



Full wwPDB EM Validation Report ⓘ

Mar 13, 2026 – 11:36 PM UTC

PDB ID : 9LVK / pdb_00009lvk
EMDB ID : EMD-63422
Title : Cryo-EM structure of CASTOR1 bound human GATOR2 complex
Authors : Su, M.-Y.
Deposited on : 2025-02-12
Resolution : 3.59 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

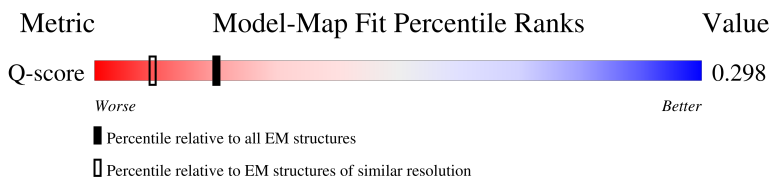
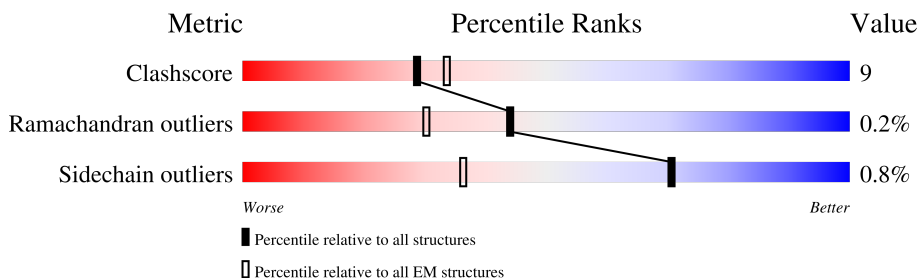
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12565 (3.09 - 4.09)

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	

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Mol	Chain	Length	Quality of chain
2	C	790	
2	M	790	
3	D	974	
3	N	974	
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	329	
6	V	329	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 51417 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	745	Total	C	N	O	S	0	0
			4650	2897	874	851	28		
1	K	737	Total	C	N	O	S	0	0
			4667	2921	869	849	28		
1	L	744	Total	C	N	O	S	0	0
			5164	3307	923	904	30		
1	B	743	Total	C	N	O	S	0	0
			4926	3141	886	874	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	577	Total	C	N	O	S	0	0
			4098	2598	742	719	39		
2	M	577	Total	C	N	O	S	0	0
			3968	2499	728	706	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	247	Total	C	N	O	S	0	0
			1714	1088	316	296	14		
3	N	261	Total	C	N	O	S	0	0
			1735	1096	323	297	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	304	Total	C	N	O	S	0	0
			2164	1397	396	360	11		
4	F	307	Total	C	N	O	S	0	0
			1965	1256	367	337	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	302	Total	C	N	O	S	0	0
			2224	1427	402	383	12		
4	O	302	Total	C	N	O	S	0	0
			2175	1400	395	370	10		
4	P	295	Total	C	N	O		0	0
			1679	1048	323	308			
4	Q	302	Total	C	N	O	S	0	0
			2188	1402	392	382	12		

- Molecule 5 is a protein called Isoform 3 of Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	285	Total	C	N	O	S	0	0
			1988	1266	357	359	6		
5	R	285	Total	C	N	O	S	0	0
			1945	1255	354	333	3		

- Molecule 6 is a protein called Cytosolic arginine sensor for mTORC1 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	292	Total	C	N	O	S	0	0
			2102	1381	350	365	6		
6	V	282	Total	C	N	O	S	0	0
			2034	1335	342	351	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	304	ALA	ASP	engineered mutation	UNP Q8WTX7
V	304	ALA	ASP	engineered mutation	UNP Q8WTX7

- 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	C	4	Total	Zn	0
			4	4	
7	D	3	Total	Zn	0
			3	3	

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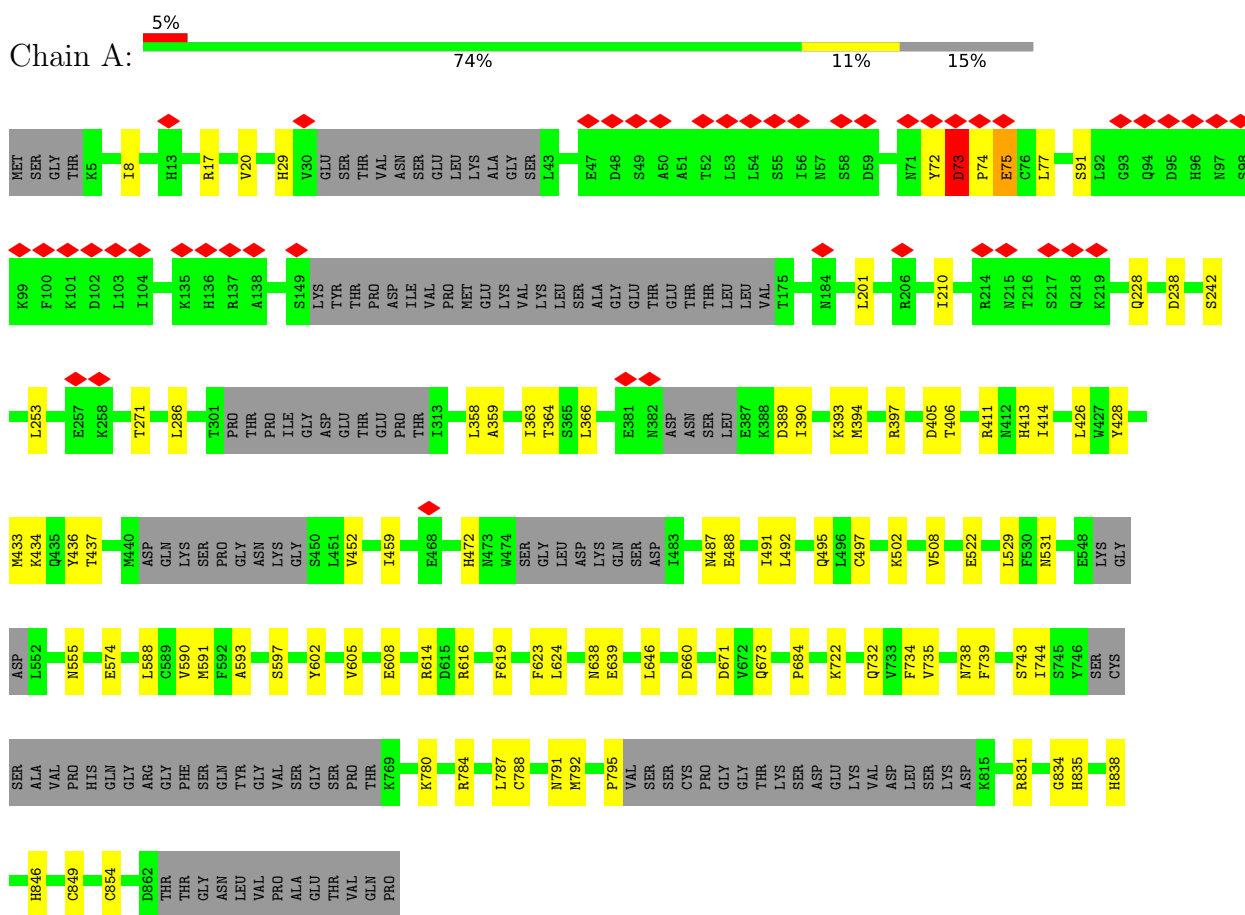
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Mol	Chain	Residues	Atoms		AltConf
7	K	4	Total 4	Zn 4	0
7	M	4	Total 4	Zn 4	0
7	N	4	Total 4	Zn 4	0
7	L	4	Total 4	Zn 4	0
7	B	4	Total 4	Zn 4	0

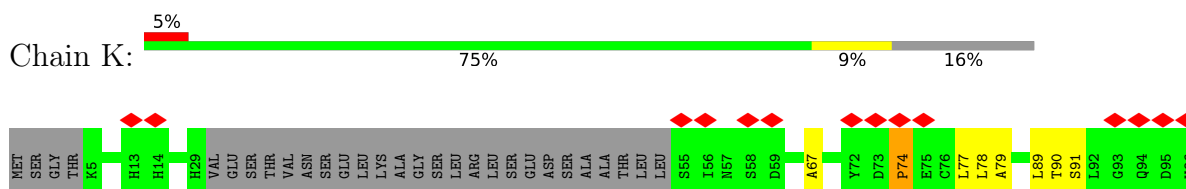
3 Residue-property plots [i](#)

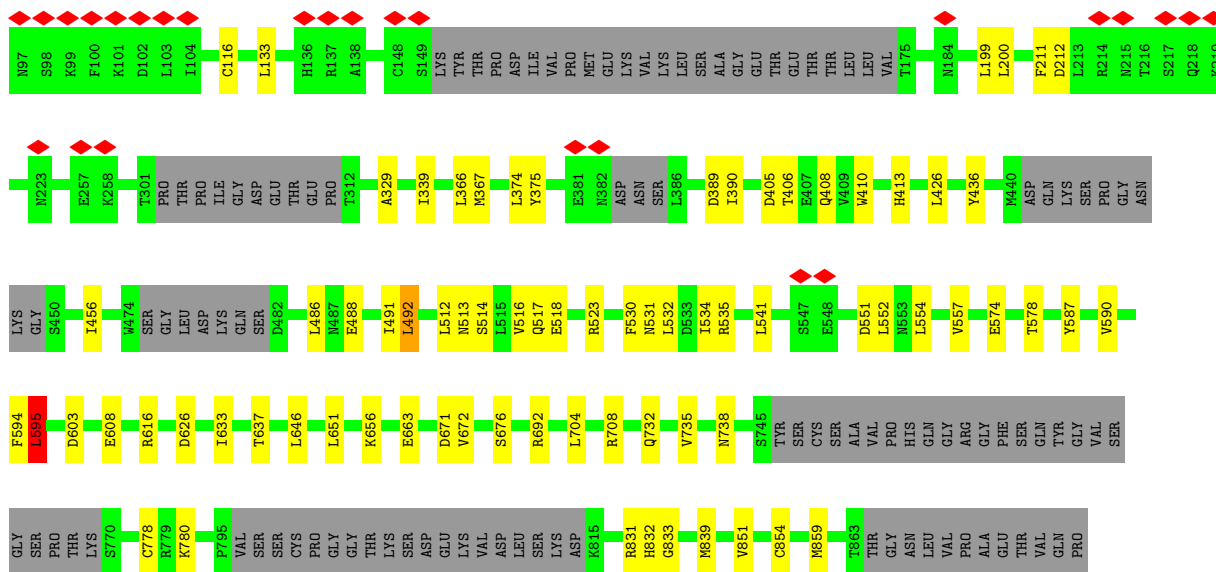
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: GATOR2 complex protein MIOS

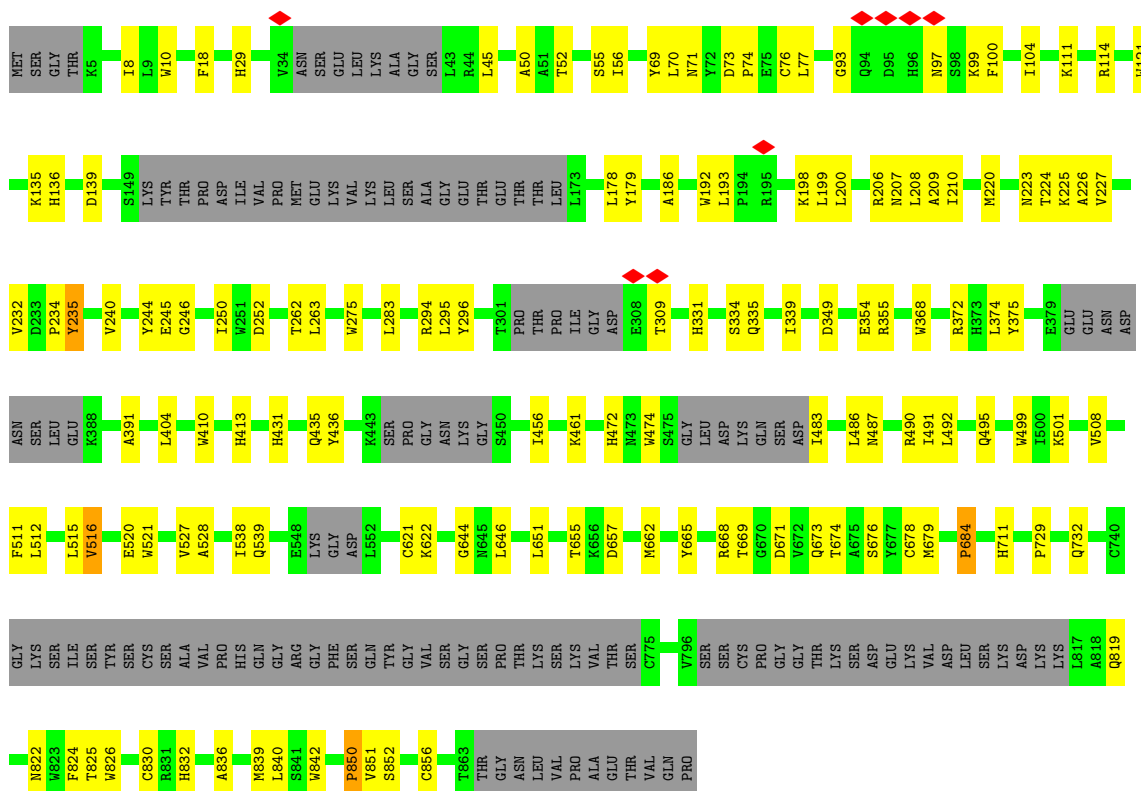


• Molecule 1: GATOR2 complex protein MIOS



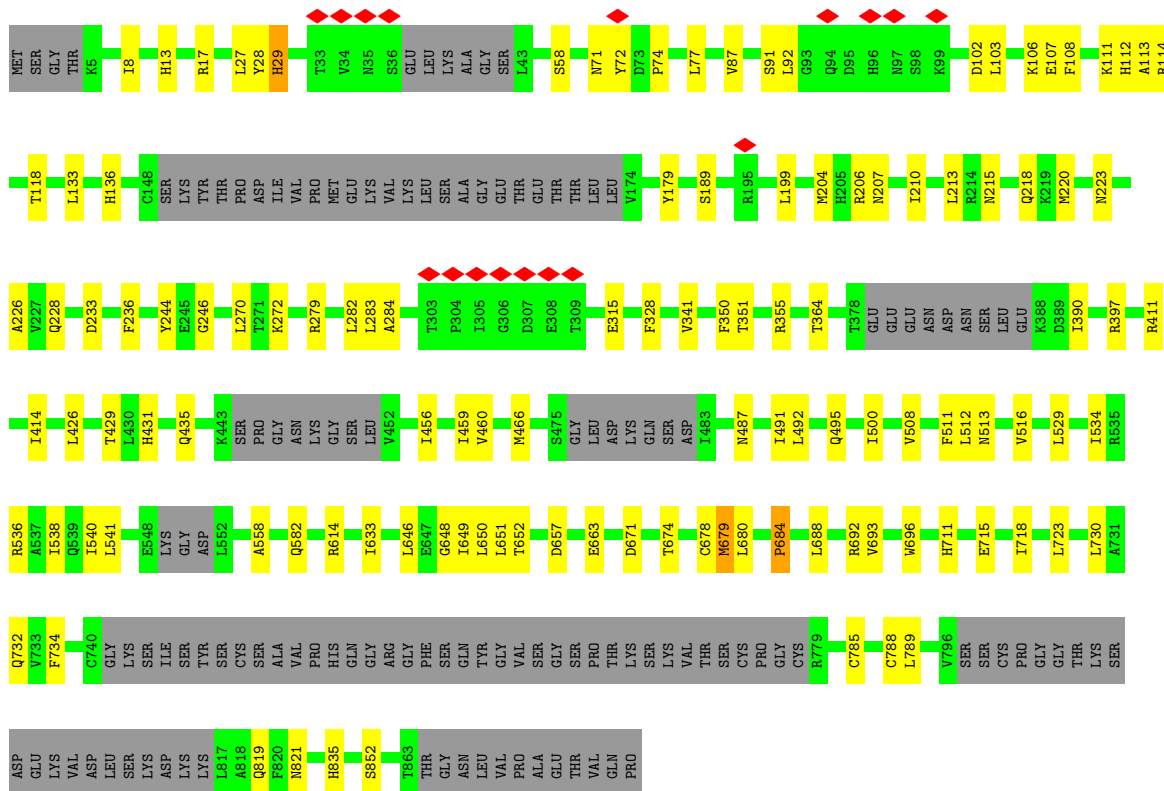


• Molecule 1: GATOR2 complex protein MIOS

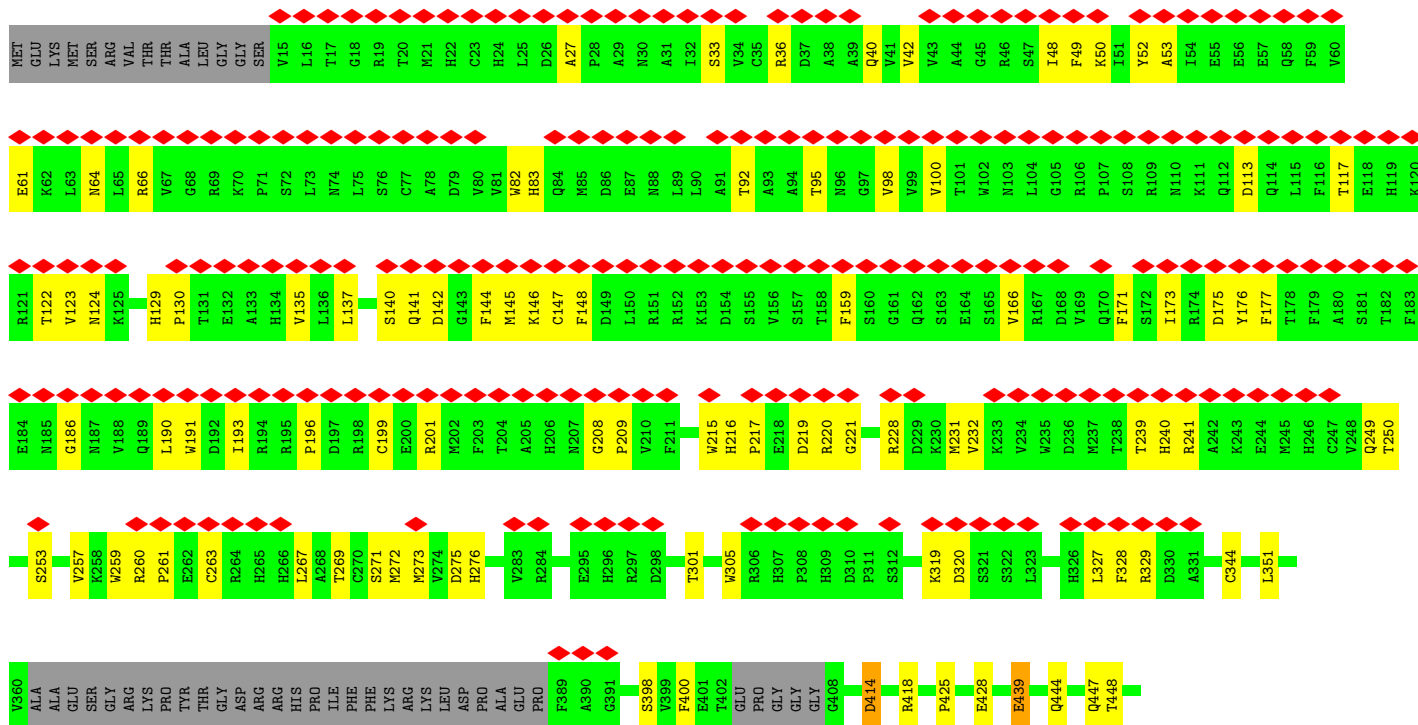


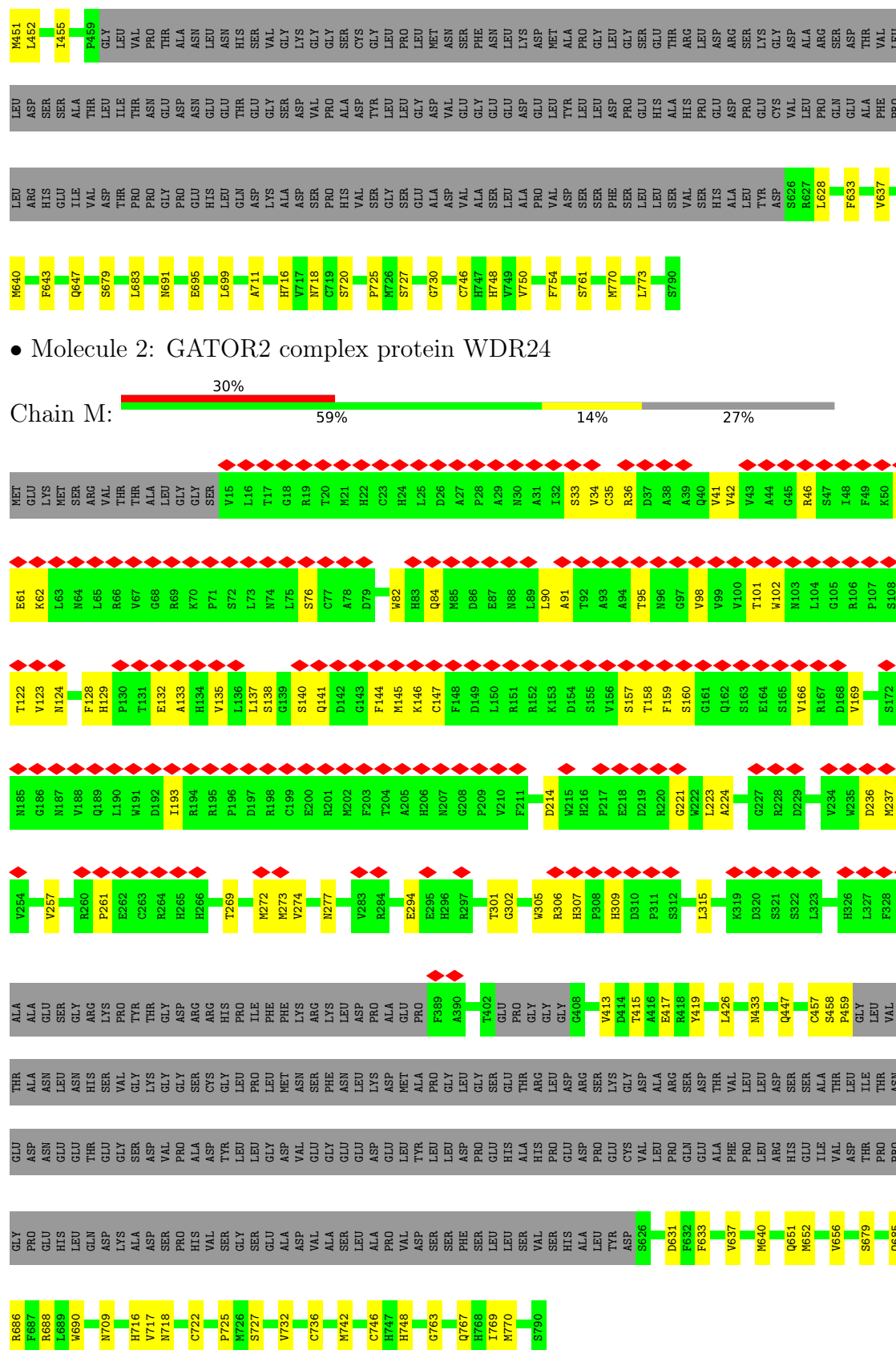
• Molecule 1: GATOR2 complex protein MIOS



