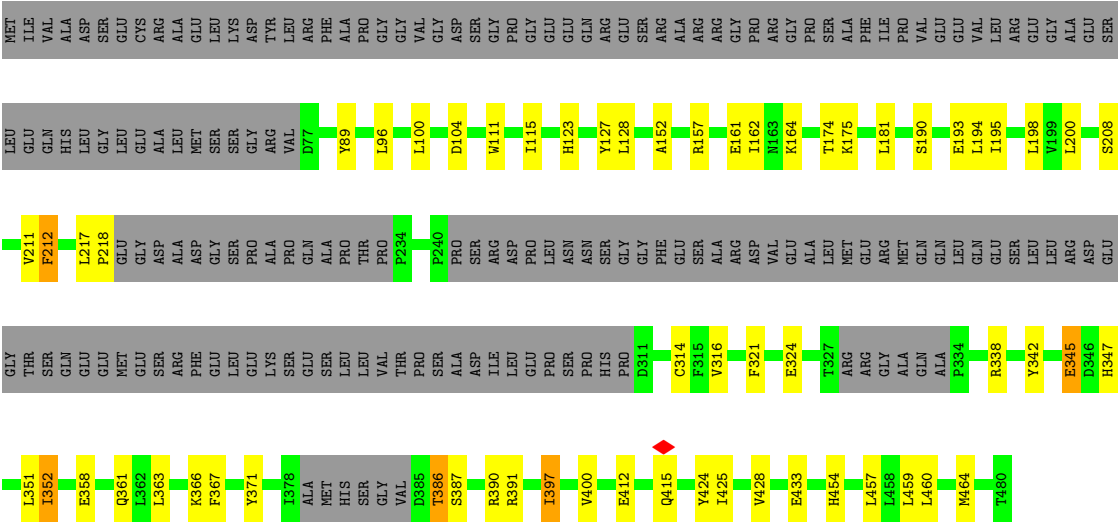
• Molecule 4: Isoform B of Nucleoporin SEH1

Chain Q: 59% 12% 28%





• Molecule 6: Sestrin-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190375	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.41	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.649	Depositor
Minimum map value	-0.175	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.101	Depositor
Map size (\AA)	493.0, 493.0, 493.0	wwPDB
Map dimensions	580, 580, 580	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.19	0/4525	0.40	1/6228 (0.0%)
1	B	0.18	0/3748	0.46	3/5217 (0.1%)
1	K	0.18	0/4255	0.38	1/5881 (0.0%)
1	L	0.17	0/3663	0.36	1/5088 (0.0%)
2	C	0.22	0/4317	0.48	1/5890 (0.0%)
2	M	0.26	0/4223	0.49	2/5775 (0.0%)
3	D	0.22	0/1883	0.46	0/2571
3	N	0.35	2/1825 (0.1%)	0.52	3/2495 (0.1%)
4	E	0.20	0/2157	0.41	0/2965
4	F	0.11	0/1486	0.26	0/2065
4	G	0.23	0/2361	0.44	0/3224
4	O	0.19	0/2113	0.36	0/2907
4	P	0.13	0/1516	0.32	0/2108
4	Q	0.22	0/2355	0.40	0/3214
5	H	0.19	0/1844	0.45	0/2547
5	R	0.15	0/1647	0.34	0/2286
6	U	0.20	0/2416	0.47	2/3299 (0.1%)
6	V	0.24	0/2325	0.45	0/3181
All	All	0.21	2/48659 (0.0%)	0.43	14/66941 (0.0%)

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
6	U	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	960	CYS	N-CA	6.06	1.54	1.46
3	N	960	CYS	CA-CB	5.84	1.62	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	780	LYS	CA-C-N	14.56	138.03	119.84
1	B	780	LYS	C-N-CA	14.56	138.03	119.84
1	K	74	PRO	CA-N-CD	-9.09	98.77	111.50
3	N	960	CYS	CA-CB-SG	9.03	135.18	114.40
1	A	74	PRO	CA-N-CD	-9.00	98.89	111.50
1	L	74	PRO	CA-N-CD	-8.99	98.92	111.50
2	M	107	PRO	CA-N-CD	-8.30	100.38	112.00
1	B	725	PRO	CA-N-CD	-8.13	100.62	112.00
2	C	294	GLU	CA-CB-CG	6.19	126.48	114.10
3	N	959	VAL	CA-C-N	5.79	135.93	121.80
3	N	959	VAL	C-N-CA	5.79	135.93	121.80
6	U	216	ILE	CA-C-N	5.26	130.93	120.94
6	U	216	ILE	C-N-CA	5.26	130.93	120.94
2	M	723	LYS	CB-CG-CD	5.22	123.30	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	U	448	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	4468	0	3028	97	0
1	B	3726	0	1854	56	0
1	K	4204	0	2561	55	0
1	L	3665	0	1672	47	0
2	C	4210	0	3777	103	0
2	M	4115	0	3624	100	0
3	D	1843	0	1564	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1788	0	1477	46	0
4	E	2099	0	1783	35	0
4	F	1490	0	685	42	0
4	G	2299	0	2157	59	0
4	O	2057	0	1686	31	0
4	P	1519	0	698	26	0
4	Q	2293	0	2151	50	0
5	H	1802	0	1370	48	0
5	R	1616	0	971	15	0
6	U	2350	0	2123	56	0
6	V	2261	0	1987	50	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
7	D	4	0	0	0	0
7	K	4	0	0	0	0
7	L	4	0	0	0	0
7	M	4	0	0	0	0
7	N	4	0	0	1	0
All	All	47837	0	35168	883	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 11.

