Full wwPDB EM Validation Report ⓘ

Sep 24, 2025 – 08:22 AM EDT

PDB ID	:	9OTI / pdb_00009oti
EMDB ID	:	EMD-70833
Title	:	GATOR2 complex bound to arginine sensor CASTOR1
Authors	:	Jansen, R.M.; Hurley, J.H.
Deposited on	:	2025-05-27
Resolution	:	3.50 Å(reported)

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

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

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

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

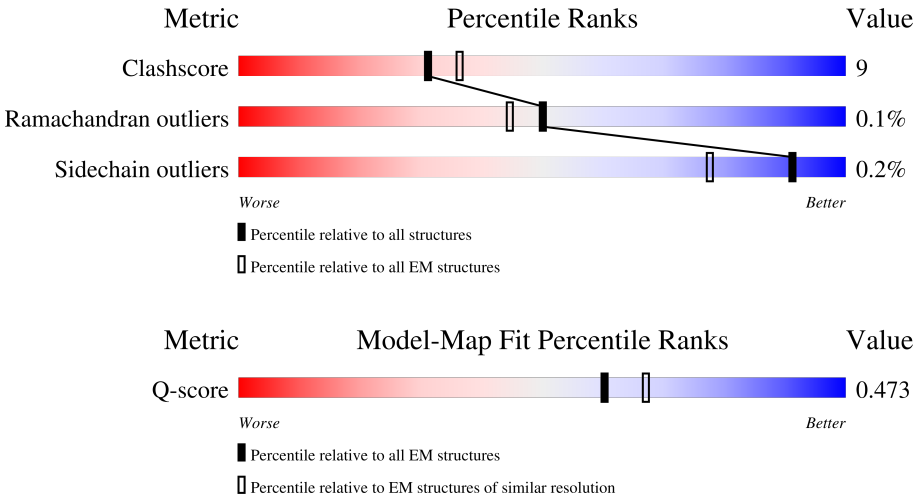
EMDB validation analysis	:	0.0.1.dev129
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



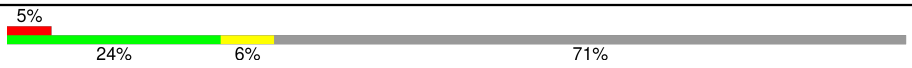
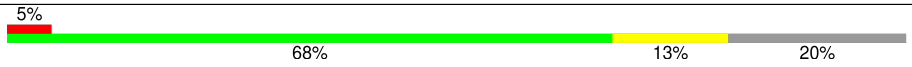
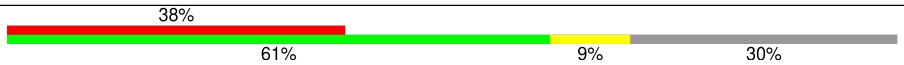
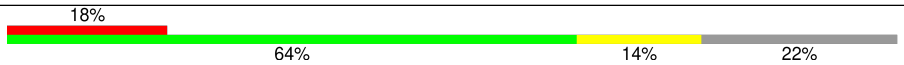
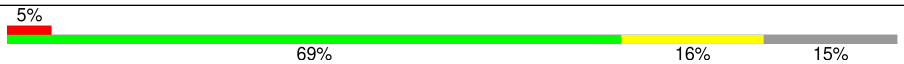
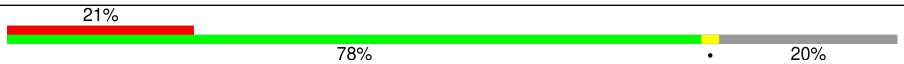
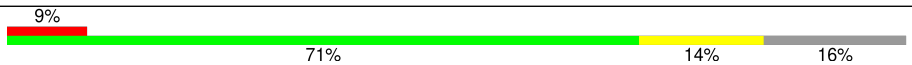
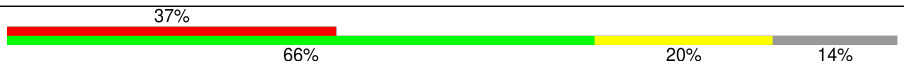
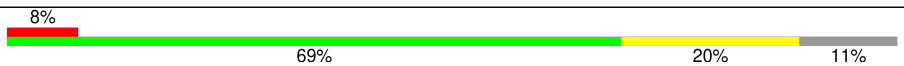
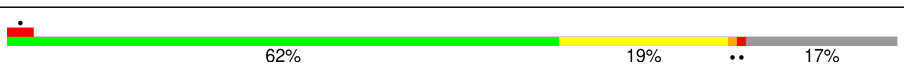
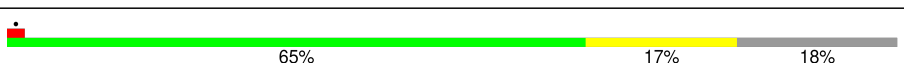
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	875	8% 38% 11% 50%
1	B	875	9% 65% 13% 21%
1	L	875	42% 10% 48%
1	T	875	12% 69% 10% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	790	
2	M	790	
3	D	974	
3	N	974	
4	E	360	
4	F	360	
4	G	360	
4	O	360	
4	P	360	
4	Q	360	
5	H	322	
5	R	322	
6	U	329	
6	V	329	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 43325 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	434	Total	C	N	O	S	0	0
			3232	2053	567	582	30		
1	B	689	Total	C	N	O	S	0	0
			4768	3056	846	842	24		
1	L	454	Total	C	N	O	S	0	0
			3498	2213	618	635	32		
1	T	697	Total	C	N	O	S	0	0
			4771	3048	853	847	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	233	Total	C	N	O	S	0	0
			1668	1065	299	283	21		
2	M	243	Total	C	N	O	S	0	0
			1870	1178	334	335	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	241	Total	C	N	O	S	0	0
			1657	1050	303	287	17		
3	N	248	Total	C	N	O	S	0	0
			1881	1187	336	339	19		

- Molecule 4 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	289	Total	C	N	O	S	0	0
			2017	1295	353	356	13		
4	F	251	Total	C	N	O	S	0	0
			1464	923	278	261	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	282	Total	C	N	O	S	0	0
			2062	1310	356	382	14		
4	O	307	Total	C	N	O	S	0	0
			2352	1483	420	434	15		
4	P	288	Total	C	N	O	S	0	0
			1660	1041	318	300	1		
4	Q	304	Total	C	N	O	S	0	0
			2343	1482	413	431	17		

- Molecule 5 is a protein called Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	278	Total	C	N	O	S	0	0
			1989	1271	339	367	12		
5	R	285	Total	C	N	O	S	0	0
			2171	1374	382	403	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	272	Total	C	N	O	S	0	0
			1946	1287	321	332	6		
6	V	270	Total	C	N	O	S	0	0
			1947	1294	317	329	7		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	111	ALA	SER	engineered mutation	UNP Q8WTX7
U	304	ALA	ASP	engineered mutation	UNP Q8WTX7
V	111	ALA	SER	engineered mutation	UNP Q8WTX7
V	304	ALA	ASP	engineered mutation	UNP Q8WTX7

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	

Continued on next page...

Continued from previous page...

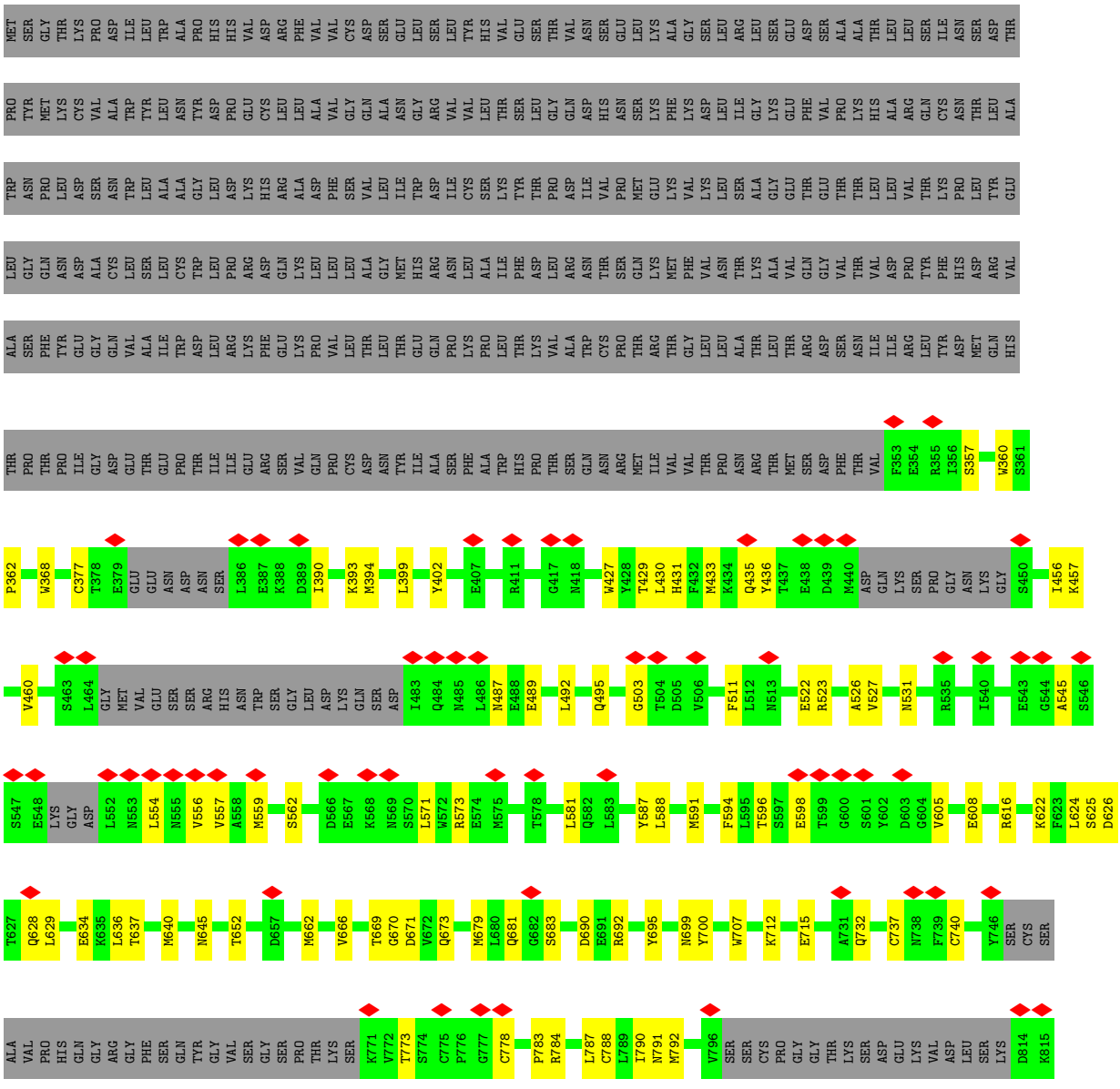
Mol	Chain	Residues	Atoms	AltConf
7	D	3	Total Zn 3 3	0
7	L	4	Total Zn 4 4	0
7	M	4	Total Zn 4 4	0
7	N	3	Total Zn 3 3	0
7	T	3	Total Zn 3 3	0