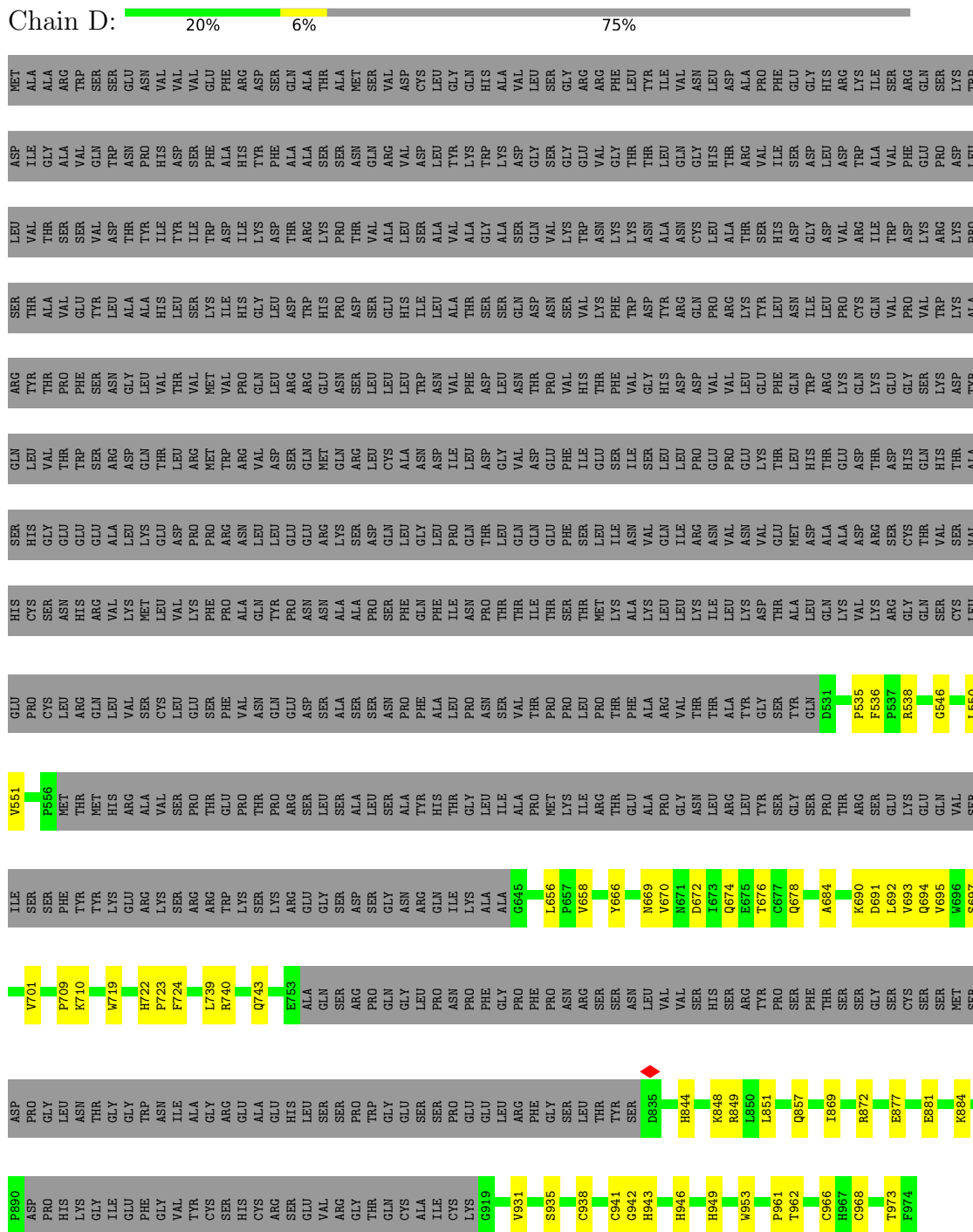


- Molecule 2: GATOR2 complex protein WDR24

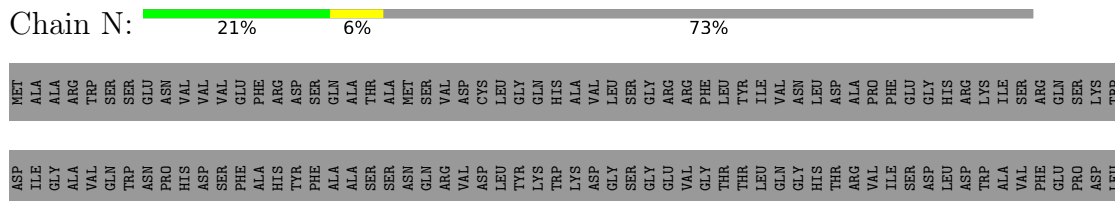


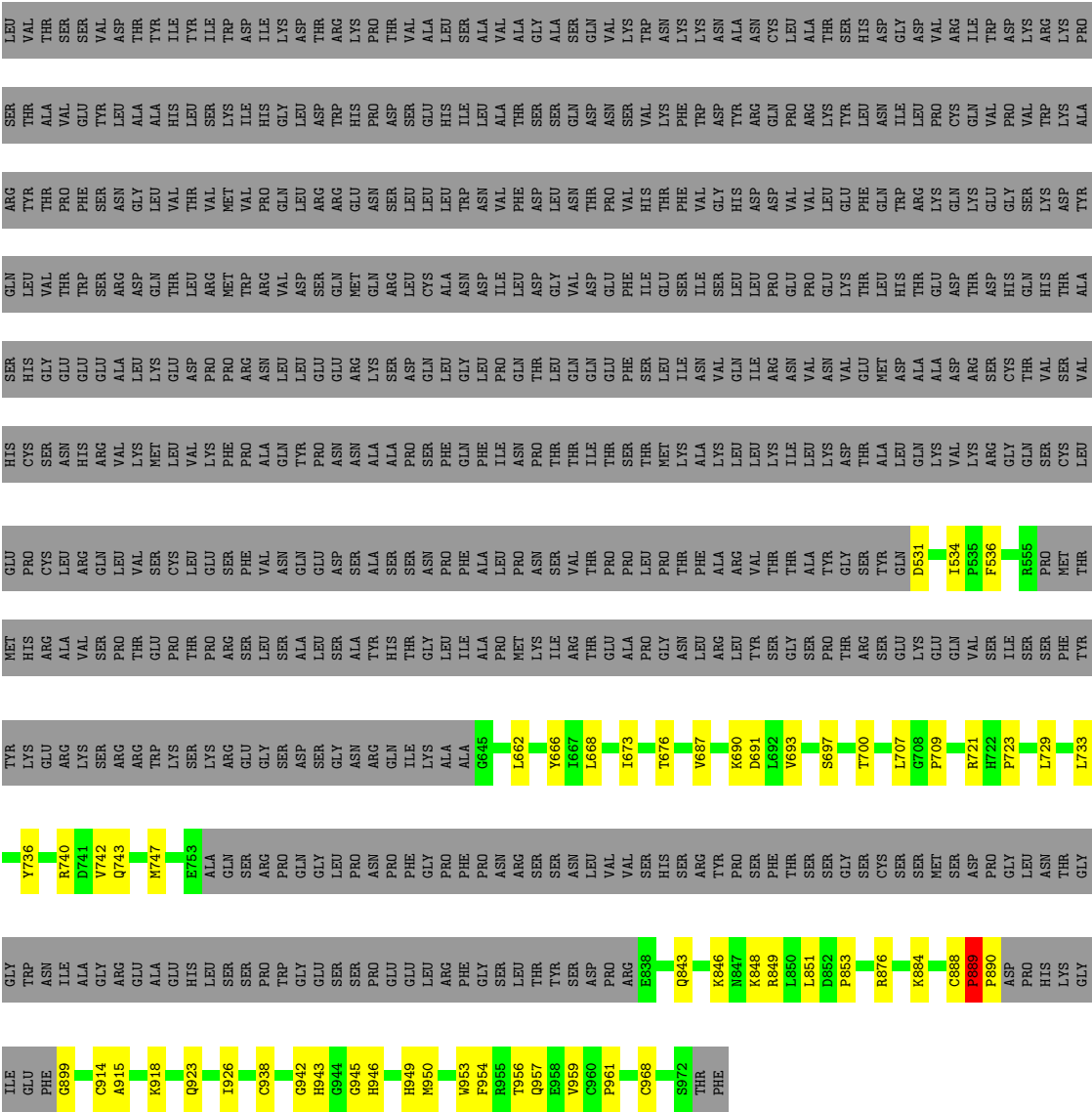


• Molecule 3: GATOR2 complex protein WDR59

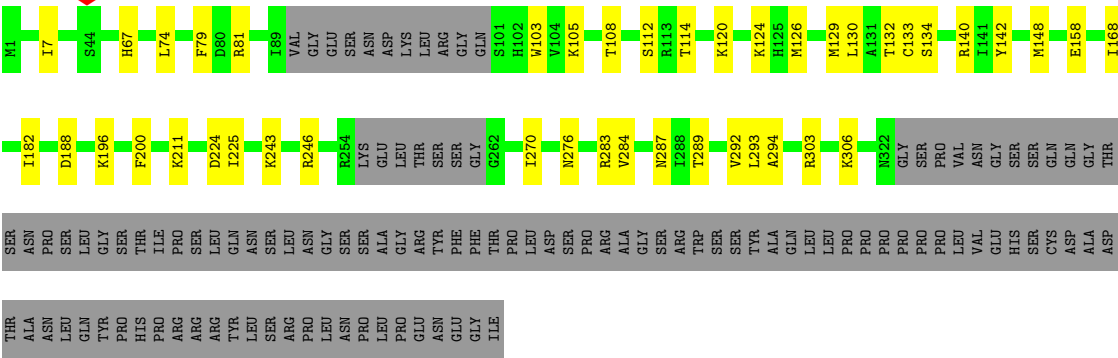


- Molecule 3: GATOR2 complex protein WDR59



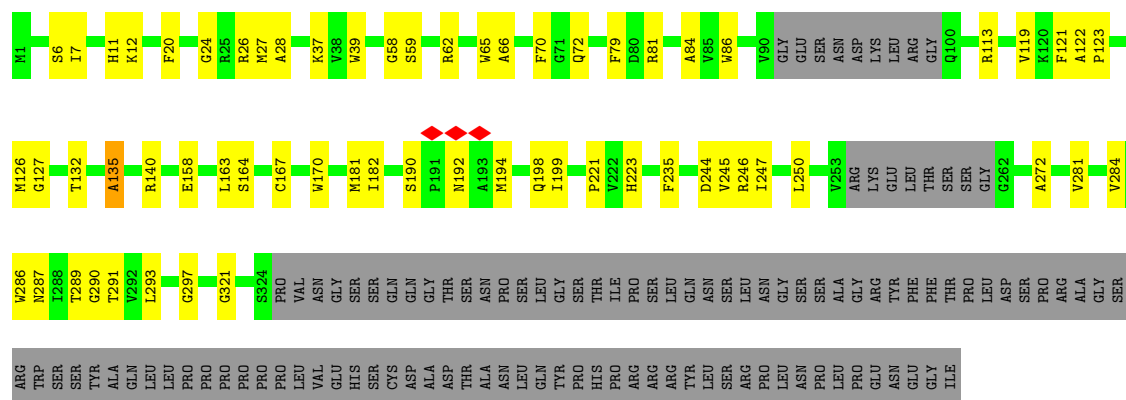


● Molecule 4: Isoform B of Nucleoporin SEH1



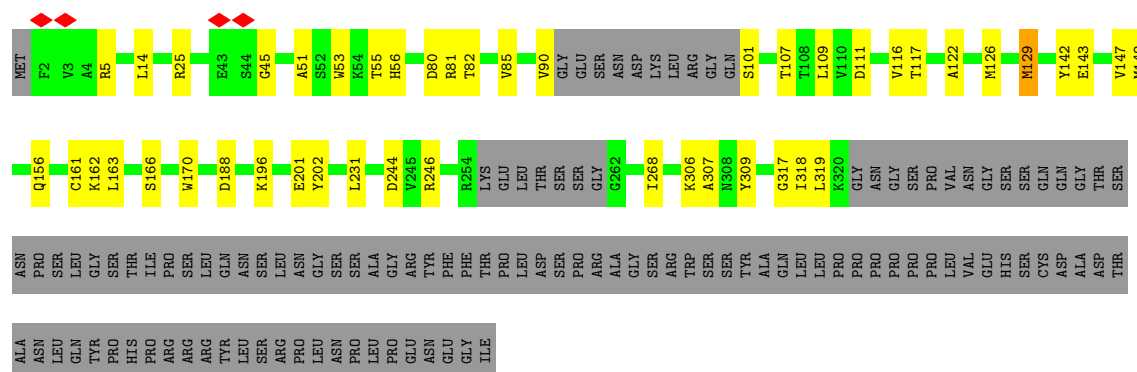
● Molecule 4: Isoform B of Nucleoporin SEH1

Chain F:  58% 15% 27%



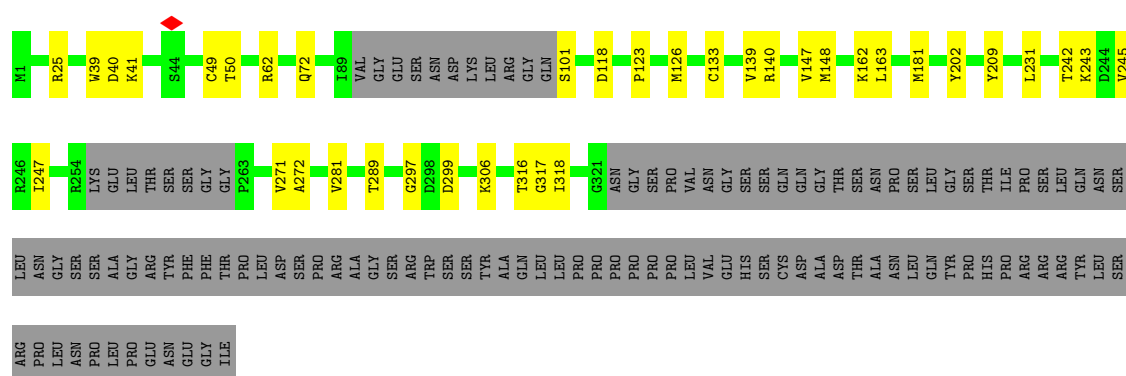
• Molecule 4: Isoform B of Nucleoporin SEH1

Chain G:  61% 11% 28%



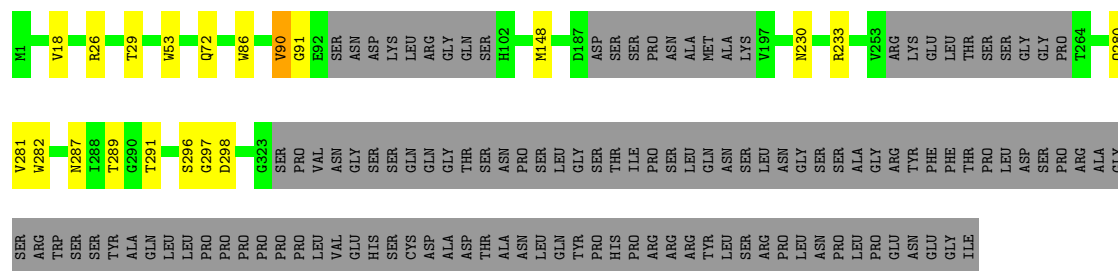
• Molecule 4: Isoform B of Nucleoporin SEH1

Chain O:  63% 9% 28%

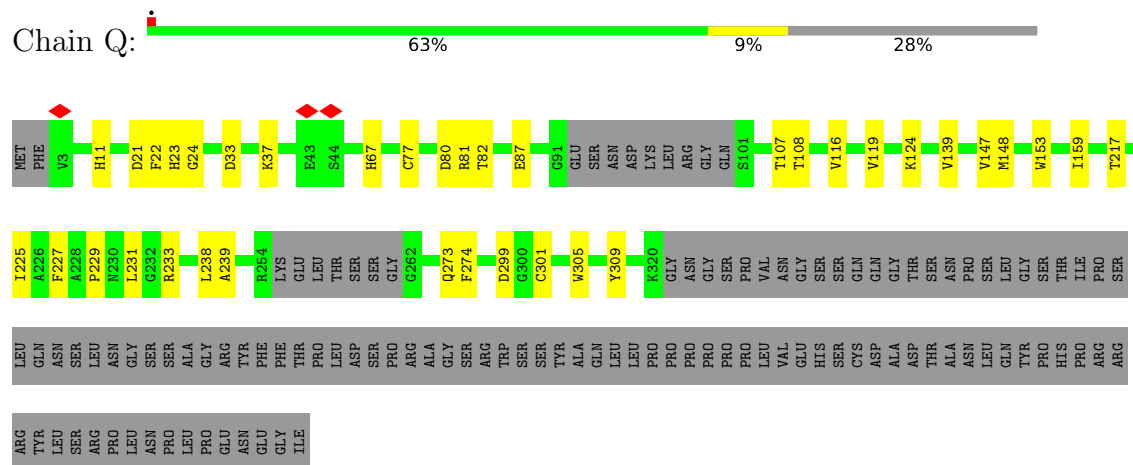


• Molecule 4: Isoform B of Nucleoporin SEH1

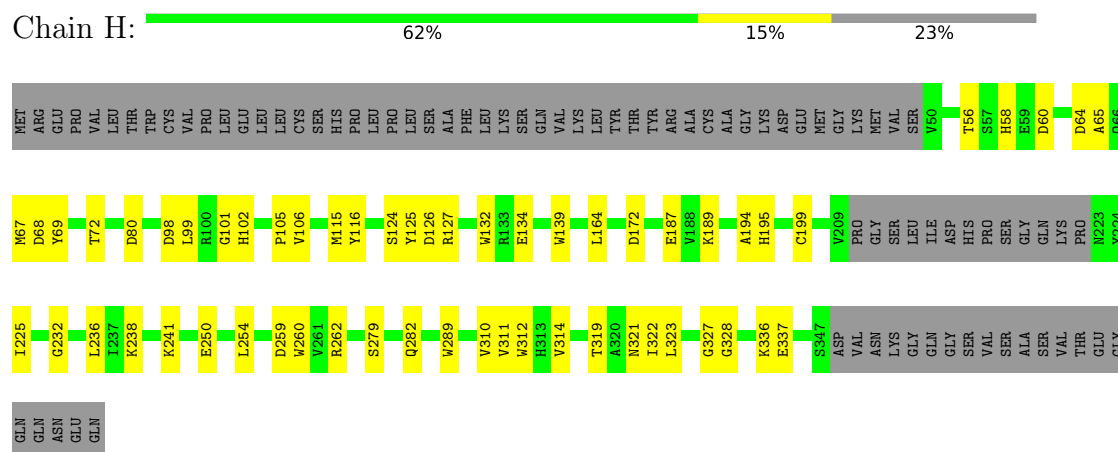
Chain P:  65% 5% 30%



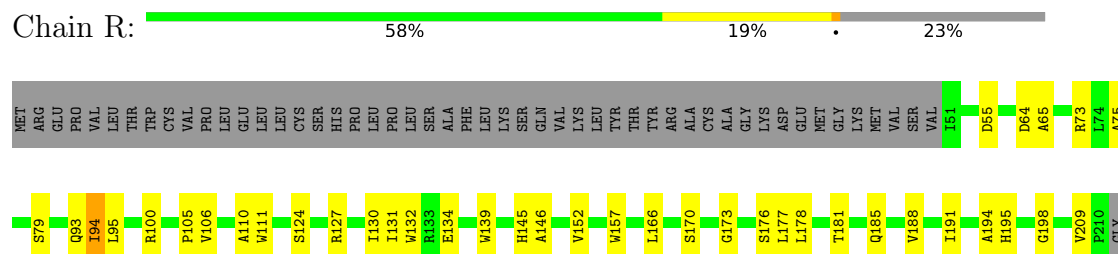
• Molecule 4: Isoform B of Nucleoporin SEH1

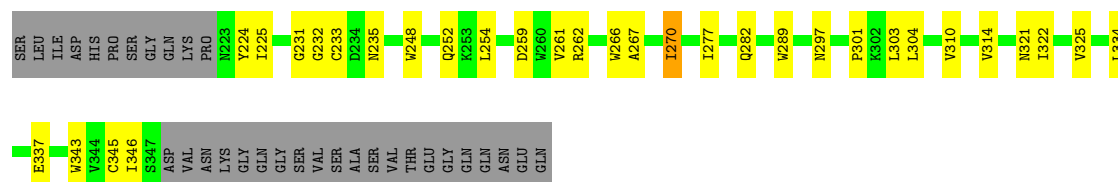


• Molecule 5: Isoform 3 of Protein SEC13 homolog



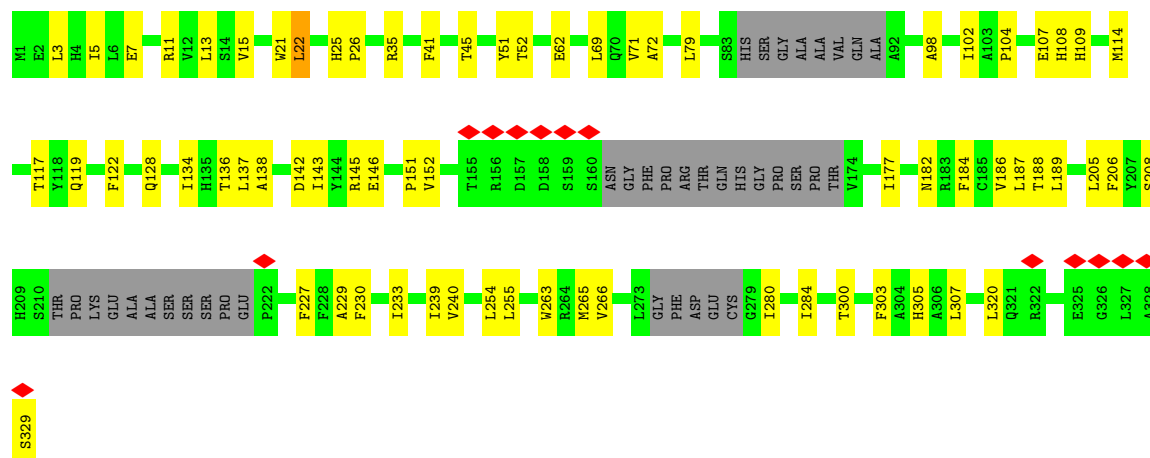
• Molecule 5: Isoform 3 of Protein SEC13 homolog