All (883) 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)
6:V:162:ILE:CD1	6:V:181:LEU:HD11	1.23	1.60
6:V:162:ILE:CD1	6:V:181:LEU:CD1	2.01	1.36
1:B:780:LYS:CB	1:B:781:PRO:HD3	1.44	1.35
6:V:162:ILE:HD11	6:V:181:LEU:CD1	1.70	1.18
1:B:780:LYS:CB	1:B:781:PRO:CD	2.21	1.17
3:N:960:CYS:SG	7:N:1004:ZN:ZN	1.39	1.11
6:V:162:ILE:HD13	6:V:181:LEU:HD11	1.33	1.07
6:V:162:ILE:HD12	6:V:181:LEU:HD11	1.17	1.06
2:M:445:VAL:HG23	2:M:652:MET:HE1	1.40	0.99
6:V:162:ILE:HD11	6:V:181:LEU:HD12	1.46	0.97
1:A:74:PRO:HG2	1:A:77:LEU:CB	1.95	0.96
2:M:107:PRO:HD2	2:M:108:SER:H	1.38	0.88
6:V:162:ILE:HD13	6:V:181:LEU:CD1	1.96	0.85
1:L:145:TRP:HA	1:L:178:LEU:H	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:189:GLN:NE2	2:C:202:MET:SD	2.51	0.83
1:B:710:TRP:HA	1:B:713:ARG:HE	1.44	0.83
2:M:207:ASN:C	2:M:207:ASN:HD22	1.86	0.83
2:M:207:ASN:ND2	2:M:207:ASN:O	2.11	0.83
4:Q:7:ILE:HD11	4:Q:47:TRP:HD1	1.44	0.83
5:H:113:HIS:HD2	5:H:114:PRO:HD2	1.44	0.82
1:K:397:ARG:NH1	1:K:416:ALA:O	2.13	0.81
2:C:721:HIS:ND1	2:C:736:CYS:SG	2.54	0.80
1:B:781:PRO:HD2	3:D:894:LYS:O	1.82	0.80
2:M:722:CYS:HB3	2:M:736:CYS:SG	2.21	0.79
1:A:389:ASP:OD1	1:A:390:ILE:N	2.16	0.79
3:D:950:MET:SD	3:D:950:MET:N	2.54	0.78
1:B:735:VAL:HA	3:D:898:PHE:HA	1.64	0.78
2:M:760:CYS:SG	2:M:785:HIS:ND1	2.56	0.77
6:V:371:TYR:O	6:V:390:ARG:NH1	2.17	0.77
2:C:342:GLY:HA2	4:G:283:ARG:HE	1.50	0.77
1:K:771:LYS:NZ	4:Q:148:MET:O	2.15	0.77
2:C:127:CYS:SG	2:C:128:PHE:N	2.57	0.77
1:B:780:LYS:N	3:D:895:GLY:HA2	2.01	0.76
6:V:397:ILE:HD12	6:V:459:LEU:HD22	1.67	0.76
1:B:742:LYS:HE3	1:B:743:SER:H	1.50	0.76
3:N:931:VAL:O	3:N:932:ARG:NH1	2.20	0.75
1:A:390:ILE:HD12	1:A:393:LYS:HE2	1.68	0.75
4:E:284:VAL:HG13	4:E:293:LEU:HD21	1.67	0.74
4:Q:7:ILE:HD11	4:Q:47:TRP:CD1	2.22	0.74
2:M:718:ASN:HB3	2:M:725:PRO:HA	1.67	0.74
6:U:119:ALA:HB2	6:U:201:LEU:HD23	1.70	0.74
1:K:779:ARG:NH2	4:Q:148:MET:HG3	2.01	0.74
4:E:148:MET:HE3	4:E:148:MET:HA	1.69	0.74
4:F:286:TRP:HA	4:F:293:LEU:HA	1.70	0.73
4:O:250:LEU:HD22	4:O:268:ILE:HG12	1.70	0.73
5:R:173:GLY:O	5:R:194:ALA:N	2.22	0.73
4:Q:7:ILE:HD13	4:Q:47:TRP:HB2	1.71	0.73
4:Q:198:GLN:OE1	4:Q:211:LYS:NZ	2.18	0.72
1:B:780:LYS:N	3:D:895:GLY:CA	2.52	0.72
1:L:81:GLY:HA2	1:L:87:VAL:HA	1.72	0.72
4:Q:80:ASP:OD1	4:Q:82:THR:OG1	2.08	0.72
4:P:281:VAL:HA	4:P:297:GLY:HA2	1.70	0.72
4:P:35:SER:HA	4:P:54:LYS:HA	1.71	0.72
1:A:819:GLN:OE1	1:A:822:ASN:ND2	2.23	0.71
2:M:185:ASN:ND2	2:M:187:ASN:OD1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:640:MET:HB2	3:D:724:PHE:HE1	1.55	0.71
1:L:43:LEU:N	1:L:51:ALA:O	2.24	0.71
2:M:273:MET:HE1	6:V:351:LEU:HB2	1.74	0.70
1:B:730:LEU:O	3:D:943:HIS:NE2	2.24	0.70
1:L:330:TRP:HA	1:L:338:MET:HA	1.72	0.70
2:M:722:CYS:CB	2:M:736:CYS:SG	2.78	0.70
1:A:209:ALA:HA	1:A:221:PHE:HA	1.74	0.70
4:F:246:ARG:HA	4:F:273:GLN:HA	1.74	0.70
5:H:261:VAL:HA	5:H:281:SER:HA	1.73	0.70
1:A:780:LYS:HG3	1:A:781:PRO:HD2	1.72	0.69
1:K:779:ARG:CZ	4:Q:148:MET:HG3	2.21	0.69
2:C:167:ARG:NH2	6:U:346:ASP:OD1	2.24	0.69
4:F:200:PHE:HA	4:F:211:LYS:HA	1.72	0.69
4:Q:222:VAL:HG22	4:Q:242:THR:HG22	1.75	0.69
6:V:100:LEU:HD22	6:V:200:LEU:HG	1.75	0.69
1:B:128:TRP:HA	1:B:146:ASP:HA	1.75	0.69
4:G:243:LYS:NZ	4:G:244:ASP:OD1	2.24	0.69
3:N:876:ARG:HE	3:N:879:ARG:HD3	1.57	0.69
2:M:782:GLY:O	2:M:784:GLY:N	2.26	0.69
1:L:295:LEU:N	1:L:316:ARG:O	2.23	0.68
2:M:119:HIS:CE1	2:M:140:SER:HB2	2.28	0.68
1:A:356:ILE:HD12	1:A:370:CYS:HA	1.75	0.68
1:A:413:HIS:CE1	1:A:414:ILE:HG23	2.29	0.68
1:A:627:THR:O	1:A:631:ARG:NH1	2.27	0.68
1:L:241:ALA:HA	1:L:250:ILE:HA	1.75	0.68
3:N:969:LEU:O	3:N:973:THR:OG1	2.11	0.68
5:H:54:VAL:HA	5:H:93:GLN:HG2	1.75	0.68
6:U:448:ARG:HD3	6:U:450:SER:H	1.56	0.68
1:L:842:TRP:O	1:L:846:HIS:N	2.27	0.67
4:F:170:TRP:HA	4:F:182:ILE:HA	1.74	0.67
6:U:195:ILE:HD13	6:U:355:LEU:HB3	1.75	0.67
6:U:472:LEU:HA	6:U:475:ILE:HG22	1.77	0.67
2:M:437:ALA:HB1	2:M:445:VAL:HG13	1.76	0.67
1:B:296:TYR:HA	1:B:315:GLU:HA	1.76	0.67
2:C:187:ASN:HB3	2:C:202:MET:HE1	1.77	0.67
1:A:144:ILE:O	1:A:178:LEU:N	2.28	0.66
1:B:143:LEU:HA	1:B:180:GLU:HA	1.78	0.66
1:A:74:PRO:CG	1:A:77:LEU:CB	2.73	0.66
6:U:165:LEU:HD11	6:U:173:ILE:HD13	1.77	0.66
6:U:473:ARG:HD2	6:U:477:ARG:HH21	1.60	0.66
2:M:347:LEU:HD11	2:M:686:ARG:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:674:GLN:O	3:N:678:GLN:NE2	2.29	0.66
3:D:938:CYS:SG	3:D:968:CYS:CB	2.84	0.66
3:D:947:THR:HA	3:D:950:MET:HE1	1.76	0.66
6:V:123:HIS:ND1	6:V:208:SER:OG	2.24	0.66
1:A:713:ARG:NH1	2:C:747:HIS:HE1	1.93	0.66
4:G:277:HIS:ND1	4:G:299:ASP:OD1	2.29	0.66
1:A:379:GLU:O	1:A:381:GLU:N	2.29	0.65
1:K:271:THR:N	1:K:286:LEU:O	2.29	0.65
2:M:129:HIS:CE1	2:M:132:GLU:H	2.15	0.65
2:C:346:GLY:O	4:G:288:ILE:HD11	1.96	0.65
4:F:171:ASN:N	4:F:181:MET:O	2.30	0.65
4:F:182:ILE:N	4:F:200:PHE:O	2.27	0.65
4:Q:107:THR:HG21	4:Q:153:TRP:HD1	1.61	0.65
2:M:107:PRO:HD2	2:M:108:SER:N	2.07	0.65
4:Q:21:ASP:OD1	4:Q:22:PHE:N	2.27	0.65
6:V:195:ILE:HD11	6:V:352:ILE:HD11	1.78	0.65
4:G:143:GLU:OE1	4:G:156:GLN:NE2	2.31	0.64
2:C:356:LYS:HB2	2:C:359:LEU:HG	1.78	0.64
3:D:714:ASP:OD2	4:G:308:ASN:ND2	2.26	0.64
4:F:121:PHE:HA	4:F:130:LEU:HA	1.78	0.64
1:L:734:PHE:O	3:N:899:GLY:N	2.29	0.64
4:O:86:TRP:CZ3	4:O:105:LYS:HB2	2.32	0.64
4:E:228:ALA:HB3	4:E:237:ILE:HB	1.79	0.64
2:C:214:ASP:OD1	2:C:215:TRP:N	2.31	0.64
1:A:607:TYR:OH	1:A:635:LYS:NZ	2.30	0.64
4:G:31:SER:OG	4:G:33:ASP:OD1	2.16	0.64
2:M:282:ASP:O	2:M:284:ARG:N	2.30	0.64
1:A:644:GLY:O	1:A:668:ARG:NH2	2.31	0.64
1:A:843:PHE:HB3	1:A:859:MET:HE2	1.80	0.64
5:H:113:HIS:CD2	5:H:114:PRO:HD2	2.31	0.64
2:C:163:SER:OG	2:C:164:GLU:N	2.26	0.64
4:E:66:ALA:HB2	4:E:121:PHE:HE2	1.63	0.64
3:N:750:SER:HB2	3:N:885:PHE:HD1	1.61	0.64
4:E:224:ASP:OD1	4:E:225:ILE:N	2.30	0.64
1:A:787:LEU:HD12	1:A:838:HIS:HB3	1.79	0.63
1:A:737:CYS:SG	1:A:738:ASN:N	2.71	0.63
1:B:295:LEU:N	1:B:316:ARG:O	2.30	0.63
1:L:231:THR:N	1:L:241:ALA:O	2.29	0.63
5:R:73:ARG:HD2	5:R:111:TRP:HH2	1.63	0.63
1:A:790:ILE:HD11	4:G:69:GLU:HA	1.80	0.63
1:K:8:ILE:HA	1:K:20:VAL:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:732:GLN:N	3:N:942:GLY:O	2.31	0.63
1:A:785:CYS:SG	1:A:835:HIS:CE1	2.89	0.63
1:A:271:THR:N	1:A:286:LEU:O	2.30	0.62
4:E:133:CYS:HB3	4:E:139:VAL:HA	1.81	0.62
1:A:360:TRP:HD1	4:E:285:SER:HG	1.45	0.62
5:H:79:SER:HA	5:H:105:PRO:HB3	1.80	0.62
4:P:181:MET:HA	4:P:201:GLU:HA	1.80	0.62
4:F:307:ALA:HA	4:F:313:TRP:HA	1.80	0.62
1:K:860:GLN:N	1:K:860:GLN:OE1	2.32	0.62
2:C:82:TRP:CD1	2:C:83:HIS:H	2.18	0.62
4:E:315:CYS:SG	4:E:316:THR:N	2.73	0.62
4:P:39:TRP:HA	4:P:49:CYS:HA	1.80	0.62
6:V:152:ALA:O	6:V:157:ARG:NH2	2.32	0.62
4:P:199:ILE:O	4:P:212:ALA:N	2.33	0.61
2:M:172:SER:OG	2:M:175:ASP:O	2.18	0.61
1:A:10:TRP:HA	1:A:18:PHE:HA	1.81	0.61
1:K:250:ILE:O	1:K:260:VAL:N	2.34	0.61
2:M:743:CYS:SG	2:M:765:HIS:ND1	2.71	0.61
1:K:394:MET:HE1	1:K:672:VAL:HG22	1.83	0.61
6:U:171:TRP:HA	6:U:470:TYR:HE1	1.65	0.61
4:G:168:ILE:HG13	4:G:182:ILE:HD11	1.82	0.61
6:U:164:LYS:HZ3	6:U:321:PHE:HB2	1.65	0.61
1:B:852:SER:HA	3:D:884:LYS:NZ	2.14	0.61
2:M:723:LYS:HE3	2:M:723:LYS:HA	1.81	0.61
3:D:868:GLU:OE1	5:H:160:HIS:NE2	2.33	0.61
2:M:643:PHE:O	2:M:647:GLN:NE2	2.32	0.61
3:N:669:ASN:H	3:N:676:THR:HG21	1.66	0.61
6:U:122:ARG:HG3	6:U:168:HIS:HE1	1.65	0.61
1:B:129:LEU:O	1:B:145:TRP:N	2.34	0.60
1:K:708:ARG:HH22	4:O:25:ARG:HD2	1.65	0.60
1:B:67:ALA:H	1:B:79:ALA:HB3	1.66	0.60
1:B:710:TRP:HA	1:B:713:ARG:NE	2.12	0.60
4:F:202:TYR:HA	4:F:209:TYR:HA	1.83	0.60
4:Q:203:ASN:HB3	4:Q:206:THR:HG22	1.83	0.60
6:V:104:ASP:OD1	6:V:104:ASP:N	2.34	0.60
6:V:174:THR:OG1	6:V:175:LYS:N	2.29	0.60
4:O:246:ARG:HB3	4:O:248:PHE:HE2	1.66	0.60
1:A:830:CYS:HB3	1:A:832:HIS:ND1	2.17	0.60
5:H:152:VAL:HA	5:H:170:SER:HA	1.83	0.60
2:C:155:SER:OG	2:C:156:VAL:N	2.34	0.60
1:K:625:SER:O	1:K:629:LEU:N	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:74:PRO:HD2	1:L:74:PRO:O	2.02	0.60
6:U:78:ASN:N	6:U:127:TYR:HH	1.98	0.60
1:B:852:SER:HA	3:D:884:LYS:HZ1	1.66	0.60
4:F:89:ILE:O	4:F:102:HIS:N	2.34	0.60
4:F:142:TYR:HA	4:F:155:LEU:HA	1.83	0.60
4:P:86:TRP:HA	4:P:105:LYS:HA	1.84	0.60
1:B:270:LEU:HA	1:B:287:THR:HA	1.83	0.60
4:F:39:TRP:HA	4:F:49:CYS:HA	1.83	0.60
1:K:703:LEU:HD11	4:O:231:LEU:HD21	1.84	0.60
1:B:271:THR:N	1:B:286:LEU:O	2.34	0.59
6:U:364:ASP:O	6:U:368:GLN:NE2	2.35	0.59
1:K:849:CYS:HB3	1:K:854:CYS:HB3	1.84	0.59
1:L:128:TRP:HA	1:L:147:ILE:H	1.65	0.59
4:Q:7:ILE:CD1	4:Q:47:TRP:CD1	2.85	0.59
4:Q:119:VAL:HG23	4:Q:130:LEU:HD11	1.83	0.59
4:F:247:ILE:O	4:F:271:VAL:N	2.35	0.59
5:R:169:GLY:HA2	5:R:175:ILE:HA	1.83	0.59
1:L:425:SER:O	1:L:429:THR:N	2.31	0.59
6:U:195:ILE:HG21	6:U:355:LEU:HD13	1.85	0.59
2:M:164:GLU:N	2:M:164:GLU:OE1	2.35	0.59
4:Q:56:HIS:HE2	4:Q:76:SER:HG	1.48	0.59
1:A:852:SER:H	2:C:709:ASN:HD21	1.50	0.59
2:C:223:LEU:HD12	2:C:224:ALA:H	1.67	0.59
1:A:74:PRO:HD2	1:A:74:PRO:O	2.03	0.59
4:P:182:ILE:N	4:P:200:PHE:O	2.32	0.59
4:P:302:VAL:N	4:P:319:LEU:O	2.35	0.59
6:U:169:ARG:HH21	6:U:324:GLU:N	1.99	0.59
2:C:401:GLU:OE2	2:C:401:GLU:N	2.35	0.59
4:E:216:MET:HA	4:E:216:MET:HE3	1.85	0.58
4:O:83:ALA:HB3	4:O:109:LEU:HD12	1.85	0.58
1:K:74:PRO:HD2	1:K:74:PRO:O	2.01	0.58
1:A:211:PHE:HA	1:A:219:LYS:HA	1.85	0.58
2:C:733:CYS:HB3	2:C:736:CYS:HB3	1.85	0.58
4:F:281:VAL:HA	4:F:297:GLY:HA2	1.84	0.58
5:H:226:LYS:HB2	5:H:248:TRP:HH2	1.68	0.58
1:L:243:PHE:HA	1:L:248:VAL:HA	1.84	0.58
1:L:787:LEU:O	3:N:876:ARG:NH1	2.35	0.58
1:L:849:CYS:N	1:L:856:CYS:O	2.35	0.58
1:B:140:PHE:HA	1:B:183:GLN:HA	1.84	0.58
5:H:66:GLN:HG2	5:H:110:ALA:HA	1.86	0.58
4:F:224:ASP:H	4:F:241:ALA:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:305:TRP:HA	4:F:315:CYS:HA	1.86	0.58
4:Q:105:LYS:NZ	4:Q:107:THR:O	2.37	0.58
6:V:342:TYR:HA	6:V:347:HIS:NE2	2.19	0.58
6:U:171:TRP:HA	6:U:470:TYR:CE1	2.38	0.58
6:V:128:LEU:HD21	6:V:211:VAL:HG21	1.84	0.58
4:F:119:VAL:HA	4:F:132:THR:HA	1.86	0.58
6:U:89:TYR:HD1	6:U:89:TYR:O	1.86	0.58
1:A:210:ILE:N	1:A:220:MET:O	2.35	0.57
1:B:145:TRP:HA	1:B:178:LEU:H	1.69	0.57
2:M:93:ALA:HB1	2:M:123:VAL:HG23	1.86	0.57
4:P:140:ARG:HA	4:P:158:GLU:HA	1.85	0.57
6:U:364:ASP:OD1	6:U:368:GLN:NE2	2.35	0.57
6:V:212:PHE:CD2	6:V:433:GLU:HA	2.40	0.57
4:F:16:HIS:N	4:F:30:CYS:O	2.30	0.57
4:F:182:ILE:O	4:F:200:PHE:N	2.23	0.57
1:L:242:SER:N	1:L:249:ALA:O	2.30	0.57
2:M:275:ASP:OD2	2:M:279:TYR:OH	2.22	0.57
1:B:142:VAL:O	1:B:181:LEU:N	2.30	0.57
3:N:690:LYS:O	3:N:693:VAL:HG12	2.03	0.57
1:A:713:ARG:NH1	2:C:747:HIS:CE1	2.71	0.57
1:L:297:ASP:N	1:L:314:ILE:O	2.28	0.57
1:K:209:ALA:HA	1:K:221:PHE:HA	1.85	0.57
1:L:604:GLY:O	1:L:608:GLU:N	2.38	0.57
2:C:640:MET:HB2	3:D:724:PHE:CE1	2.39	0.57
4:E:171:ASN:HD22	4:E:181:MET:HE3	1.69	0.56
4:E:224:ASP:H	4:E:241:ALA:HB3	1.70	0.56
5:R:168:CYS:O	5:R:176:SER:N	2.35	0.56
6:V:111:TRP:O	6:V:115:ILE:HG23	2.05	0.56
4:O:129:MET:HE3	4:O:143:GLU:HG3	1.86	0.56
4:P:142:TYR:HA	4:P:156:GLN:H	1.69	0.56
6:V:195:ILE:CD1	6:V:352:ILE:HD11	2.35	0.56
1:L:729:PRO:O	3:N:943:HIS:NE2	2.37	0.56
2:M:644:TYR:CZ	2:M:652:MET:HE3	2.41	0.56
1:K:783:PRO:HG2	2:M:715:LEU:HD23	1.86	0.56
1:K:784:ARG:HD3	2:M:711:ALA:O	2.04	0.56
5:H:108:GLN:NE2	5:H:153:ASN:O	2.38	0.56
1:B:729:PRO:HB2	3:D:943:HIS:NE2	2.21	0.56
1:B:430:LEU:O	1:B:434:LYS:N	2.34	0.56
2:C:640:MET:HA	3:D:723:PRO:HG2	1.88	0.56
6:V:164:LYS:HD2	6:V:321:PHE:HD2	1.70	0.56
1:A:713:ARG:NH2	2:C:745:VAL:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:ARG:NH1	2:C:727:SER:O	2.32	0.56
1:A:785:CYS:SG	1:A:835:HIS:N	2.78	0.56
1:K:708:ARG:NH2	4:O:25:ARG:HD2	2.20	0.56
1:K:710:TRP:CD1	1:K:713:ARG:HH21	2.23	0.56
1:K:788:CYS:HB3	1:K:790:ILE:HG22	1.88	0.56
4:E:84:ALA:HB1	4:E:105:LYS:HE2	1.88	0.55
1:K:679:MET:HE3	1:K:679:MET:HA	1.88	0.55
3:N:691:ASP:O	3:N:695:VAL:HG13	2.06	0.55
6:U:195:ILE:HD12	6:U:356:TYR:HB2	1.87	0.55
4:G:81:ARG:NH1	4:G:113:ARG:O	2.39	0.55
6:U:89:TYR:OH	6:U:460:LEU:HD11	2.07	0.55
1:B:785:CYS:O	1:B:789:LEU:N	2.34	0.55
1:B:852:SER:O	3:D:890:PRO:HG3	2.07	0.55
4:F:35:SER:HA	4:F:54:LYS:HA	1.87	0.55
4:F:308:ASN:N	4:F:312:ASN:O	2.36	0.55
2:M:273:MET:O	2:M:275:ASP:N	2.40	0.55
5:H:164:LEU:C	5:H:165:ILE:HD13	2.32	0.55
4:O:21:ASP:O	4:O:23:HIS:N	2.39	0.55
4:P:141:ILE:N	4:P:157:HIS:O	2.35	0.55
1:A:787:LEU:HD21	1:A:850:PRO:HB3	1.89	0.55
2:C:82:TRP:HD1	2:C:83:HIS:H	1.55	0.55
2:C:125:LYS:HD3	2:C:168:ASP:HA	1.89	0.55
6:V:324:GLU:N	6:V:324:GLU:OE1	2.39	0.55
6:V:424:TYR:O	6:V:428:VAL:HG12	2.06	0.55
2:M:413:VAL:O	2:M:417:GLU:HG2	2.07	0.55
1:B:725:PRO:HD2	1:B:726:SER:N	2.21	0.55
4:G:274:PHE:HZ	4:G:313:TRP:HB2	1.72	0.54
2:M:342:GLY:HA2	4:Q:283:ARG:HD3	1.89	0.54
6:U:348:GLY:O	6:U:352:ILE:HG22	2.08	0.54
1:A:852:SER:H	2:C:709:ASN:ND2	2.05	0.54
1:A:713:ARG:CZ	2:C:747:HIS:CE1	2.90	0.54
2:C:213:CYS:SG	2:C:223:LEU:HD11	2.48	0.54
2:C:223:LEU:HD12	2:C:224:ALA:N	2.22	0.54
2:M:261:PRO:HD2	2:M:311:PRO:HB3	1.89	0.54
2:C:733:CYS:CB	2:C:736:CYS:HB3	2.37	0.54
3:D:662:LEU:HB2	3:D:743:GLN:HE22	1.72	0.54
2:C:169:VAL:HG13	2:C:179:PHE:HE1	1.73	0.54
4:E:143:GLU:HB2	4:E:156:GLN:HE22	1.73	0.54
4:F:14:LEU:O	4:F:32:SER:N	2.40	0.54
4:F:141:ILE:O	4:F:156:GLN:N	2.36	0.54
1:K:426:LEU:HD22	1:K:646:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:231:THR:O	1:L:241:ALA:N	2.40	0.54
4:F:248:PHE:HA	4:F:270:ILE:HA	1.89	0.54
4:P:42:SER:N	4:P:46:ASP:O	2.37	0.54
4:Q:122:ALA:HB1	4:Q:126:MET:HE3	1.89	0.54
4:G:288:ILE:HD12	4:G:288:ILE:H	1.73	0.54
1:K:693:VAL:HA	1:K:696:TRP:NE1	2.23	0.54
6:V:397:ILE:HA	6:V:400:VAL:HG22	1.89	0.54
1:B:369:ALA:HA	1:B:374:LEU:HA	1.89	0.54
4:G:277:HIS:HD1	4:G:299:ASP:CG	2.16	0.54
3:N:870:LEU:HD23	3:N:873:TRP:HE3	1.72	0.54
1:A:773:THR:CG2	1:A:791:ASN:HB2	2.38	0.54
1:A:820:PHE:N	2:C:788:GLU:OE1	2.42	0.53
2:C:760:CYS:SG	2:C:785:HIS:CG	2.92	0.53
1:A:394:MET:HG2	1:A:673:GLN:HE21	1.72	0.53
1:A:790:ILE:CD1	4:G:69:GLU:HA	2.39	0.53
3:D:542:ALA:HA	3:D:551:VAL:O	2.08	0.53
6:U:122:ARG:HG3	6:U:168:HIS:CE1	2.44	0.53
6:U:406:ASP:OD1	6:U:406:ASP:N	2.38	0.53
1:A:784:ARG:NH1	2:C:712:SER:OG	2.41	0.53
3:D:872:ARG:HD3	5:H:69:TYR:CD2	2.44	0.53
2:M:746:CYS:SG	2:M:765:HIS:ND1	2.73	0.53
2:C:127:CYS:SG	2:C:171:PHE:HB2	2.49	0.53
4:F:26:ARG:HA	4:F:40:ASP:HA	1.90	0.53
6:V:212:PHE:HD2	6:V:433:GLU:HA	1.73	0.53
4:E:73:VAL:HA	4:E:86:TRP:O	2.08	0.53
4:E:274:PHE:HZ	4:E:313:TRP:HB3	1.73	0.53
5:H:317:SER:OG	5:H:318:ILE:N	2.40	0.53
2:M:768:HIS:HA	2:M:771:LYS:NZ	2.24	0.53
3:D:546:GLY:O	3:D:872:ARG:NE	2.37	0.53
4:P:83:ALA:N	4:P:109:LEU:O	2.37	0.53
2:C:27:ALA:HB3	2:C:48:ILE:HD13	1.90	0.53
2:C:136:LEU:HD12	2:C:137:LEU:H	1.73	0.53
2:C:426:LEU:HD22	2:C:663:ARG:HH22	1.73	0.53
3:D:549:TYR:HD1	3:D:651:ASP:HA	1.74	0.53
2:M:442:ARG:HB2	2:M:445:VAL:CG1	2.38	0.53
2:M:652:MET:O	2:M:656:VAL:HG22	2.09	0.53
2:M:722:CYS:HB2	2:M:724:ARG:HD2	1.91	0.53
4:F:90:VAL:HA	4:F:101:SER:HA	1.89	0.53
4:F:251:LYS:O	4:F:267:GLU:N	2.32	0.53
1:L:89:LEU:O	1:L:105:GLY:N	2.38	0.53
1:L:272:LYS:O	1:L:286:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TRP:HA	1:A:260:VAL:H	1.73	0.52
2:C:95:THR:HG22	6:U:340:GLN:NE2	2.23	0.52
4:F:89:ILE:N	4:F:102:HIS:O	2.41	0.52
4:Q:107:THR:HG21	4:Q:153:TRP:CD1	2.43	0.52
1:K:826:TRP:HB3	2:M:715:LEU:HD12	1.91	0.52
1:L:733:VAL:HA	3:N:900:VAL:HA	1.91	0.52
6:V:425:ILE:HG13	6:V:459:LEU:HD11	1.92	0.52
1:A:74:PRO:HD2	1:A:77:LEU:CB	2.39	0.52
2:C:183:PHE:CE2	2:C:189:GLN:HG3	2.45	0.52
2:C:202:MET:HE3	2:C:203:PHE:N	2.24	0.52
4:E:63:VAL:HG22	4:E:76:SER:HB3	1.91	0.52
4:G:134:SER:OG	4:G:138:ILE:O	2.27	0.52
1:K:851:VAL:O	2:M:698:LYS:NZ	2.41	0.52
1:B:787:LEU:O	3:D:876:ARG:NH1	2.39	0.52
4:Q:308:ASN:C	4:Q:310:MET:H	2.17	0.52
3:D:884:LYS:HE3	3:D:884:LYS:HA	1.90	0.52
1:L:140:PHE:HA	1:L:183:GLN:HA	1.90	0.52
3:N:742:VAL:HG13	3:N:742:VAL:O	2.09	0.52
4:G:233:ARG:HD3	4:G:235:PHE:CE2	2.43	0.52
1:K:792:MET:HE3	1:K:824:PHE:CE1	2.45	0.52
6:U:78:ASN:N	6:U:127:TYR:OH	2.43	0.52
4:E:70:PHE:CD2	4:E:128:LEU:HD13	2.45	0.52
4:Q:21:ASP:CG	4:Q:22:PHE:H	2.15	0.52
5:R:289:TRP:H	5:R:289:TRP:CD1	2.28	0.52
2:C:412:PHE:HA	2:C:651:GLN:HE22	1.75	0.52
3:D:740:ARG:HH12	5:H:272:LEU:HD12	1.75	0.52
4:Q:82:THR:HG22	4:Q:110:VAL:HG12	1.92	0.52
5:R:116:TYR:HD2	5:R:164:LEU:HD12	1.74	0.52
1:L:329:ALA:N	1:L:339:ILE:O	2.40	0.52
4:P:41:LYS:HA	4:P:47:TRP:HA	1.91	0.52
1:B:781:PRO:O	3:D:895:GLY:HA3	2.09	0.51
2:C:418:ARG:HG3	2:C:418:ARG:HH11	1.75	0.51
2:M:141:GLN:HG3	2:M:165:SER:OG	2.10	0.51
1:A:704:LEU:HD23	1:A:707:TRP:HD1	1.75	0.51
2:M:743:CYS:HG	2:M:765:HIS:CE1	2.24	0.51
4:O:80:ASP:O	4:O:81:ARG:HG2	2.11	0.51
1:A:228:GLN:O	1:A:243:PHE:N	2.41	0.51
5:H:175:ILE:O	5:H:191:ILE:N	2.43	0.51
2:M:743:CYS:HG	2:M:765:HIS:HD1	1.53	0.51
6:V:363:LEU:O	6:V:367:PHE:HD1	1.93	0.51
2:C:785:HIS:CE1	2:C:787:CYS:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:552:TYR:CZ	3:D:648:ILE:HB	2.46	0.51
5:H:67:MET:HG3	5:H:74:LEU:HD12	1.92	0.51
3:N:729:LEU:HD21	3:N:851:LEU:HD23	1.92	0.51
3:N:927:CYS:SG	3:N:949:HIS:HE1	2.06	0.51
3:D:941:CYS:HB3	3:D:966:CYS:SG	2.51	0.51
4:G:107:THR:HG21	4:G:153:TRP:CD1	2.46	0.51
4:G:66:ALA:HB3	4:G:73:VAL:HG13	1.92	0.51
2:M:46:ARG:NH2	6:V:338:ARG:HD3	2.25	0.51
4:O:14:LEU:O	4:O:32:SER:N	2.43	0.51
3:N:689:ARG:HE	3:N:692:LEU:HD23	1.75	0.51
5:R:321:ASN:HB3	5:R:322:ILE:HD12	1.93	0.51
1:A:360:TRP:CD1	4:E:285:SER:HG	2.25	0.51
1:A:733:VAL:CG1	2:C:717:VAL:HG13	2.40	0.51
4:E:70:PHE:HD2	4:E:128:LEU:HD13	1.75	0.51
2:C:411:TRP:H	2:C:411:TRP:CD1	2.27	0.50
4:E:271:VAL:HG12	4:E:313:TRP:HD1	1.77	0.50
2:M:163:SER:OG	2:M:185:ASN:OD1	2.29	0.50
1:B:340:VAL:O	1:B:348:SER:N	2.41	0.50
3:D:677:CYS:HB3	3:D:700:THR:HB	1.91	0.50
2:M:785:HIS:ND1	2:M:787:CYS:SG	2.82	0.50
4:Q:305:TRP:HZ3	4:Q:315:CYS:HG	1.58	0.50
6:V:89:TYR:OH	6:V:460:LEU:HD13	2.11	0.50
4:G:106:ARG:HB3	4:G:150:LEU:O	2.12	0.50
4:G:246:ARG:HG3	4:G:246:ARG:HH11	1.75	0.50
2:M:140:SER:OG	2:M:141:GLN:N	2.44	0.50
2:M:442:ARG:HB2	2:M:445:VAL:HG12	1.93	0.50
4:Q:167:CYS:SG	4:Q:224:ASP:HA	2.51	0.50
4:P:305:TRP:HA	4:P:315:CYS:HA	1.93	0.50
6:U:190:SER:H	6:U:193:GLU:HG2	1.76	0.50
5:H:310:VAL:O	5:H:328:GLY:N	2.44	0.50
5:H:312:TRP:CH2	5:H:328:GLY:HA2	2.47	0.50
1:K:779:ARG:HD2	1:K:779:ARG:C	2.36	0.50
1:B:116:CYS:HA	1:B:133:LEU:HA	1.94	0.50
1:B:297:ASP:N	1:B:314:ILE:O	2.43	0.50
5:H:289:TRP:CZ3	5:H:301:PRO:HD3	2.46	0.50
5:H:314:VAL:HG22	5:H:323:LEU:HD11	1.93	0.50
1:K:713:ARG:NH1	2:M:747:HIS:CE1	2.79	0.50
1:L:339:ILE:HA	1:L:349:ASP:HA	1.92	0.50
4:O:128:LEU:HB3	4:O:144:ALA:HB3	1.92	0.50
5:R:338:SER:N	5:R:342:GLN:O	2.45	0.50
1:A:699:ASN:ND2	4:E:231:LEU:HA	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:845:ASP:HA	3:D:848:LYS:NZ	2.27	0.50
1:L:649:ILE:O	1:L:653:GLY:N	2.42	0.50
2:M:93:ALA:HB2	2:M:126:VAL:CG2	2.42	0.50
4:F:41:LYS:HA	4:F:47:TRP:HA	1.94	0.50
2:M:772:TRP:O	2:M:776:SER:OG	2.24	0.50
2:C:290:ALA:O	2:C:333:GLN:NE2	2.28	0.49
1:K:603:ASP:HA	1:K:606:LEU:HB2	1.93	0.49
2:M:121:ARG:HH12	6:V:391:ARG:NH2	2.10	0.49
2:M:644:TYR:CE2	2:M:652:MET:HE3	2.47	0.49
2:M:743:CYS:SG	2:M:765:HIS:N	2.80	0.49
6:U:448:ARG:HD3	6:U:448:ARG:C	2.37	0.49
1:B:842:TRP:O	1:B:846:HIS:N	2.44	0.49
2:C:54:ILE:HG21	2:C:306:ARG:HE	1.77	0.49
1:A:862:ASP:OD2	2:C:765:HIS:NE2	2.38	0.49
1:B:209:ALA:HA	1:B:221:PHE:HA	1.94	0.49
2:C:171:PHE:CE1	2:C:179:PHE:HB2	2.47	0.49
4:G:242:THR:HG22	4:G:243:LYS:H	1.77	0.49
4:P:202:TYR:HA	4:P:209:TYR:HA	1.94	0.49
1:B:780:LYS:N	1:B:781:PRO:HD2	2.27	0.49
2:C:171:PHE:HE1	2:C:179:PHE:HB2	1.77	0.49
4:G:11:HIS:NE2	4:G:37:LYS:HD3	2.27	0.49
1:L:80:VAL:O	1:L:88:VAL:N	2.26	0.49
1:L:391:ALA:O	1:L:393:LYS:N	2.45	0.49
1:A:358:LEU:HD22	1:A:366:LEU:HD11	1.95	0.49
4:E:271:VAL:HG12	4:E:313:TRP:CD1	2.48	0.49
1:K:375:TYR:HD1	4:O:6:SER:HA	1.78	0.49
3:N:924:CYS:SG	3:N:927:CYS:N	2.70	0.49
5:R:261:VAL:HA	5:R:281:SER:HA	1.95	0.49
2:C:168:ASP:OD2	2:C:213:CYS:N	2.46	0.49