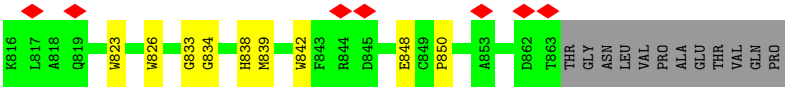
3 Residue-property plots (i)

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

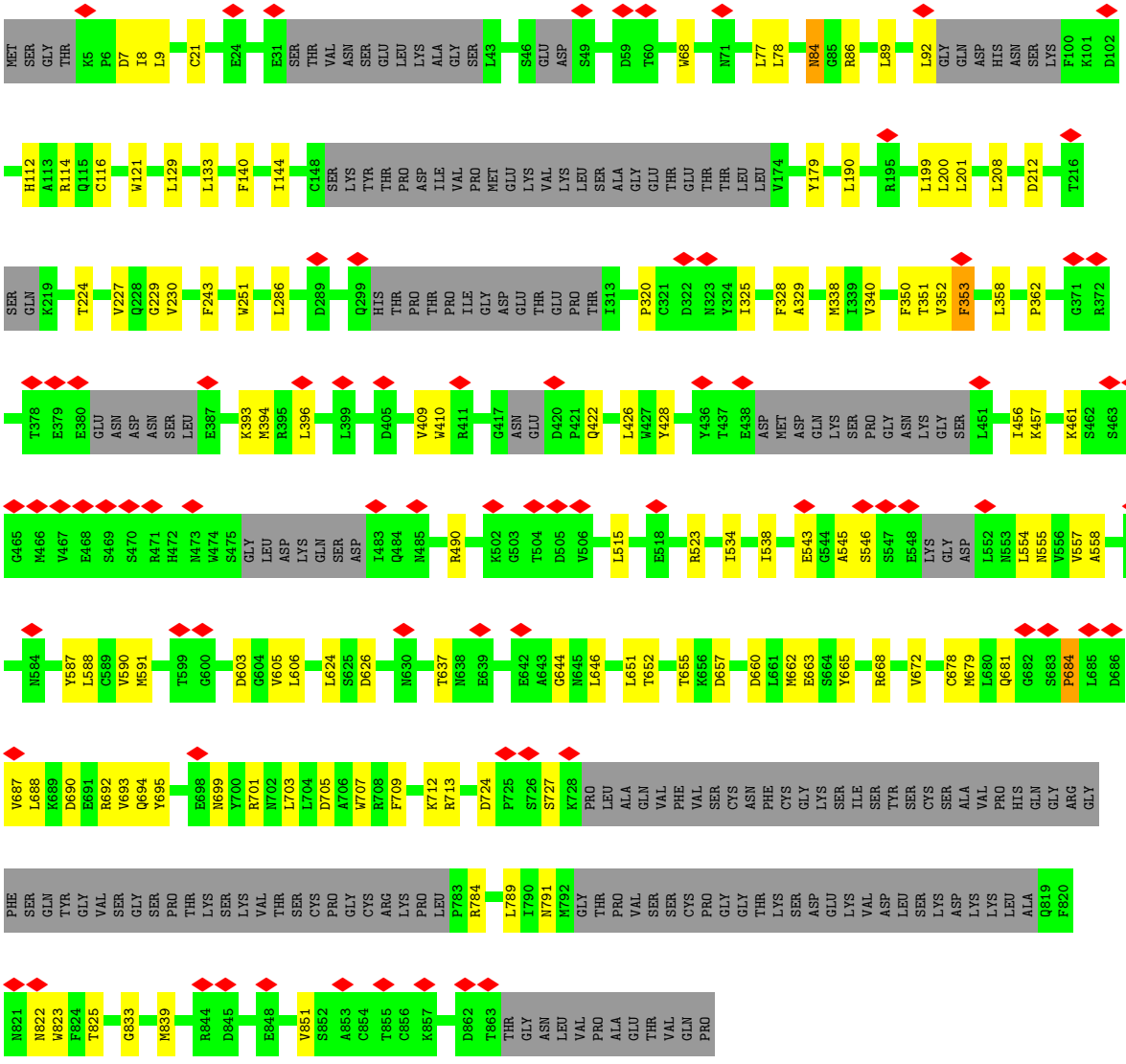
Chain A:





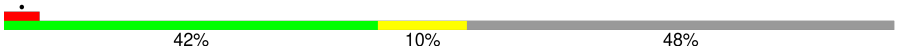
• Molecule 1: GATOR2 complex protein MIOS

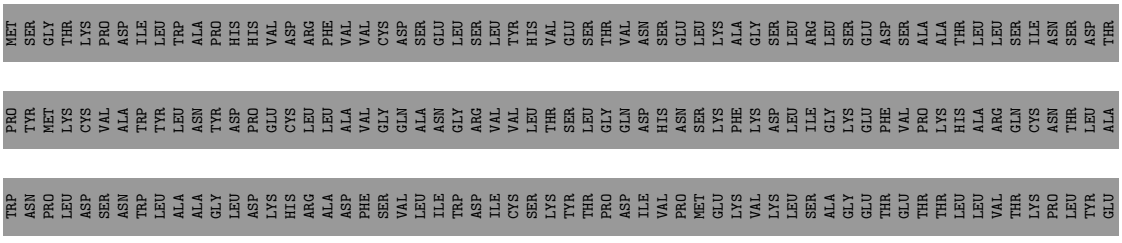
Chain B:

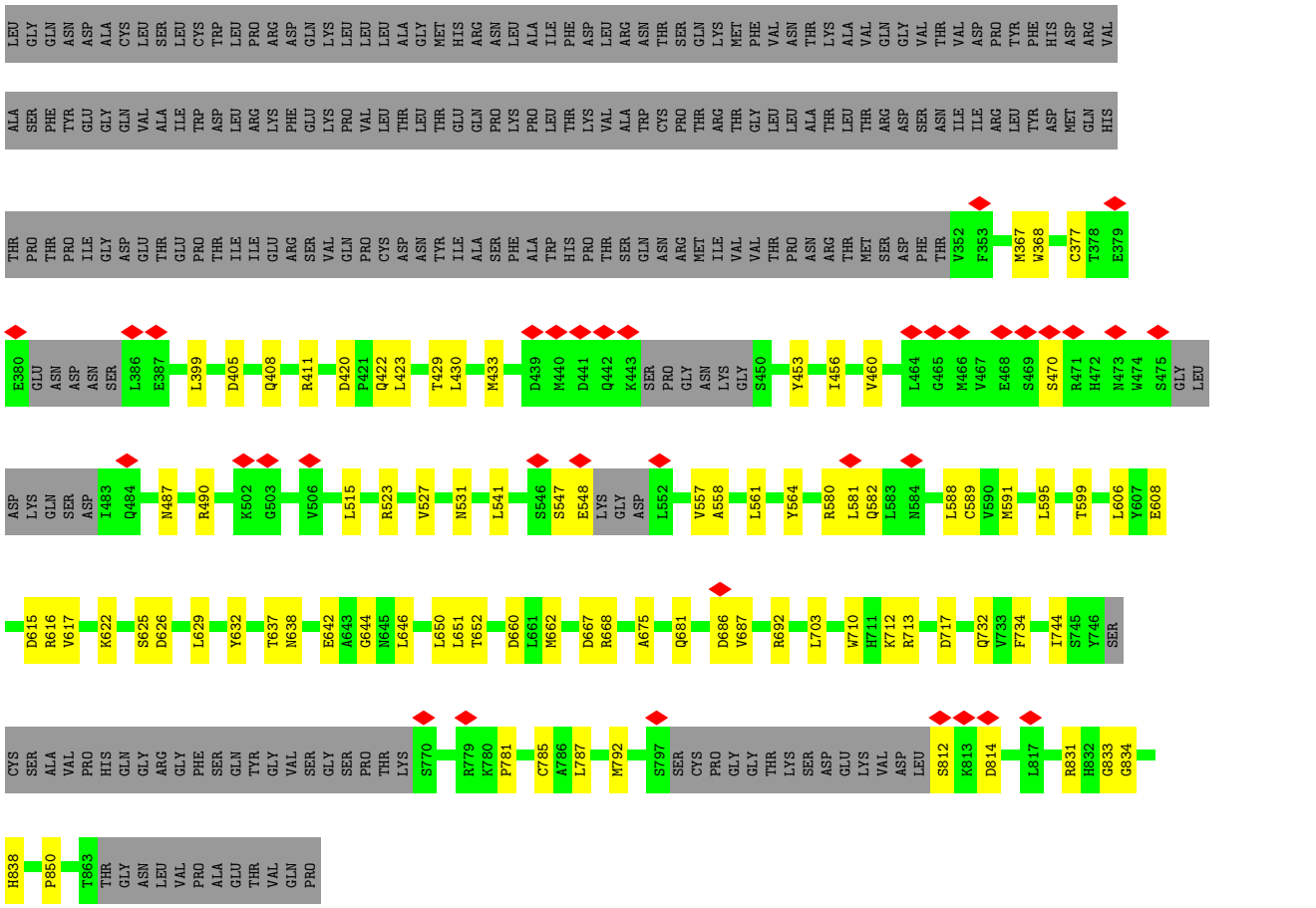


• Molecule 1: GATOR2 complex protein MIOS

Chain L:

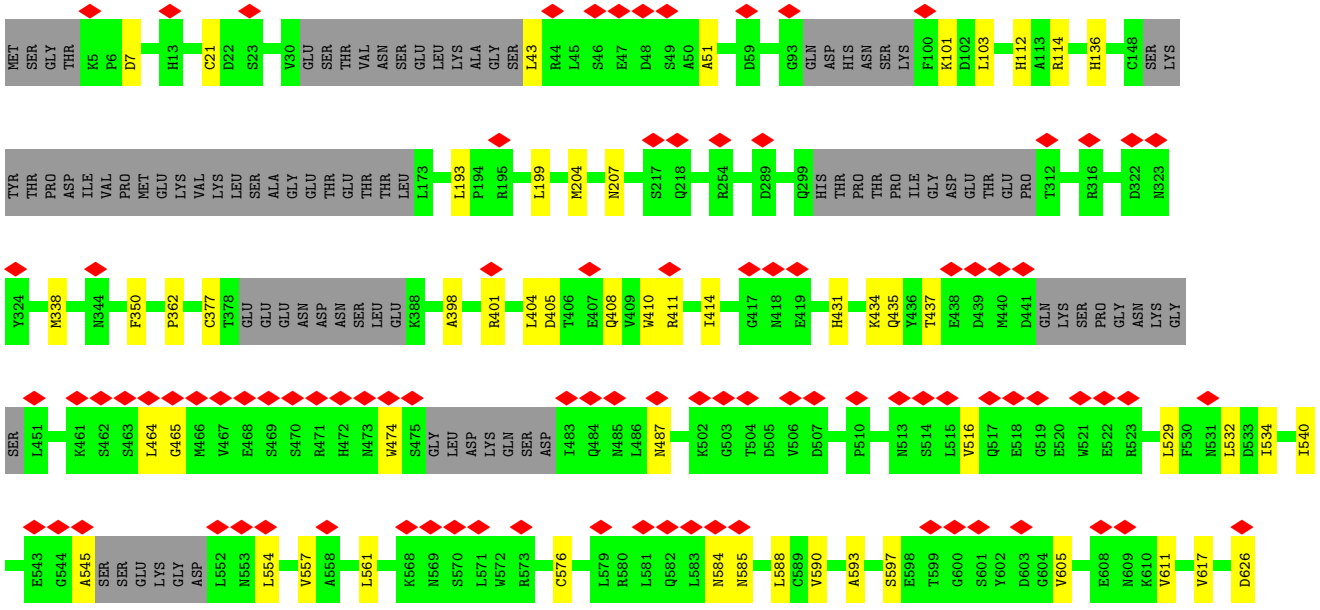


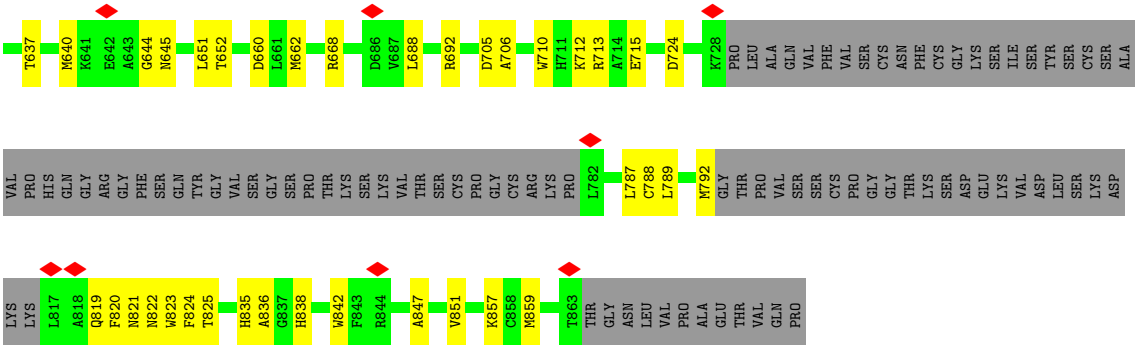




• Molecule 1: GATOR2 complex protein MIOS

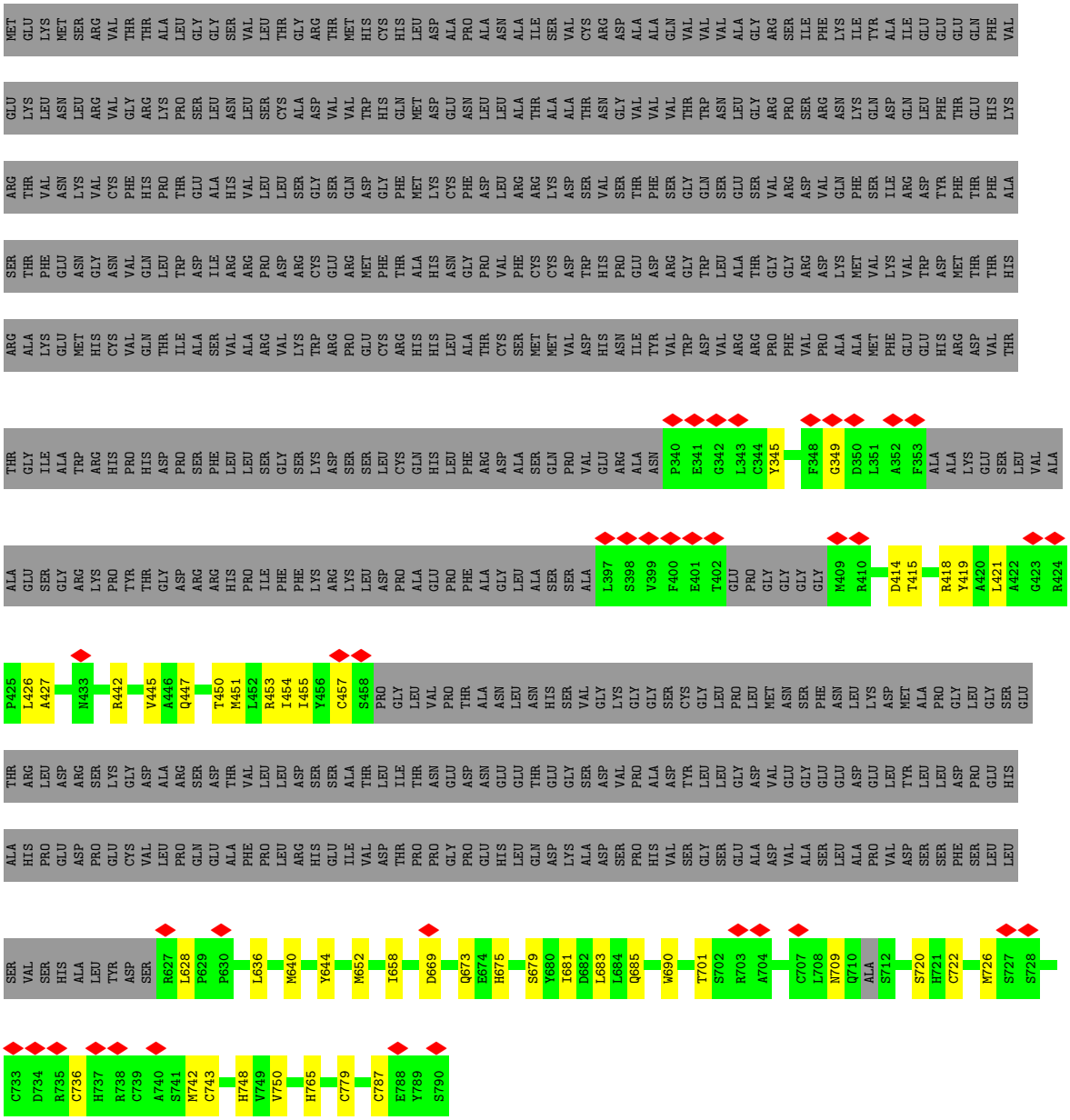
Chain T:





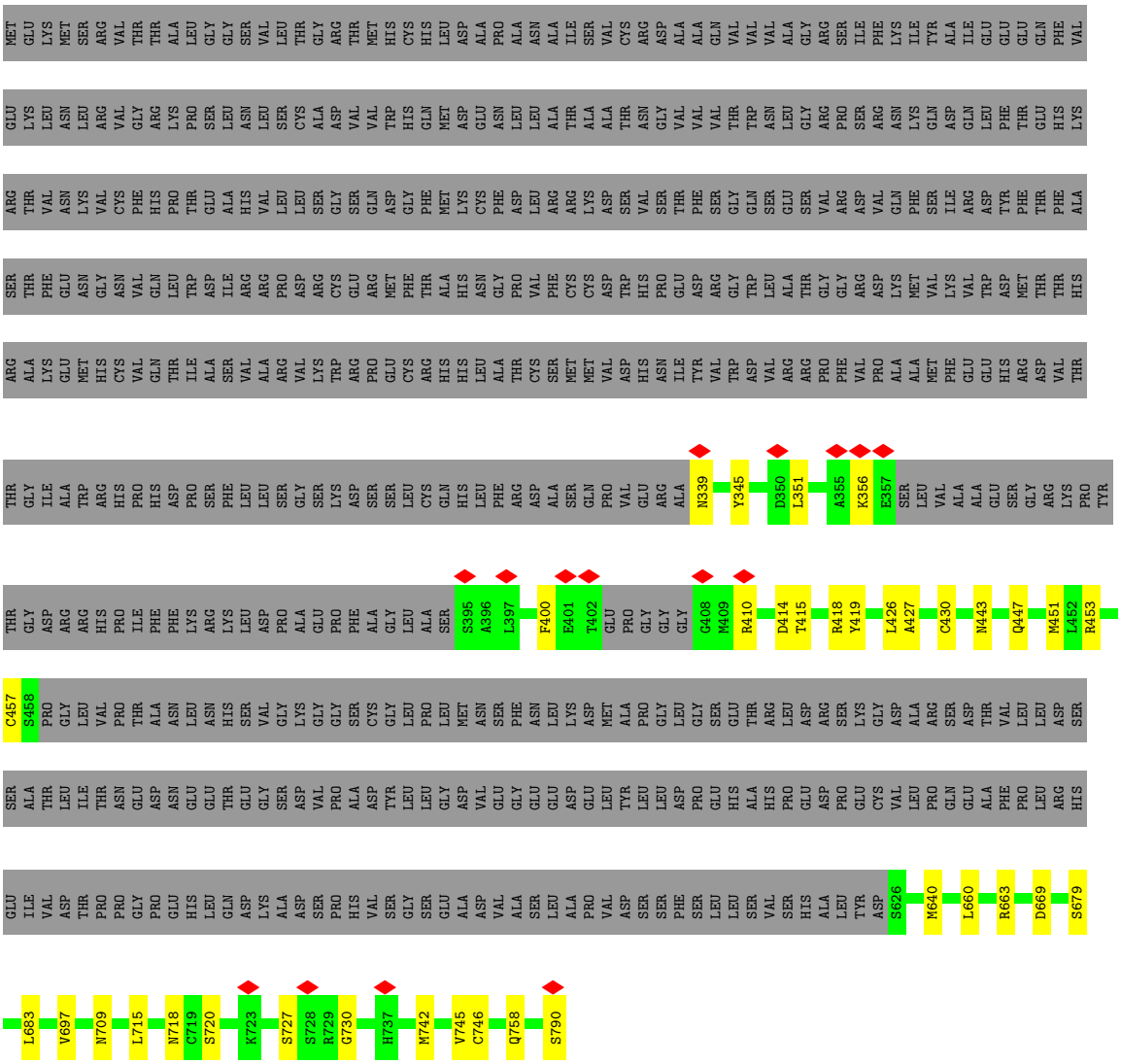
• Molecule 2: GATOR complex protein WDR24