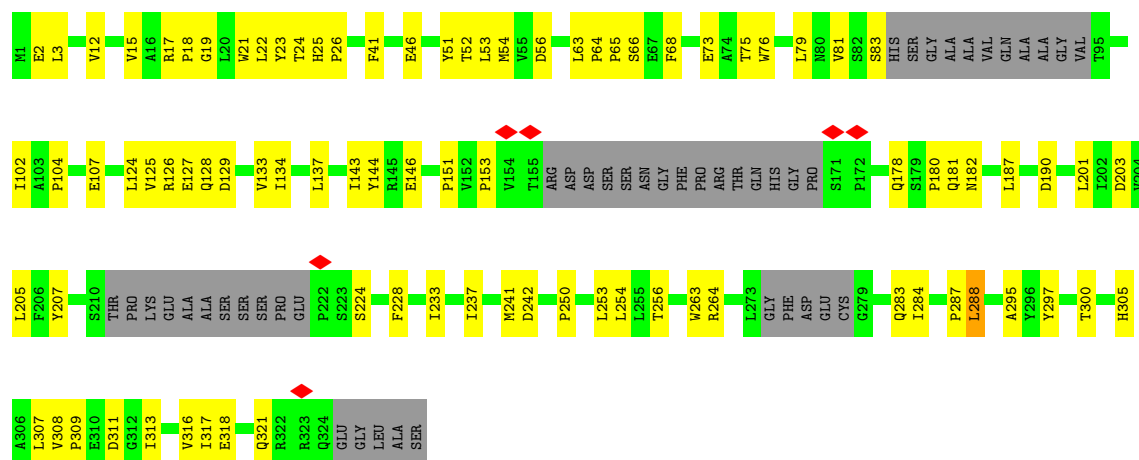
- Molecule 6: Cytosolic arginine sensor for mTORC1 subunit 1

Chain U: 67% 21% 11%



- Molecule 6: Cytosolic arginine sensor for mTORC1 subunit 1

Chain V: 59% 26% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	760701	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 ($e^-/\text{\AA}^2$)	51.52	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	0.694	Depositor
Minimum map value	-0.216	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0958	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.23	1/4714 (0.0%)	0.52	8/6474 (0.1%)
1	B	0.19	0/5028	0.41	1/6926 (0.0%)
1	K	0.23	0/4737	0.46	1/6500 (0.0%)
1	L	0.32	2/5283 (0.0%)	0.58	6/7257 (0.1%)
2	C	0.17	0/4205	0.39	0/5760
2	M	0.16	0/4064	0.37	0/5575
3	D	0.23	0/1755	0.50	0/2398
3	N	0.22	0/1771	0.44	0/2421
4	E	0.21	0/2224	0.47	0/3054
4	F	0.25	0/2013	0.55	0/2783
4	G	0.19	0/2286	0.41	0/3131
4	O	0.21	0/2237	0.41	0/3068
4	P	0.18	0/1711	0.39	2/2378 (0.1%)
4	Q	0.17	0/2249	0.36	0/3084
5	H	0.19	0/2045	0.45	0/2813
5	R	0.21	0/2004	0.58	1/2769 (0.0%)
6	U	0.24	0/2151	0.59	1/2951 (0.0%)
6	V	0.26	0/2081	0.57	0/2858
All	All	0.22	3/52558 (0.0%)	0.47	20/72200 (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
1	A	0	1
1	B	0	1
3	N	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	850	PRO	CG-CD	-6.46	1.28	1.50
1	L	349	ASP	C-O	-5.99	1.16	1.23
1	A	75	GLU	CA-C	-5.15	1.46	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	850	PRO	CA-N-CD	-13.57	93.01	112.00
1	L	684	PRO	CA-N-CD	-10.69	97.03	112.00
1	K	74	PRO	CA-N-CD	-9.12	98.73	111.50
1	L	850	PRO	N-CD-CG	-8.69	90.17	103.20
1	A	73	ASP	CA-C-N	8.66	130.66	119.84
1	A	73	ASP	C-N-CA	8.66	130.66	119.84
1	A	73	ASP	N-CA-C	7.84	122.58	108.55
1	A	72	TYR	N-CA-C	7.65	120.51	111.71
1	L	73	ASP	CA-C-N	7.46	144.90	127.00
1	L	73	ASP	C-N-CA	7.46	144.90	127.00
1	B	74	PRO	CA-N-CD	-6.79	102.50	112.00
1	L	73	ASP	C-N-CD	-6.51	106.27	120.60
4	P	91	GLY	N-CA-C	6.24	121.77	111.59
1	A	722	LYS	N-CA-C	-5.88	107.34	114.75
4	P	90	VAL	N-CA-C	5.74	121.29	109.34
1	A	684	PRO	CA-N-CD	-5.52	104.27	112.00
6	U	109	HIS	N-CA-C	5.44	117.27	110.91
5	R	270	ILE	N-CA-C	-5.35	108.63	113.71
1	A	75	GLU	O-C-N	5.32	129.47	122.93
1	A	639	GLU	N-CA-C	-5.13	106.35	113.18

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	ASP	Peptide
1	B	71	ASN	Peptide
3	N	889	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4650	0	3408	65	0
1	B	4926	0	4028	89	0
1	K	4667	0	3506	54	0
1	L	5164	0	4390	107	0
2	C	4098	0	3573	90	0
2	M	3968	0	3361	76	0
3	D	1714	0	1469	47	0
3	N	1735	0	1437	43	0
4	E	2164	0	1932	32	0
4	F	1965	0	1496	45	0
4	G	2224	0	2031	33	0
4	O	2175	0	1930	25	0
4	P	1679	0	1008	10	0
4	Q	2188	0	1965	25	0
5	H	1988	0	1649	42	0
5	R	1945	0	1597	51	0
6	U	2102	0	1994	52	0
6	V	2034	0	1915	62	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
7	D	3	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	0	0
All	All	51417	0	42689	881	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 9.