3:D:699:ALA:O	3:D:703:THR:HG23	2.12	0.49
1:B:672:VAL:O	1:B:676:SER:N	2.37	0.49
2:C:114:GLN:HB2	2:C:116:PHE:HE1	1.78	0.49
2:C:456:TYR:HE2	2:C:660:LEU:HD13	1.77	0.49
2:C:95:THR:O	2:C:122:THR:HG23	2.12	0.49
2:C:447:GLN:HG3	3:D:707:LEU:HD11	1.95	0.49
3:D:675:GLU:HA	3:D:678:GLN:OE1	2.13	0.49
4:G:17:ASP:OD2	4:G:62:ARG:HD2	2.13	0.49
1:L:128:TRP:HA	1:L:146:ASP:HA	1.94	0.49
3:N:721:ARG:NH1	4:Q:309:TYR:HD1	2.11	0.49
6:U:110:SER:HB2	6:U:136:PHE:HE1	1.78	0.49
6:U:456:ASN:HA	6:U:459:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:167:CYS:SG	4:G:224:ASP:HA	2.53	0.49
1:L:787:LEU:O	3:N:876:ARG:CZ	2.61	0.49
1:A:849:CYS:HB3	1:A:854:CYS:HB3	1.94	0.48
2:C:228:ARG:NH1	6:U:345:GLU:O	2.45	0.48
2:C:453:ARG:HE	2:C:454:ILE:HD13	1.77	0.48
4:E:77:CYS:HB2	4:E:116:VAL:HG13	1.93	0.48
2:M:167:ARG:NH1	6:V:345:GLU:OE2	2.46	0.48
4:O:150:LEU:O	4:O:153:TRP:NE1	2.39	0.48
4:Q:46:ASP:OD1	4:Q:46:ASP:N	2.46	0.48
6:V:127:TYR:HD2	6:V:128:LEU:HD23	1.78	0.48
4:E:66:ALA:HB2	4:E:121:PHE:CE2	2.45	0.48
5:H:75:ALA:HB1	5:H:109:VAL:HG21	1.95	0.48
1:K:144:ILE:O	1:K:178:LEU:N	2.46	0.48
6:U:165:LEU:HB2	6:U:169:ARG:O	2.12	0.48
1:A:74:PRO:CD	1:A:77:LEU:CB	2.90	0.48
2:C:294:GLU:O	2:C:294:GLU:CD	2.57	0.48
1:L:144:ILE:O	1:L:178:LEU:N	2.47	0.48
6:U:448:ARG:HH11	6:U:449:HIS:H	1.61	0.48
2:C:324:CYS:SG	2:C:326:HIS:NE2	2.87	0.48
4:G:286:TRP:CE2	4:G:293:LEU:HD13	2.48	0.48
1:A:735:VAL:HG13	1:A:744:ILE:HD13	1.96	0.48
1:L:735:VAL:O	1:L:744:ILE:N	2.36	0.48
2:M:706:SER:O	2:M:706:SER:OG	2.30	0.48
4:O:200:PHE:HE1	4:O:211:LYS:HG2	1.78	0.48
3:D:657:PRO:HB2	3:D:741:ASP:HB3	1.96	0.48
4:Q:268:ILE:HD12	4:Q:268:ILE:H	1.79	0.48
1:A:83:ALA:O	1:A:115:GLN:HA	2.14	0.48
2:C:97:GLY:HA2	2:C:123:VAL:HG23	1.96	0.48
4:G:241:ALA:HB1	4:G:281:VAL:HG12	1.94	0.48
5:H:106:VAL:HA	5:H:124:SER:HA	1.95	0.48
3:N:870:LEU:HD23	3:N:873:TRP:CE3	2.49	0.48
6:V:386:THR:OG1	6:V:387:SER:N	2.46	0.48
2:C:250:THR:OG1	2:C:251:ILE:N	2.46	0.48
2:M:121:ARG:HH12	6:V:391:ARG:CZ	2.26	0.48
2:C:314:LEU:O	2:C:326:HIS:N	2.43	0.48
4:E:27:MET:HG3	4:E:39:TRP:HB2	1.96	0.48
4:F:169:SER:N	4:F:183:ALA:O	2.38	0.47
3:D:953:TRP:NE1	3:D:961:PRO:HD3	2.30	0.47
5:H:131:ILE:HD11	5:H:166:LEU:HD22	1.96	0.47
5:H:141:LYS:HD2	5:H:142:SER:H	1.80	0.47
4:G:301:CYS:SG	4:G:303:ARG:NH1	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:190:SER:OG	6:V:193:GLU:HG3	2.13	0.47
1:B:725:PRO:HD2	1:B:726:SER:H	1.79	0.47
4:E:16:HIS:HB2	4:E:30:CYS:SG	2.55	0.47
4:F:296:SER:HA	4:F:302:VAL:HA	1.95	0.47
4:G:275:ASP:O	4:G:275:ASP:OD2	2.33	0.47
1:B:780:LYS:N	1:B:781:PRO:CD	2.75	0.47
1:K:410:TRP:HB3	1:K:431:HIS:HD2	1.80	0.47
1:A:358:LEU:HD23	1:A:368:TRP:HB3	1.96	0.47
1:A:464:LEU:HA	1:A:626:ASP:OD2	2.15	0.47
4:G:274:PHE:CD1	4:G:305:TRP:CE3	3.03	0.47
5:H:107:TRP:HB2	5:H:108:GLN:NE2	2.30	0.47
2:M:409:MET:HA	2:M:411:TRP:CZ3	2.50	0.47
4:O:109:LEU:HD22	4:O:142:TYR:CE2	2.50	0.47
4:O:121:PHE:CE1	4:O:130:LEU:HD13	2.49	0.47
6:U:175:LYS:HD2	6:U:478:TYR:HA	1.95	0.47
5:H:313:HIS:ND1	5:H:314:VAL:N	2.62	0.47
3:N:871:TYR:HB2	3:N:879:ARG:HE	1.78	0.47
6:V:464:MET:O	6:V:464:MET:HG2	2.15	0.47
2:C:246:HIS:CD2	2:C:283:VAL:HG22	2.49	0.47
3:D:674:GLN:HE21	3:D:678:GLN:HE22	1.63	0.47
6:V:194:LEU:O	6:V:198:LEU:HG	2.15	0.47
4:F:285:SER:O	4:F:294:ALA:N	2.45	0.47
5:H:141:LYS:HD2	5:H:142:SER:N	2.29	0.47
4:O:66:ALA:HB2	4:O:121:PHE:HE2	1.80	0.47
2:C:174:ARG:NH1	2:C:218:GLU:O	2.48	0.46
3:D:844:HIS:O	3:D:848:LYS:HG3	2.16	0.46
1:L:294:ARG:HA	1:L:317:SER:HA	1.96	0.46
4:P:88:GLU:HA	4:P:103:TRP:HA	1.97	0.46
1:B:204:MET:N	1:B:207:ASN:O	2.48	0.46
2:C:306:ARG:O	2:C:306:ARG:HG2	2.15	0.46
3:D:938:CYS:SG	3:D:968:CYS:HB2	2.51	0.46
5:H:277:ILE:HB	5:H:289:TRP:HB2	1.97	0.46
5:H:334:LEU:C	5:H:335:TRP:HD1	2.24	0.46
3:N:960:CYS:C	3:N:962:THR:H	2.23	0.46
1:A:789:LEU:HD21	2:C:708:LEU:HB3	1.96	0.46
4:G:88:GLU:HB2	4:G:103:TRP:CD2	2.51	0.46
1:L:67:ALA:HB3	1:L:79:ALA:HB3	1.98	0.46
1:L:326:ALA:N	1:L:341:VAL:O	2.35	0.46
1:B:144:ILE:N	1:B:179:TYR:O	2.30	0.46
2:M:303:ILE:HB	2:M:314:LEU:HD21	1.98	0.46
2:M:341:GLU:OE1	4:Q:282:TRP:HD1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:396:TYR:HA	6:U:399:CYS:SG	2.56	0.46
1:A:819:GLN:CD	1:A:819:GLN:H	2.23	0.46
3:D:696:TRP:O	3:D:700:THR:HG22	2.16	0.46
1:L:487:ASN:O	1:L:491:ILE:N	2.35	0.46
6:U:195:ILE:CD1	6:U:356:TYR:HB2	2.46	0.46
2:C:451:MET:O	2:C:455:ILE:HG13	2.16	0.46
3:D:669:ASN:H	3:D:676:THR:HG21	1.80	0.46
1:K:16:ASP:O	1:K:30:VAL:N	2.43	0.46
1:L:329:ALA:O	1:L:339:ILE:N	2.35	0.46
2:C:731:TRP:CZ3	4:E:148:MET:HE1	2.51	0.46
1:B:193:LEU:N	1:B:199:LEU:O	2.47	0.46
2:C:410:ARG:HH21	2:C:413:VAL:HG21	1.80	0.46
3:D:914:CYS:HB3	3:D:917:CYS:SG	2.55	0.46
1:K:695:TYR:CE1	4:O:175:SER:HA	2.50	0.46
2:M:32:ILE:CD1	2:M:317:GLY:H	2.29	0.46
4:Q:268:ILE:HD12	4:Q:268:ILE:N	2.31	0.46
1:A:145:TRP:HA	1:A:178:LEU:H	1.79	0.46
3:D:941:CYS:HB2	3:D:943:HIS:CE1	2.51	0.46
4:F:86:TRP:HA	4:F:105:LYS:HA	1.98	0.46
4:G:34:GLN:HA	4:G:60:VAL:HG23	1.98	0.46
4:G:268:ILE:N	4:G:268:ILE:HD12	2.30	0.46
2:M:273:MET:SD	6:V:347:HIS:HB2	2.56	0.46
3:N:932:ARG:HA	3:N:932:ARG:NE	2.31	0.46
4:Q:316:THR:O	4:Q:316:THR:OG1	2.30	0.46
3:D:741:ASP:OD2	3:D:744:THR:HG22	2.16	0.46
1:K:67:ALA:O	1:K:79:ALA:N	2.38	0.46
2:M:16:LEU:HD23	2:M:16:LEU:HA	1.79	0.46
3:N:697:SER:O	3:N:700:THR:OG1	2.28	0.46
1:K:230:VAL:HA	1:K:241:ALA:O	2.15	0.45
4:O:178:HIS:NE2	4:O:236:HIS:HE1	2.14	0.45
4:P:203:ASN:O	4:P:207:ARG:N	2.49	0.45
5:R:337:GLU:HA	5:R:343:TRP:HA	1.98	0.45
6:U:195:ILE:HG13	6:U:196:GLN:N	2.31	0.45
1:B:731:ALA:O	3:D:942:GLY:HA3	2.17	0.45
4:G:166:SER:HB2	4:G:187:ASP:HB2	1.97	0.45
2:C:695:GLU:O	2:C:699:LEU:HD12	2.17	0.45
4:F:88:GLU:HA	4:F:103:TRP:HA	1.97	0.45
4:F:168:ILE:HA	4:F:184:VAL:HA	1.97	0.45
2:M:273:MET:CE	6:V:351:LEU:HB2	2.46	0.45
3:N:941:CYS:HB3	3:N:966:CYS:SG	2.56	0.45
6:U:421:LEU:O	6:U:425:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:243:LYS:HG3	4:G:244:ASP:OD1	2.17	0.45
5:H:115:MET:HE2	5:H:115:MET:HA	1.99	0.45
4:O:114:THR:HB	4:O:135:ALA:HB3	1.97	0.45
1:A:210:ILE:O	1:A:220:MET:N	2.50	0.45
1:A:360:TRP:HD1	4:E:285:SER:OG	1.99	0.45
3:D:662:LEU:HB2	3:D:743:GLN:NE2	2.32	0.45
5:H:113:HIS:C	5:H:115:MET:H	2.24	0.45
1:K:779:ARG:NH1	4:Q:148:MET:SD	2.89	0.45
3:N:960:CYS:C	3:N:962:THR:N	2.74	0.45
4:O:168:ILE:HA	4:O:183:ALA:O	2.16	0.45
5:R:133:ARG:NH1	5:R:142:SER:OG	2.43	0.45
6:V:358:GLU:HA	6:V:361:GLN:HE22	1.81	0.45
2:C:121:ARG:NH1	2:C:142:ASP:OD1	2.50	0.45
2:C:224:ALA:HB2	2:C:259:TRP:HZ2	1.82	0.45
4:E:17:ASP:O	4:E:29:THR:HG22	2.17	0.45
4:G:288:ILE:HD12	4:G:288:ILE:N	2.32	0.45
4:Q:308:ASN:OD1	4:Q:308:ASN:O	2.34	0.45
1:B:824:PHE:O	3:D:936:ASN:HA	2.16	0.45
5:H:337:GLU:HA	5:H:343:TRP:HA	1.98	0.45
2:M:685:GLN:HG2	2:M:690:TRP:CZ3	2.51	0.45
4:O:66:ALA:HB2	4:O:121:PHE:CE2	2.51	0.45
4:Q:119:VAL:CG2	4:Q:130:LEU:HD11	2.46	0.45
2:M:159:PHE:CZ	2:M:179:PHE:HZ	2.35	0.45
4:O:33:ASP:O	4:O:54:LYS:NZ	2.47	0.45
1:A:401:ARG:HB3	1:A:401:ARG:NH1	2.32	0.45
1:B:453:TYR:O	1:B:654:LEU:N	2.46	0.45
5:H:157:TRP:CE2	5:H:166:LEU:HD13	2.52	0.45
2:M:694:ASN:C	2:M:694:ASN:HD22	2.25	0.45
3:N:876:ARG:O	3:N:879:ARG:HG2	2.16	0.45
6:V:314:CYS:O	6:V:316:VAL:HG23	2.17	0.45
3:D:937:PHE:CD1	3:D:937:PHE:C	2.95	0.44
4:F:295:SER:O	4:F:303:ARG:N	2.33	0.44
4:P:199:ILE:N	4:P:213:GLU:O	2.40	0.44
5:H:189:LYS:HE3	5:H:189:LYS:HB2	1.75	0.44
2:M:65:LEU:HD23	2:M:65:LEU:HA	1.74	0.44
6:U:89:TYR:CD2	6:U:457:LEU:HD11	2.52	0.44
6:U:164:LYS:NZ	6:U:321:PHE:HB2	2.32	0.44
6:U:453:VAL:O	6:U:457:LEU:HB3	2.17	0.44
2:C:80:VAL:HG12	2:C:92:THR:HB	1.99	0.44
4:G:26:ARG:HE	4:G:40:ASP:CG	2.25	0.44
1:K:367:MET:HE3	1:K:367:MET:HB2	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:267:LEU:O	2:M:280:VAL:HA	2.17	0.44
1:B:128:TRP:HA	1:B:147:ILE:H	1.83	0.44
5:H:270:ILE:HD11	5:H:319:THR:HG22	1.99	0.44
5:H:335:TRP:N	5:H:335:TRP:CD1	2.86	0.44
1:K:733:VAL:HG13	2:M:740:ALA:HB1	1.99	0.44
1:L:785:CYS:N	1:L:790:ILE:O	2.50	0.44
3:N:878:LYS:HA	3:N:881:GLU:HG3	1.99	0.44
3:N:941:CYS:HB3	3:N:966:CYS:CB	2.47	0.44
4:Q:169:SER:HB3	4:Q:225:ILE:HG22	1.99	0.44
1:A:86:ARG:HA	1:A:109:VAL:HA	1.99	0.44
1:A:204:MET:N	1:A:207:ASN:O	2.43	0.44
1:A:330:TRP:HA	1:A:338:MET:HA	2.00	0.44
1:A:394:MET:HE3	1:A:671:ASP:HA	1.99	0.44
1:B:742:LYS:HE3	1:B:743:SER:N	2.27	0.44
4:F:139:VAL:O	4:F:159:ILE:N	2.43	0.44
4:G:21:ASP:HB2	4:G:26:ARG:HB2	2.00	0.44
1:K:790:ILE:HD12	4:Q:69:GLU:HA	2.00	0.44
6:U:175:LYS:HB3	6:U:175:LYS:HE3	1.71	0.44
1:A:408:GLN:O	1:A:408:GLN:HG3	2.16	0.44
1:B:570:SER:O	1:B:574:GLU:N	2.47	0.44
2:M:147:CYS:HB3	2:M:157:SER:OG	2.17	0.44
4:P:198:GLN:HA	4:P:214:THR:HA	2.00	0.44
6:U:79:LEU:N	6:U:127:TYR:OH	2.46	0.44
6:U:325:ASP:O	6:U:326:PHE:HB2	2.18	0.44
2:C:216:HIS:HD2	2:C:217:PRO:HD2	1.82	0.44
2:M:70:LYS:O	2:M:72:SER:N	2.49	0.44
2:M:442:ARG:O	2:M:445:VAL:HG12	2.18	0.44
4:O:121:PHE:CD1	4:O:130:LEU:HD13	2.53	0.44
4:O:122:ALA:HB3	4:O:129:MET:HB2	2.00	0.44
4:P:307:ALA:HA	4:P:313:TRP:HA	1.99	0.44
4:Q:308:ASN:O	4:Q:310:MET:N	2.51	0.44
1:B:528:ALA:O	1:B:532:LEU:N	2.50	0.44
1:B:742:LYS:HD2	1:B:742:LYS:HA	1.82	0.44
5:H:316:TRP:CZ3	5:H:323:LEU:HB2	2.53	0.44
1:L:144:ILE:O	1:L:179:TYR:N	2.35	0.44
2:M:760:CYS:HB3	2:M:762:HIS:CD2	2.52	0.44
1:A:87:VAL:O	1:A:108:PHE:N	2.49	0.44
5:H:124:SER:OG	5:H:126:ASP:O	2.36	0.44
3:N:871:TYR:HB2	3:N:879:ARG:NE	2.32	0.44
4:Q:37:LYS:HG2	4:Q:52:SER:HB2	2.00	0.44
4:Q:197:VAL:HG21	4:Q:240:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:GLU:H	1:A:354:GLU:CD	2.26	0.43
1:A:411:ARG:O	1:A:414:ILE:HG12	2.18	0.43
1:B:742:LYS:C	1:B:744:ILE:H	2.26	0.43
2:C:698:LYS:HB3	2:C:698:LYS:HE3	1.69	0.43
4:F:137:GLY:O	4:F:161:CYS:N	2.39	0.43
5:H:67:MET:HE2	5:H:71:GLY:HA2	2.00	0.43
6:V:412:GLU:HA	6:V:415:GLN:NE2	2.33	0.43
1:A:422:GLN:OE1	1:A:422:GLN:HA	2.18	0.43
4:E:119:VAL:HG23	4:E:132:THR:HG22	2.01	0.43
2:M:272:MET:O	2:M:273:MET:HG2	2.18	0.43
3:N:677:CYS:HB3	3:N:700:THR:HG23	2.00	0.43
3:N:750:SER:HB2	3:N:885:PHE:CD1	2.46	0.43
4:Q:16:HIS:NE2	4:Q:32:SER:HB2	2.33	0.43
6:U:453:VAL:O	6:U:457:LEU:CB	2.66	0.43
4:G:58:GLY:HA3	4:G:79:PHE:HB3	2.01	0.43
1:K:241:ALA:HA	1:K:250:ILE:HA	2.00	0.43
1:L:736:SER:HA	1:L:743:SER:HA	2.00	0.43
3:N:932:ARG:HA	3:N:932:ARG:CZ	2.48	0.43
5:H:77:CYS:SG	5:H:109:VAL:HG13	2.58	0.43
3:N:875:LEU:O	3:N:878:LYS:N	2.51	0.43
3:N:888:CYS:HA	3:N:889:PRO:HD2	1.74	0.43
4:Q:308:ASN:O	4:Q:309:TYR:CD2	2.71	0.43
3:D:741:ASP:OD2	3:D:741:ASP:C	2.62	0.43
1:A:745:SER:OG	2:C:758:GLN:O	2.27	0.43
4:G:245:VAL:HG23	4:G:281:VAL:HG21	2.01	0.43
1:K:732:GLN:NE2	2:M:763:GLY:O	2.51	0.43
2:M:660:LEU:HD13	2:M:664:VAL:HG11	2.00	0.43
6:V:96:LEU:HD23	6:V:366:LYS:HZ3	1.82	0.43
6:V:217:LEU:HA	6:V:218:PRO:HD2	1.82	0.43
2:C:351:LEU:HD12	2:C:351:LEU:HA	1.81	0.43
5:H:240:TRP:CD1	5:H:250:GLU:HA	2.53	0.43
1:A:325:ILE:HA	1:A:342:THR:HA	2.00	0.43
1:A:409:VAL:HB	1:A:431:HIS:HB2	2.01	0.43
1:A:852:SER:HB3	2:C:698:LYS:HA	2.01	0.43
2:C:66:ARG:HD2	2:C:75:LEU:HB3	2.01	0.43
2:C:688:ARG:HE	4:G:23:HIS:CE1	2.37	0.43
3:D:902:CYS:N	3:D:907:SER:O	2.47	0.43
4:F:42:SER:N	4:F:46:ASP:O	2.44	0.43
3:N:880:ALA:O	3:N:884:LYS:HG2	2.19	0.43
4:P:89:ILE:O	4:P:102:HIS:N	2.47	0.43
5:R:119:ILE:HG12	5:R:133:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:ALA:O	2:C:32:ILE:HD12	2.19	0.43
2:C:265:HIS:HD2	2:C:284:ARG:NH1	2.16	0.43
3:D:878:LYS:HD2	3:D:878:LYS:HA	1.80	0.43
1:K:394:MET:CE	1:K:672:VAL:H	2.32	0.43
2:M:307:HIS:CG	2:M:308:PRO:HD2	2.54	0.43
5:R:260:TRP:O	5:R:282:GLN:N	2.35	0.43
6:U:103:THR:O	6:U:112:ARG:NH1	2.37	0.43
3:D:914:CYS:CB	3:D:917:CYS:SG	3.07	0.43
3:D:927:CYS:SG	3:D:949:HIS:HE1	2.30	0.43
4:G:85:VAL:HG12	4:G:85:VAL:O	2.18	0.43
4:G:221:PRO:HB2	4:G:223:HIS:NE2	2.34	0.43
4:G:222:VAL:C	4:G:223:HIS:HD2	2.27	0.43
5:H:311:VAL:HA	5:H:327:GLY:HA2	2.01	0.43
2:M:651:GLN:HG3	2:M:680:TYR:CZ	2.54	0.43
4:Q:208:LYS:HB2	4:Q:208:LYS:HE2	1.66	0.43
6:V:162:ILE:CD1	6:V:181:LEU:HD12	2.11	0.43
1:A:662:MET:O	1:A:666:VAL:HG23	2.18	0.42
2:C:261:PRO:HG2	2:C:310:ASP:O	2.18	0.42
3:D:742:VAL:HG21	5:H:270:ILE:HD12	2.01	0.42
4:E:225:ILE:HG23	4:E:238:LEU:HD21	2.01	0.42
4:E:287:ASN:HB2	4:E:292:VAL:HG23	2.01	0.42
1:K:132:GLY:HA2	1:K:142:VAL:HA	2.00	0.42
2:M:161:GLY:O	2:M:163:SER:N	2.51	0.42
6:U:167:ALA:HB2	6:U:205:HIS:NE2	2.34	0.42
1:A:733:VAL:HG11	2:C:717:VAL:HG13	2.00	0.42
4:E:143:GLU:HB2	4:E:156:GLN:NE2	2.34	0.42
4:G:169:SER:HB2	4:G:225:ILE:HG23	1.99	0.42
2:M:731:TRP:HD1	2:M:739:CYS:SG	2.41	0.42
4:P:81:ARG:H	4:P:115:SER:HA	1.84	0.42
4:Q:267:GLU:N	4:Q:267:GLU:OE1	2.52	0.42
1:A:635:LYS:HE3	1:A:635:LYS:HB2	1.74	0.42
2:C:179:PHE:HD2	2:C:191:TRP:HB2	1.84	0.42
2:C:326:HIS:C	2:C:327:LEU:HD12	2.45	0.42
3:D:726:ARG:O	3:D:730:GLU:HG3	2.19	0.42
4:G:66:ALA:HB2	4:G:121:PHE:CZ	2.53	0.42
1:K:713:ARG:CZ	2:M:747:HIS:CE1	3.02	0.42
2:M:164:GLU:HB2	2:M:184:GLU:HB3	2.01	0.42
1:A:705:ASP:HA	1:A:710:TRP:HZ3	1.83	0.42
1:A:847:ALA:C	1:A:857:LYS:HZ2	2.26	0.42
2:C:273:MET:HE1	6:U:351:LEU:HD12	2.01	0.42
4:O:249:THR:C	4:O:250:LEU:HD23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ARG:HG2	1:A:401:ARG:O	2.19	0.42
2:C:339:ASN:HA	2:C:340:PRO:HD3	1.89	0.42
3:D:540:SER:HA	3:D:553:PHE:O	2.18	0.42
3:D:713:PRO:O	4:G:309:TYR:HE1	2.02	0.42
5:H:107:TRP:HB2	5:H:108:GLN:CD	2.44	0.42
5:H:130:ILE:HD12	5:H:141:LYS:NZ	2.34	0.42
2:M:19:ARG:NH1	2:M:56:GLU:O	2.53	0.42
2:M:267:LEU:HD23	2:M:267:LEU:HA	1.85	0.42
6:U:128:LEU:O	6:U:132:HIS:HB2	2.19	0.42
1:K:781:PRO:HB3	4:Q:148:MET:HE1	2.01	0.42
6:V:161:GLU:OE1	6:V:162:ILE:HG13	2.20	0.42
2:C:39:ALA:O	2:C:54:ILE:N	2.33	0.42
4:F:195:ALA:HB2	4:F:216:MET:HA	2.01	0.42
1:L:204:MET:N	1:L:207:ASN:O	2.50	0.42
2:M:718:ASN:OD1	2:M:718:ASN:N	2.53	0.42
3:N:882:VAL:HG12	3:N:883:LEU:HD23	2.01	0.42
1:A:662:MET:HE2	1:A:662:MET:HB2	1.85	0.42
3:D:685:LEU:HD23	3:D:685:LEU:HA	1.82	0.42
3:D:879:ARG:HA	3:D:882:VAL:HG12	2.01	0.42
1:K:787:LEU:HD21	1:K:850:PRO:HB3	2.01	0.42
6:U:89:TYR:OH	6:U:366:LYS:NZ	2.53	0.42
6:U:342:TYR:CE2	6:U:473:ARG:HA	2.55	0.42
4:G:276:ASN:HD21	4:G:305:TRP:HH2	1.68	0.42
1:K:665:TYR:CD1	1:K:665:TYR:C	2.98	0.42
1:L:250:ILE:O	1:L:260:VAL:N	2.44	0.42
2:M:754:PHE:CE1	2:M:764:GLY:HA2	2.54	0.42
3:N:694:GLN:O	3:N:697:SER:OG	2.31	0.42
1:A:843:PHE:CZ	1:A:858:CYS:HB2	2.55	0.42
2:C:31:ALA:C	2:C:32:ILE:HD12	2.45	0.42
2:C:762:HIS:HE1	2:C:783:CYS:SG	2.42	0.42
4:E:231:LEU:HD22	4:E:289:THR:HA	2.02	0.42
4:G:110:VAL:HG23	4:G:110:VAL:O	2.20	0.42
2:M:19:ARG:O	2:M:21:MET:HG3	2.20	0.42
3:N:950:MET:SD	3:N:951:MET:N	2.93	0.42
4:Q:231:LEU:HD22	4:Q:289:THR:HG22	2.01	0.42
1:A:733:VAL:HG13	2:C:717:VAL:HG13	2.01	0.41
4:F:117:THR:N	4:F:133:CYS:O	2.53	0.41
1:K:788:CYS:CB	1:K:790:ILE:HG22	2.50	0.41
1:A:28:TYR:HA	1:A:53:LEU:HA	2.01	0.41
4:G:113:ARG:H	4:G:113:ARG:HG2	1.53	0.41
2:M:755:VAL:O	2:M:763:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:5:ARG:NH1	4:Q:45:GLY:O	2.49	0.41
4:Q:274:PHE:HD1	4:Q:305:TRP:CZ3	2.38	0.41
1:A:744:ILE:HG23	1:A:776:PRO:HD3	2.02	0.41
4:O:34:GLN:HE22	4:O:57:SER:C	2.28	0.41
6:U:125:CYS:HA	6:U:212:PHE:CZ	2.55	0.41
1:K:695:TYR:HE1	4:O:175:SER:HA	1.84	0.41
1:K:720:ARG:O	1:K:724:ASP:N	2.49	0.41
4:O:74:LEU:HB2	4:O:86:TRP:HB2	2.03	0.41
4:P:284:VAL:HA	4:P:295:SER:HA	2.01	0.41
6:U:210:PHE:CE1	6:U:457:LEU:HD23	2.56	0.41
2:C:136:LEU:HD12	2:C:137:LEU:N	2.34	0.41
2:C:310:ASP:C	2:C:310:ASP:OD1	2.63	0.41
2:C:669:ASP:OD2	2:C:672:THR:OG1	2.33	0.41
3:D:684:ALA:HB1	3:D:692:LEU:HB2	2.02	0.41
2:M:129:HIS:HB3	2:M:135:VAL:CG2	2.50	0.41
4:Q:197:VAL:HG23	4:Q:222:VAL:HG21	2.02	0.41
1:A:250:ILE:O	1:A:260:VAL:N	2.54	0.41
4:G:231:LEU:HD12	4:G:289:THR:HA	2.01	0.41
2:M:760:CYS:HB3	2:M:762:HIS:HD2	1.85	0.41
3:N:692:LEU:HD13	3:N:692:LEU:HA	1.91	0.41
4:P:243:LYS:HA	4:P:280:GLN:HA	2.03	0.41
6:U:136:PHE:O	6:U:139:THR:HG22	2.20	0.41
2:C:400:PHE:HE1	4:G:4:ALA:HB2	1.85	0.41
4:G:226:ALA:O	4:G:238:LEU:HD12	2.20	0.41
1:K:646:LEU:HD23	1:K:646:LEU:HA	1.95	0.41
2:M:183:PHE:CE1	2:M:189:GLN:HG3	2.55	0.41
2:M:253:SER:OG	2:M:272:MET:HB3	2.21	0.41
3:N:724:PHE:O	3:N:728:LEU:HB3	2.21	0.41
6:U:101:LEU:HD23	6:U:101:LEU:HA	1.89	0.41
1:A:733:VAL:HG23	2:C:740:ALA:O	2.21	0.41
1:B:729:PRO:HB2	3:D:943:HIS:HE2	1.85	0.41
4:Q:225:ILE:CD1	4:Q:240:ILE:HG12	2.51	0.41
1:A:25:LEU:N	1:A:57:ASN:O	2.52	0.41
1:A:820:PHE:CE2	2:C:770:MET:HG3	2.55	0.41
1:A:857:LYS:HB3	1:A:857:LYS:HE3	1.82	0.41
1:B:560:ALA:HA	1:K:560:ALA:HA	2.02	0.41
2:C:426:LEU:HD22	2:C:663:ARG:NH2	2.35	0.41
3:D:883:LEU:HD23	3:D:883:LEU:HA	1.89	0.41
4:G:34:GLN:O	4:G:54:LYS:HG3	2.21	0.41
4:G:88:GLU:HB2	4:G:103:TRP:CE2	2.55	0.41
1:L:74:PRO:O	1:L:74:PRO:CD	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:655:THR:O	1:L:659:VAL:N	2.52	0.41
2:M:273:MET:HE2	6:V:347:HIS:O	2.20	0.41
2:M:280:VAL:HG22	2:M:291:ALA:HB3	2.02	0.41
4:O:4:ALA:HB2	4:O:319:LEU:HD13	2.02	0.41
5:R:85:ILE:HD13	5:R:85:ILE:HA	1.84	0.41
6:U:207:LEU:HD23	6:U:207:LEU:HA	1.89	0.41
6:V:89:TYR:CD2	6:V:457:LEU:HD11	2.56	0.41
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.85	0.41
3:D:544:PHE:HA	3:D:550:LEU:HD12	2.02	0.41
3:D:953:TRP:NE1	3:D:959:VAL:O	2.46	0.41
4:E:21:ASP:CG	4:E:22:PHE:H	2.26	0.41
4:F:201:GLU:N	4:F:210:ALA:O	2.36	0.41
4:G:246:ARG:HG3	4:G:246:ARG:NH1	2.36	0.41
4:G:276:ASN:ND2	4:G:305:TRP:HH2	2.19	0.41
4:P:82:THR:HA	4:P:110:VAL:HA	2.02	0.41
2:M:722:CYS:O	2:M:723:LYS:HB2	2.21	0.40
6:U:433:GLU:OE1	6:U:433:GLU:N	2.53	0.40
6:V:390:ARG:HG3	6:V:391:ARG:N	2.35	0.40
1:B:342:THR:N	1:B:346:THR:O	2.45	0.40
4:G:242:THR:HB	4:G:246:ARG:HH12	1.87	0.40
1:L:593:ALA:O	1:L:597:SER:N	2.55	0.40
2:M:176:TYR:O	2:M:177:PHE:HD1	2.04	0.40
3:N:721:ARG:HH12	4:Q:309:TYR:HD1	1.68	0.40
1:A:16:ASP:O	1:A:30:VAL:N	2.41	0.40
1:A:394:MET:HA	1:A:673:GLN:NE2	2.37	0.40
1:A:453:TYR:CE2	1:A:682:GLY:HA3	2.56	0.40
2:C:284:ARG:HE	2:C:284:ARG:HB2	1.75	0.40
3:D:740:ARG:HG3	3:D:740:ARG:HH11	1.87	0.40
5:H:118:ASN:C	5:H:119:ILE:HD12	2.47	0.40
2:M:107:PRO:CD	2:M:108:SER:N	2.82	0.40
2:M:297:ARG:NH1	2:M:297:ARG:HB2	2.37	0.40
5:R:242:GLU:HA	5:R:248:TRP:HA	2.02	0.40
1:A:646:LEU:HD23	1:A:646:LEU:HA	1.93	0.40
1:B:853:ALA:HB3	3:D:890:PRO:HD3	2.02	0.40
2:C:260:ARG:NE	2:C:260:ARG:HA	2.36	0.40
4:G:80:ASP:O	4:G:82:THR:N	2.52	0.40
2:M:333:GLN:HA	2:M:334:PRO:HD3	1.96	0.40
2:M:667:ASP:C	2:M:668:ILE:HD13	2.46	0.40
3:N:876:ARG:CZ	3:N:876:ARG:HB2	2.52	0.40
4:Q:7:ILE:CD1	4:Q:47:TRP:HB2	2.46	0.40
1:A:74:PRO:O	1:A:74:PRO:CD	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:ASP:CG	2:C:765:HIS:HE2	2.28	0.40
4:G:253:VAL:HG22	4:G:265:LYS:O	2.21	0.40
5:H:66:GLN:HG3	5:H:111:TRP:CD1	2.56	0.40
5:H:173:GLY:O	5:H:194:ALA:N	2.42	0.40
1:K:145:TRP:HA	1:K:177:PRO:HA	2.04	0.40
1:K:773:THR:O	1:K:773:THR:OG1	2.40	0.40
2:M:305:TRP:CH2	2:M:314:LEU:HD12	2.56	0.40
6:U:195:ILE:HA	6:U:198:LEU:HG	2.03	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	726/875 (83%)	682 (94%)	43 (6%)	1 (0%)	48	80
1	B	700/875 (80%)	655 (94%)	45 (6%)	0	100	100
1	K	717/875 (82%)	684 (95%)	33 (5%)	0	100	100
1	L	708/875 (81%)	672 (95%)	35 (5%)	1 (0%)	48	80
2	C	565/790 (72%)	508 (90%)	55 (10%)	2 (0%)	30	65
2	M	564/790 (71%)	514 (91%)	49 (9%)	1 (0%)	44	74
3	D	267/974 (27%)	252 (94%)	15 (6%)	0	100	100
3	N	263/974 (27%)	239 (91%)	23 (9%)	1 (0%)	30	65
4	E	296/421 (70%)	274 (93%)	22 (7%)	0	100	100
4	F	293/421 (70%)	277 (94%)	16 (6%)	0	100	100
4	G	297/421 (70%)	270 (91%)	27 (9%)	0	100	100
4	O	296/421 (70%)	281 (95%)	15 (5%)	0	100	100
4	P	301/421 (72%)	289 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	298/421 (71%)	281 (94%)	16 (5%)	1 (0%)	37	70
5	H	280/368 (76%)	252 (90%)	28 (10%)	0	100	100
5	R	281/368 (76%)	254 (90%)	27 (10%)	0	100	100
6	U	303/480 (63%)	278 (92%)	24 (8%)	1 (0%)	37	70
6	V	297/480 (62%)	272 (92%)	23 (8%)	2 (1%)	19	54
All	All	7452/11250 (66%)	6934 (93%)	508 (7%)	10 (0%)	50	80