Chain C:



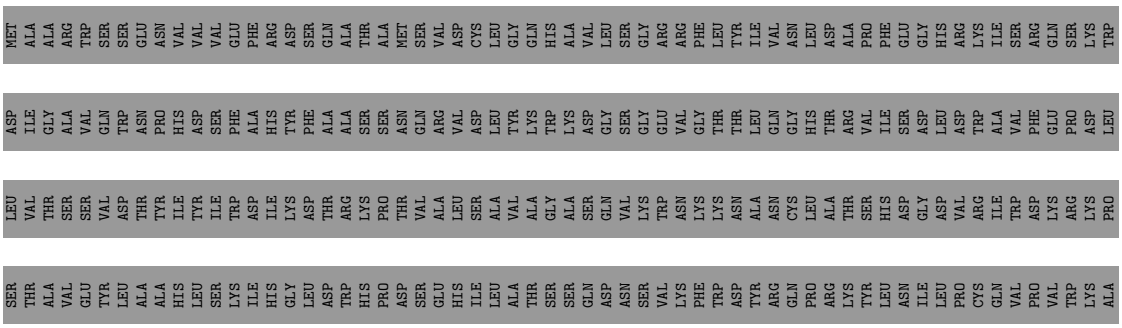
• Molecule 2: GATOR complex protein WDR24

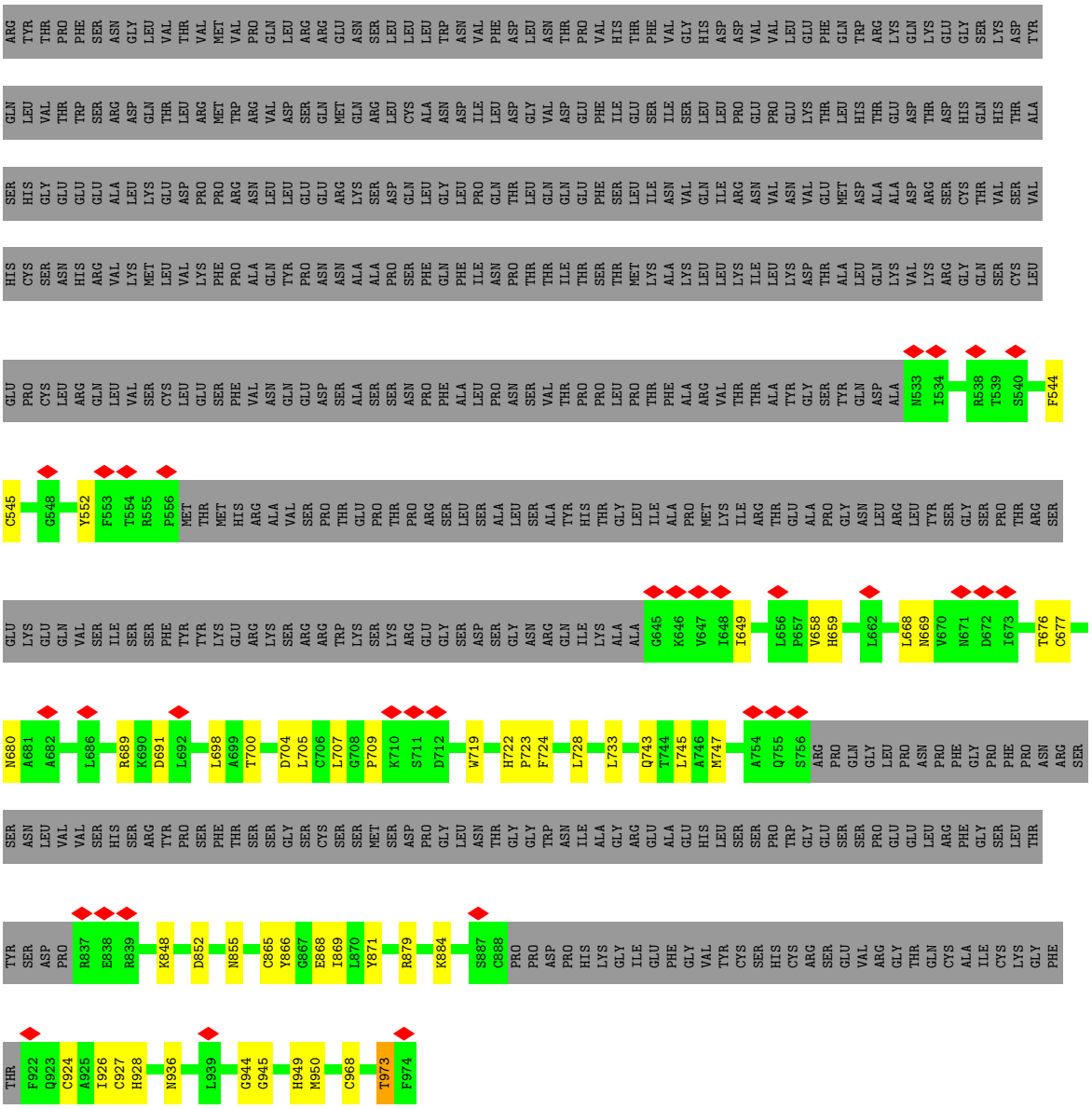
Chain M:



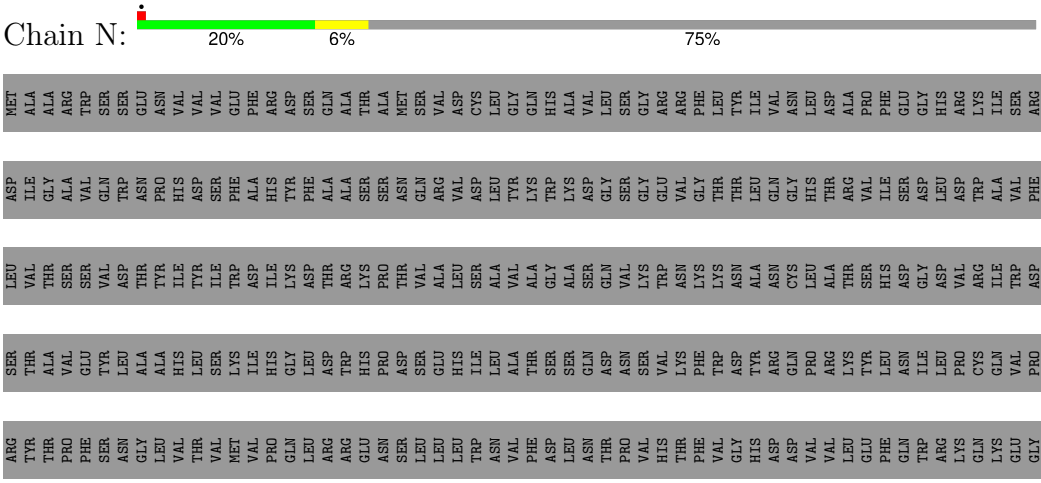
• Molecule 3: GATOR complex protein WDR59

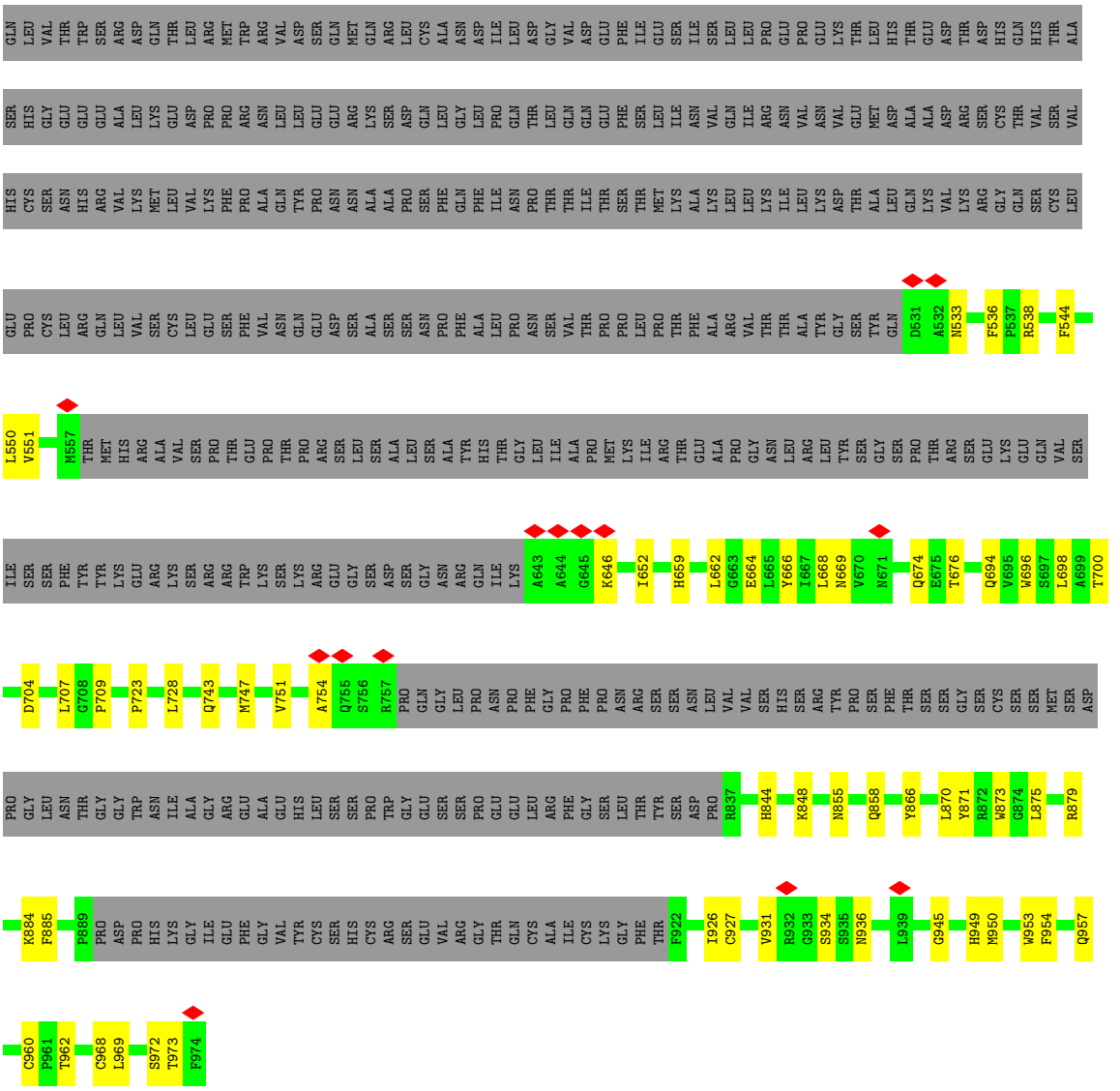
Chain D:





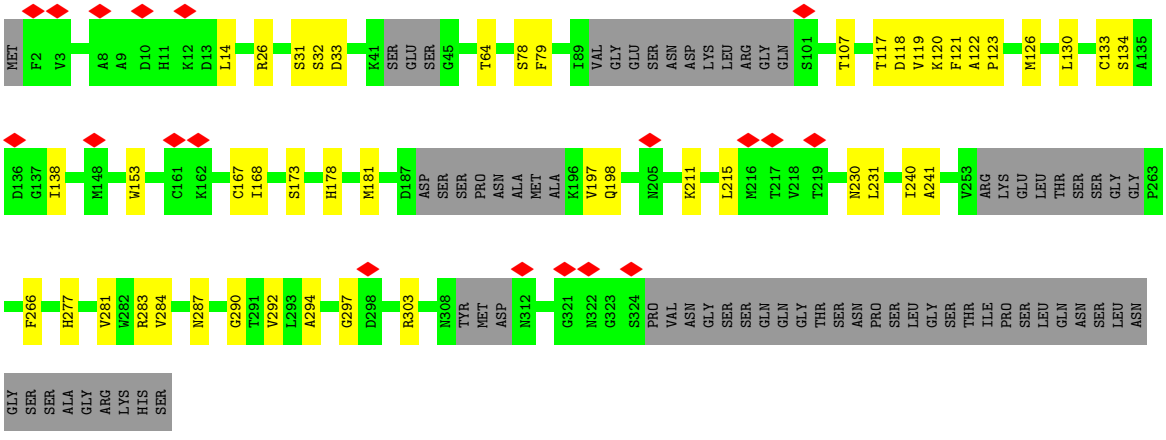
• Molecule 3: GATOR complex protein WDR59





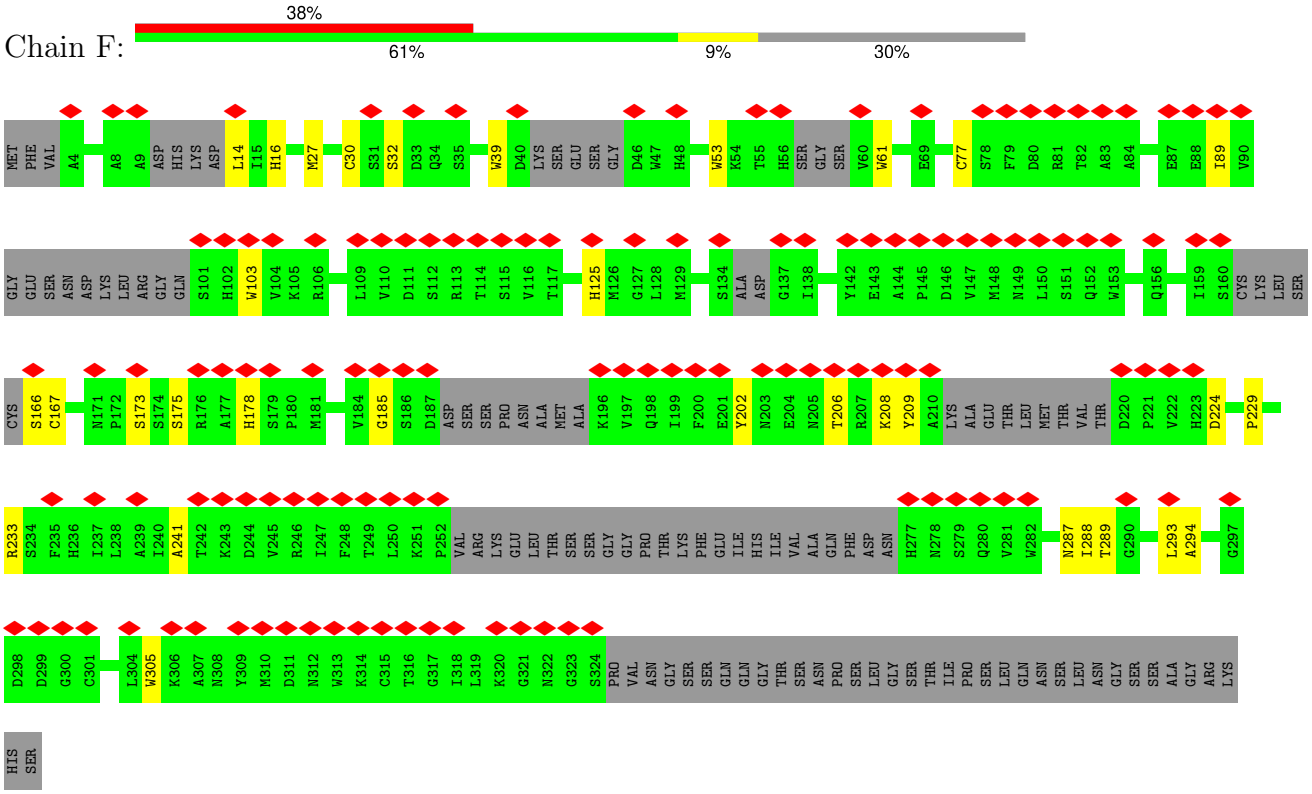
• Molecule 4: Nucleoporin SEH1

Chain E:



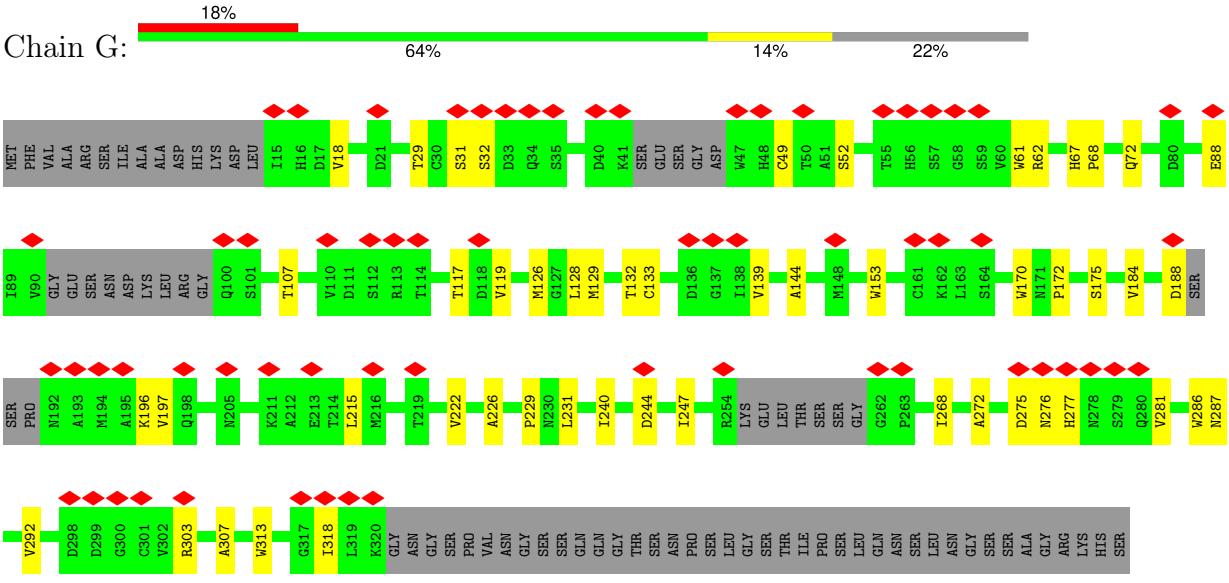
• Molecule 4: Nucleoporin SEH1

Chain F:



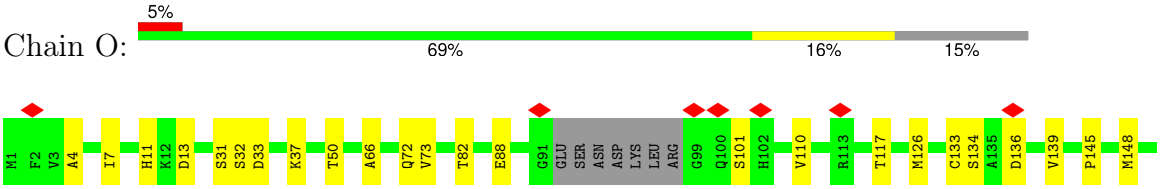
• Molecule 4: Nucleoporin SEH1

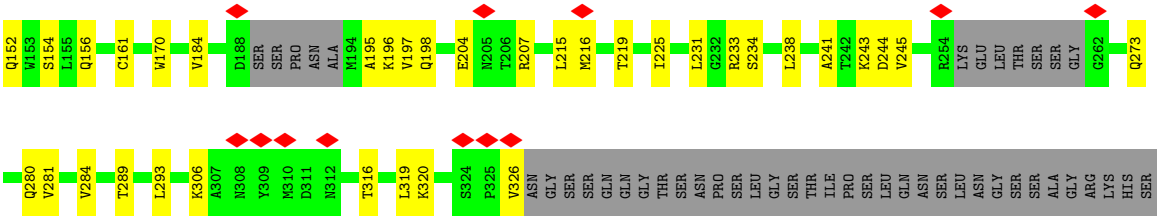
Chain G:



• Molecule 4: Nucleoporin SEH1

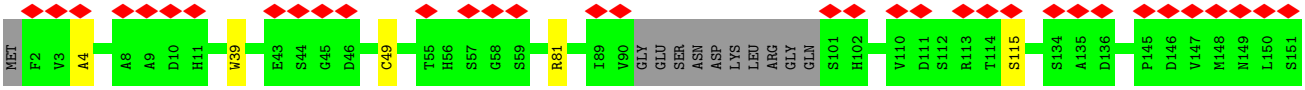
Chain O:

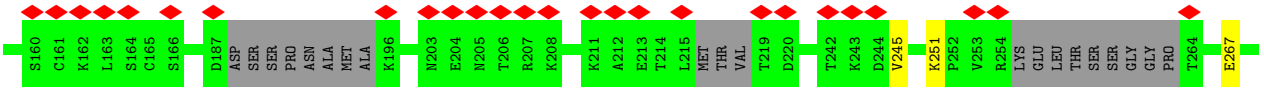


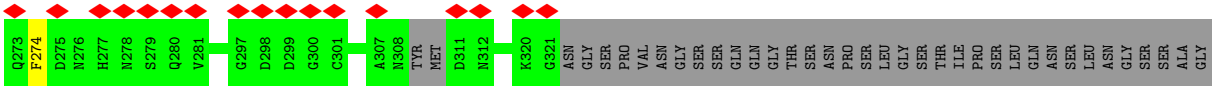


• Molecule 4: Nucleoporin SEH1

Chain P:

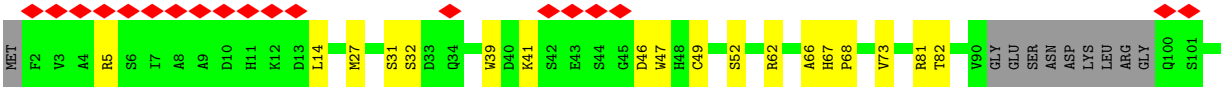


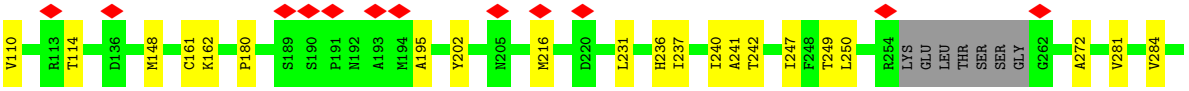


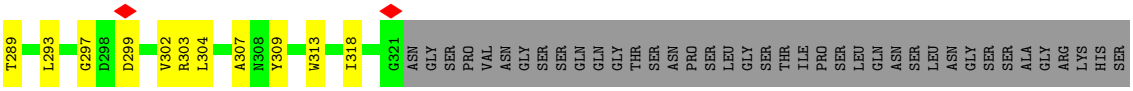


• Molecule 4: Nucleoporin SEH1

Chain Q:

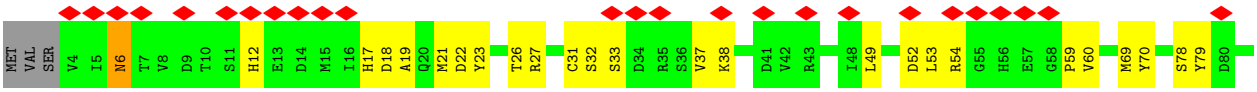


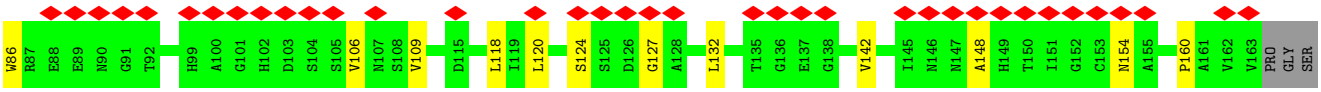


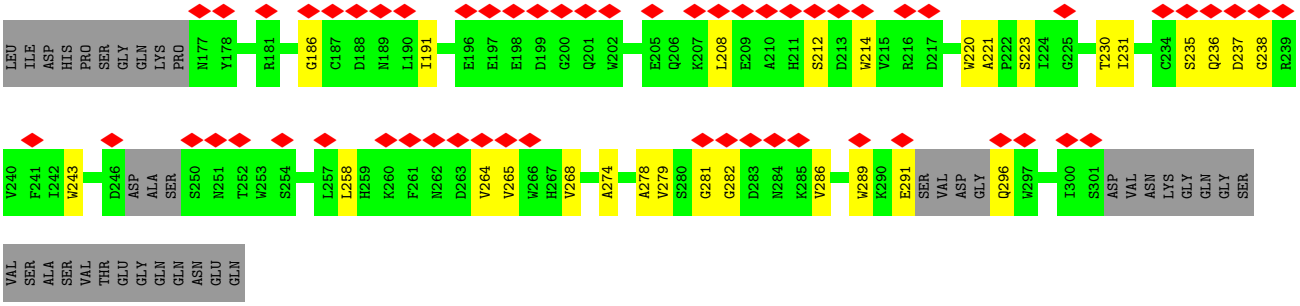


• Molecule 5: Protein SEC13 homolog

Chain H:

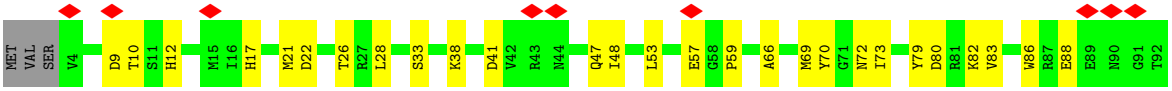


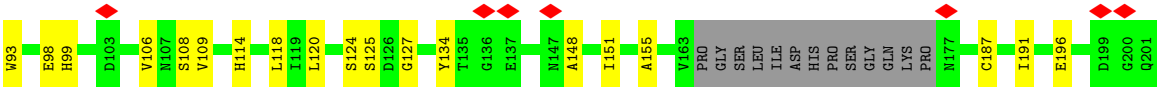


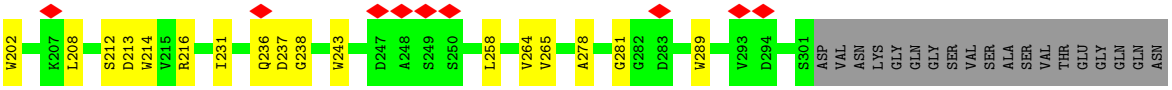


• Molecule 5: Protein SEC13 homolog

Chain R:

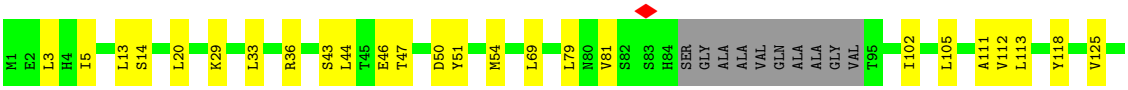


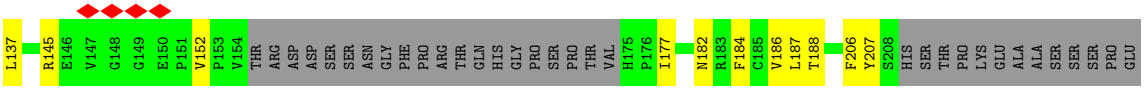


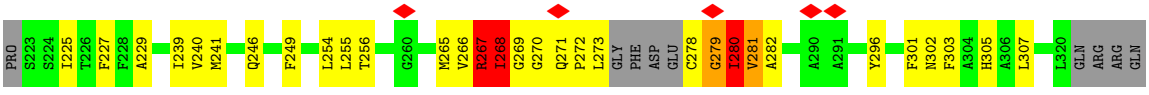


• Molecule 6: Cytosolic arginine sensor for mTORC1 subunit 1

Chain U:

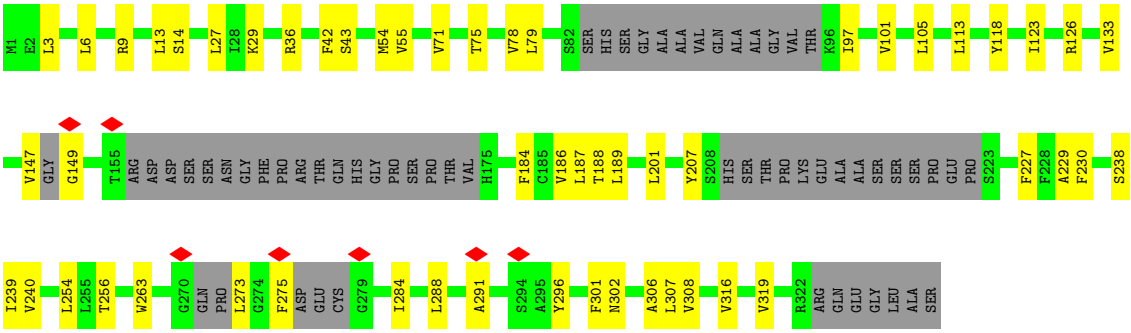






• Molecule 6: Cytosolic arginine sensor for mTORC1 subunit 1

Chain V:


M1 E2 L3 L6 R9 L13 S14 L27 I28 K29 R36 F42 S43 M54 V55 V71 T75 V78 L79 S82 SER HIS SER GLY ALA ALA VAL GLN ALA ALA GLY VAL THR K96 I97 V101 L105 L113 Y118 I123 R126 V133
V147 GLY G149 T155 ARG ASP ASP SER SER ASN GLY PHE PRO ARG THR GLN HIS GLY PRO SER PRO THR VAL H175 F184 C185 V186 L187 T188 L189 L201 Y207 S208 HIS SER THR PRO LYS GLU ALA ALA SER SER SER PRO GLU PRO S223 F227 F228 A229 F230 S238
I239 V240 L254 L255 T256 W263 G270 GLN PRO L273 G274 F275 ASP GLU CYS G279 T284 L288 A291 S294 A295 Y296 F301 N302 A306 L307 V308 V316 V319 R322 ARG GLN GLU GLY LEU ALA SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch Motion Corr. was used for motion correction and Patch CTF estimated (multi) was used for CTF determination.	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.203	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	588.0, 588.0, 588.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.10	0/3301	0.27	0/4496
1	B	0.11	0/4868	0.29	2/6674 (0.0%)
1	L	0.10	0/3571	0.23	0/4841
1	T	0.09	0/4877	0.24	0/6702
2	C	0.11	0/1710	0.28	0/2335
2	M	0.12	0/1915	0.26	0/2597
3	D	0.12	0/1694	0.26	0/2317
3	N	0.10	0/1921	0.24	0/2607
4	E	0.09	0/2072	0.24	0/2848
4	F	0.10	0/1493	0.26	0/2066
4	G	0.09	0/2116	0.25	0/2903
4	O	0.09	0/2413	0.23	0/3285
4	P	0.09	0/1693	0.23	0/2350
4	Q	0.09	0/2406	0.24	0/3276
5	H	0.09	0/2048	0.24	0/2822
5	R	0.09	0/2233	0.26	0/3055
6	U	0.21	0/1994	0.37	0/2742
6	V	0.12	0/1993	0.28	0/2735
All	All	0.11	0/44318	0.26	2/60651 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	684	PRO	CA-N-CD	-5.66	104.08	112.00
1	B	684	PRO	N-CD-CG	-5.55	94.87	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3232	0	2979	70	0
1	B	4768	0	4044	83	0
1	L	3498	0	3325	58	0
1	T	4771	0	3926	67	0
2	C	1668	0	1463	36	0
2	M	1870	0	1756	37	0
3	D	1657	0	1436	42	0
3	N	1881	0	1796	46	0
4	E	2017	0	1744	29	0
4	F	1464	0	882	18	0
4	G	2062	0	1852	33	0
4	O	2352	0	2234	34	0
4	P	1660	0	995	5	0
4	Q	2343	0	2233	33	0
5	H	1989	0	1719	45	0
5	R	2171	0	2014	44	0
6	U	1946	0	1849	60	0
6	V	1947	0	1875	46	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	L	4	0	0	0	0
7	M	4	0	0	0	0
7	N	3	0	0	0	0
7	T	3	0	0	0	0
All	All	43325	0	38122	696	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 (696) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:722:CYS:HB3	2:C:736:CYS:SG	2.07	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:269:GLY:HA3	6:U:280:ILE:HG23	1.52	0.90
6:U:272:PRO:HA	6:U:302:ASN:HA	1.52	0.89
6:V:189:LEU:HD21	6:V:254:LEU:HD23	1.52	0.89
6:V:189:LEU:HD12	6:V:239:ILE:HD11	1.55	0.88
6:U:270:GLY:HA2	6:U:303:PHE:CE1	2.15	0.81
1:A:740:CYS:HB3	1:A:778:CYS:SG	2.23	0.79
1:T:114:ARG:HD3	1:T:136:HIS:HB2	1.64	0.79
1:B:789:LEU:HB3	5:H:69:MET:HG3	1.66	0.77
1:L:405:ASP:OD2	1:L:411:ARG:NH1	2.19	0.76
6:U:111:ALA:HA	6:U:278:CYS:CB	2.16	0.76
6:V:189:LEU:CD1	6:V:239:ILE:CD1	2.65	0.74
1:B:545:ALA:HB2	1:B:554:LEU:HB2	1.70	0.74
4:F:175:SER:HB2	4:F:178:HIS:HB2	1.69	0.73
1:A:557:VAL:HG21	1:A:588:LEU:HD13	1.73	0.70
1:A:571:LEU:HD21	1:T:534:ILE:HG21	1.75	0.69
1:T:617:VAL:HG21	1:T:651:LEU:HD21	1.72	0.69
3:N:871:TYR:HB2	3:N:879:ARG:HD2	1.74	0.69
6:V:189:LEU:HD12	6:V:239:ILE:CD1	2.22	0.69
6:V:308:VAL:HG21	6:V:316:VAL:HG11	1.75	0.69
6:V:187:LEU:HD23	6:V:256:THR:HB	1.75	0.68
1:A:357:SER:HA	4:E:283:ARG:HG3	1.75	0.68
6:V:189:LEU:HD11	6:V:239:ILE:HD12	1.75	0.68
4:G:303:ARG:HG3	4:G:318:ILE:HA	1.76	0.68
1:L:637:THR:HG23	1:L:652:THR:HG22	1.74	0.68
6:V:189:LEU:CD1	6:V:239:ILE:HD11	2.24	0.68
2:C:451:MET:HE1	3:D:728:LEU:HD22	1.75	0.67
4:E:117:THR:OG1	4:E:133:CYS:SG	2.54	0.66
3:N:969:LEU:HD13	1:T:819:GLN:HE21	1.61	0.66
3:N:927:CYS:SG	3:N:949:HIS:HE1	2.16	0.66
4:G:197:VAL:HG21	4:G:240:ILE:HD13	1.77	0.66
1:B:358:LEU:HD13	4:F:294:ALA:HB1	1.77	0.66
4:G:49:CYS:HG	4:G:52:SER:HG	1.40	0.65
3:N:669:ASN:H	3:N:676:THR:HG21	1.60	0.65
4:O:117:THR:HG1	4:O:133:CYS:HG	1.39	0.65
3:D:680:ASN:HD21	3:D:747:MET:HE2	1.60	0.65
1:A:826:TRP:HA	1:A:833:GLY:HA3	1.79	0.64
1:T:431:HIS:O	1:T:435:GLN:NE2	2.31	0.64
1:A:842:TRP:NE1	1:A:848:GLU:O	2.30	0.64
6:V:189:LEU:CD1	6:V:239:ILE:HD12	2.27	0.64
2:M:730:GLY:HA2	4:O:148:MET:HE1	1.79	0.64
5:R:109:VAL:HB	5:R:120:LEU:HD11	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ILE:HG23	1:B:558:ALA:HB1	1.79	0.64
1:L:527:VAL:O	1:L:531:ASN:ND2	2.29	0.64
3:N:844:HIS:HD1	4:Q:309:TYR:HH	1.46	0.63
1:T:408:GLN:HE21	1:T:410:TRP:HE1	1.46	0.63
6:V:189:LEU:HD11	6:V:239:ILE:CD1	2.27	0.63
6:U:187:LEU:HD13	6:U:254:LEU:HD22	1.79	0.63
1:B:590:VAL:HB	1:B:605:VAL:HG23	1.81	0.63
4:P:39:TRP:HA	4:P:49:CYS:HA	1.81	0.63
1:B:833:GLY:HA2	1:B:839:MET:HE3	1.81	0.62
1:L:792:MET:HE1	2:M:715:LEU:HD11	1.81	0.62
1:B:114:ARG:NH2	1:B:140:PHE:O	2.32	0.62
4:Q:5:ARG:HH22	4:Q:46:ASP:HA	1.65	0.62
2:M:447:GLN:HG3	3:N:707:LEU:HD11	1.82	0.62
1:T:398:ALA:O	1:T:712:LYS:NZ	2.26	0.62
6:U:33:LEU:HB3	6:U:36:ARG:HG3	1.82	0.62
1:B:822:ASN:HB2	3:D:973:THR:HG23	1.82	0.61
6:U:278:CYS:O	6:U:279:GLY:C	2.43	0.61
1:A:531:ASN:OD1	1:A:622:LYS:NZ	2.33	0.61
6:U:265:MET:HG3	6:U:266:VAL:N	2.15	0.61
1:L:644:GLY:O	1:L:668:ARG:NH1	2.34	0.61
4:O:243:LYS:HA	4:O:280:GLN:HA	1.82	0.60
1:A:390:ILE:HD12	1:A:393:LYS:HD3	1.83	0.60
2:C:679:SER:HB3	4:G:231:LEU:HD12	1.82	0.60
1:B:84:ASN:HD22	1:B:86:ARG:H	1.50	0.60
1:T:644:GLY:O	1:T:668:ARG:NH1	2.34	0.60
3:D:927:CYS:SG	3:D:949:HIS:HE1	2.18	0.60
4:O:82:THR:HG22	4:O:110:VAL:HG12	1.84	0.60
4:Q:303:ARG:HG2	4:Q:318:ILE:HG12	1.83	0.60
6:V:186:VAL:HG22	6:V:240:VAL:HG22	1.83	0.59
4:E:287:ASN:HD22	4:E:292:VAL:HG12	1.67	0.59
2:M:351:LEU:HD21	4:Q:302:VAL:HG11	1.83	0.59
4:O:145:PRO:HD2	4:O:152:GLN:HE22	1.65	0.59
6:U:267:ARG:HD2	6:U:305:HIS:CE1	2.36	0.59
6:U:182:ASN:ND2	6:U:225:ILE:O	2.36	0.59
5:R:9:ASP:HB3	5:R:47:GLN:HE22	1.67	0.59
6:U:20:LEU:HD21	6:U:206:PHE:HD1	1.68	0.59
6:U:225:ILE:CD1	6:U:267:ARG:HD3	2.32	0.59