All (881) 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:B:788:CYS:SG	1:B:835:HIS:CE1	2.41	1.13
5:H:106:VAL:HA	5:H:124:SER:HB2	1.49	0.93
3:N:938:CYS:SG	3:N:968:CYS:HB3	2.07	0.93
2:C:301:THR:HG21	2:C:319:LYS:HE3	1.49	0.92
1:L:830:CYS:SG	1:L:856:CYS:CB	2.60	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:266:TRP:HD1	5:R:267:ALA:H	1.24	0.83
5:R:266:TRP:CD1	5:R:267:ALA:H	1.97	0.82
6:U:255:LEU:HD22	1:B:113:ALA:HB1	1.62	0.81
1:A:605:VAL:HG11	1:A:619:PHE:HE1	1.45	0.80
3:D:941:CYS:SG	3:D:966:CYS:HB3	2.25	0.76
2:C:643:PHE:O	2:C:647:GLN:NE2	2.19	0.76
6:V:182:ASN:HD21	6:V:224:SER:HA	1.52	0.75
5:H:194:ALA:O	5:H:238:LYS:NZ	2.21	0.74
1:K:541:LEU:HD21	1:K:557:VAL:HG13	1.67	0.74
5:H:56:THR:HG23	5:H:58:HIS:H	1.51	0.74
5:H:64:ASP:OD2	5:H:65:ALA:N	2.20	0.74
1:K:77:LEU:HA	1:K:91:SER:HA	1.70	0.72
5:R:252:GLN:HE22	5:R:297:ASN:HD22	1.37	0.72
1:L:210:ILE:HG23	1:L:220:MET:HE2	1.70	0.72
5:H:199:CYS:HA	5:H:232:GLY:HA2	1.71	0.71
2:M:245:MET:SD	2:M:245:MET:N	2.64	0.71
1:A:788:CYS:SG	1:A:835:HIS:HE1	2.14	0.71
4:F:244:ASP:O	4:F:246:ARG:N	2.24	0.71
4:G:80:ASP:OD1	4:G:82:THR:OG1	2.08	0.71
6:U:128:GLN:N	6:U:128:GLN:OE1	2.22	0.71
2:M:679:SER:HB3	4:Q:231:LEU:HD23	1.74	0.70
6:U:117:THR:HG22	6:U:119:GLN:H	1.56	0.70
2:C:52:TYR:HA	2:C:61:GLU:HA	1.73	0.70
6:V:187:LEU:HD11	6:V:254:LEU:HD12	1.73	0.69
2:C:36:ARG:NH1	2:C:83:HIS:O	2.25	0.69
3:N:889:PRO:HB2	3:N:890:PRO:HD3	1.75	0.69
5:H:124:SER:OG	5:H:126:ASP:OD1	2.10	0.69
1:L:104:ILE:HD12	1:L:104:ILE:H	1.57	0.69
5:R:314:VAL:HG12	5:R:325:VAL:HG22	1.75	0.69
6:V:79:LEU:HD11	6:V:125:VAL:HG22	1.74	0.69
1:A:574:GLU:OE2	1:A:574:GLU:N	2.26	0.69
1:L:76:CYS:HB2	1:L:93:GLY:H	1.57	0.69
6:U:7:GLU:N	6:U:7:GLU:OE2	2.26	0.68
1:L:114:ARG:NH1	1:L:139:ASP:OD2	2.26	0.68
1:B:431:HIS:NE2	1:B:435:GLN:OE1	2.27	0.68
4:F:284:VAL:HG13	4:F:293:LEU:HD11	1.75	0.68
2:M:52:TYR:HA	2:M:61:GLU:HA	1.74	0.68
5:R:64:ASP:OD1	5:R:65:ALA:N	2.27	0.68
2:C:730:GLY:HA3	4:E:148:MET:HE1	1.75	0.68
6:V:264:ARG:HD3	6:V:313:ILE:HG13	1.74	0.68
1:L:114:ARG:HD3	1:L:136:HIS:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:536:PHE:O	5:R:262:ARG:NH2	2.26	0.67
1:L:29:HIS:O	1:L:52:THR:OG1	2.13	0.67
1:B:118:THR:HG21	1:B:189:SER:HA	1.77	0.67
1:A:734:PHE:HE2	1:A:743:SER:HB2	1.60	0.67
3:D:941:CYS:SG	3:D:966:CYS:CB	2.82	0.67
3:N:926:ILE:HD12	3:N:949:HIS:HB3	1.76	0.66
6:U:52:THR:HG21	6:U:300:THR:HB	1.78	0.66
5:R:282:GLN:HA	5:R:310:VAL:HG13	1.78	0.66
1:L:220:MET:SD	1:L:220:MET:N	2.68	0.66
2:C:447:GLN:N	2:C:447:GLN:OE1	2.28	0.66
1:B:13:HIS:NE2	1:B:72:TYR:O	2.28	0.66
6:U:230:PHE:HA	6:U:239:ILE:HG22	1.78	0.65
4:E:105:LYS:NZ	4:E:108:THR:OG1	2.29	0.65
3:N:899:GLY:N	1:B:734:PHE:O	2.30	0.65
4:P:281:VAL:HA	4:P:297:GLY:HA2	1.77	0.65
5:R:195:HIS:HE1	5:R:231:GLY:HA2	1.62	0.65
6:V:313:ILE:HA	6:V:316:VAL:HG12	1.78	0.65
6:U:104:PRO:HA	6:U:107:GLU:HG2	1.79	0.64
6:V:73:GLU:OE2	6:V:73:GLU:N	2.28	0.64
1:L:644:GLY:O	1:L:668:ARG:NH1	2.31	0.64
1:B:426:LEU:HD23	1:B:649:ILE:HG21	1.80	0.64
3:D:710:LYS:O	3:D:848:LYS:NZ	2.31	0.64
4:E:292:VAL:HG12	4:E:306:LYS:HB2	1.80	0.64
5:H:187:GLU:OE2	5:H:189:LYS:NZ	2.29	0.64
4:F:289:THR:HG23	4:F:291:THR:HG23	1.80	0.63
1:K:663:GLU:OE1	1:K:692:ARG:NH1	2.30	0.63
2:M:419:TYR:HD1	2:M:433:ASN:HD22	1.45	0.63
1:A:358:LEU:HD12	4:E:283:ARG:HB3	1.79	0.63
1:A:495:GLN:HE22	1:A:502:LYS:HA	1.63	0.63
2:M:34:VAL:HG23	2:M:41:VAL:HG12	1.80	0.63
5:H:126:ASP:OD1	5:H:126:ASP:N	2.27	0.63
1:L:368:TRP:HB2	1:L:375:TYR:H	1.64	0.63
1:B:204:MET:HG3	1:B:206:ARG:H	1.63	0.63
4:O:306:LYS:HB3	4:O:316:THR:HG21	1.81	0.63
2:C:257:VAL:HG22	2:C:269:THR:HG22	1.80	0.62
2:C:455:ILE:HD11	2:C:633:PHE:CD2	2.34	0.62
1:A:608:GLU:O	1:A:616:ARG:NH1	2.32	0.62
4:E:284:VAL:HG13	4:E:293:LEU:HD11	1.82	0.62
5:R:106:VAL:HA	5:R:124:SER:HA	1.80	0.62
3:D:938:CYS:HB2	3:D:941:CYS:HB2	1.80	0.62
1:A:393:LYS:O	1:A:397:ARG:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:942:GLY:O	1:L:732:GLN:N	2.31	0.62
4:E:126:MET:O	4:E:129:MET:HE3	1.99	0.62
4:G:147:VAL:HG23	4:G:148:MET:HE2	1.82	0.62
4:E:140:ARG:NH1	4:E:158:GLU:OE2	2.33	0.62
1:A:74:PRO:HB2	1:A:77:LEU:CB	2.29	0.62
1:B:111:LYS:O	1:B:112:HIS:ND1	2.33	0.62
1:A:795:PRO:HB3	4:G:90:VAL:HG11	1.81	0.61
1:K:456:ILE:HG22	1:K:651:LEU:HA	1.80	0.61
2:C:129:HIS:HB2	2:C:135:VAL:HB	1.82	0.61
3:D:684:ALA:HB3	3:D:693:VAL:HG13	1.81	0.61
4:E:276:ASN:O	4:E:303:ARG:NH1	2.32	0.61
5:H:68:ASP:OD1	5:H:72:THR:N	2.33	0.61
1:L:671:ASP:OD1	1:L:674:THR:OG1	2.18	0.61
2:C:123:VAL:HA	2:C:140:SER:HA	1.83	0.61
1:L:208:LEU:HD13	1:L:227:VAL:HG12	1.82	0.61
4:O:25:ARG:HH11	4:O:41:LYS:HD3	1.66	0.60
2:M:722:CYS:HB3	2:M:736:CYS:SG	2.40	0.60
1:B:819:GLN:O	1:B:819:GLN:NE2	2.32	0.60
1:A:17:ARG:HA	1:A:29:HIS:HA	1.83	0.60
5:H:98:ASP:OD1	5:H:99:LEU:N	2.34	0.60
3:N:697:SER:O	3:N:700:THR:OG1	2.18	0.60
5:R:152:VAL:HA	5:R:170:SER:HA	1.83	0.60
6:V:128:GLN:NE2	6:V:129:ASP:OD1	2.33	0.60
6:V:308:VAL:HG21	6:V:316:VAL:HG21	1.82	0.60
1:A:77:LEU:HA	1:A:91:SER:HA	1.82	0.60
4:O:123:PRO:HG2	4:O:126:MET:HE3	1.83	0.60
6:V:76:TRP:HD1	6:V:124:LEU:HB3	1.66	0.60
1:A:738:ASN:OD1	2:C:716:HIS:ND1	2.34	0.60
5:R:55:ASP:N	5:R:93:GLN:OE1	2.29	0.60
6:V:25:HIS:HB3	6:V:26:PRO:HD3	1.83	0.60
1:A:426:LEU:HD22	1:A:646:LEU:HD13	1.82	0.60
4:G:5:ARG:NH2	4:G:45:GLY:O	2.35	0.60
1:K:390:ILE:HD11	1:K:671:ASP:HB2	1.84	0.60
4:F:140:ARG:NE	4:F:158:GLU:OE2	2.35	0.60
2:C:145:MET:O	2:C:159:PHE:N	2.26	0.59
1:L:111:LYS:HE3	1:L:111:LYS:HA	1.83	0.59
6:U:13:LEU:HD12	6:U:69:LEU:HD11	1.84	0.59
2:C:92:THR:OG1	2:C:100:VAL:O	2.20	0.59
6:V:19:GLY:HA3	6:V:68:PHE:CE2	2.37	0.59
1:L:232:VAL:HG22	1:L:240:VAL:HG12	1.84	0.59
4:F:122:ALA:HA	4:F:170:TRP:HE1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:MET:HG3	1:B:207:ASN:H	1.67	0.59
5:R:75:ALA:HB2	5:R:111:TRP:HE1	1.67	0.59
1:L:70:LEU:HD23	1:L:70:LEU:H	1.67	0.59
2:C:191:TRP:CZ3	2:C:199:CYS:HA	2.38	0.59
1:K:832:HIS:HE1	1:K:854:CYS:SG	2.26	0.59
2:M:54:ILE:HA	2:M:59:PHE:HA	1.84	0.59
1:A:434:LYS:O	1:A:437:THR:OG1	2.18	0.59
6:V:203:ASP:HA	6:V:207:TYR:HD1	1.68	0.59
4:G:201:GLU:HG2	4:G:202:TYR:H	1.68	0.58
4:O:62:ARG:NE	4:O:118:ASP:OD1	2.35	0.58
1:L:331:HIS:CE1	1:L:334:SER:H	2.21	0.58
5:R:345:CYS:SG	5:R:346:ILE:N	2.75	0.58
6:U:329:SER:O	6:U:329:SER:OG	2.21	0.58
5:R:110:ALA:O	5:R:157:TRP:NE1	2.36	0.58
2:M:98:VAL:HG23	2:M:117:THR:HG22	1.84	0.58
2:M:306:ARG:HB2	2:M:315:LEU:HD21	1.86	0.58
1:K:389:ASP:OD1	1:K:390:ILE:N	2.36	0.58
6:V:41:PHE:HB3	6:V:56:ASP:OD1	2.04	0.58
1:B:678:CYS:SG	1:B:679:MET:HE2	2.44	0.58
2:C:95:THR:HA	2:C:122:THR:HG23	1.86	0.57
4:G:306:LYS:NZ	4:G:307:ALA:O	2.30	0.57
1:K:594:PHE:O	1:K:595:LEU:HB2	2.02	0.57
6:V:250:PRO:HB2	6:V:253:LEU:HD13	1.84	0.57
4:G:244:ASP:OD2	4:G:246:ARG:NH1	2.36	0.57
4:Q:80:ASP:OD2	4:Q:82:THR:OG1	2.16	0.57
1:B:272:LYS:NZ	1:B:328:PHE:O	2.37	0.57
6:V:187:LEU:HD23	6:V:256:THR:HB	1.86	0.57
4:F:26:ARG:NH1	4:F:72:GLN:OE1	2.36	0.57
4:F:7:ILE:N	1:L:374:LEU:O	2.36	0.57
5:H:116:TYR:HD2	5:H:164:LEU:HD13	1.69	0.57
3:N:662:LEU:HD21	3:N:687:VAL:HG11	1.85	0.57
2:C:50:LYS:HA	2:C:64:ASN:HA	1.87	0.57
6:U:137:LEU:H	6:U:137:LEU:HD23	1.69	0.57
1:A:411:ARG:HG3	1:A:414:ILE:HD11	1.86	0.57
4:F:281:VAL:HA	4:F:297:GLY:HA2	1.86	0.57
1:K:74:PRO:HD2	1:K:74:PRO:O	2.05	0.57
2:M:447:GLN:HG3	3:N:707:LEU:HD21	1.85	0.57
1:A:831:ARG:NH1	2:C:727:SER:O	2.33	0.56
2:C:201:ARG:HH22	2:C:240:HIS:C	2.13	0.56
3:D:691:ASP:O	3:D:695:VAL:HG23	2.05	0.56
2:M:631:ASP:OD1	2:M:631:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:139:VAL:HG12	4:Q:159:ILE:HB	1.88	0.56
6:V:3:LEU:HD22	6:V:137:LEU:HD12	1.88	0.56
1:L:830:CYS:SG	1:L:856:CYS:HB3	2.38	0.56
1:B:199:LEU:HD12	1:B:210:ILE:HD11	1.86	0.56
2:C:27:ALA:HB3	2:C:48:ILE:HB	1.85	0.56
5:H:259:ASP:OD1	5:H:259:ASP:N	2.38	0.56
2:M:307:HIS:HE1	2:M:309:HIS:HB2	1.70	0.56
4:Q:147:VAL:HG23	4:Q:148:MET:HE2	1.88	0.56
2:C:444:GLN:O	2:C:448:THR:OG1	2.20	0.56
3:D:536:PHE:O	3:D:538:ARG:N	2.36	0.56
1:L:495:GLN:NE2	1:L:501:LYS:O	2.39	0.56
4:E:112:SER:HA	4:E:140:ARG:HH21	1.70	0.56
4:F:119:VAL:HG22	4:F:132:THR:HG22	1.86	0.56
2:M:732:VAL:HG22	4:O:148:MET:HE2	1.87	0.56
4:F:62:ARG:NH2	4:F:167:CYS:SG	2.78	0.56
5:R:157:TRP:CZ3	5:R:166:LEU:HB2	2.40	0.56
4:E:133:CYS:SG	4:E:134:SER:N	2.79	0.56
4:G:306:LYS:HG2	4:G:307:ALA:H	1.70	0.56
5:H:195:HIS:CE1	5:H:199:CYS:HB2	2.41	0.56
6:V:178:GLN:OE1	6:V:178:GLN:N	2.38	0.56
1:L:206:ARG:CZ	1:L:223:ASN:HB2	2.35	0.56
2:C:679:SER:HB3	4:G:231:LEU:HD12	1.87	0.56
3:D:931:VAL:HG23	3:D:946:HIS:CD2	2.41	0.56
2:C:452:LEU:O	2:C:455:ILE:HG22	2.06	0.55
1:K:738:ASN:OD1	2:M:716:HIS:ND1	2.38	0.55
1:B:648:GLY:O	1:B:652:THR:HG23	2.06	0.55
2:C:177:PHE:HB3	2:C:193:ILE:HG22	1.87	0.55
4:F:170:TRP:HE3	4:F:182:ILE:HG13	1.71	0.55
4:P:230:ASN:O	4:P:233:ARG:HG2	2.06	0.55
6:U:62:GLU:N	6:U:62:GLU:OE1	2.39	0.55
5:H:99:LEU:HA	5:H:132:TRP:HH2	1.71	0.55
2:C:451:MET:O	2:C:455:ILE:HB	2.06	0.55
1:K:672:VAL:O	1:K:676:SER:OG	2.24	0.55
2:M:95:THR:HA	2:M:122:THR:HG23	1.87	0.55
1:B:429:THR:HG21	1:B:650:LEU:HA	1.88	0.55
4:F:11:HIS:O	1:L:372:ARG:NH1	2.40	0.55
4:Q:67:HIS:CE1	4:Q:124:LYS:HE2	2.42	0.55
5:R:322:ILE:HD12	5:R:334:LEU:HD12	1.89	0.55
6:V:190:ASP:OD1	6:V:190:ASP:N	2.37	0.55
4:G:143:GLU:OE1	4:G:156:GLN:NE2	2.40	0.55
4:O:242:THR:OG1	4:O:243:LYS:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ASN:ND2	2:C:166:VAL:O	2.36	0.55
3:N:876:ARG:HH22	1:B:788:CYS:C	2.14	0.55
6:V:311:ASP:OD1	6:V:311:ASP:N	2.39	0.55
1:B:534:ILE:O	1:B:538:ILE:HG23	2.07	0.55
1:A:487:ASN:OD1	1:A:488:GLU:N	2.40	0.55
2:C:439:GLU:N	2:C:439:GLU:OE1	2.40	0.55
3:N:884:LYS:HA	1:B:852:SER:HB3	1.88	0.55
1:K:530:PHE:HZ	1:K:590:VAL:HG11	1.72	0.54
4:Q:67:HIS:NE2	4:Q:124:LYS:HE2	2.22	0.54
1:L:224:THR:OG1	1:L:225:LYS:N	2.40	0.54
2:M:145:MET:HG2	2:M:159:PHE:HB2	1.88	0.54
1:B:283:LEU:HD23	1:B:284:ALA:N	2.22	0.54
1:A:784:ARG:HA	1:A:791:ASN:HA	1.88	0.54
2:M:419:TYR:HD1	2:M:433:ASN:ND2	2.05	0.54
1:L:135:LYS:HB3	1:L:186:ALA:HB2	1.88	0.54
1:L:490:ARG:NH1	1:L:621:CYS:O	2.40	0.54
1:L:512:LEU:HD11	1:L:528:ALA:HB2	1.89	0.54
1:A:784:ARG:NH1	2:C:711:ALA:O	2.33	0.54
2:M:129:HIS:HB3	2:M:135:VAL:HB	1.90	0.54
6:V:283:GLN:O	6:V:287:PRO:HD2	2.08	0.54
1:L:491:ILE:HD12	1:L:491:ILE:H	1.72	0.54
1:A:602:TYR:O	1:A:605:VAL:HG12	2.07	0.54
3:D:674:GLN:O	3:D:678:GLN:HG3	2.08	0.54
1:B:456:ILE:HG12	1:B:651:LEU:HA	1.90	0.54
2:C:275:ASP:OD1	2:C:276:HIS:N	2.40	0.54
1:B:397:ARG:HG3	1:B:397:ARG:HH11	1.73	0.54
2:M:129:HIS:CD2	2:M:132:GLU:H	2.26	0.54
2:M:239:THR:OG1	2:M:241:ARG:O	2.26	0.54
5:R:277:ILE:HG23	5:R:289:TRP:HB2	1.90	0.54
2:M:237:MET:HE3	2:M:237:MET:N	2.23	0.54
6:U:265:MET:HE1	6:U:305:HIS:CD2	2.43	0.54
4:Q:11:HIS:CE1	4:Q:37:LYS:HD2	2.43	0.53
6:U:108:HIS:NE2	6:U:136:THR:OG1	2.35	0.53
1:L:10:TRP:HZ2	1:L:339:ILE:HG23	1.72	0.53
4:E:129:MET:HB3	4:E:142:TYR:O	2.08	0.53
2:M:147:CYS:HB3	2:M:157:SER:HB3	1.89	0.53
5:R:134:GLU:HA	5:R:139:TRP:HA	1.88	0.53
6:V:46:GLU:N	6:V:228:PHE:O	2.39	0.53
1:B:114:ARG:HD3	1:B:136:HIS:HB2	1.90	0.53
1:K:551:ASP:O	1:K:554:LEU:N	2.41	0.53
3:D:546:GLY:O	3:D:872:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:656:LYS:O	1:K:656:LYS:HD3	2.09	0.53
4:P:72:GLN:N	4:P:72:GLN:OE1	2.42	0.53
6:U:177:ILE:HD12	6:U:177:ILE:H	1.74	0.53
6:V:318:GLU:HA	6:V:321:GLN:HG2	1.90	0.53
1:A:846:HIS:CE1	2:C:691:ASN:HD21	2.27	0.53
3:D:691:ASP:OD1	3:D:692:LEU:HD22	2.07	0.53
1:K:78:LEU:N	1:K:90:THR:O	2.39	0.53
3:N:849:ARG:HG2	3:N:851:LEU:H	1.73	0.53
3:N:918:LYS:O	4:P:148:MET:N	2.41	0.53
1:A:739:PHE:HD2	1:A:780:LYS:HD3	1.73	0.53
4:E:293:LEU:HD12	4:E:294:ALA:N	2.24	0.53
1:K:200:LEU:O	1:K:211:PHE:N	2.42	0.53
6:U:186:VAL:HG22	6:U:240:VAL:HG22	1.90	0.53
1:K:408:GLN:OE1	1:K:410:TRP:NE1	2.40	0.53
2:M:123:VAL:HA	2:M:140:SER:HA	1.90	0.53
1:A:522:GLU:OE2	1:A:588:LEU:HG	2.09	0.52
5:H:126:ASP:O	5:H:127:ARG:HB2	2.09	0.52
4:P:282:TRP:N	4:P:296:SER:O	2.33	0.52
5:R:178:LEU:HG	5:R:188:VAL:HG22	1.92	0.52
3:D:694:GLN:O	3:D:697:SER:OG	2.22	0.52
4:O:39:TRP:CZ3	4:O:49:CYS:HB2	2.43	0.52
1:A:590:VAL:HG13	1:A:605:VAL:HG23	1.91	0.52
2:C:98:VAL:HB	2:C:117:THR:HG23	1.91	0.52
2:C:239:THR:OG1	2:C:241:ARG:O	2.26	0.52
4:E:120:LYS:HB2	4:E:168:ILE:HD11	1.90	0.52
6:V:180:PRO:O	6:V:264:ARG:NH1	2.43	0.52
6:V:181:GLN:HA	6:V:264:ARG:HH12	1.74	0.52
1:L:825:THR:OG1	1:L:826:TRP:N	2.38	0.52
2:C:398:SER:HB2	2:C:400:PHE:HE2	1.74	0.52
2:C:398:SER:HB2	2:C:400:PHE:CE2	2.45	0.52
1:B:233:ASP:OD2	1:B:236:PHE:N	2.41	0.52
5:H:314:VAL:HG23	5:H:323:LEU:HD21	1.91	0.52
4:F:12:LYS:O	1:L:372:ARG:NH2	2.43	0.52
4:G:55:THR:HG23	4:G:56:HIS:HD2	1.75	0.52
2:M:214:ASP:OD1	2:M:214:ASP:N	2.42	0.52
1:L:456:ILE:HG12	1:L:651:LEU:HA	1.91	0.52
1:B:541:LEU:HD23	1:B:558:ALA:HB2	1.90	0.52
4:G:14:LEU:HD12	4:G:14:LEU:H	1.75	0.52
1:A:555:ASN:ND2	1:B:582:GLN:OE1	2.42	0.52
1:L:193:LEU:HD11	1:L:210:ILE:HD11	1.91	0.52
1:A:495:GLN:NE2	1:A:502:LYS:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:872:ARG:HD3	5:H:69:TYR:CZ	2.45	0.52
5:H:225:ILE:HD11	5:H:241:LYS:HE2	1.92	0.52
6:V:144:TYR:CD2	6:V:153:PRO:HB3	2.45	0.52
1:B:614:ARG:HG2	1:B:650:LEU:HD22	1.92	0.52
1:A:787:LEU:HD12	1:A:838:HIS:HB3	1.92	0.51
2:M:122:THR:O	2:M:141:GLN:N	2.39	0.51
3:N:953:TRP:HE3	1:B:711:HIS:CD2	2.29	0.51
5:R:177:LEU:HD21	5:R:248:TRP:CZ2	2.46	0.51
6:U:5:ILE:HG12	6:U:79:LEU:HD22	1.93	0.51
1:L:55:SER:O	1:L:56:ILE:HD13	2.10	0.51
2:C:231:MET:SD	2:C:232:VAL:N	2.83	0.51
1:L:45:LEU:H	1:L:50:ALA:HA	1.75	0.51
1:A:619:PHE:HE2	1:A:623:PHE:CD2	2.28	0.51
1:K:512:LEU:O	1:K:516:VAL:HG23	2.10	0.51
1:K:851:VAL:HA	2:M:709:ASN:ND2	2.25	0.51
3:N:923:GLN:N	3:N:923:GLN:OE1	2.44	0.51
1:L:684:PRO:HD2	1:L:684:PRO:O	2.08	0.51
4:O:242:THR:O	4:O:281:VAL:HG22	2.11	0.51
1:A:413:HIS:CE1	1:A:414:ILE:HG23	2.45	0.51
4:G:318:ILE:HG22	4:G:318:ILE:O	2.10	0.51
3:N:890:PRO:O	1:B:852:SER:OG	2.29	0.51
1:L:825:THR:HG22	1:L:836:ALA:HA	1.93	0.51
3:D:535:PRO:HB2	5:H:262:ARG:HH21	1.76	0.51
5:R:181:THR:OG1	5:R:185:GLN:O	2.26	0.51
5:R:198:GLY:H	5:R:233:CYS:CB	2.24	0.51
1:L:69:TYR:CZ	1:L:71:ASN:HB2	2.45	0.51
4:G:51:ALA:HB1	4:G:53:TRP:HZ3	1.75	0.51
5:R:289:TRP:CZ3	5:R:301:PRO:HG3	2.46	0.51
1:A:389:ASP:OD1	1:A:390:ILE:N	2.44	0.51
4:E:246:ARG:HD3	4:E:270:ILE:HD11	1.93	0.51
5:H:279:SER:HB2	5:H:289:TRP:HE1	1.75	0.51
5:H:312:TRP:CZ2	5:H:328:GLY:HA2	2.46	0.51
4:O:231:LEU:HD22	4:O:289:THR:HG23	1.93	0.51
4:G:122:ALA:HB1	4:G:126:MET:HE2	1.93	0.50
1:B:785:CYS:HB3	1:B:789:LEU:H	1.76	0.50
1:K:523:ARG:HG3	1:K:587:TYR:CE1	2.46	0.50
6:U:21:TRP:CZ3	6:U:22:LEU:HD12	2.46	0.50
6:V:76:TRP:CD1	6:V:124:LEU:HB3	2.45	0.50
3:D:872:ARG:HD3	5:H:69:TYR:CE2	2.46	0.50
4:E:287:ASN:OD1	4:E:289:THR:N	2.42	0.50
1:B:426:LEU:HD11	1:B:646:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:685:GLN:HG2	2:M:690:TRP:HZ3	1.76	0.50
5:R:79:SER:HA	5:R:105:PRO:HB3	1.93	0.50
1:L:431:HIS:NE2	1:L:435:GLN:OE1	2.44	0.50
1:B:491:ILE:HG13	1:B:492:LEU:N	2.25	0.50
3:D:935:SER:O	1:L:825:THR:OG1	2.24	0.50
5:R:195:HIS:CE1	5:R:231:GLY:HA2	2.45	0.50
4:E:224:ASP:OD1	4:E:225:ILE:N	2.45	0.50
2:M:51:ILE:O	2:M:62:LYS:N	2.44	0.50
6:U:71:VAL:HG13	6:U:72:ALA:N	2.27	0.50
6:V:263:TRP:CD1	6:V:307:LEU:HB3	2.46	0.50
1:B:226:ALA:HA	1:B:244:TYR:HB2	1.92	0.50
1:A:405:ASP:OD1	1:A:406:THR:N	2.45	0.50
5:H:99:LEU:O	5:H:101:GLY:N	2.44	0.50
2:M:128:PHE:HZ	2:M:133:ALA:HA	1.75	0.50
2:M:177:PHE:HB3	2:M:193:ILE:HG22	1.94	0.50
3:N:945:GLY:N	3:N:950:MET:HE2	2.27	0.50
1:L:499:TRP:CZ2	1:L:527:VAL:HG23	2.47	0.50
2:M:144:PHE:HE1	2:M:160:SER:HB2	1.76	0.49
3:N:914:CYS:SG	3:N:915:ALA:N	2.85	0.49
1:L:99:LYS:HG3	1:L:100:PHE:CE2	2.47	0.49
3:D:941:CYS:HB3	3:D:943:HIS:ND1	2.27	0.49
4:F:81:ARG:NH1	4:F:113:ARG:O	2.45	0.49
1:B:17:ARG:HG3	1:B:17:ARG:HH11	1.75	0.49
1:B:102:ASP:OD1	1:B:102:ASP:N	2.33	0.49
3:D:690:LYS:HA	3:D:693:VAL:HG22	1.95	0.49
4:F:58:GLY:HA3	4:F:79:PHE:HB2	1.94	0.49
2:M:146:LYS:HA	2:M:158:THR:HA	1.94	0.49
4:O:140:ARG:HG3	4:O:140:ARG:HH11	1.78	0.49
5:H:102:HIS:ND1	5:H:126:ASP:OD2	2.45	0.49
1:K:436:TYR:CZ	1:K:492:LEU:HD11	2.47	0.49
5:R:321:ASN:O	5:R:322:ILE:HG12	2.12	0.49
6:V:242:ASP:OD1	6:V:242:ASP:N	2.38	0.49
1:L:538:ILE:HG13	1:L:539:GLN:N	2.26	0.49
2:C:33:SER:HB3	2:C:42:VAL:HG23	1.93	0.49
6:U:11:ARG:HH21	6:U:72:ALA:HB3	1.78	0.49
6:V:308:VAL:HG11	6:V:316:VAL:HG11	1.93	0.49
6:U:303:PHE:HB3	6:U:305:HIS:CE1	2.47	0.49
1:B:411:ARG:O	1:B:414:ILE:HG13	2.12	0.49
1:A:619:PHE:HE2	1:A:623:PHE:HD2	1.59	0.49
4:F:221:PRO:O	4:F:223:HIS:ND1	2.46	0.49
1:L:836:ALA:O	1:L:840:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:VAL:HG13	1:B:108:PHE:HD1	1.78	0.49
1:B:220:MET:SD	1:B:220:MET:N	2.86	0.49
4:G:268:ILE:H	4:G:268:ILE:HD12	1.78	0.49
4:F:6:SER:HA	1:L:375:TYR:HA	1.95	0.49
1:K:79:ALA:HA	1:K:89:LEU:HA	1.94	0.49
2:M:307:HIS:HD1	2:M:309:HIS:H	1.60	0.49
6:U:263:TRP:CE3	6:U:307:LEU:HB3	2.47	0.49
6:U:25:HIS:CD2	6:V:207:TYR:HE2	2.31	0.48
1:B:715:GLU:O	1:B:718:ILE:HG22	2.12	0.48
3:N:942:GLY:O	1:B:732:GLN:N	2.28	0.48
4:Q:107:THR:OG1	4:Q:108:THR:N	2.46	0.48
1:L:245:GLU:OE1	1:L:246:GLY:N	2.45	0.48
4:G:55:THR:HG23	4:G:56:HIS:CD2	2.48	0.48
2:M:145:MET:SD	2:M:145:MET:N	2.87	0.48
2:C:142:ASP:OD1	2:C:144:PHE:N	2.43	0.48
3:D:844:HIS:ND1	4:G:309:TYR:OH	2.46	0.48
6:V:52:THR:HG21	6:V:300:THR:OG1	2.14	0.48
1:L:456:ILE:HD11	1:L:651:LEU:HG	1.95	0.48
1:B:179:TYR:HD2	1:B:213:LEU:HD12	1.78	0.48
4:F:247:ILE:H	4:F:272:ALA:HB3	1.79	0.48
4:Q:273:GLN:C	4:Q:274:PHE:HD2	2.21	0.48
6:U:41:PHE:CE1	6:U:233:ILE:HD12	2.49	0.48
4:F:286:TRP:CZ3	4:F:293:LEU:HB2	2.49	0.48
1:K:833:GLY:HA2	1:K:839:MET:CE	2.43	0.48
3:N:662:LEU:HD22	3:N:666:TYR:HE1	1.79	0.48
6:U:188:THR:OG1	6:U:189:LEU:N	2.42	0.48
6:V:53:LEU:HD23	6:V:53:LEU:HA	1.76	0.48
6:V:134:ILE:HD12	6:V:143:ILE:HG21	1.96	0.48
2:C:301:THR:HG21	2:C:319:LYS:CE	2.33	0.48
4:F:123:PRO:HG2	4:F:126:MET:HE2	1.96	0.48
1:B:189:SER:OG	1:B:228:GLN:O	2.32	0.48
1:A:488:GLU:O	1:A:491:ILE:HG22	2.14	0.48
2:C:249:GLN:NE2	2:C:250:THR:O	2.47	0.48
4:P:287:ASN:HD21	1:B:364:THR:HG22	1.77	0.48
4:Q:238:LEU:HD12	4:Q:239:ALA:H	1.79	0.48
6:U:266:VAL:O	6:U:266:VAL:HG23	2.13	0.48
6:V:305:HIS:N	6:V:305:HIS:CD2	2.81	0.48
4:F:287:ASN:OD1	4:F:290:GLY:N	2.47	0.48
4:F:289:THR:HG21	1:L:391:ALA:HB2	1.95	0.48
2:M:128:PHE:CZ	2:M:133:ALA:HA	2.48	0.48
6:U:187:LEU:HB2	6:U:255:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:THR:N	1:A:286:LEU:O	2.45	0.47
1:A:605:VAL:HG11	1:A:619:PHE:CE1	2.37	0.47
4:E:182:ILE:HG22	4:E:200:PHE:HB2	1.96	0.47
4:G:111:ASP:OD1	4:G:111:ASP:N	2.44	0.47
3:N:740:ARG:HG3	5:R:321:ASN:HD21	1.79	0.47
4:O:101:SER:O	4:O:101:SER:OG	2.31	0.47
4:P:53:TRP:HZ2	4:P:86:TRP:CD1	2.32	0.47
5:R:289:TRP:H	5:R:289:TRP:CD1	2.31	0.47
4:G:148:MET:HE3	4:G:148:MET:HB2	1.78	0.47
4:Q:225:ILE:HG23	4:Q:238:LEU:HD11	1.96	0.47
1:L:263:LEU:HD12	1:L:296:TYR:HE2	1.79	0.47
1:L:499:TRP:HA	1:L:511:PHE:HD2	1.80	0.47
1:A:73:ASP:HA	1:A:75:GLU:N	2.28	0.47
2:C:327:LEU:HD23	2:C:329:ARG:H	1.80	0.47
2:M:277:ASN:HD21	2:M:294:GLU:HG2	1.79	0.47
3:D:740:ARG:HD3	5:H:319:THR:O	2.14	0.47
4:F:84:ALA:HB1	4:F:86:TRP:NE1	2.29	0.47
2:M:214:ASP:OD1	2:M:224:ALA:HB3	2.15	0.47
5:R:254:LEU:HB3	5:R:289:TRP:CZ3	2.50	0.47
1:L:226:ALA:HA	1:L:244:TYR:CB	2.44	0.47
1:L:842:TRP:NE1	1:L:850:PRO:HD3	2.30	0.47
2:C:137:LEU:HD12	2:C:145:MET:HE2	1.97	0.47
4:G:126:MET:HE1	4:G:170:TRP:CZ3	2.49	0.47
5:H:105:PRO:HD2	5:H:125:TYR:HB3	1.97	0.47
2:M:124:ASN:ND2	2:M:166:VAL:O	2.41	0.47
2:M:257:VAL:HG22	2:M:269:THR:HG22	1.96	0.47
1:B:426:LEU:HG	1:B:646:LEU:HG	1.95	0.47
3:N:742:VAL:HG21	5:R:270:ILE:HD12	1.97	0.47
1:L:226:ALA:HA	1:L:244:TYR:HB2	1.96	0.47
1:B:8:ILE:HD13	1:B:341:VAL:HG21	1.96	0.47
2:C:451:MET:HE1	3:D:719:TRP:HZ2	1.80	0.47
1:K:116:CYS:HA	1:K:133:LEU:HA	1.95	0.47
2:M:685:GLN:HG2	2:M:690:TRP:CZ3	2.49	0.47
3:N:843:GLN:HA	3:N:846:LYS:NZ	2.29	0.47
5:R:177:LEU:HD21	5:R:248:TRP:HZ2	1.78	0.47
1:L:295:LEU:C	1:L:296:TYR:HD1	2.21	0.47