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	GLU
2	C	153	LYS
1	L	392	THR
2	M	783	CYS
3	N	889	PRO
6	U	326	PHE
6	V	345	GLU
6	V	386	THR
2	C	109	ARG
4	Q	287	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/771 (28%)	209 (99%)	3 (1%)	62	76
1	B	40/771 (5%)	40 (100%)	0	100	100
1	K	137/771 (18%)	137 (100%)	0	100	100
1	L	9/771 (1%)	9 (100%)	0	100	100
2	C	392/677 (58%)	385 (98%)	7 (2%)	54	71
2	M	361/677 (53%)	355 (98%)	6 (2%)	56	72
3	D	144/858 (17%)	143 (99%)	1 (1%)	81	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	136/858 (16%)	134 (98%)	2 (2%)	60	75
4	E	170/365 (47%)	170 (100%)	0	100	100
4	G	238/365 (65%)	237 (100%)	1 (0%)	89	92
4	O	142/365 (39%)	139 (98%)	3 (2%)	48	67
4	Q	232/365 (64%)	228 (98%)	4 (2%)	56	72
5	H	109/313 (35%)	109 (100%)	0	100	100
5	R	43/313 (14%)	43 (100%)	0	100	100
6	U	210/410 (51%)	210 (100%)	0	100	100
6	V	193/410 (47%)	189 (98%)	4 (2%)	48	67
All	All	2768/9060 (31%)	2737 (99%)	31 (1%)	69	79

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	SER
1	A	627	THR
1	A	841	SER
2	C	48	ILE
2	C	163	SER
2	C	222	TRP
2	C	301	THR
2	C	309	HIS
2	C	328	PHE
2	C	726	MET
3	D	742	VAL
4	G	316	THR
2	M	64	ASN
2	M	158	THR
2	M	207	ASN
2	M	249	GLN
2	M	694	ASN
2	M	713	THR
3	N	730	GLU
3	N	961	PRO
4	O	121	PHE
4	O	270	ILE
4	O	316	THR
4	Q	5	ARG
4	Q	245	VAL

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Mol	Chain	Res	Type
4	Q	295	SER
4	Q	305	TRP
6	V	212	PHE
6	V	352	ILE
6	V	397	ILE
6	V	454	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	HIS
1	A	431	HIS
1	A	673	GLN
1	A	699	ASN
1	A	711	HIS
2	C	134	HIS
2	C	189	GLN
2	C	651	GLN
2	C	694	ASN
2	C	709	ASN
2	C	747	HIS
3	D	674	GLN
4	E	34	GLN
4	E	171	ASN
4	G	157	HIS
4	G	205	ASN
2	M	22	HIS
2	M	119	HIS
2	M	207	ASN
2	M	307	HIS
2	M	710	GLN
3	N	735	HIS
4	O	230	ASN
4	O	236	HIS
4	Q	156	GLN
6	U	102	HIS
6	U	177	HIS
6	U	398	HIS
6	V	353	GLN
6	V	398	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

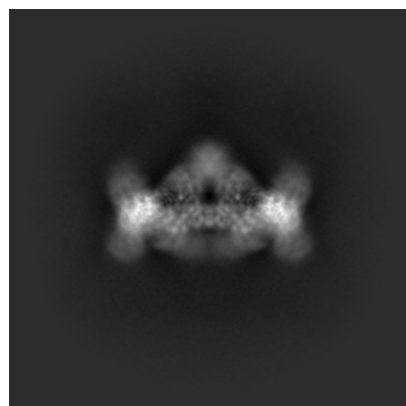
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63421. These allow visual inspection of the internal detail of the map and identification of artifacts.