1:B:27:LEU:C	1:B:28:TYR:HD2	2.23	0.47
1:B:204:MET:HE2	1:B:206:ARG:N	2.29	0.47
2:C:173:ILE:HD11	2:C:217:PRO:HA	1.97	0.47
2:C:219:ASP:OD1	2:C:221:GLY:N	2.39	0.47
1:K:67:ALA:O	1:K:79:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:426:LEU:HD22	1:K:646:LEU:HD13	1.96	0.47
4:O:317:GLY:C	4:O:318:ILE:HD13	2.39	0.47
1:L:275:TRP:CE2	1:L:283:LEU:HD21	2.49	0.47
4:E:188:ASP:O	4:E:196:LYS:NZ	2.48	0.47
4:E:287:ASN:OD1	4:E:287:ASN:C	2.57	0.47
4:G:85:VAL:HB	4:G:107:THR:HG22	1.96	0.47
5:H:321:ASN:CG	5:H:322:ILE:HG13	2.40	0.47
1:A:433:MET:HG3	1:A:452:VAL:HG12	1.97	0.46
2:C:216:HIS:HB3	2:C:219:ASP:O	2.14	0.46
6:U:184:PHE:HE2	6:U:227:PHE:CD2	2.33	0.46
1:L:824:PHE:CE2	1:L:826:TRP:HZ3	2.33	0.46
5:R:145:HIS:NE2	5:R:188:VAL:HG11	2.30	0.46
1:L:678:CYS:SG	1:L:679:MET:N	2.88	0.46
1:K:735:VAL:HG12	2:M:717:VAL:HG12	1.96	0.46
2:M:33:SER:HB3	2:M:42:VAL:HG23	1.96	0.46
6:V:63:LEU:O	6:V:65:PRO:HD3	2.14	0.46
3:D:697:SER:O	3:D:701:VAL:HG22	2.15	0.46
5:R:232:GLY:HA2	5:R:261:VAL:HG12	1.96	0.46
6:V:263:TRP:HD1	6:V:307:LEU:HB3	1.80	0.46
1:L:662:MET:HE2	1:L:662:MET:HB2	1.78	0.46
1:B:102:ASP:O	1:B:106:LYS:NZ	2.48	0.46
2:C:746:CYS:SG	2:C:748:HIS:HB2	2.56	0.46
6:V:3:LEU:HD12	6:V:81:VAL:HG22	1.97	0.46
6:V:64:PRO:O	6:V:66:SER:N	2.49	0.46
1:B:91:SER:C	1:B:92:LEU:HD23	2.41	0.46
2:C:142:ASP:OD1	2:C:142:ASP:C	2.58	0.46
3:D:942:GLY:C	1:L:732:GLN:H	2.24	0.46
4:G:81:ARG:HA	4:G:116:VAL:HG23	1.98	0.46
1:L:207:ASN:HD21	1:L:209:ALA:HB2	1.80	0.46
1:B:680:LEU:HG	1:B:723:LEU:HD12	1.97	0.46
1:B:788:CYS:SG	1:B:835:HIS:HE1	2.13	0.46
3:D:722:HIS:CE1	3:D:724:PHE:HB2	2.50	0.46
4:E:276:ASN:OD1	4:E:276:ASN:N	2.48	0.46
4:Q:299:ASP:OD2	4:Q:301:CYS:N	2.48	0.46
6:V:146:GLU:HA	6:V:151:PRO:HA	1.98	0.46
3:D:535:PRO:HB2	5:H:262:ARG:HE	1.81	0.46
3:D:884:LYS:NZ	1:L:852:SER:HA	2.31	0.46
1:K:199:LEU:HA	1:K:212:ASP:HA	1.98	0.46
1:K:405:ASP:OD1	1:K:406:THR:N	2.49	0.46
6:U:182:ASN:OD1	6:U:182:ASN:C	2.59	0.46
2:C:260:ARG:HG2	2:C:263:CYS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:750:VAL:HG11	2:C:754:PHE:HD1	1.80	0.46
2:C:770:MET:HE2	2:C:770:MET:HB3	1.75	0.46
1:K:859:MET:HE3	2:M:767:GLN:HE22	1.80	0.46
2:M:343:LEU:HD21	2:M:351:LEU:HD11	1.97	0.46
1:L:665:TYR:O	1:L:669:THR:HG22	2.16	0.46
5:R:235:ASN:ND2	5:R:259:ASP:O	2.47	0.46
1:A:646:LEU:HD23	1:A:646:LEU:HA	1.84	0.45
2:C:695:GLU:O	2:C:699:LEU:HD12	2.16	0.45
4:F:235:PHE:HB2	4:F:250:LEU:O	2.16	0.45
5:R:173:GLY:O	5:R:194:ALA:N	2.47	0.45
5:R:303:LEU:HD23	5:R:304:LEU:N	2.31	0.45
1:L:192:TRP:CZ3	1:L:200:LEU:HB2	2.51	0.45
3:D:962:THR:O	1:L:729:PRO:HG3	2.15	0.45
3:N:721:ARG:HH22	4:Q:309:TYR:HB2	1.80	0.45
4:O:245:VAL:HG23	4:O:281:VAL:HG11	1.99	0.45
4:P:18:VAL:HG22	4:P:29:THR:HG22	1.98	0.45
1:B:821:ASN:OD1	1:B:821:ASN:N	2.49	0.45
1:A:614:ARG:HG3	1:A:614:ARG:HH11	1.80	0.45
1:K:608:GLU:O	1:K:616:ARG:NH1	2.49	0.45
3:N:888:CYS:O	3:N:889:PRO:C	2.59	0.45
3:N:950:MET:O	3:N:954:PHE:HB2	2.16	0.45
4:Q:274:PHE:HD1	4:Q:305:TRP:CZ3	2.34	0.45
5:R:100:ARG:HB2	5:R:100:ARG:NH1	2.31	0.45
6:V:17:ARG:N	6:V:18:PRO:HD2	2.30	0.45
2:C:730:GLY:CA	4:E:148:MET:HE1	2.45	0.45
4:F:20:PHE:HE1	4:F:24:GLY:HA2	1.80	0.45
4:F:27:MET:SD	4:F:27:MET:N	2.88	0.45
2:M:221:GLY:O	2:M:236:ASP:HA	2.16	0.45
6:U:45:THR:HA	6:U:229:ALA:HA	1.98	0.45
6:U:263:TRP:HE3	6:U:307:LEU:HB3	1.80	0.45
1:B:671:ASP:OD1	1:B:674:THR:OG1	2.34	0.45
1:A:660:ASP:OD1	1:A:660:ASP:N	2.47	0.45
3:D:953:TRP:HE3	1:L:711:HIS:CE1	2.35	0.45
2:M:119:HIS:NE2	2:M:138:SER:O	2.50	0.45
6:V:2:GLU:H	6:V:83:SER:CB	2.29	0.45
6:V:41:PHE:CD1	6:V:233:ILE:HG12	2.52	0.45
1:L:819:GLN:NE2	1:L:822:ASN:HD21	2.13	0.45
1:B:460:VAL:HG11	1:B:633:ILE:HG13	1.98	0.45
1:A:792:MET:HE1	1:A:834:GLY:C	2.41	0.45
2:C:190:LEU:HD11	2:C:215:TRP:HZ2	1.81	0.45
3:D:709:PRO:HB2	3:D:848:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:81:ARG:HG3	4:E:114:THR:O	2.17	0.45
4:G:101:SER:O	4:G:101:SER:OG	2.32	0.45
5:R:94:ILE:HG22	5:R:95:LEU:H	1.81	0.45
5:R:191:ILE:HD11	5:R:248:TRP:HB2	1.98	0.45
6:V:104:PRO:O	6:V:107:GLU:HG2	2.17	0.45
1:B:684:PRO:O	1:B:688:LEU:HB2	2.17	0.45
2:C:36:ARG:HH12	2:C:82:TRP:CD1	2.34	0.45
3:D:550:LEU:HD23	3:D:551:VAL:N	2.32	0.45
4:E:103:TRP:H	4:E:103:TRP:CD1	2.34	0.45
2:M:413:VAL:O	2:M:417:GLU:HG3	2.16	0.45
2:M:770:MET:HE2	2:M:770:MET:HB3	1.86	0.45
2:C:261:PRO:HD3	2:C:305:TRP:CD1	2.52	0.45
4:O:40:ASP:OD1	4:O:41:LYS:N	2.49	0.45
5:R:130:ILE:HB	5:R:132:TRP:HE1	1.82	0.45
1:K:626:ASP:OD1	1:K:626:ASP:N	2.50	0.45
4:O:133:CYS:HB3	4:O:139:VAL:HG12	1.97	0.45
6:U:102:ILE:HD12	6:U:102:ILE:HA	1.78	0.45
1:L:515:LEU:HD22	1:L:520:GLU:HB2	1.99	0.45
1:B:77:LEU:HD12	1:B:77:LEU:HA	1.79	0.45
1:A:238:ASP:O	1:A:253:LEU:N	2.35	0.45
2:C:272:MET:N	2:C:272:MET:HE3	2.32	0.45
4:F:70:PHE:HZ	4:F:127:GLY:HA2	1.81	0.45
4:O:299:ASP:C	4:O:299:ASP:OD2	2.60	0.45
1:L:335:GLN:OE1	1:L:335:GLN:HA	2.17	0.45
1:B:536:ARG:O	1:B:540:ILE:HG12	2.16	0.45
2:C:319:LYS:HA	2:C:319:LYS:HD3	1.80	0.44
2:C:400:PHE:CD1	4:G:319:LEU:HD22	2.52	0.44
2:C:633:PHE:O	2:C:637:VAL:HG23	2.18	0.44
5:H:60:ASP:N	5:H:80:ASP:OD2	2.48	0.44
1:K:329:ALA:O	1:K:339:ILE:N	2.48	0.44
2:M:237:MET:HE3	2:M:237:MET:H	1.81	0.44
6:V:15:VAL:HG23	6:V:51:TYR:HB2	2.00	0.44
4:E:81:ARG:HD3	4:E:81:ARG:N	2.33	0.44
5:H:236:LEU:O	5:H:238:LYS:HG2	2.17	0.44
2:M:137:LEU:HD21	2:M:169:VAL:HB	2.00	0.44
1:B:508:VAL:O	1:B:511:PHE:N	2.51	0.44
2:C:260:ARG:HA	2:C:305:TRP:NE1	2.32	0.44
3:D:849:ARG:HG2	3:D:851:LEU:H	1.82	0.44
4:P:280:GLN:O	4:P:298:ASP:N	2.51	0.44
1:B:215:ASN:OD1	1:B:218:GLN:N	2.38	0.44
4:F:181:MET:C	4:F:182:ILE:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:718:ASN:OD1	2:M:718:ASN:N	2.51	0.44
3:N:956:THR:OG1	3:N:957:GLN:N	2.50	0.44
4:Q:229:PRO:O	4:Q:233:ARG:NH2	2.51	0.44
1:B:246:GLY:O	1:B:270:LEU:HD11	2.17	0.44
1:B:648:GLY:O	1:B:651:LEU:HG	2.18	0.44
1:B:693:VAL:HA	1:B:696:TRP:CE3	2.52	0.44
2:C:718:ASN:HD22	2:C:725:PRO:HA	1.83	0.44
4:F:12:LYS:HA	1:L:372:ARG:HH22	1.83	0.44
5:H:115:MET:HG2	5:H:116:TYR:CE1	2.53	0.44
4:Q:77:CYS:SG	4:Q:119:VAL:HG12	2.57	0.44
5:R:224:TYR:C	5:R:225:ILE:HD13	2.42	0.44
6:V:228:PHE:HE1	6:V:241:MET:HE2	1.82	0.44
2:C:761:SER:O	2:C:761:SER:OG	2.31	0.44
2:M:90:LEU:O	2:M:102:TRP:N	2.50	0.44
3:N:743:GLN:HG2	3:N:747:MET:HE1	1.99	0.44
1:B:426:LEU:HA	1:B:649:ILE:HG21	1.99	0.44
1:K:488:GLU:O	1:K:491:ILE:HG22	2.18	0.44
1:K:708:ARG:NH2	4:O:25:ARG:HH21	2.14	0.44
6:U:11:ARG:HD2	6:U:11:ARG:HA	1.79	0.44
6:U:25:HIS:HB2	6:V:24:THR:HG21	1.98	0.44
2:C:175:ASP:OD1	2:C:176:TYR:N	2.47	0.44
2:C:773:LEU:HD23	2:C:773:LEU:O	2.18	0.44
3:D:672:ASP:O	3:D:676:THR:HG23	2.18	0.44
4:F:27:MET:SD	4:F:39:TRP:HB2	2.57	0.44
3:N:709:PRO:HB2	3:N:848:LYS:HD2	1.98	0.44
4:Q:33:ASP:OD1	4:Q:33:ASP:C	2.61	0.44
4:F:287:ASN:HD21	4:F:289:THR:HG22	1.83	0.44
4:G:129:MET:HE2	4:G:129:MET:HB3	1.79	0.44
1:K:574:GLU:O	1:K:578:THR:HG23	2.17	0.44
2:M:688:ARG:HH21	4:Q:23:HIS:CG	2.36	0.44
2:M:746:CYS:SG	2:M:748:HIS:HB2	2.57	0.44
3:N:953:TRP:NE1	3:N:959:VAL:O	2.49	0.44
4:Q:309:TYR:C	4:Q:309:TYR:CD2	2.96	0.44
5:R:270:ILE:HD13	5:R:270:ILE:HA	1.85	0.44
6:U:3:LEU:N	6:U:142:ASP:O	2.47	0.44
2:C:159:PHE:HE1	2:C:196:PRO:HA	1.83	0.43
6:U:146:GLU:HA	6:U:151:PRO:HA	1.99	0.43
1:L:516:VAL:HG23	1:L:521:TRP:HZ3	1.82	0.43
3:D:877:GLU:O	3:D:881:GLU:HG3	2.18	0.43
2:M:415:THR:HG23	2:M:651:GLN:HE22	1.83	0.43
6:V:317:ILE:O	6:V:321:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:404:LEU:HA	1:L:404:LEU:HD23	1.76	0.43
2:C:40:GLN:HA	2:C:53:ALA:HA	2.01	0.43
4:F:58:GLY:HA3	4:F:79:PHE:CG	2.53	0.43
4:F:65:TRP:HE3	4:F:66:ALA:H	1.66	0.43
3:N:946:HIS:HB2	3:N:949:HIS:CG	2.53	0.43
6:V:182:ASN:HD21	6:V:224:SER:CA	2.26	0.43
1:B:513:ASN:HA	1:B:516:VAL:HG12	2.00	0.43
1:A:436:TYR:O	1:A:436:TYR:CD2	2.71	0.43
1:A:795:PRO:CB	4:G:90:VAL:HG11	2.49	0.43
3:D:656:LEU:H	3:D:656:LEU:HD12	1.81	0.43
4:F:190:SER:O	4:F:192:ASN:N	2.46	0.43
5:H:238:LYS:HD2	5:H:250:GLU:OE1	2.19	0.43
1:K:513:ASN:O	1:K:517:GLN:HG3	2.18	0.43
6:U:15:VAL:HB	6:U:51:TYR:HB2	1.99	0.43
1:A:359:ALA:O	1:A:366:LEU:HD12	2.18	0.43
1:A:624:LEU:HD23	1:A:624:LEU:HA	1.87	0.43
3:D:953:TRP:CE2	3:D:961:PRO:HG3	2.53	0.43
5:H:260:TRP:HB2	5:H:282:GLN:HB2	2.01	0.43
5:H:336:LYS:HG2	5:H:337:GLU:H	1.83	0.43
6:U:35:ARG:H	6:U:35:ARG:HG2	1.51	0.43
6:U:134:ILE:HD12	6:U:134:ILE:HA	1.87	0.43
1:L:655:THR:HG23	1:L:657:ASP:H	1.83	0.43
1:B:58:SER:O	1:B:58:SER:OG	2.27	0.43
2:C:273:MET:O	2:C:275:ASP:N	2.49	0.43
4:E:7:ILE:HD12	4:E:7:ILE:HA	1.84	0.43
1:K:534:ILE:HG13	1:K:535:ARG:HD2	2.01	0.43
1:L:206:ARG:NH2	1:L:223:ASN:HD22	2.15	0.43
1:L:492:LEU:HD12	1:L:492:LEU:HA	1.77	0.43
1:A:735:VAL:HB	1:A:744:ILE:HD11	1.99	0.43
5:H:310:VAL:O	5:H:328:GLY:N	2.38	0.43
1:K:633:ILE:O	1:K:637:THR:OG1	2.25	0.43
2:M:458:SER:HA	2:M:459:PRO:HD2	1.77	0.43
6:V:126:ARG:HE	6:V:127:GLU:H	1.67	0.43
1:L:8:ILE:HG21	1:L:339:ILE:HD11	1.99	0.43
1:L:832:HIS:CG	1:L:851:VAL:HG11	2.54	0.43
1:B:111:LYS:O	1:B:112:HIS:CG	2.71	0.43
2:C:49:PHE:HB2	2:C:66:ARG:HE	1.83	0.43
4:E:200:PHE:HD1	4:E:211:LYS:HA	1.82	0.43
5:H:259:ASP:C	5:H:260:TRP:HD1	2.27	0.43
1:K:374:LEU:C	1:K:375:TYR:HD2	2.27	0.43
2:M:36:ARG:NH1	2:M:84:GLN:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:131:ILE:HD12	5:R:131:ILE:N	2.34	0.43
1:B:103:LEU:HA	1:B:106:LYS:NZ	2.33	0.43
1:B:283:LEU:HD23	1:B:284:ALA:H	1.83	0.43
1:B:508:VAL:HG22	1:B:512:LEU:HD23	2.01	0.43
1:B:652:THR:HB	1:B:657:ASP:HB2	2.01	0.43
1:A:529:LEU:HD23	1:A:591:MET:HB2	2.01	0.43
4:E:243:LYS:HB2	4:E:243:LYS:HE2	1.83	0.43
4:F:20:PHE:CE1	4:F:24:GLY:HA2	2.53	0.43
1:L:436:TYR:CD2	1:L:436:TYR:C	2.97	0.43
4:F:135:ALA:O	4:F:164:SER:HA	2.19	0.43
4:G:188:ASP:O	4:G:196:LYS:HE2	2.19	0.43
1:K:708:ARG:HH22	4:O:25:ARG:NH2	2.17	0.43
2:C:425:PRO:HD2	2:C:428:GLU:OE2	2.18	0.42
5:R:132:TRP:CD1	5:R:132:TRP:N	2.87	0.42
5:R:252:GLN:NE2	5:R:297:ASN:HB3	2.34	0.42
6:U:205:LEU:HD12	6:U:205:LEU:HA	1.80	0.42
1:L:250:ILE:N	1:L:250:ILE:HD12	2.34	0.42
1:L:673:GLN:O	1:L:676:SER:OG	2.35	0.42
1:B:487:ASN:O	1:B:491:ILE:HG23	2.19	0.42
1:A:363:ILE:O	1:A:364:THR:OG1	2.27	0.42
2:C:271:SER:HB3	2:C:275:ASP:HB3	2.01	0.42
5:H:134:GLU:HB3	5:H:139:TRP:CE3	2.54	0.42
5:H:311:VAL:HA	5:H:327:GLY:HA3	2.00	0.42
4:Q:107:THR:HG21	4:Q:153:TRP:NE1	2.33	0.42
1:L:472:HIS:HB2	1:L:474:TRP:CH2	2.54	0.42
3:D:658:VAL:HG12	3:D:743:GLN:HB2	2.02	0.42
4:E:79:PHE:O	4:E:79:PHE:CG	2.73	0.42
5:H:199:CYS:HA	5:H:232:GLY:CA	2.47	0.42
5:R:337:GLU:HB3	5:R:343:TRP:CD2	2.53	0.42
1:B:456:ILE:HA	1:B:459:ILE:HD12	2.01	0.42
1:A:739:PHE:CD2	1:A:780:LYS:HD3	2.54	0.42
2:C:147:CYS:SG	2:C:148:PHE:N	2.93	0.42
1:K:514:SER:O	1:K:518:GLU:CB	2.68	0.42
2:M:91:ALA:HA	2:M:101:THR:HA	2.01	0.42
2:M:633:PHE:O	2:M:637:VAL:HG23	2.19	0.42
4:Q:21:ASP:OD1	4:Q:24:GLY:N	2.53	0.42
4:Q:81:ARG:HA	4:Q:116:VAL:HG23	2.02	0.42
6:U:71:VAL:CG1	6:U:72:ALA:N	2.82	0.42
1:L:296:TYR:CD1	1:L:296:TYR:N	2.88	0.42
2:C:130:PRO:HD3	2:C:171:PHE:HD2	1.83	0.42
3:D:938:CYS:SG	3:D:968:CYS:HB3	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:67:HIS:CE1	4:E:124:LYS:HD3	2.55	0.42
4:G:117:THR:HG21	4:G:166:SER:HA	2.01	0.42
1:K:366:LEU:HD12	1:K:367:MET:N	2.34	0.42
2:M:95:THR:O	2:M:122:THR:OG1	2.24	0.42
6:V:12:VAL:HG22	6:V:54:MET:HG3	2.00	0.42
1:L:296:TYR:HD1	1:L:296:TYR:N	2.18	0.42
1:B:8:ILE:HD12	1:B:8:ILE:HA	1.83	0.42
1:B:17:ARG:HG3	1:B:17:ARG:NH1	2.34	0.42
1:B:350:PHE:HD1	1:B:351:THR:H	1.68	0.42
4:G:317:GLY:O	4:G:318:ILE:HD13	2.19	0.42
1:K:374:LEU:HD23	1:K:374:LEU:HA	1.81	0.42
6:U:280:ILE:O	6:U:284:ILE:HG13	2.20	0.42
6:V:102:ILE:H	6:V:102:ILE:HD12	1.85	0.42
6:V:133:VAL:HG13	6:V:134:ILE:HG12	2.01	0.42
6:V:181:GLN:O	6:V:181:GLN:NE2	2.48	0.42
6:V:284:ILE:O	6:V:288:LEU:HB2	2.18	0.42
2:C:259:TRP:CD1	2:C:267:LEU:HD23	2.55	0.42
4:F:28:ALA:HA	4:F:37:LYS:O	2.19	0.42
1:K:514:SER:HA	1:K:517:GLN:HE21	1.84	0.42
2:M:652:MET:HE3	2:M:656:VAL:HG21	2.02	0.42
4:O:49:CYS:SG	4:O:50:THR:N	2.92	0.42
6:V:308:VAL:HG13	6:V:309:PRO:HD2	2.02	0.42
1:L:461:LYS:HE2	1:L:461:LYS:HB2	1.77	0.42
1:L:646:LEU:HD23	1:L:646:LEU:HA	1.83	0.42
2:C:122:THR:O	2:C:141:GLN:N	2.51	0.42
3:D:857:GLN:OE1	3:D:857:GLN:HA	2.19	0.42
3:N:943:HIS:NE2	1:B:730:LEU:O	2.53	0.42
5:R:100:ARG:HB2	5:R:100:ARG:CZ	2.50	0.42
5:R:254:LEU:HD13	5:R:289:TRP:CE3	2.55	0.42
1:L:139:ASP:OD2	1:L:139:ASP:C	2.62	0.42
2:C:414:ASP:OD1	2:C:418:ARG:NH1	2.53	0.42
1:K:831:ARG:NH1	2:M:727:SER:O	2.53	0.42
2:M:769:ILE:HD13	2:M:769:ILE:HA	1.93	0.42
3:N:729:LEU:O	3:N:733:LEU:HG	2.20	0.42
4:O:140:ARG:HG3	4:O:140:ARG:NH1	2.35	0.42
5:R:73:ARG:HD2	5:R:111:TRP:HH2	1.85	0.42
6:U:134:ILE:HD11	6:U:143:ILE:HG21	2.02	0.42
6:V:75:THR:O	6:V:75:THR:OG1	2.34	0.42
1:A:734:PHE:CE2	1:A:743:SER:HB2	2.47	0.42
2:C:209:PRO:HD2	2:C:228:ARG:HG2	2.02	0.42
2:C:628:LEU:HD23	2:C:628:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:640:MET:HA	3:D:723:PRO:HG2	2.02	0.42
4:E:130:LEU:HD23	4:E:132:THR:H	1.85	0.42
4:G:25:ARG:HA	4:G:25:ARG:HD2	1.75	0.42
1:K:514:SER:HA	1:K:517:GLN:NE2	2.34	0.42
1:K:704:LEU:HD23	1:K:704:LEU:HA	1.91	0.42
6:U:114:MET:HG2	6:U:122:PHE:O	2.20	0.42
1:L:234:PRO:HG2	1:L:235:TYR:CE2	2.55	0.42
1:B:223:ASN:C	1:B:223:ASN:OD1	2.63	0.42
1:B:270:LEU:H	1:B:270:LEU:HD12	1.85	0.42
1:K:833:GLY:HA2	1:K:839:MET:HE3	2.02	0.41
3:N:666:TYR:CE2	3:N:747:MET:HE3	2.55	0.41
3:N:673:ILE:HD13	3:N:673:ILE:HA	1.91	0.41
3:N:676:THR:O	3:N:676:THR:OG1	2.37	0.41
4:O:247:ILE:HB	4:O:272:ALA:HB3	2.02	0.41
6:V:182:ASN:ND2	6:V:224:SER:HA	2.29	0.41
1:B:459:ILE:H	1:B:459:ILE:HG13	1.69	0.41
1:B:723:LEU:HA	1:B:723:LEU:HD23	1.70	0.41
1:B:785:CYS:O	1:B:789:LEU:HA	2.20	0.41
1:A:497:CYS:O	1:A:614:ARG:HD2	2.20	0.41
1:A:638:ASN:OD1	1:A:638:ASN:N	2.52	0.41
1:A:849:CYS:HB3	1:A:854:CYS:HB3	2.02	0.41
4:E:74:LEU:HD23	4:E:74:LEU:HA	1.86	0.41
4:F:119:VAL:HG22	4:F:132:THR:CG2	2.49	0.41
1:K:732:GLN:NE2	2:M:742:MET:O	2.52	0.41
4:Q:227:PHE:CD1	4:Q:238:LEU:HD13	2.55	0.41
5:R:127:ARG:O	5:R:146:ALA:HA	2.20	0.41
5:R:176:SER:C	5:R:177:LEU:HD12	2.45	0.41
1:B:87:VAL:O	1:B:107:GLU:HA	2.20	0.41
1:A:508:VAL:HG11	1:A:531:ASN:ND2	2.36	0.41
2:C:186:GLY:HA2	2:C:208:GLY:O	2.19	0.41
3:D:946:HIS:HB2	3:D:949:HIS:CG	2.56	0.41
4:G:109:LEU:HD13	4:G:142:TYR:CE1	2.55	0.41
2:M:272:MET:SD	2:M:273:MET:SD	3.17	0.41
6:V:19:GLY:HA3	6:V:68:PHE:CD2	2.54	0.41
6:V:23:TYR:CE1	6:V:64:PRO:HD2	2.55	0.41
1:L:839:MET:HA	1:L:842:TRP:HB3	2.01	0.41
2:M:46:ARG:HA	2:M:76:SER:HA	2.02	0.41
2:M:101:THR:OG1	2:M:102:TRP:N	2.51	0.41
6:U:145:ARG:O	6:U:152:VAL:N	2.49	0.41
1:L:252:ASP:OD2	1:L:252:ASP:C	2.63	0.41
1:L:456:ILE:CG1	1:L:651:LEU:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:487:ASN:OD1	1:L:487:ASN:N	2.52	0.41
2:C:320:ASP:OD2	2:C:320:ASP:C	2.63	0.41
4:F:59:SER:H	4:F:79:PHE:HD2	1.66	0.41
4:F:122:ALA:HA	4:F:170:TRP:NE1	2.31	0.41
5:H:99:LEU:HA	5:H:132:TRP:CH2	2.53	0.41
1:K:778:CYS:HB3	1:K:780:LYS:HB2	2.03	0.41
4:P:291:THR:HG21	1:B:390:ILE:HG21	2.02	0.41
6:V:21:TRP:O	6:V:24:THR:HG22	2.20	0.41
3:D:849:ARG:CZ	3:D:849:ARG:HB2	2.50	0.41
1:L:10:TRP:CZ3	1:L:331:HIS:CD2	3.09	0.41
1:L:18:PHE:CD1	1:L:18:PHE:C	2.99	0.41
1:A:459:ILE:CD1	1:A:492:LEU:HD22	2.51	0.41
3:D:669:ASN:OD1	3:D:670:VAL:N	2.54	0.41
4:F:140:ARG:HE	4:F:140:ARG:HB2	1.72	0.41
4:G:161:CYS:O	4:G:163:LEU:N	2.54	0.41
2:M:261:PRO:HD3	2:M:305:TRP:CE2	2.55	0.41
2:M:718:ASN:HB3	2:M:725:PRO:HA	2.03	0.41
1:L:97:ASN:OD1	1:L:97:ASN:O	2.39	0.41
1:L:224:THR:C	1:L:225:LYS:HD3	2.46	0.41
1:A:394:MET:HG2	1:A:673:GLN:OE1	2.21	0.41
2:C:191:TRP:HZ3	2:C:199:CYS:HA	1.82	0.41
4:F:163:LEU:HD12	4:F:164:SER:H	1.85	0.41
4:F:170:TRP:CE3	4:F:182:ILE:HG13	2.53	0.41
5:H:254:LEU:HB3	5:H:289:TRP:CZ3	2.56	0.41
6:U:187:LEU:HD11	6:U:254:LEU:HD22	2.01	0.41
6:U:320:LEU:HD12	6:U:320:LEU:O	2.20	0.41
1:L:76:CYS:HB2	1:L:93:GLY:N	2.31	0.41
1:L:198:LYS:O	1:L:199:LEU:HD22	2.20	0.41
1:L:410:TRP:O	1:L:413:HIS:HD2	2.02	0.41
1:L:819:GLN:HE22	1:L:822:ASN:HD21	1.69	0.41
1:B:495:GLN:NE2	1:B:500:ILE:O	2.53	0.41
1:A:8:ILE:HA	1:A:20:VAL:HA	2.03	0.41
1:A:436:TYR:HD2	1:A:452:VAL:HG21	1.85	0.41
2:C:145:MET:HE3	2:C:146:LYS:N	2.36	0.41
3:D:869:ILE:O	3:D:872:ARG:HB2	2.20	0.41
5:H:67:MET:HB3	5:H:67:MET:HE3	1.77	0.41
2:M:301:THR:OG1	2:M:302:GLY:N	2.53	0.41
2:M:426:LEU:HD23	2:M:457:CYS:HB2	2.02	0.41
3:N:668:LEU:HD11	3:N:747:MET:HG3	2.03	0.41
3:N:953:TRP:NE1	3:N:961:PRO:HD3	2.36	0.41
4:O:162:LYS:O	4:O:163:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:274:PHE:N	4:Q:274:PHE:CD2	2.89	0.41
6:U:25:HIS:HB3	6:U:26:PRO:HD3	2.03	0.41
6:V:201:LEU:O	6:V:205:LEU:HD12	2.21	0.41
1:L:178:LEU:HG	1:L:179:TYR:CE2	2.55	0.41
1:L:294:ARG:CB	1:L:296:TYR:HE1	2.33	0.41
1:A:228:GLN:O	1:A:242:SER:HA	2.20	0.41
2:C:451:MET:HE1	3:D:719:TRP:CZ2	2.55	0.41
4:F:198:GLN:C	4:F:199:ILE:HD13	2.45	0.41
2:M:272:MET:N	2:M:272:MET:HE3	2.35	0.41
3:N:690:LYS:HA	3:N:693:VAL:HG23	2.02	0.41
4:O:281:VAL:HA	4:O:297:GLY:HA2	2.01	0.41
6:U:254:LEU:HD23	6:U:254:LEU:HA	1.86	0.41
1:L:69:TYR:HB2	1:L:121:TRP:CZ2	2.55	0.41
1:L:262:THR:O	1:L:263:LEU:HD22	2.20	0.41
1:L:622:LYS:HB3	1:L:622:LYS:HE3	1.80	0.41
1:B:29:HIS:C	1:B:29:HIS:ND1	2.78	0.41
2:C:327:LEU:HD23	2:C:328:PHE:N	2.36	0.40
2:C:683:LEU:HD23	2:C:683:LEU:HA	1.84	0.40
4:F:66:ALA:HB2	4:F:121:PHE:CE2	2.57	0.40
1:K:531:ASN:C	1:K:532:LEU:HD12	2.46	0.40
6:U:108:HIS:ND1	6:U:108:HIS:N	2.69	0.40
1:L:69:TYR:HB3	1:L:77:LEU:HB3	2.03	0.40
1:B:315:GLU:OE1	1:B:315:GLU:N	2.54	0.40
1:A:201:LEU:HA	1:A:210:ILE:HA	2.02	0.40
1:A:593:ALA:O	1:A:597:SER:N	2.54	0.40
1:A:732:GLN:O	2:C:720:SER:OG	2.36	0.40
2:C:219:ASP:OD1	2:C:220:ARG:N	2.54	0.40
2:C:344:CYS:O	2:C:351:LEU:HD12	2.22	0.40
4:E:112:SER:HA	4:E:140:ARG:NH2	2.34	0.40
1:L:354:GLU:O	1:L:355:ARG:HG2	2.20	0.40
1:L:508:VAL:HG23	1:L:512:LEU:HD23	2.02	0.40
2:M:686:ARG:HG2	4:Q:22:PHE:CZ	2.56	0.40
4:O:202:TYR:HB2	4:O:209:TYR:CE1	2.57	0.40
6:V:295:ALA:HB1	6:V:297:TYR:CE1	2.56	0.40
2:C:253:SER:O	2:C:272:MET:HE1	2.22	0.40
2:C:455:ILE:HD11	2:C:633:PHE:CE2	2.57	0.40
3:D:739:LEU:HD12	3:D:739:LEU:HA	1.93	0.40
1:K:534:ILE:HD12	1:K:535:ARG:HH11	1.87	0.40
1:K:732:GLN:NE2	2:M:763:GLY:O	2.54	0.40
3:N:531:ASP:N	3:N:534:ILE:O	2.54	0.40
3:N:691:ASP:OD1	3:N:736:TYR:OH	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:843:GLN:HA	3:N:846:LYS:HZ3	1.86	0.40
1:L:483:ILE:HA	1:L:486:LEU:HD13	2.03	0.40
1:B:663:GLU:OE2	1:B:692:ARG:HG2	2.22	0.40
1:A:671:ASP:OD1	1:A:671:ASP:C	2.63	0.40
2:C:176:TYR:HB3	2:C:177:PHE:CE2	2.57	0.40
3:D:973:THR:OG1	1:L:822:ASN:ND2	2.54	0.40
2:M:35:CYS:HA	2:M:82:TRP:CE2	2.57	0.40
2:M:640:MET:HA	3:N:723:PRO:HG2	2.04	0.40
3:N:846:LYS:HB3	3:N:853:PRO:HG2	2.03	0.40
4:O:72:GLN:OE1	4:O:72:GLN:HA	2.21	0.40
6:U:98:ALA:O	6:U:102:ILE:HG22	2.21	0.40
6:U:134:ILE:O	6:U:138:ALA:HB2	2.21	0.40
6:U:208:SER:O	6:U:208:SER:OG	2.32	0.40
1:B:114:ARG:NH2	1:B:133:LEU:HD22	2.36	0.40
1:B:279:ARG:HH21	1:B:282:LEU:CB	2.35	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	725/875 (83%)	670 (92%)	55 (8%)	0	100	100
1	B	725/875 (83%)	653 (90%)	69 (10%)	3 (0%)	30	61
1	K	719/875 (82%)	666 (93%)	51 (7%)	2 (0%)	36	65
1	L	724/875 (83%)	643 (89%)	79 (11%)	2 (0%)	36	65
2	C	569/790 (72%)	541 (95%)	28 (5%)	0	100	100
2	M	569/790 (72%)	553 (97%)	15 (3%)	1 (0%)	43	72
3	D	239/974 (24%)	220 (92%)	19 (8%)	0	100	100
3	N	253/974 (26%)	246 (97%)	6 (2%)	1 (0%)	30	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	298/421 (71%)	282 (95%)	16 (5%)	0	100	100
4	F	301/421 (72%)	250 (83%)	47 (16%)	4 (1%)	9	39
4	G	296/421 (70%)	280 (95%)	15 (5%)	1 (0%)	36	65
4	O	296/421 (70%)	279 (94%)	17 (6%)	0	100	100
4	P	287/421 (68%)	261 (91%)	24 (8%)	2 (1%)	18	51
4	Q	296/421 (70%)	285 (96%)	11 (4%)	0	100	100
5	H	281/368 (76%)	257 (92%)	24 (8%)	0	100	100
5	R	281/368 (76%)	239 (85%)	41 (15%)	1 (0%)	30	61
6	U	282/329 (86%)	257 (91%)	25 (9%)	0	100	100
6	V	272/329 (83%)	240 (88%)	32 (12%)	0	100	100
All	All	7413/10948 (68%)	6822 (92%)	574 (8%)	17 (0%)	44	72

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	135	ALA
4	F	245	VAL
1	K	595	LEU
3	N	889	PRO
4	P	26	ARG
4	P	90	VAL
1	L	309	THR
1	B	466	MET
1	B	684	PRO
4	G	162	LYS
1	K	552	LEU
4	F	194	MET
1	L	74	PRO
4	F	321	GLY
5	R	209	VAL
1	B	355	ARG
2	M	274	VAL

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	269/771 (35%)	267 (99%)	2 (1%)	76	78
1	B	361/771 (47%)	358 (99%)	3 (1%)	73	77
1	K	286/771 (37%)	281 (98%)	5 (2%)	53	69
1	L	415/771 (54%)	413 (100%)	2 (0%)	81	80
2	C	367/677 (54%)	364 (99%)	3 (1%)	73	77
2	M	336/677 (50%)	335 (100%)	1 (0%)	86	83
3	D	142/858 (17%)	141 (99%)	1 (1%)	76	78
3	N	131/858 (15%)	131 (100%)	0	100	100
4	E	184/365 (50%)	184 (100%)	0	100	100
4	F	116/365 (32%)	116 (100%)	0	100	100
4	G	206/365 (56%)	205 (100%)	1 (0%)	81	80
4	O	188/365 (52%)	185 (98%)	3 (2%)	55	69
4	P	52/365 (14%)	51 (98%)	1 (2%)	50	67
4	Q	200/365 (55%)	198 (99%)	2 (1%)	68	75
5	H	156/313 (50%)	155 (99%)	1 (1%)	78	79
5	R	139/313 (44%)	138 (99%)	1 (1%)	76	78
6	U	199/285 (70%)	197 (99%)	2 (1%)	68	75
6	V	189/285 (66%)	186 (98%)	3 (2%)	55	69
All	All	3936/9540 (41%)	3905 (99%)	31 (1%)	70	77

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

Mol	Chain	Res	Type
1	A	428	TYR
1	A	472	HIS
2	C	113	ASP
2	C	414	ASP
2	C	439	GLU
3	D	666	TYR
4	G	129	MET
5	H	172	ASP
1	K	413	HIS
1	K	486	LEU
1	K	492	LEU

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Mol	Chain	Res	Type
1	K	595	LEU
1	K	603	ASP
2	M	223	LEU
4	O	147	VAL
4	O	181	MET
4	O	271	VAL
4	P	289	THR
4	Q	87	GLU
4	Q	217	THR
5	R	94	ILE
6	U	22	LEU
6	U	206	PHE
6	V	22	LEU
6	V	237	ILE
6	V	288	LEU
1	L	235	TYR
1	L	516	VAL
1	B	29	HIS
1	B	529	LEU
1	B	679	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	GLN
1	A	555	ASN
1	A	846	HIS
2	C	119	HIS
3	D	847	ASN
4	E	277	HIS
4	G	16	HIS
5	H	195	HIS
1	K	435	GLN
1	K	702	ASN
1	K	732	GLN
2	M	189	GLN
2	M	433	ASN
2	M	447	GLN
2	M	651	GLN
2	M	675	HIS
2	M	694	ASN
2	M	748	HIS

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Mol	Chain	Res	Type
4	O	156	GLN
4	Q	230	ASN
4	Q	277	HIS
5	R	102	HIS
5	R	195	HIS
5	R	252	GLN
6	U	4	HIS
6	V	182	ASN
1	L	14	HIS
1	L	82	GLN
1	L	207	ASN
1	L	319	GLN
1	L	412	ASN
1	L	413	HIS
1	L	542	ASN
1	L	673	GLN
1	L	719	HIS
1	L	822	ASN
1	B	413	HIS
1	B	495	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 31 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

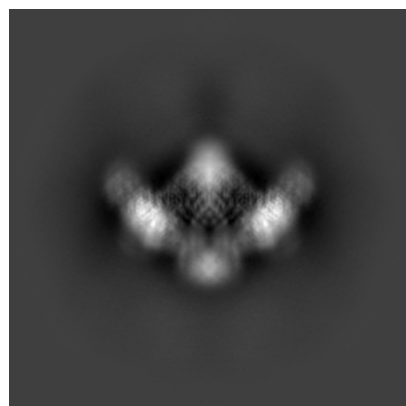
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63422. These allow visual inspection of the internal detail of the map and identification of artifacts.

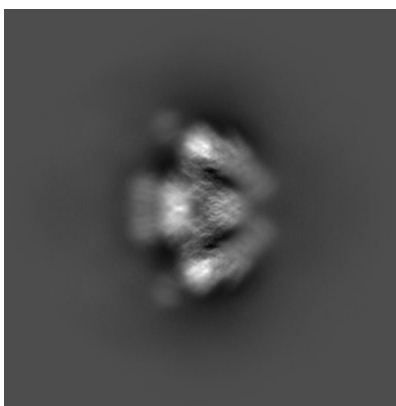
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

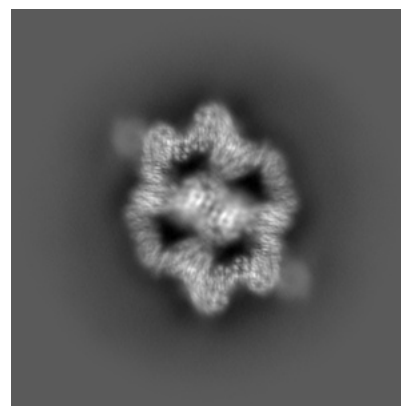
6.1.1 Primary map



X

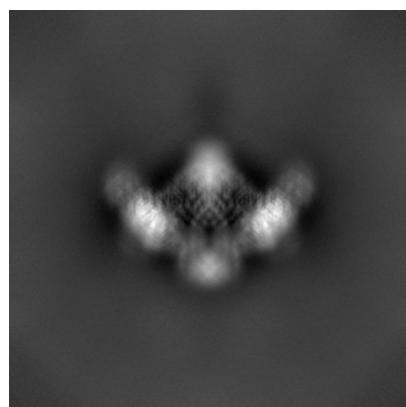


Y

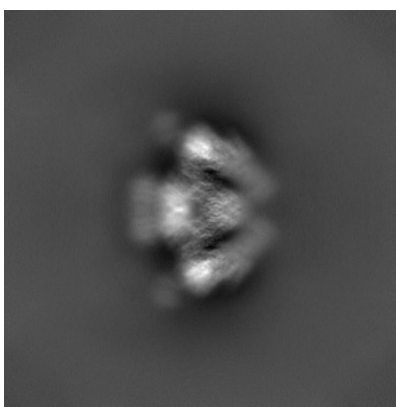


Z

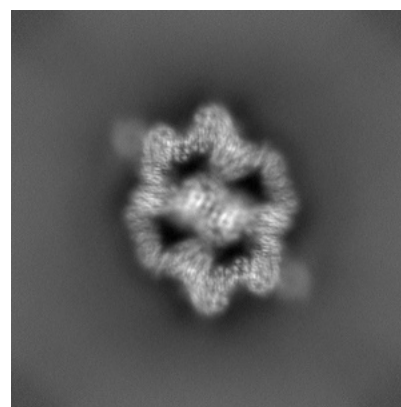
6.1.2 Raw map



X



Y

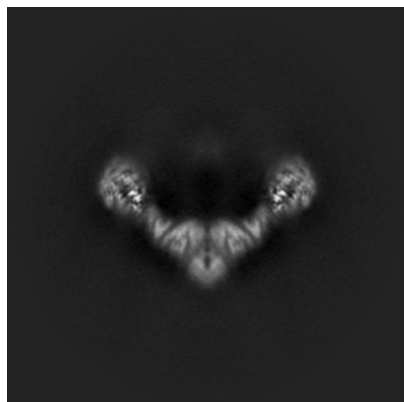


Z

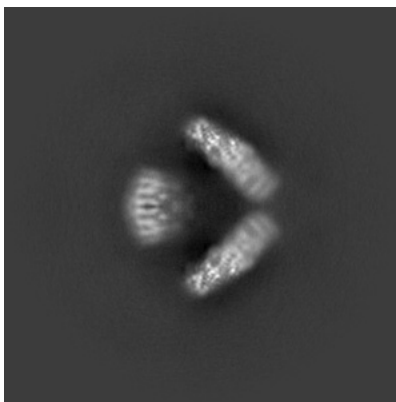
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

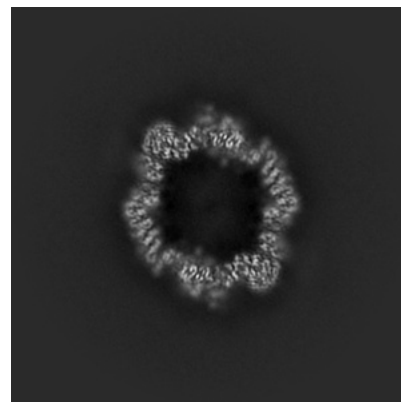
6.2.1 Primary map



X Index: 290

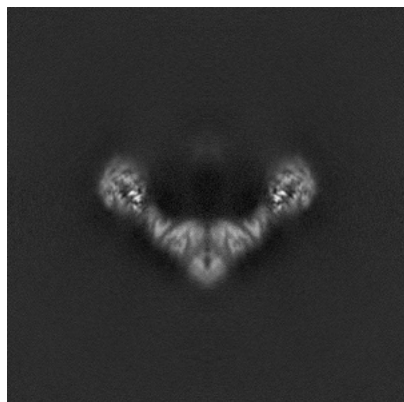


Y Index: 290

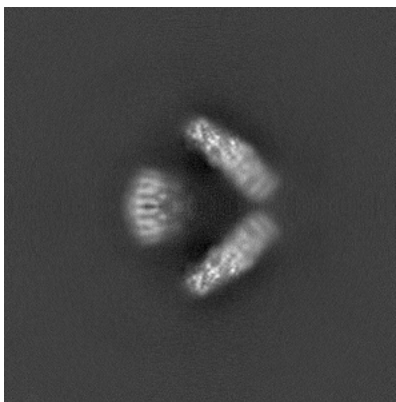


Z Index: 290

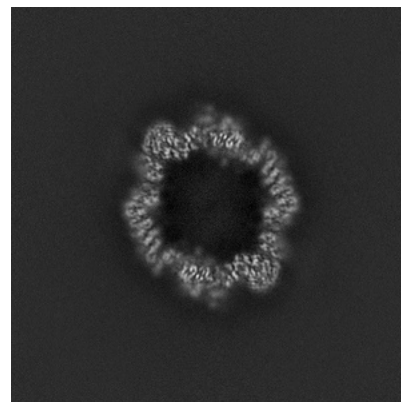
6.2.2 Raw map



X Index: 290



Y Index: 290

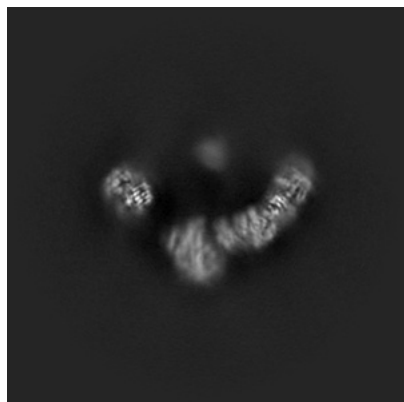


Z Index: 290

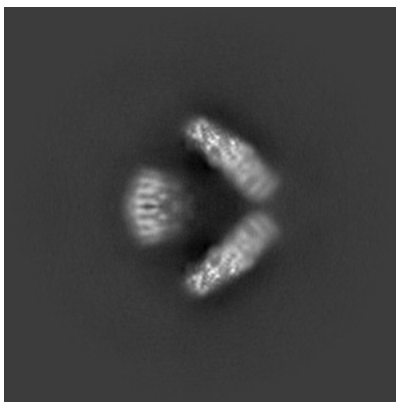
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