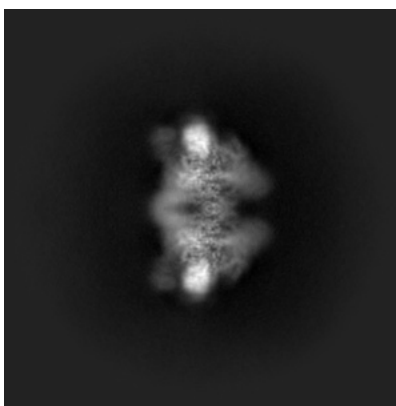
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

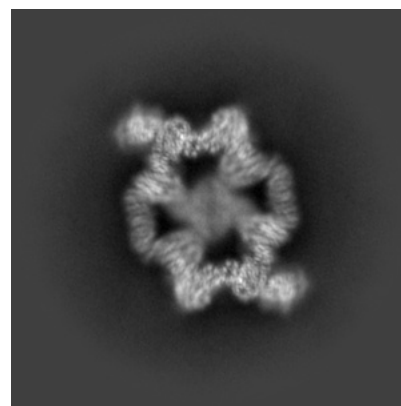
6.1.1 Primary map



X

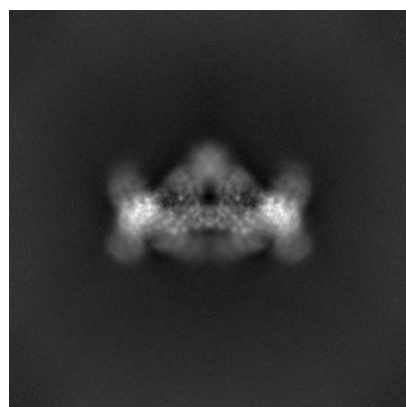


Y

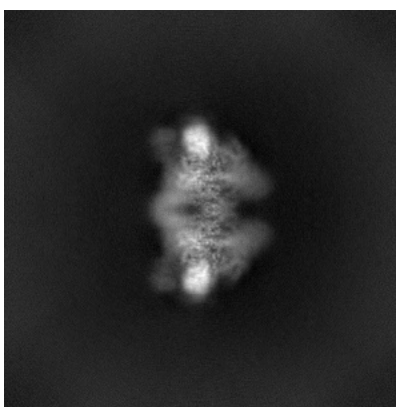


Z

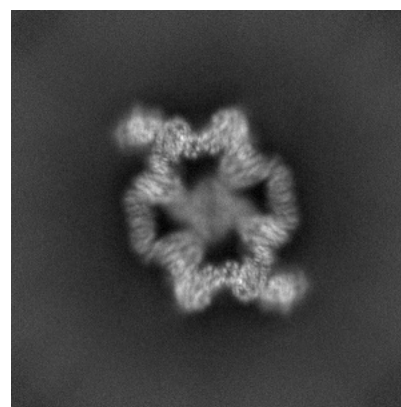
6.1.2 Raw map



X



Y

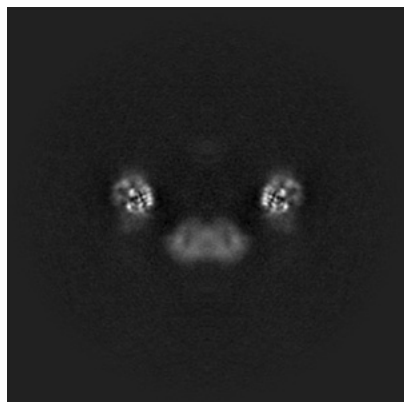


Z

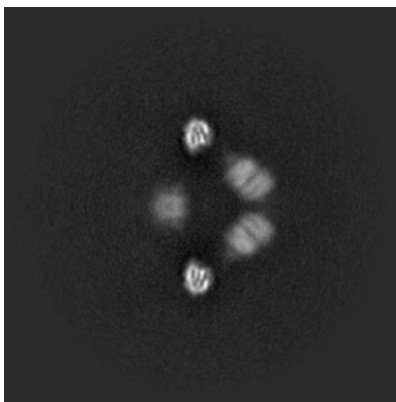
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

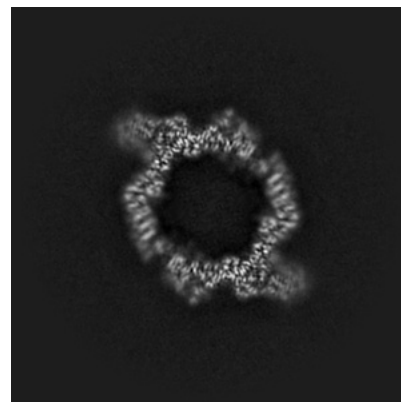
6.2.1 Primary map



X Index: 290



Y Index: 290

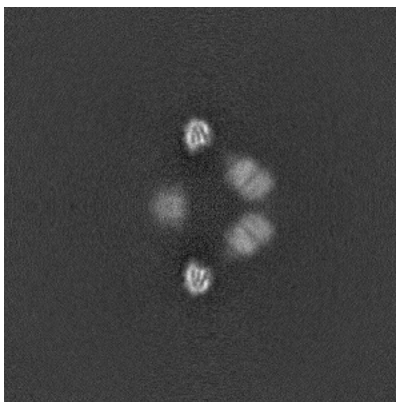


Z Index: 290

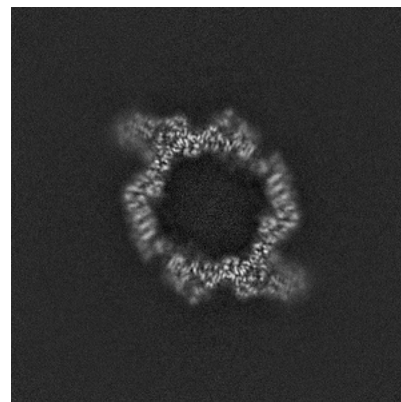
6.2.2 Raw map



X Index: 290



Y Index: 290

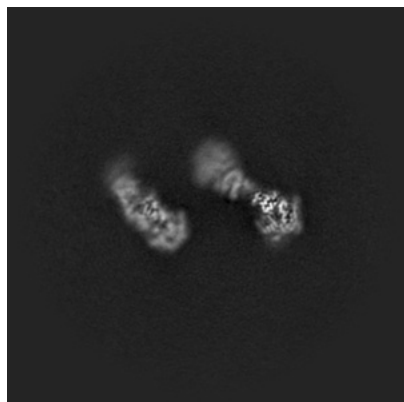


Z Index: 290

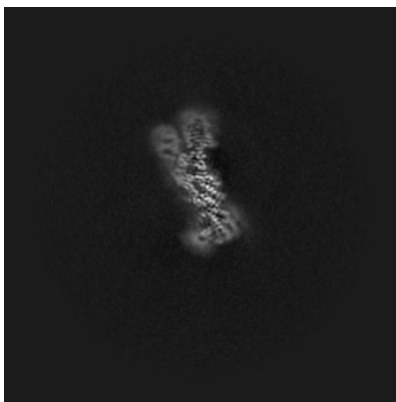
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

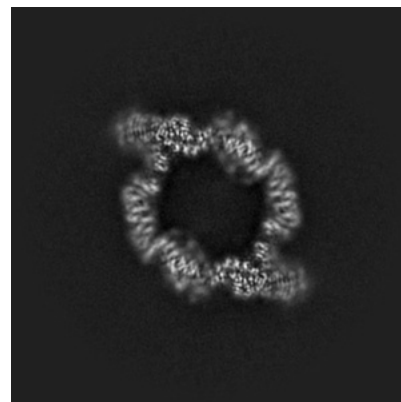
6.3.1 Primary map



X Index: 242



Y Index: 186

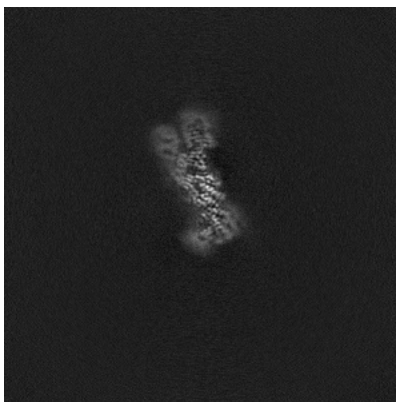


Z Index: 284

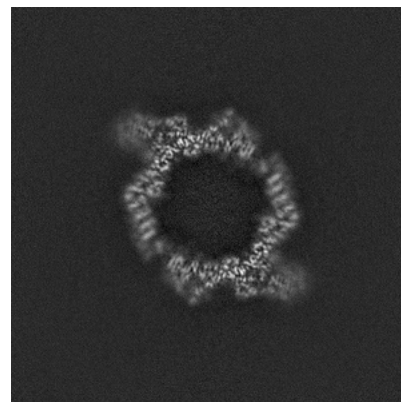
6.3.2 Raw map



X Index: 338



Y Index: 187

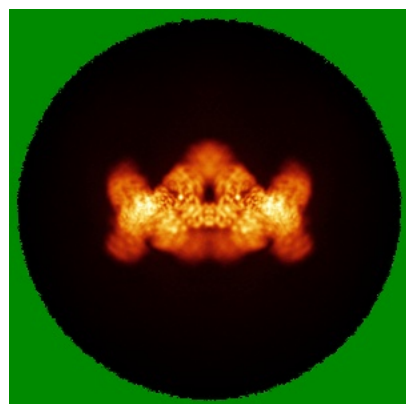


Z Index: 291

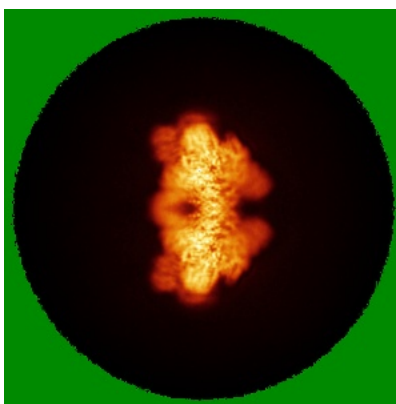
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

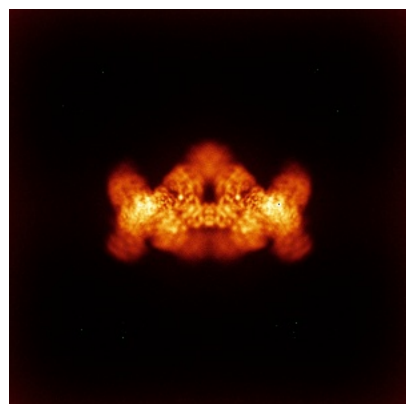


Y

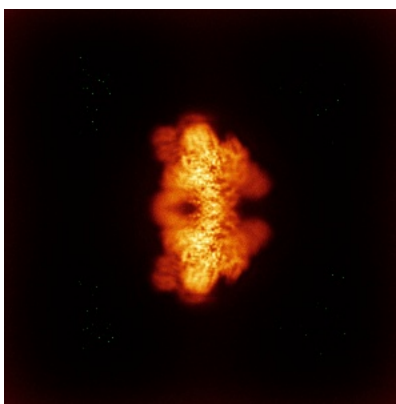


Z

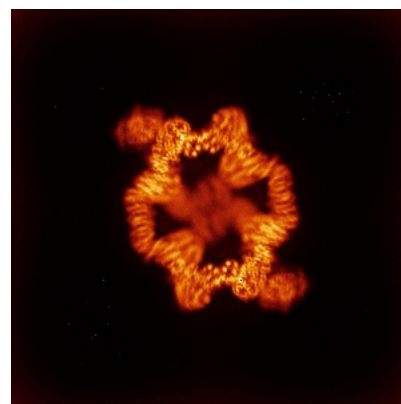
6.4.2 Raw map



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.

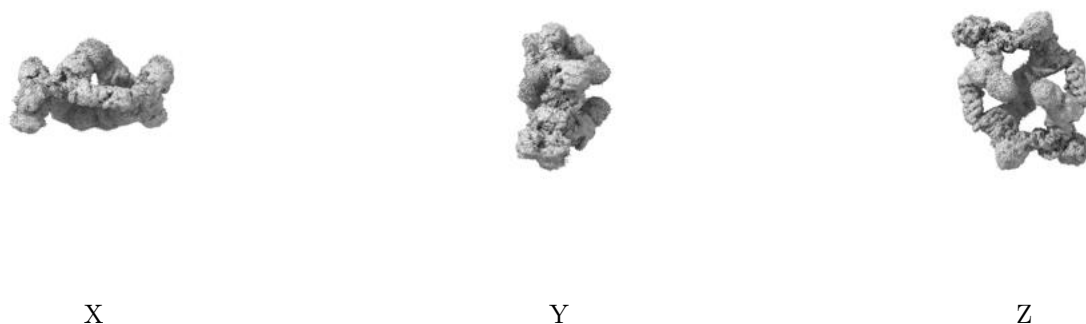
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.101. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

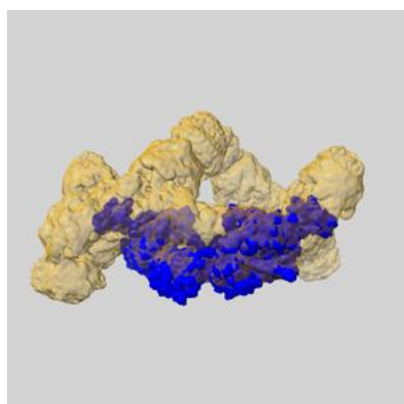
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

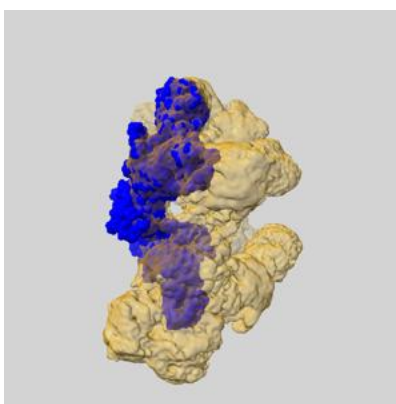
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

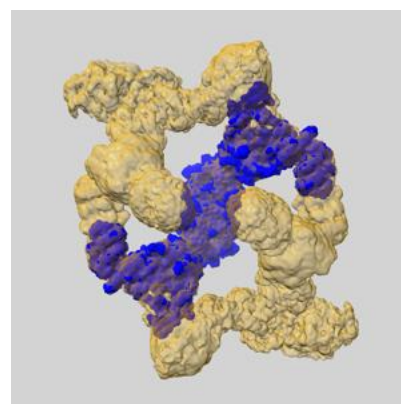
6.6.1 emd_63421_msk_1.map [i](#)



X

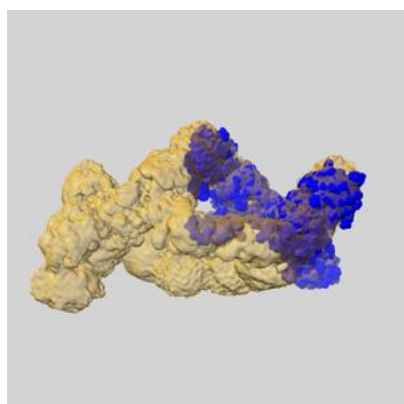


Y

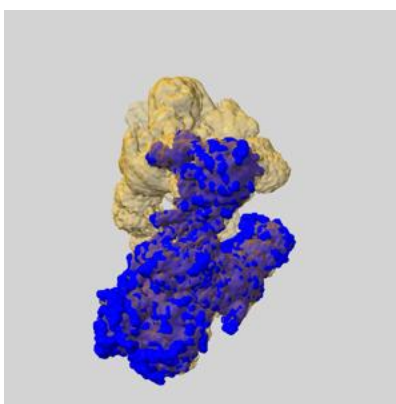


Z

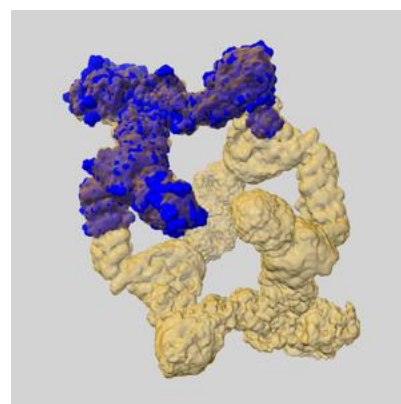
6.6.2 emd_63421_msk_2.map [i](#)



X

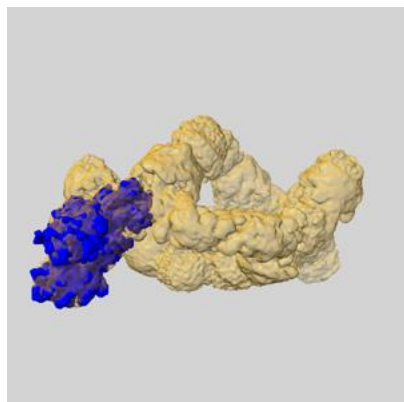


Y

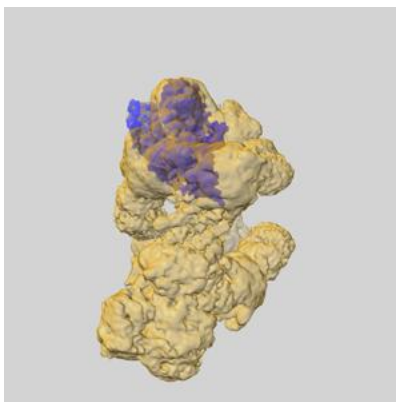


Z

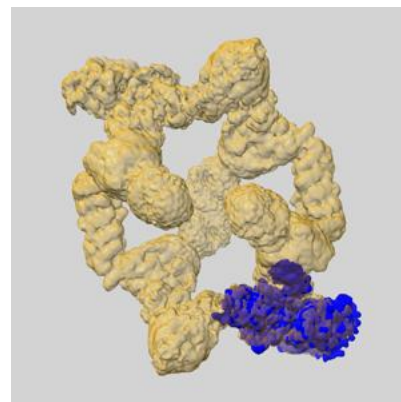
6.6.3 emd_63421_msk_3.map [i](#)