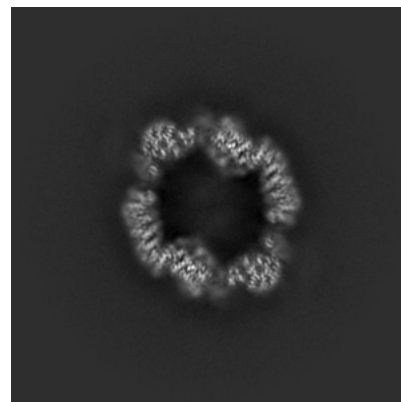
6.3.1 Primary map



X Index: 306

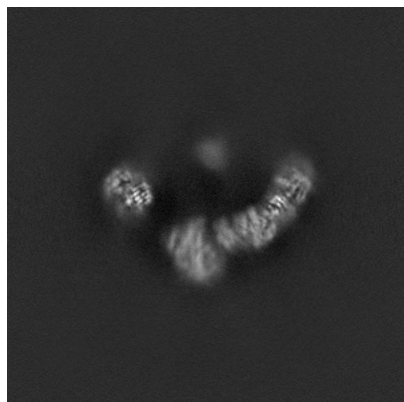


Y Index: 290

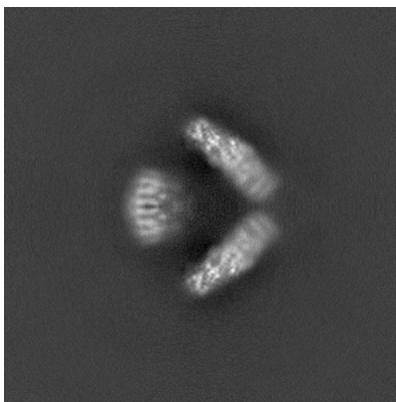


Z Index: 282

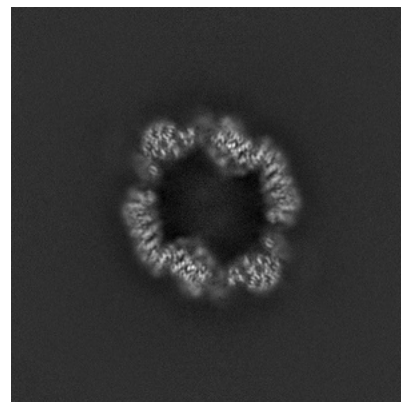
6.3.2 Raw map



X Index: 306



Y Index: 290

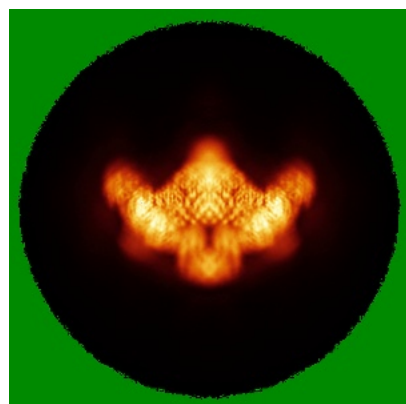


Z Index: 282

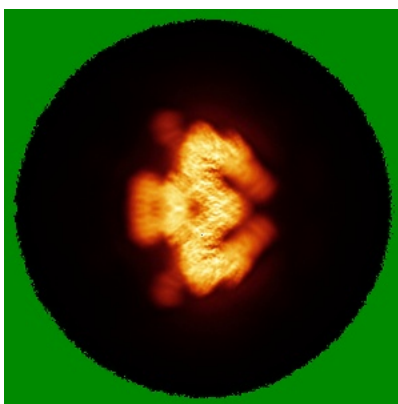
The images above show the largest variance slices of the map in three orthogonal directions.

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

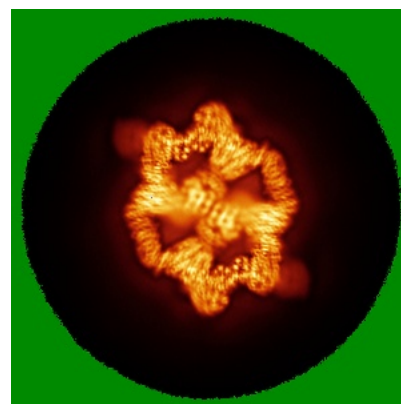
6.4.1 Primary map



X

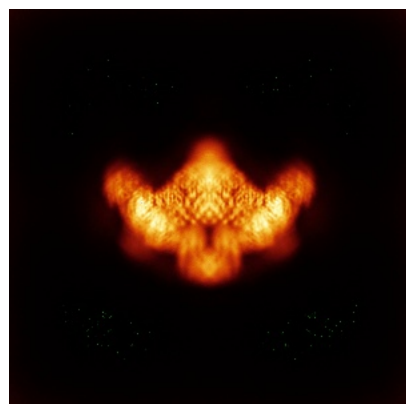


Y

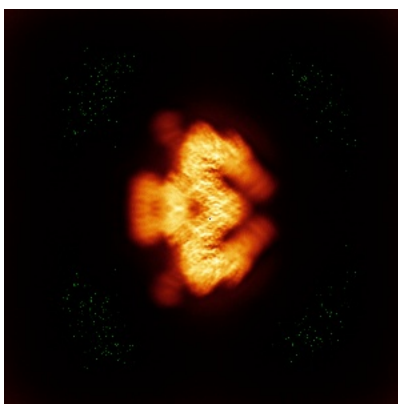


Z

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.

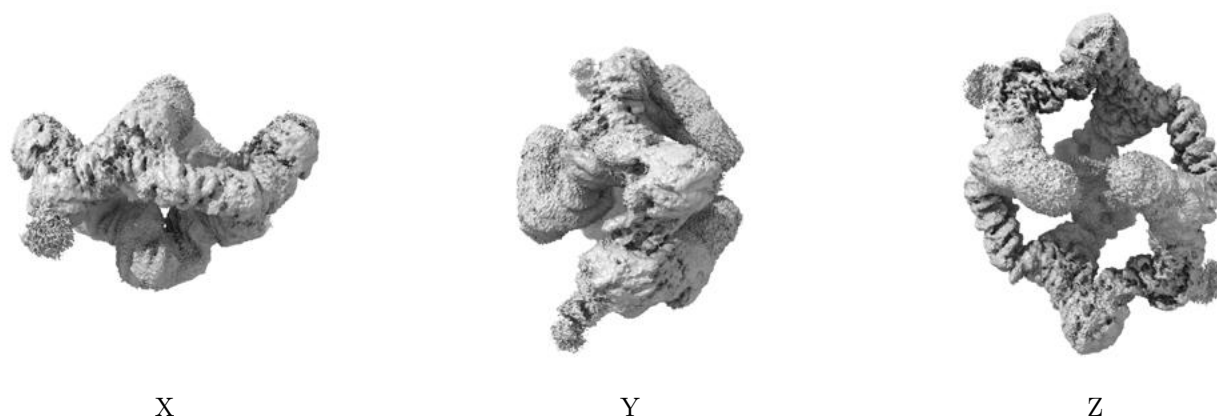
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0958. 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.

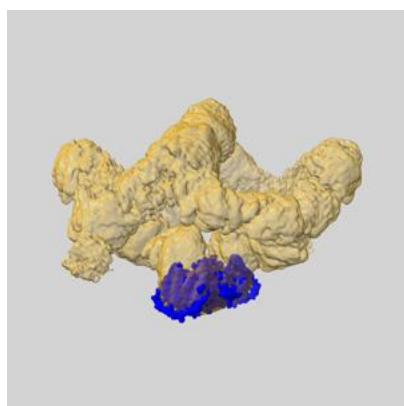
6.6 Mask visualisation [i](#)

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

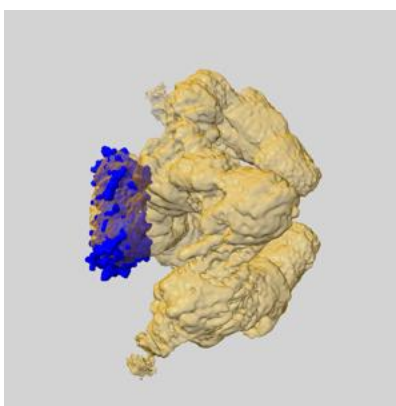
A mask typically either:

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

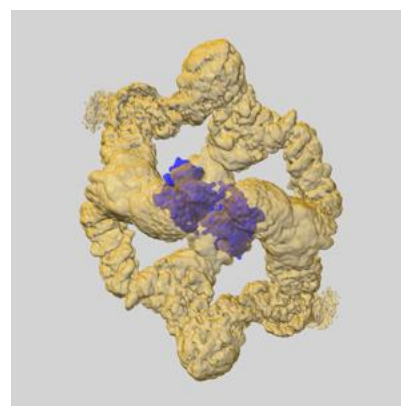
6.6.1 emd_63422_msk_1.map [i](#)



X

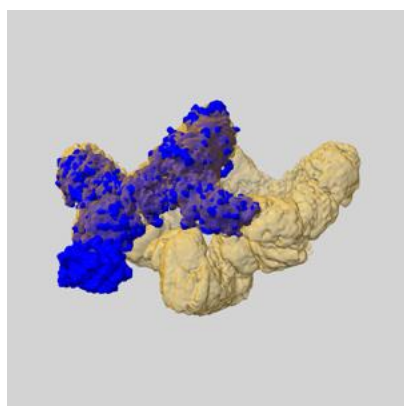


Y

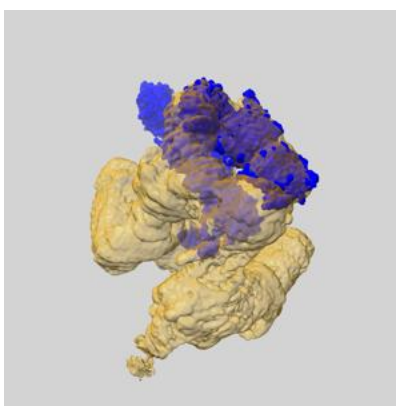


Z

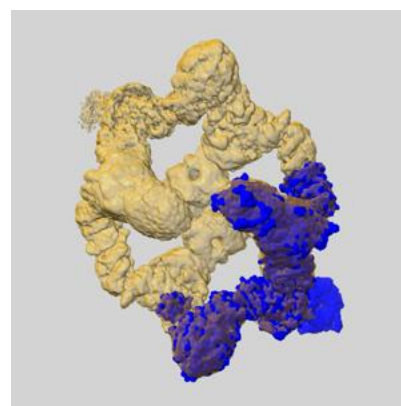
6.6.2 emd_63422_msk_2.map [i](#)



X

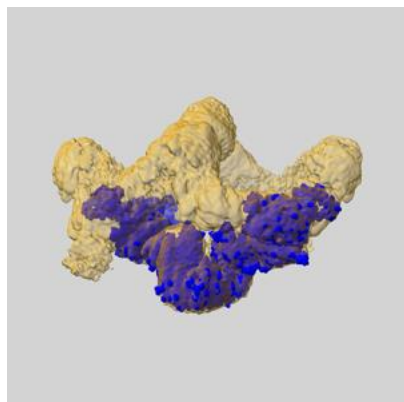


Y

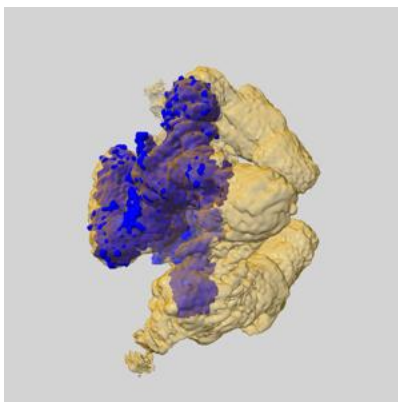


Z

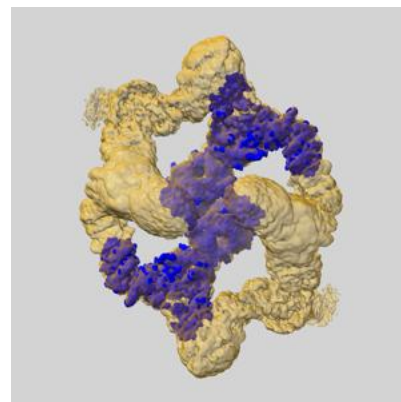
6.6.3 emd_63422_msk_3.map [i](#)



X

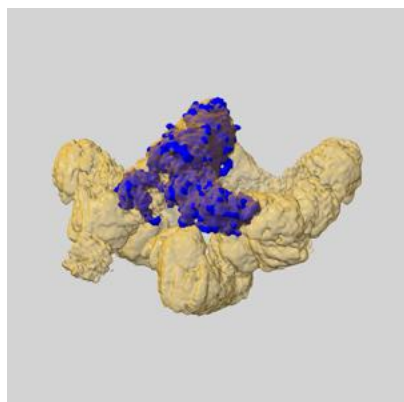


Y

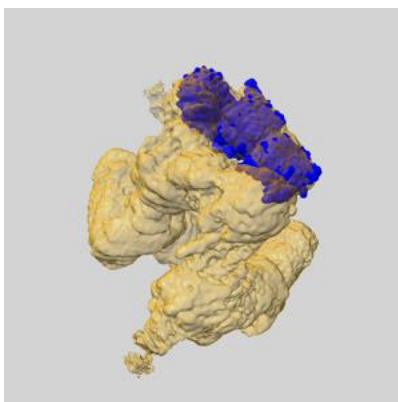


Z

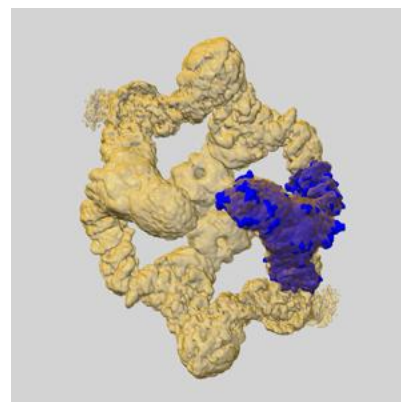
6.6.4 emd_63422_msk_4.map [i](#)



X

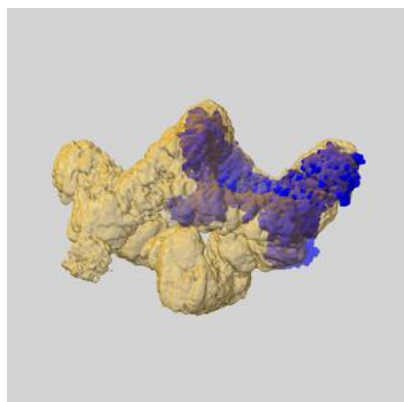


Y

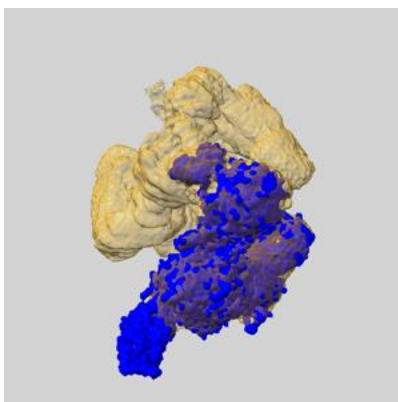


Z

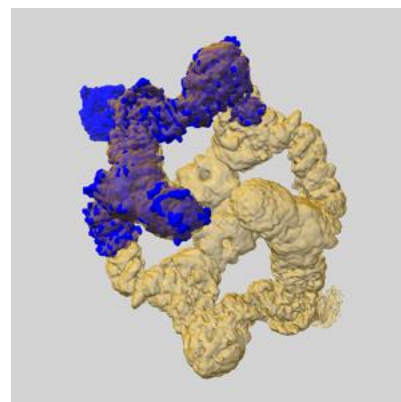
6.6.5 emd_63422_msk_5.map [i](#)



X

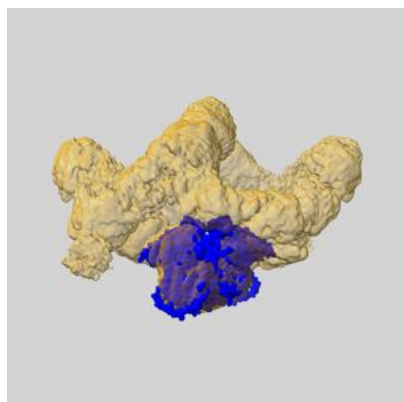


Y

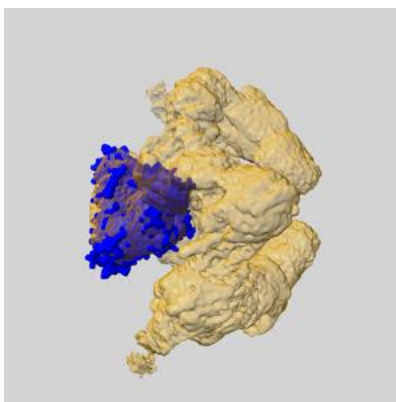


Z

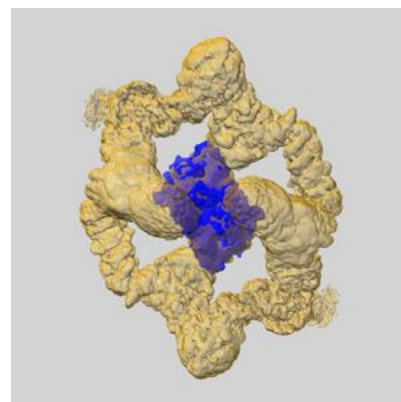
6.6.6 emd_63422_msk_6.map [i](#)



X

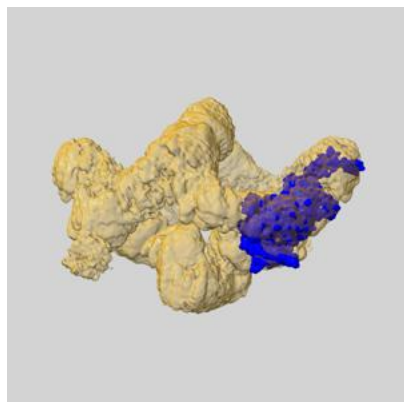


Y

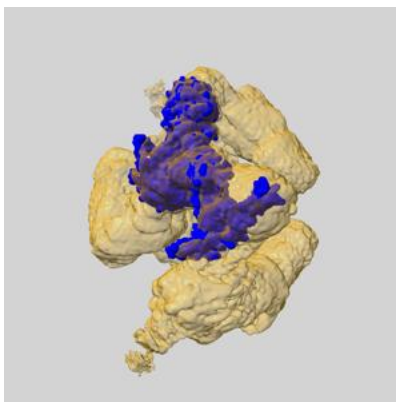


Z

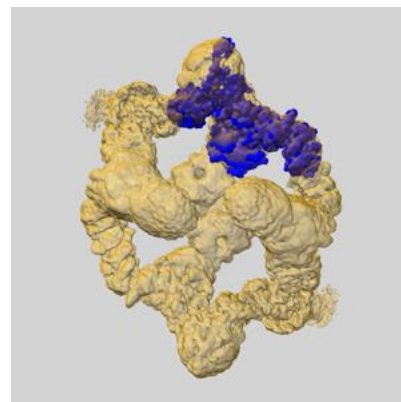
6.6.7 emd_63422_msk_7.map [i](#)