X

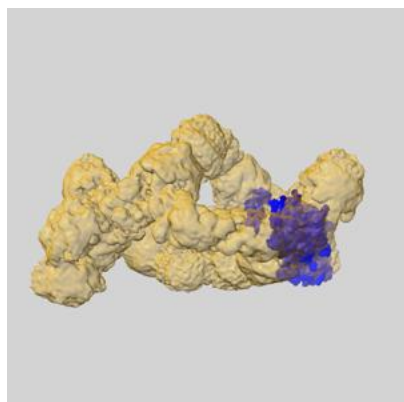


Y

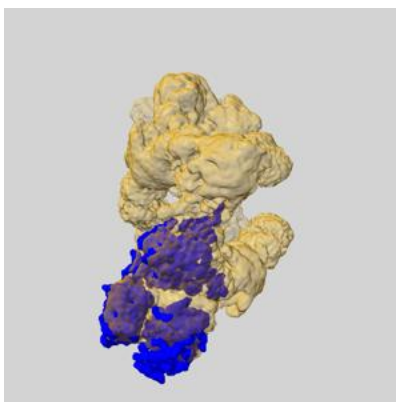


Z

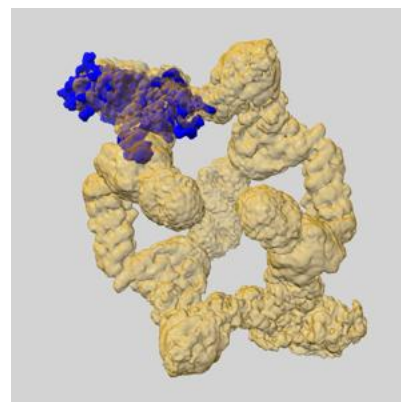
6.6.4 emd_63421_msk_4.map [i](#)



X

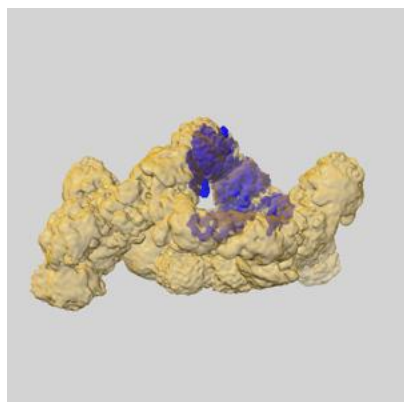


Y

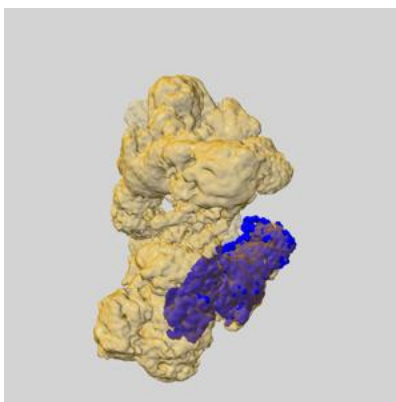


Z

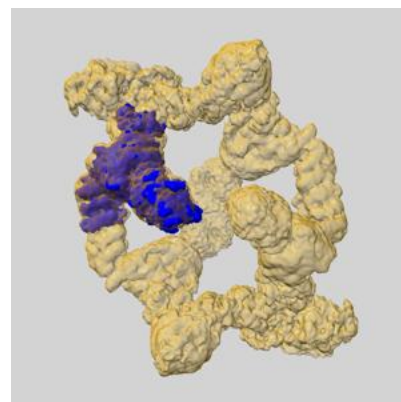
6.6.5 emd_63421_msk_5.map [i](#)



X

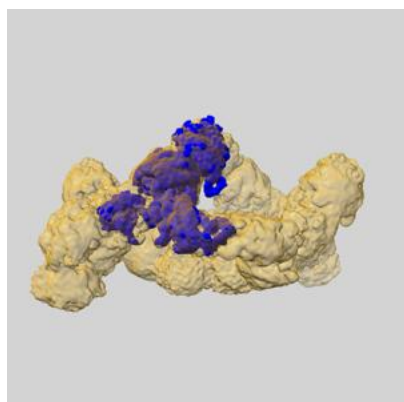


Y

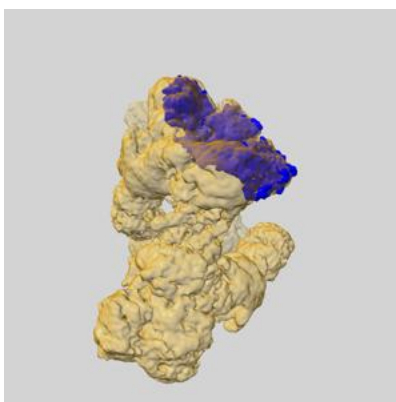


Z

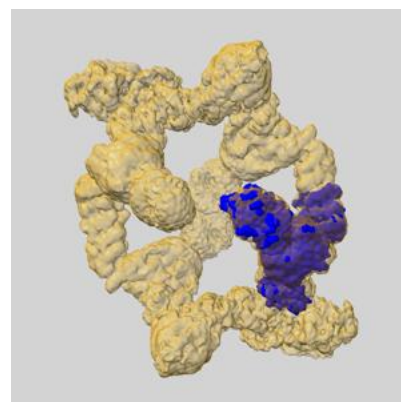
6.6.6 emd_63421_msk_6.map [i](#)



X

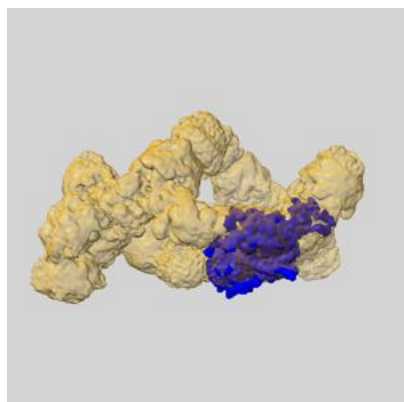


Y

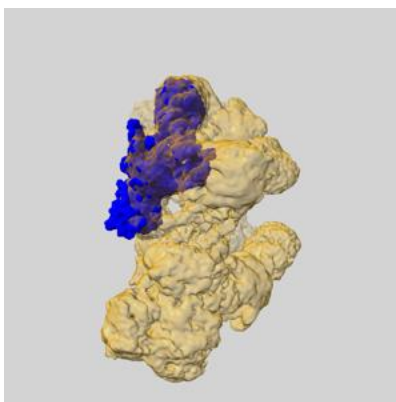


Z

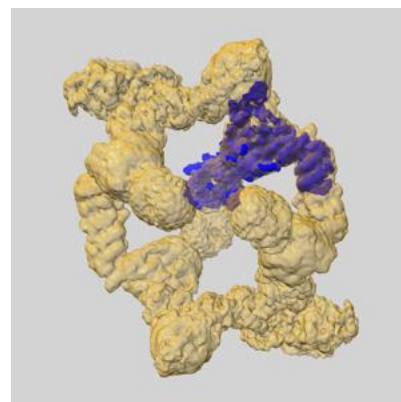
6.6.7 emd_63421_msk_7.map [i](#)



X

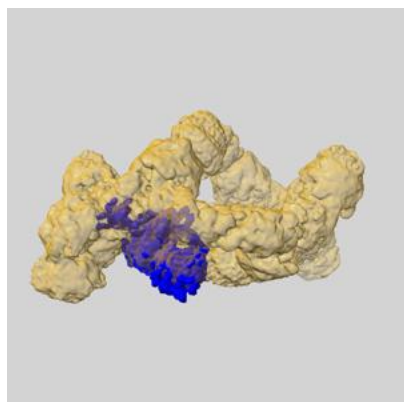


Y

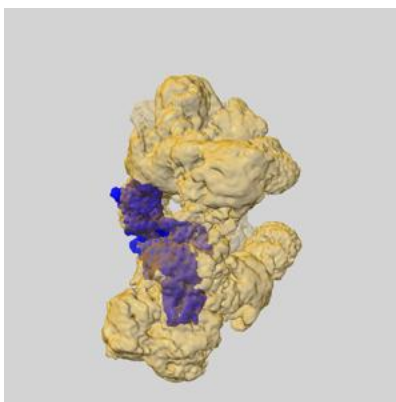


Z

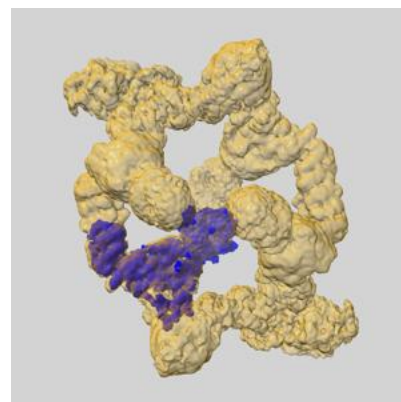
6.6.8 emd_63421_msk_8.map [i](#)



X



Y

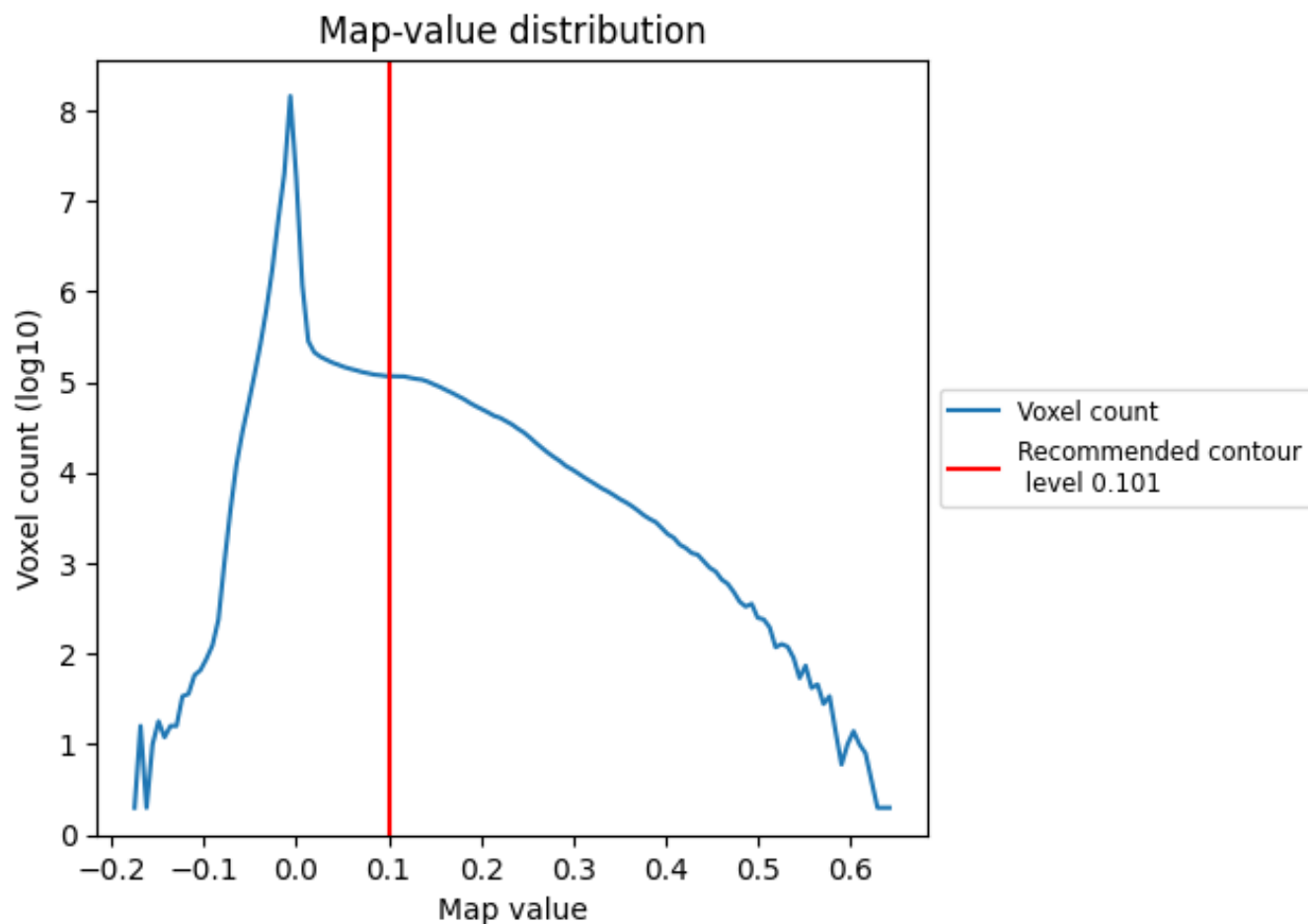


Z

7 Map analysis [i](#)

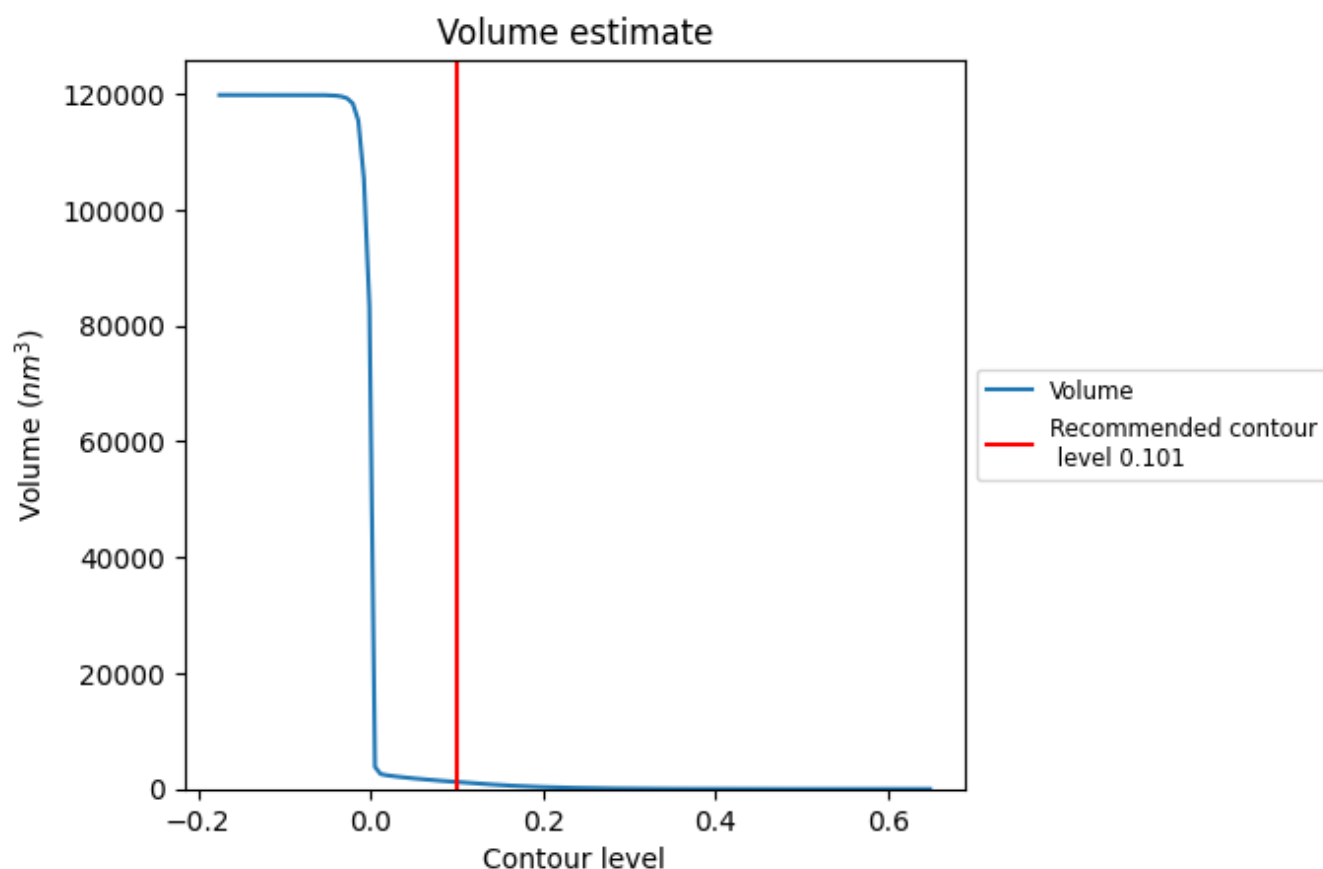
This section contains the results of statistical analysis of the map.

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.