X



Y

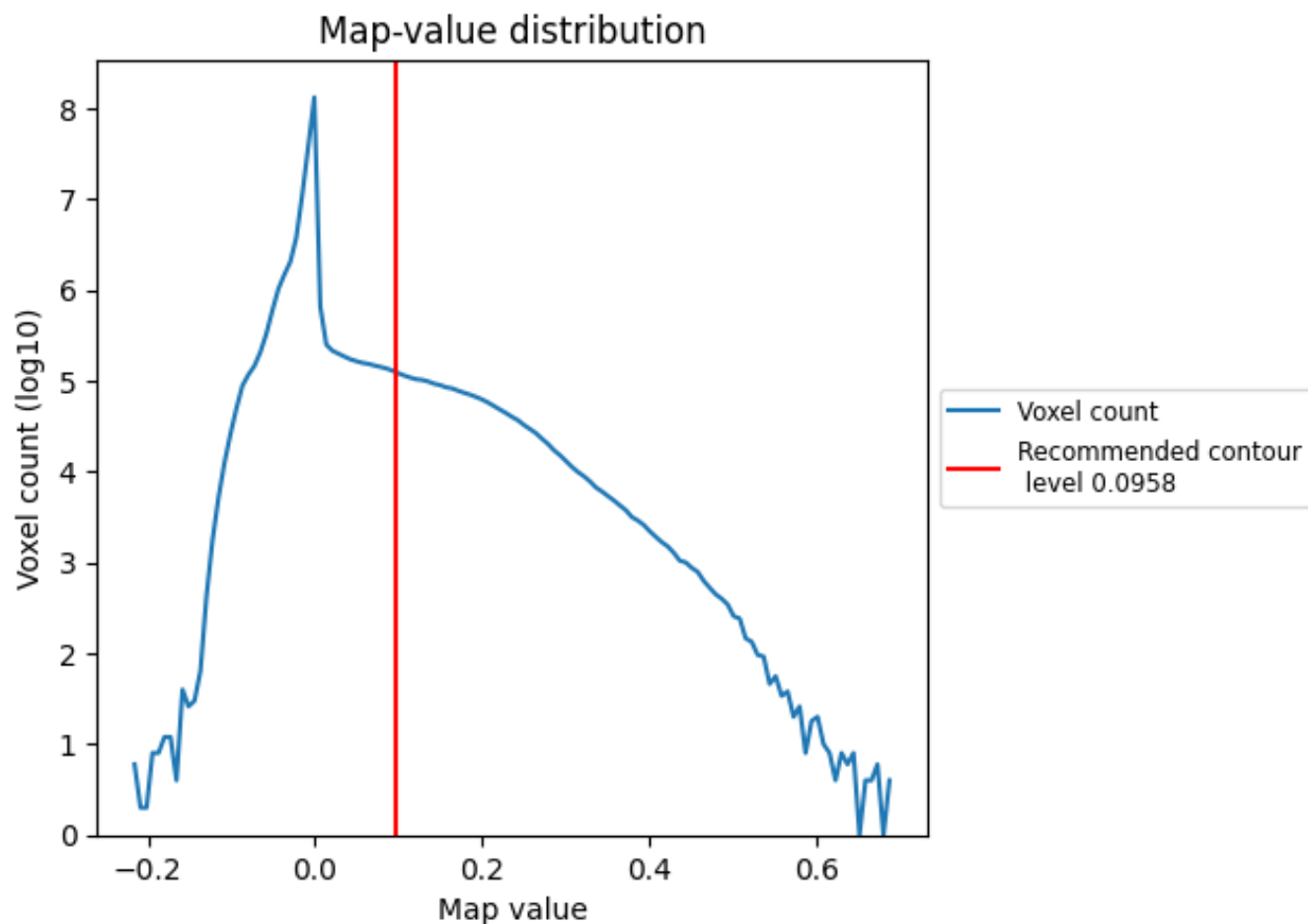


Z

7 Map analysis [i](#)

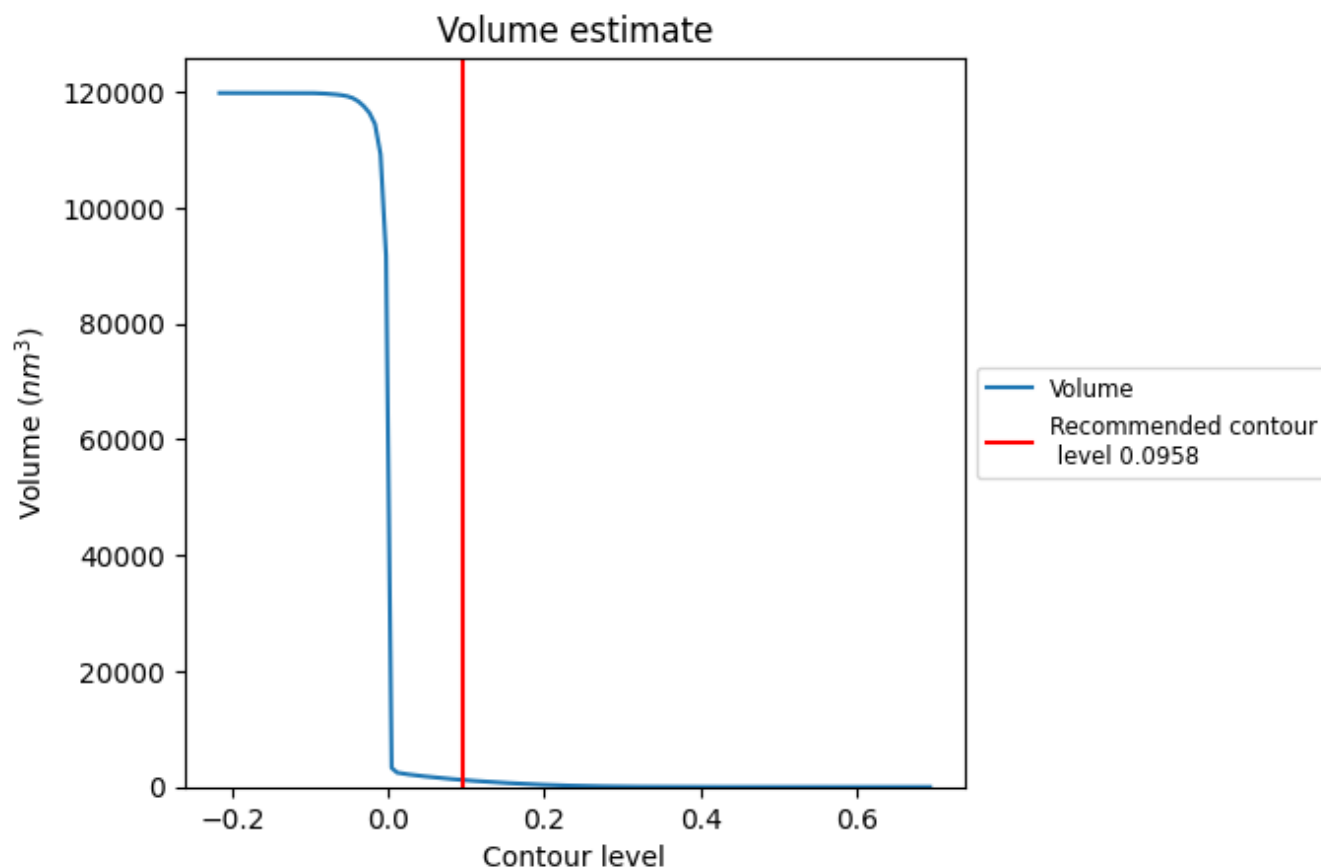
This section contains the results of statistical analysis of the map.

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.

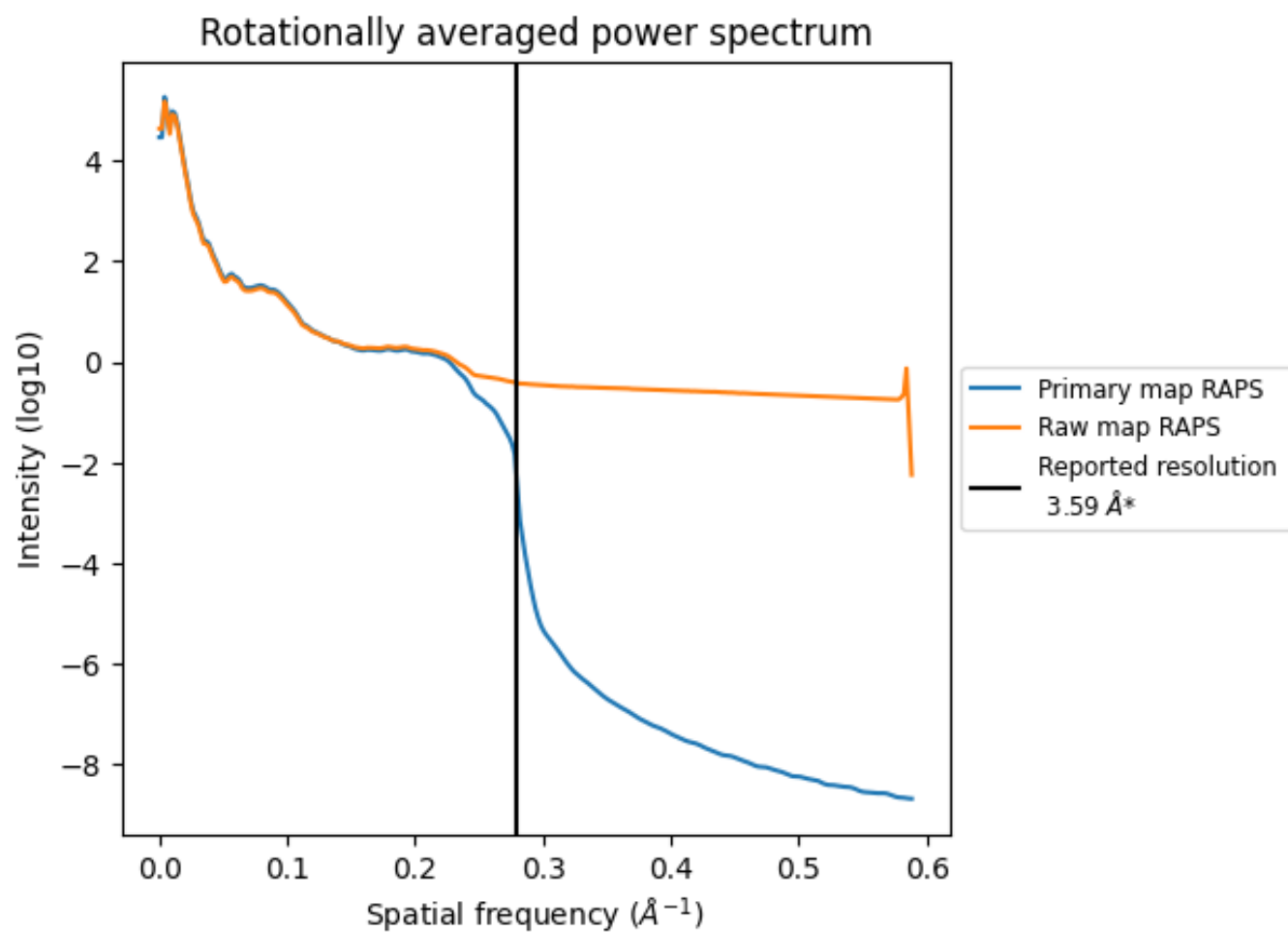
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1202 nm³; this corresponds to an approximate mass of 1085 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 ⓘ

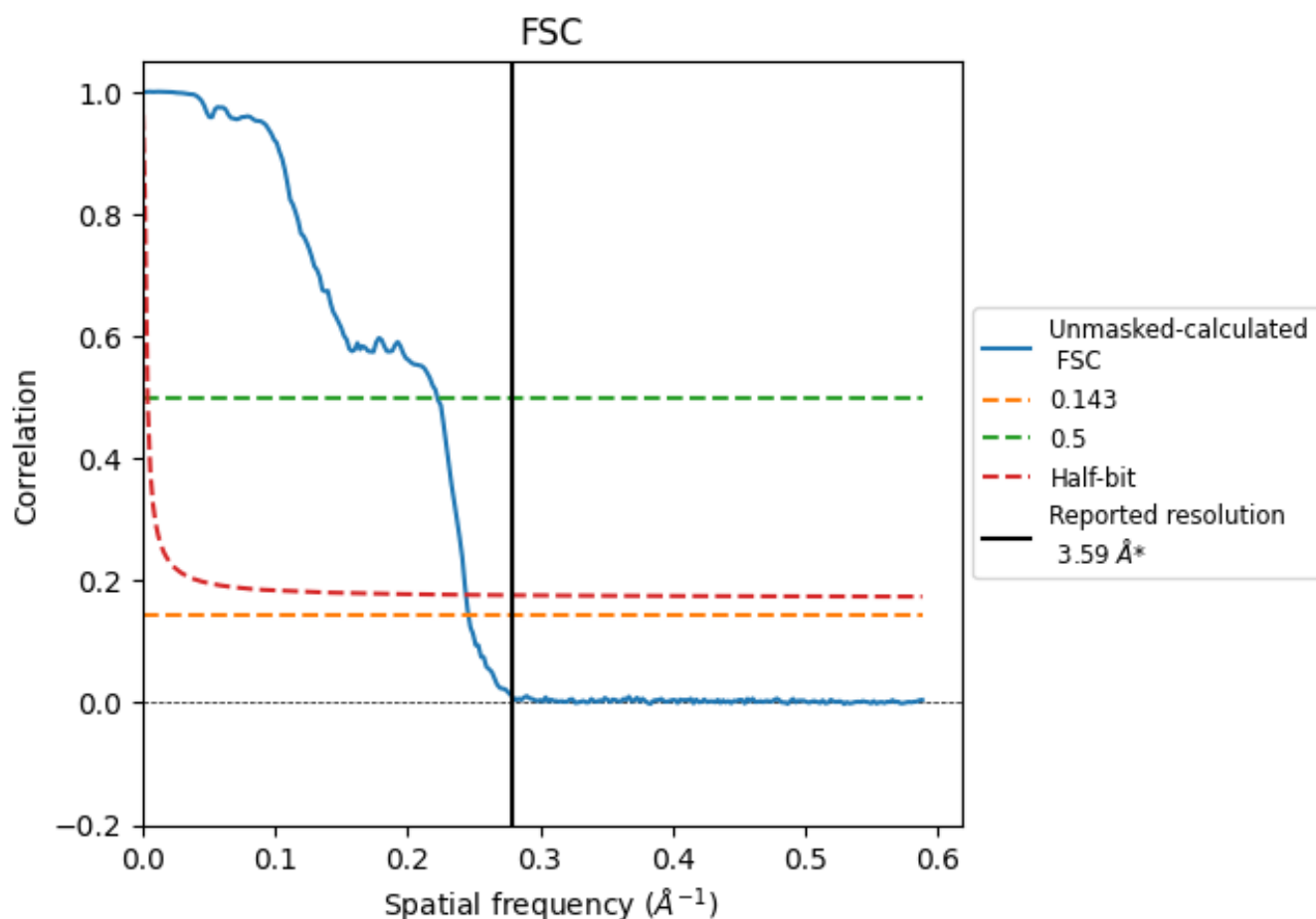


*Reported resolution corresponds to spatial frequency of 0.279 $\text{\AA}^{-1}$

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 0.279 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

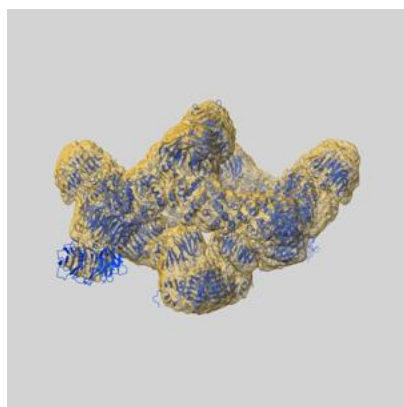
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	4.49	4.10

*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 4.06 differs from the reported value 3.59 by more than 10 %

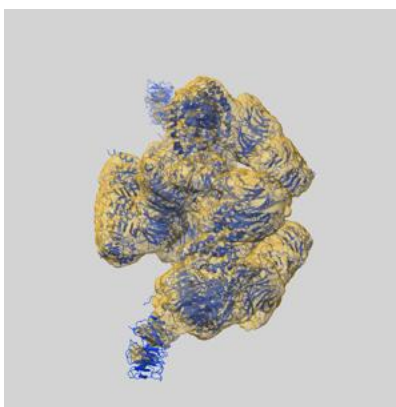
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63422 and PDB model 9LVK. Per-residue inclusion information can be found in section 3 on page 7.

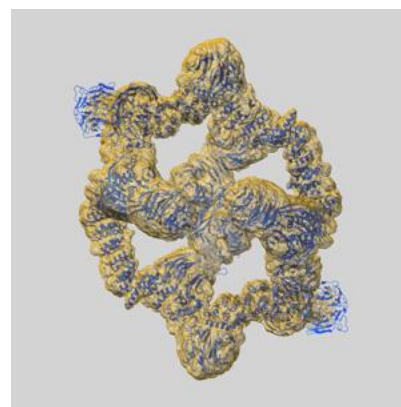
9.1 Map-model overlay [i](#)



X



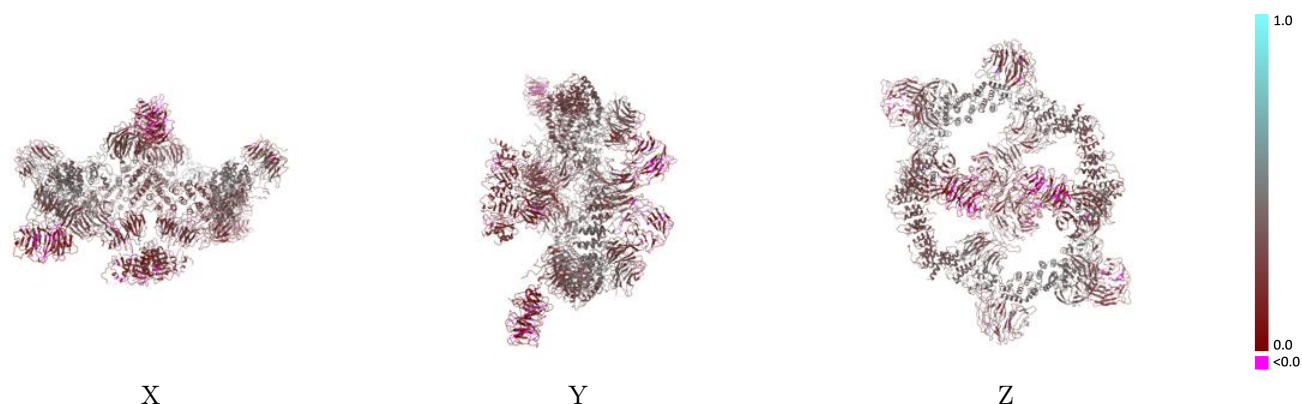
Y



Z

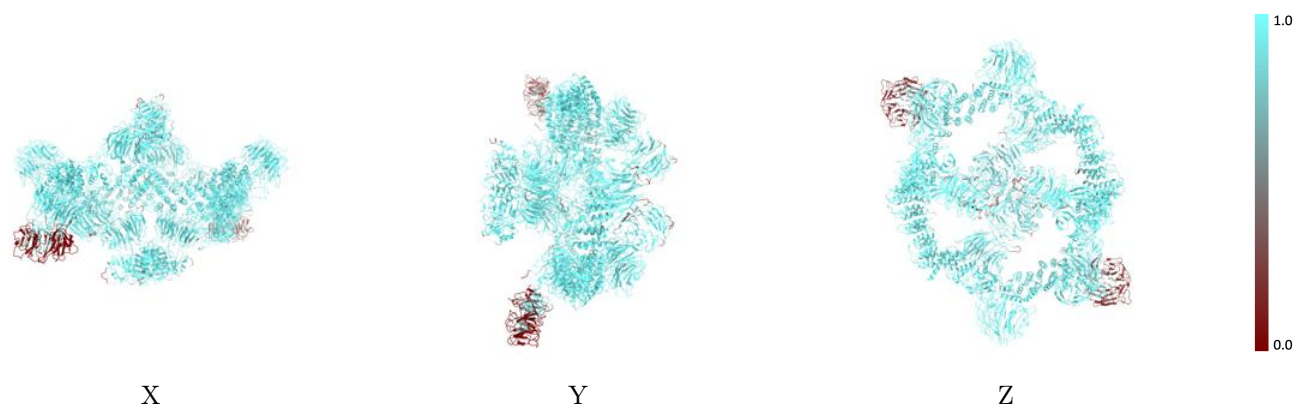
The images above show the 3D surface view of the map at the recommended contour level 0.0958 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



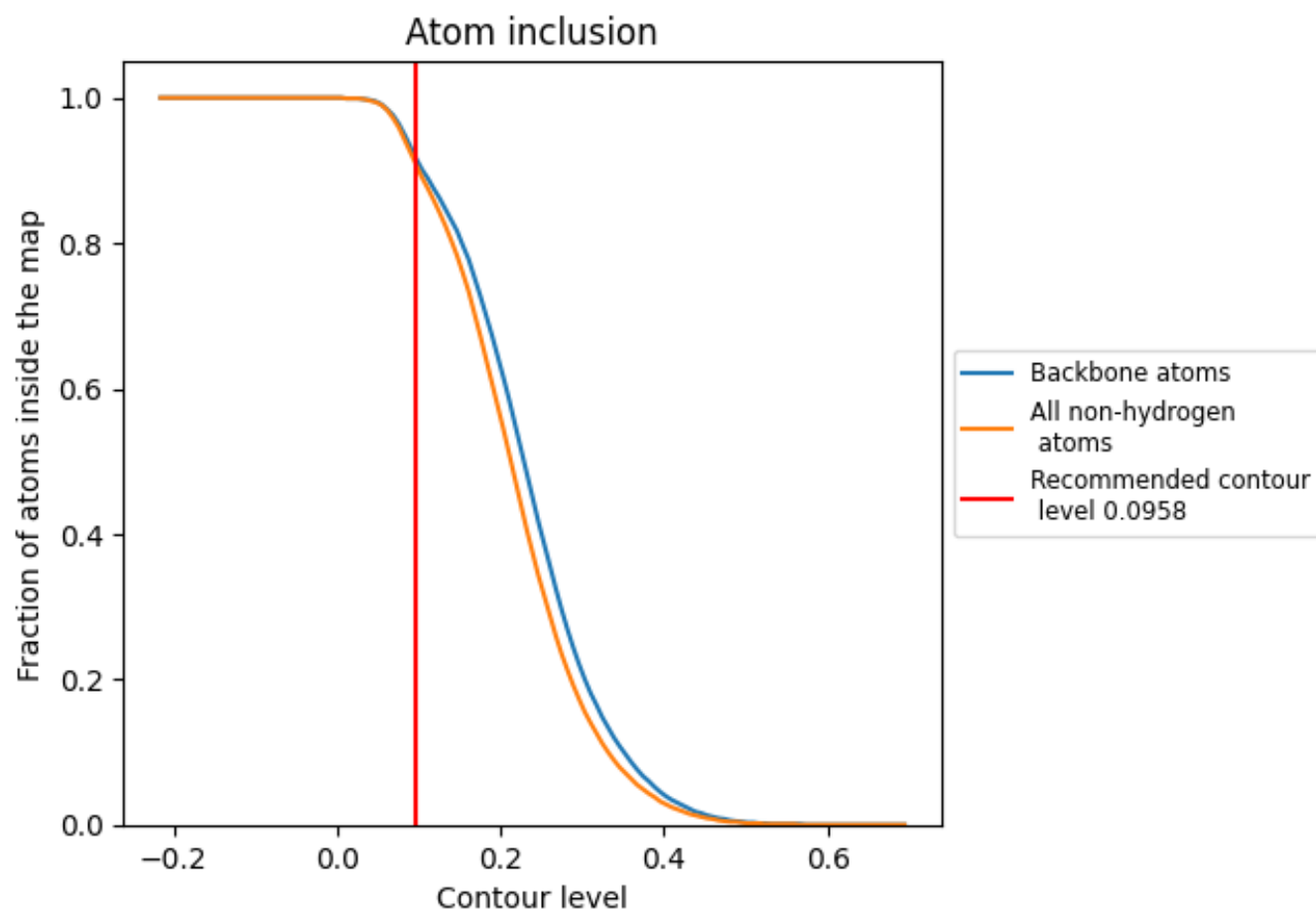
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0958).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.0958) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9100	 0.2980
A	 0.9380	 0.2860
B	 0.9720	 0.2920
C	 0.5800	 0.2690
D	 0.9820	 0.3930
E	 0.9930	 0.3100
F	 0.9860	 0.3080
G	 0.9670	 0.3620
H	 0.9850	 0.3190
K	 0.9410	 0.2830
L	 0.9800	 0.2940
M	 0.5910	 0.2780
N	 0.9870	 0.3870
O	 0.9910	 0.3080
P	 0.9960	 0.3490
Q	 0.9770	 0.3670
R	 0.9870	 0.3380
U	 0.9480	 0.1650
V	 0.9650	 0.1750