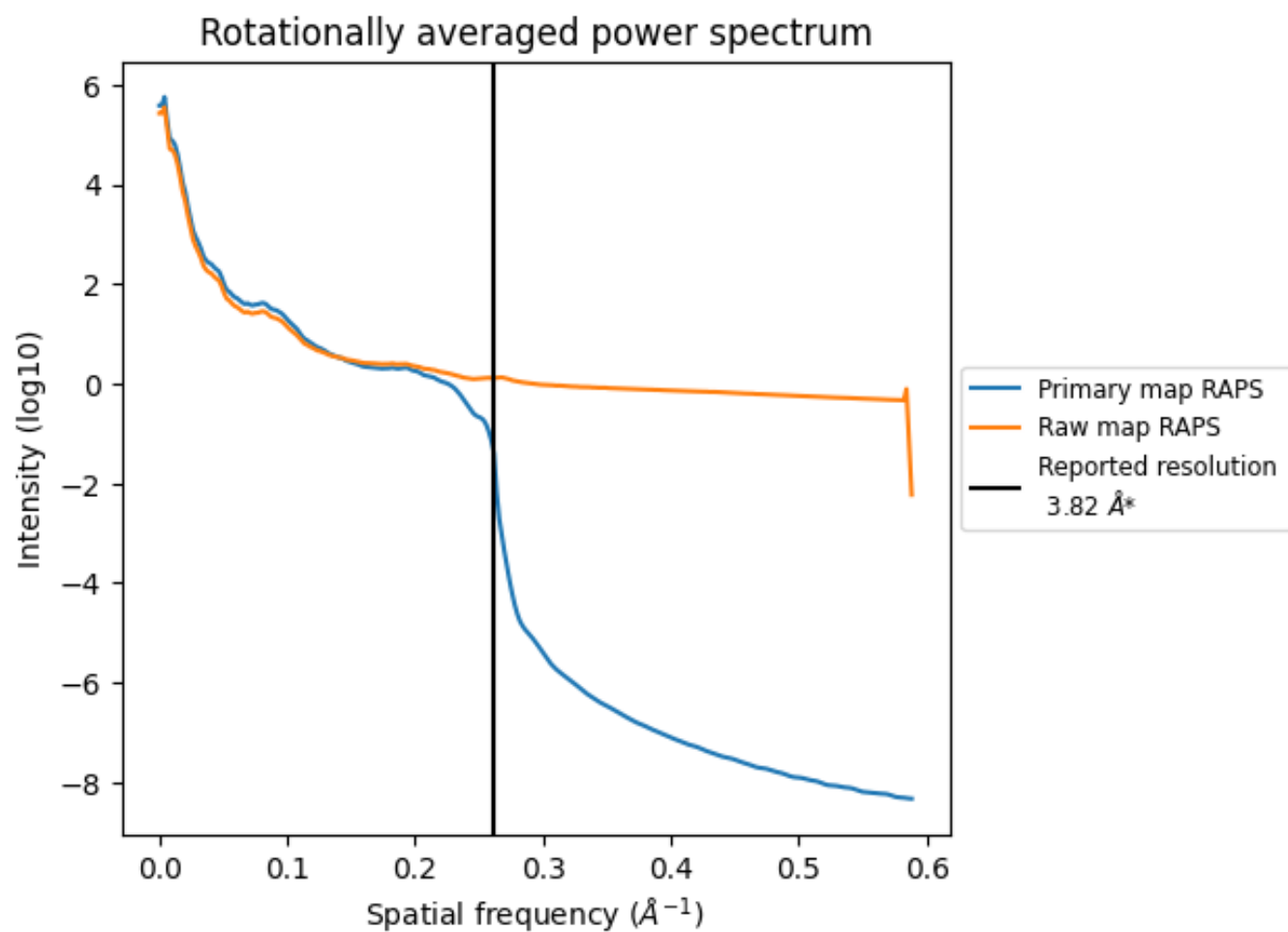
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1197 nm^3 ; this corresponds to an approximate mass of 1081 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

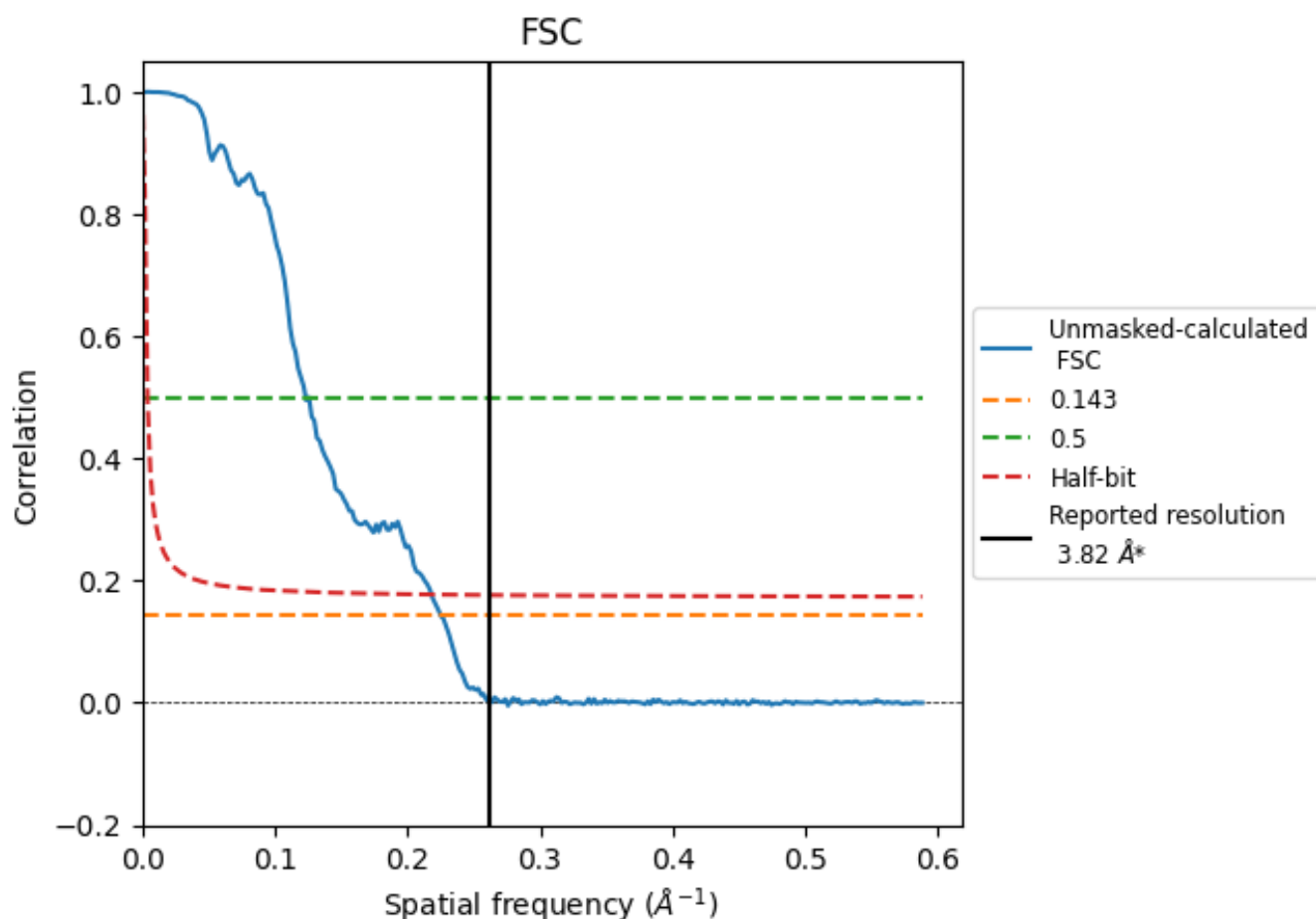


*Reported resolution corresponds to spatial frequency of 0.262 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.262 \AA^{-1}

8.2 Resolution estimates [i](#)

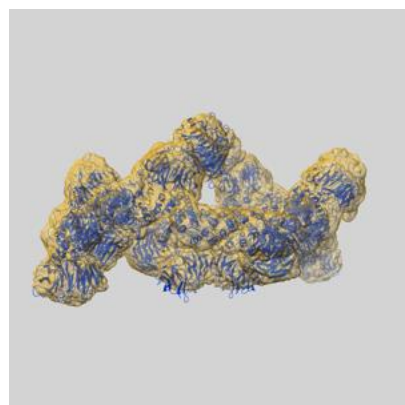
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	8.11	4.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.82 by more than 10 %

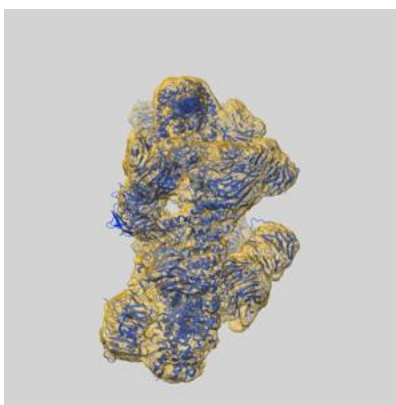
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63421 and PDB model 9LVJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

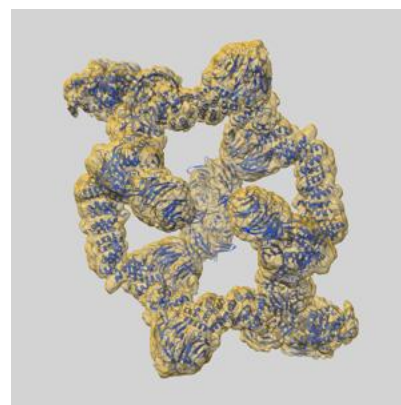
9.1 Map-model overlay [i](#)



X



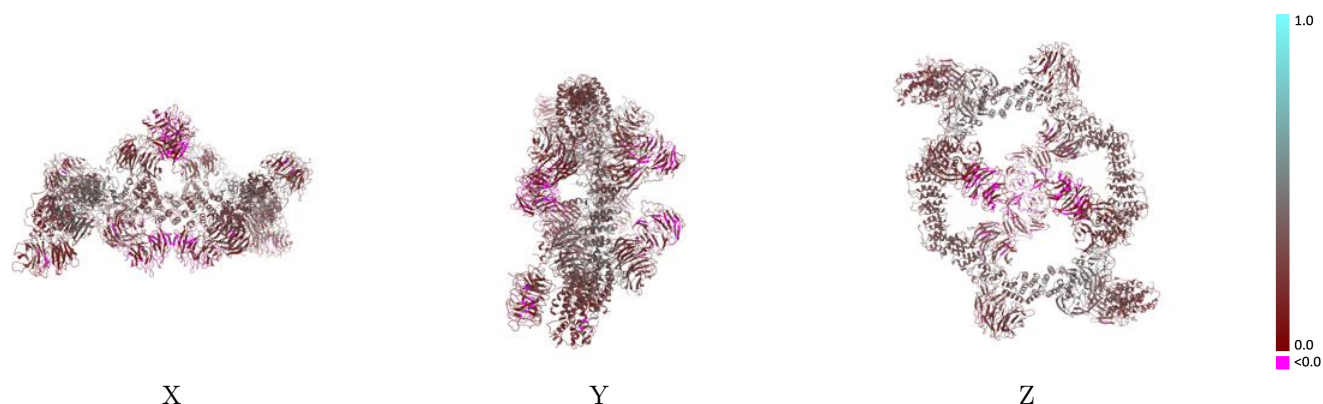
Y



Z

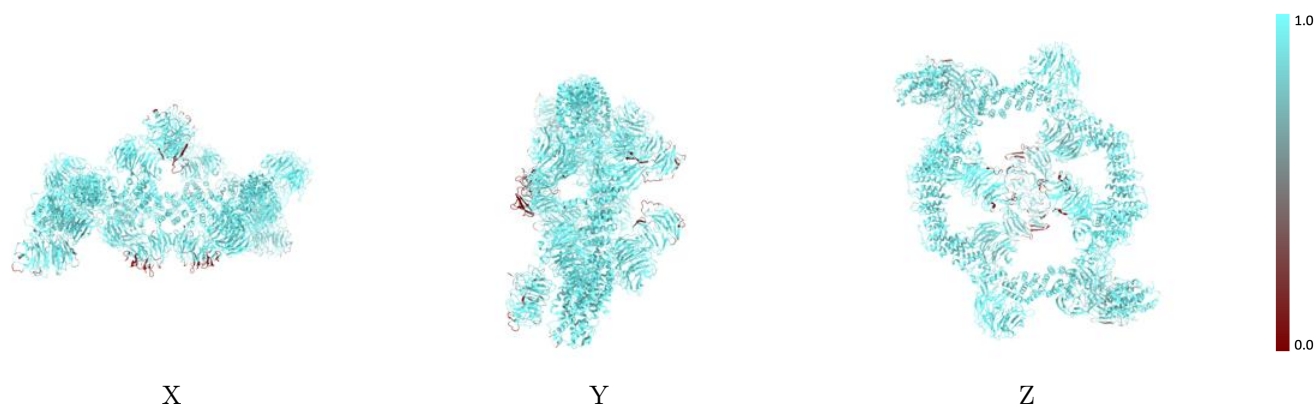
The images above show the 3D surface view of the map at the recommended contour level 0.101 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



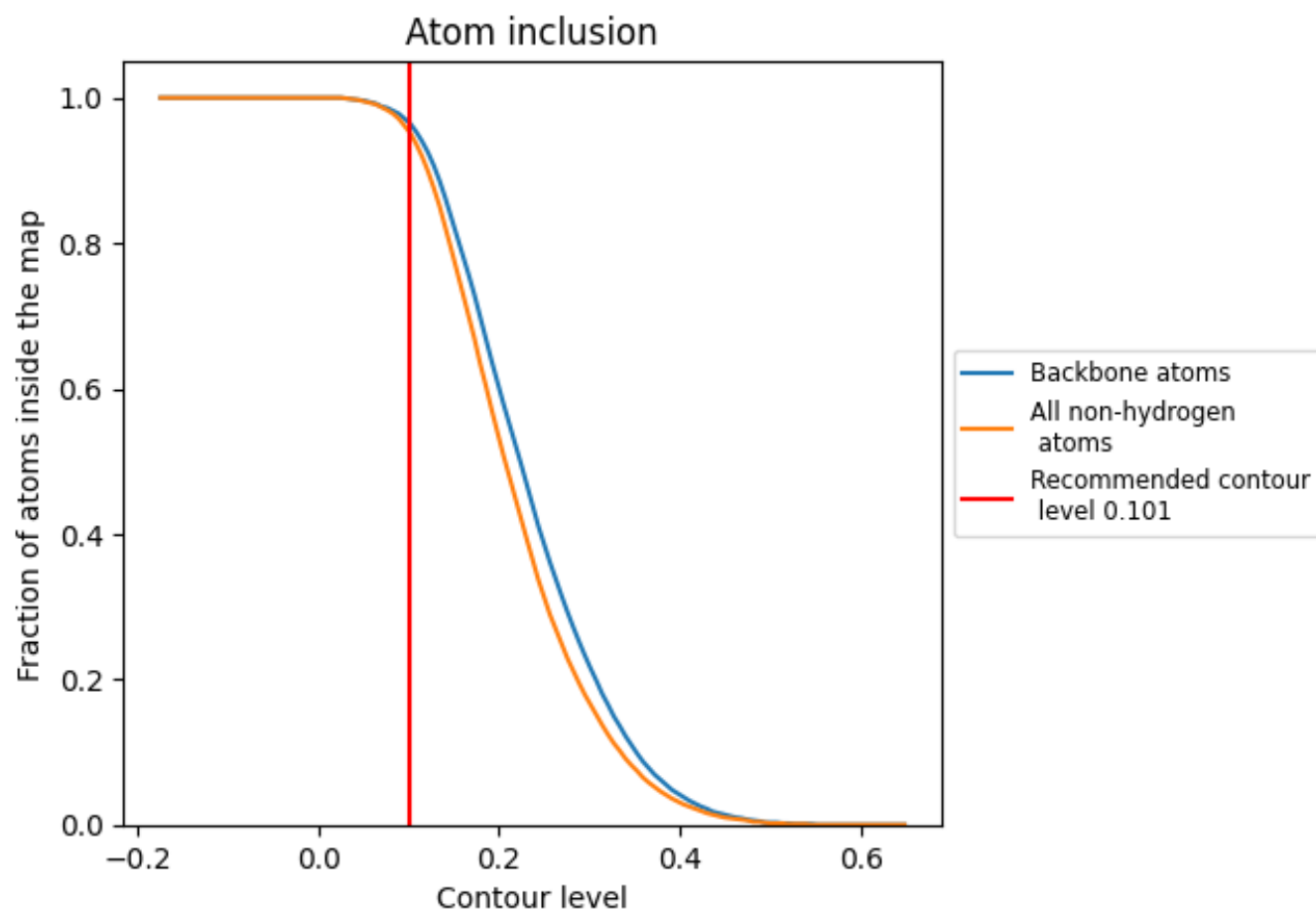
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.101).







































9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9520	 0.2740
A	 0.9520	 0.2580
B	 0.9050	 0.2230
C	 0.9240	 0.2830
D	 0.9880	 0.3340
E	 0.9910	 0.2670
F	 0.9950	 0.2140
G	 0.9780	 0.3650
H	 0.9900	 0.2790
K	 0.9300	 0.2530
L	 0.9120	 0.2210
M	 0.9310	 0.2930
N	 0.9860	 0.3360
O	 0.9900	 0.2700
P	 0.9850	 0.1850
Q	 0.9820	 0.3770
R	 0.9990	 0.2950
U	 0.9390	 0.2550
V	 0.9440	 0.2690