1:A:624:LEU:HG	1:A:628:GLN:HG3	1.83	0.59
1:A:737:CYS:HB3	1:A:740:CYS:SG	2.43	0.59
1:B:644:GLY:O	1:B:668:ARG:NH1	2.36	0.59
2:M:679:SER:HB3	4:Q:231:LEU:HD12	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:47:THR:OG1	6:U:50:ASP:O	2.21	0.59
6:V:296:TYR:HB2	6:V:307:LEU:HB2	1.84	0.59
1:B:515:LEU:HD11	1:B:523:ARG:HH11	1.68	0.58
2:C:640:MET:HA	3:D:723:PRO:HG2	1.85	0.58
4:O:306:LYS:HE2	4:O:316:THR:HG21	1.85	0.58
4:G:61:TRP:C	4:G:62:ARG:HD2	2.28	0.58
4:O:4:ALA:HB2	4:O:319:LEU:HD23	1.85	0.58
1:B:352:VAL:HG13	1:B:353:PHE:H	1.68	0.58
4:F:53:TRP:HE1	4:F:103:TRP:H	1.52	0.58
1:L:408:GLN:HE21	1:L:411:ARG:NH2	2.00	0.58
1:A:399:LEU:HD23	1:A:712:LYS:HE3	1.84	0.58
1:A:792:MET:HE1	1:A:834:GLY:HA2	1.86	0.58
4:E:118:ASP:OD1	4:E:119:VAL:N	2.37	0.58
2:C:644:TYR:OH	3:D:722:HIS:NE2	2.28	0.58
1:A:788:CYS:SG	1:A:838:HIS:HE1	2.19	0.58
4:F:89:ILE:H	4:F:103:TRP:CD1	2.22	0.58
5:R:17:HIS:NE2	5:R:33:SER:OG	2.28	0.58
5:R:57:GLU:N	5:R:80:ASP:OD2	2.37	0.57
4:G:287:ASN:HB2	4:G:292:VAL:H	1.68	0.57
4:G:117:THR:HG1	4:G:133:CYS:HG	1.52	0.57
4:G:197:VAL:HG23	4:G:222:VAL:HG21	1.86	0.57
1:B:684:PRO:HD2	1:B:687:VAL:HB	1.87	0.57
5:H:22:ASP:OD1	5:H:26:THR:N	2.34	0.57
3:N:704:ASP:HB3	3:N:707:LEU:HD13	1.86	0.57
1:A:556:VAL:HA	1:A:559:MET:SD	2.44	0.57
5:R:231:ILE:HB	5:R:243:TRP:HB2	1.87	0.57
5:H:33:SER:HA	5:H:59:PRO:HB3	1.86	0.57
6:U:5:ILE:HG12	6:U:79:LEU:HD22	1.87	0.57
1:A:527:VAL:O	1:A:531:ASN:ND2	2.33	0.57
3:D:865:CYS:O	3:D:869:ILE:HG12	2.05	0.57
2:M:451:MET:HE3	3:N:698:LEU:HD22	1.86	0.57
4:E:287:ASN:OD1	4:E:290:GLY:N	2.37	0.57
1:A:545:ALA:HB2	1:A:554:LEU:HB2	1.87	0.57
1:L:713:ARG:NH1	1:L:717:ASP:OD2	2.38	0.57
3:D:668:LEU:HG	3:D:747:MET:HE1	1.87	0.56
4:F:287:ASN:ND2	4:F:289:THR:OG1	2.38	0.56
6:V:187:LEU:HD22	6:V:254:LEU:HB3	1.86	0.56
2:M:351:LEU:O	2:M:400:PHE:N	2.32	0.56
4:Q:49:CYS:SG	4:Q:52:SER:OG	2.62	0.56
1:B:201:LEU:HD22	1:B:230:VAL:HG11	1.87	0.56
1:B:655:THR:OG1	1:B:657:ASP:OD1	2.19	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:973:THR:HB	1:T:822:ASN:HB2	1.88	0.56
1:L:429:THR:O	1:L:433:MET:HG3	2.05	0.56
5:R:127:GLY:O	5:R:148:ALA:N	2.38	0.56
5:R:21:MET:HG2	5:R:28:LEU:HB2	1.87	0.56
1:A:390:ILE:HG23	1:A:394:MET:HE1	1.87	0.56
1:B:224:THR:HG21	1:B:251:TRP:HH2	1.70	0.56
3:D:649:ILE:HB	5:H:6:ASN:HB3	1.86	0.56
6:U:177:ILE:HG22	6:U:268:ILE:HG13	1.88	0.56
6:V:147:VAL:O	6:V:149:GLY:N	2.39	0.56
3:N:533:ASN:ND2	5:R:125:SER:O	2.38	0.56
4:Q:82:THR:HG22	4:Q:110:VAL:HG12	1.87	0.56
1:A:573:ARG:NH2	1:A:596:THR:O	2.38	0.56
1:L:399:LEU:HA	1:L:712:LYS:HE2	1.88	0.56
1:A:368:TRP:HZ3	1:A:377:CYS:HB2	1.71	0.55
4:G:188:ASP:O	4:G:196:LYS:NZ	2.38	0.55
4:O:225:ILE:HD11	4:O:238:LEU:HD21	1.89	0.55
4:G:119:VAL:HG23	4:G:132:THR:HG22	1.87	0.55
5:H:231:ILE:HB	5:H:243:TRP:HB2	1.87	0.55
5:R:191:ILE:HB	5:R:208:LEU:HB2	1.87	0.55
5:H:127:GLY:O	5:H:148:ALA:N	2.39	0.55
1:T:788:CYS:SG	1:T:838:HIS:HE1	2.24	0.55
1:A:495:GLN:NE2	1:A:503:GLY:O	2.40	0.55
1:A:587:TYR:O	1:A:591:MET:HG2	2.06	0.55
3:N:664:GLU:HG3	3:N:875:LEU:HD11	1.88	0.55
4:O:244:ASP:OD2	4:O:273:GLN:NE2	2.33	0.55
4:Q:236:HIS:HB2	4:Q:250:LEU:HB2	1.89	0.55
1:L:850:PRO:O	2:M:709:ASN:ND2	2.39	0.55
1:T:545:ALA:HB2	1:T:554:LEU:HB2	1.89	0.55
5:H:268:VAL:HG12	5:H:279:VAL:HG22	1.89	0.55
4:G:117:THR:OG1	4:G:133:CYS:SG	2.63	0.55
5:H:52:ASP:OD2	5:H:54:ARG:NH1	2.40	0.55
3:N:544:PHE:HE1	5:R:278:ALA:HB2	1.72	0.55
3:N:844:HIS:ND1	4:Q:309:TYR:OH	2.37	0.55
1:T:705:ASP:OD1	1:T:713:ARG:NH1	2.40	0.55
5:H:17:HIS:NE2	5:H:33:SER:OG	2.34	0.55
2:M:640:MET:HA	3:N:723:PRO:HG2	1.89	0.55
3:N:551:VAL:HG21	5:R:21:MET:HG3	1.89	0.55
6:U:225:ILE:HG21	6:U:265:MET:HE3	1.89	0.55
6:U:296:TYR:HB3	6:U:307:LEU:HB2	1.89	0.54
3:D:659:HIS:HE1	3:D:689:ARG:HD2	1.72	0.54
5:R:69:MET:HE3	1:T:789:LEU:HD13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:HD12	1:B:328:PHE:HD1	1.72	0.54
1:B:422:GLN:HB3	1:B:646:LEU:HB2	1.89	0.54
2:C:451:MET:HE2	3:D:724:PHE:HB3	1.88	0.54
6:U:268:ILE:CG1	6:U:269:GLY:H	2.20	0.54
1:A:787:LEU:HD12	1:A:838:HIS:HB3	1.90	0.54
1:L:831:ARG:NH1	2:M:727:SER:O	2.38	0.54
3:D:709:PRO:HB3	3:D:848:LYS:HB2	1.90	0.54
6:U:187:LEU:N	6:U:239:ILE:O	2.41	0.54
1:A:457:LYS:NZ	1:A:634:GLU:HA	2.23	0.54
2:C:742:MET:HA	2:C:742:MET:HE2	1.89	0.54
3:N:936:ASN:HD21	1:T:825:THR:HG22	1.73	0.54
1:A:608:GLU:O	1:A:616:ARG:NH1	2.41	0.54
1:B:555:ASN:ND2	1:L:582:GLN:OE1	2.41	0.54
5:H:236:GLN:HA	5:H:264:VAL:HG13	1.89	0.54
6:U:267:ARG:HG2	6:U:305:HIS:ND1	2.23	0.54
6:U:187:LEU:HD22	6:U:254:LEU:HB3	1.90	0.54
4:Q:281:VAL:HA	4:Q:297:GLY:HA2	1.90	0.54
1:T:401:ARG:HD3	1:T:404:LEU:HD12	1.90	0.54
6:U:272:PRO:HA	6:U:302:ASN:CA	2.33	0.54
1:T:7:ASP:O	1:T:21:CYS:N	2.41	0.53
1:B:144:ILE:HB	1:B:179:TYR:HB2	1.89	0.53
1:L:399:LEU:HD23	1:L:712:LYS:HE2	1.89	0.53
1:L:686:ASP:OD1	1:L:687:VAL:N	2.41	0.53
6:U:184:PHE:CE2	6:U:265:MET:HE2	2.44	0.53
2:M:697:VAL:HG11	2:M:709:ASN:HB2	1.89	0.53
1:T:112:HIS:O	6:V:118:TYR:OH	2.26	0.53
6:U:273:LEU:HD12	6:U:301:PHE:HA	1.90	0.53
4:E:117:THR:HG1	4:E:133:CYS:HG	1.55	0.53
1:A:823:TRP:CZ2	2:C:787:CYS:HB3	2.44	0.53
1:T:464:LEU:O	1:T:487:ASN:ND2	2.42	0.53
1:L:814:ASP:O	2:M:790:SER:OG	2.19	0.53
2:M:410:ARG:NH2	2:M:414:ASP:OD1	2.42	0.53
6:U:186:VAL:O	6:U:256:THR:HG21	2.09	0.53
5:H:69:MET:HE3	5:H:70:TYR:CE1	2.44	0.53
4:O:139:VAL:HG21	4:O:184:VAL:HG21	1.91	0.53
1:L:561:LEU:HD13	1:L:591:MET:HE3	1.89	0.53
6:V:187:LEU:HD13	6:V:254:LEU:HD22	1.91	0.53
1:B:557:VAL:HG11	1:B:588:LEU:HD22	1.91	0.52
6:U:269:GLY:HA3	6:U:280:ILE:CG2	2.31	0.52
6:U:278:CYS:O	6:U:280:ILE:N	2.42	0.52
3:N:754:ALA:HB2	3:N:885:PHE:HE2	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:237:ASP:OD1	5:R:238:GLY:N	2.42	0.52
1:B:713:ARG:NH2	3:D:926:ILE:O	2.42	0.52
4:G:172:PRO:HG2	4:G:229:PRO:HA	1.90	0.52
5:H:106:VAL:HA	5:H:124:SER:HA	1.91	0.52
1:B:603:ASP:OD1	1:B:603:ASP:N	2.42	0.52
4:F:224:ASP:H	4:F:241:ALA:HB3	1.75	0.52
5:R:196:GLU:HB3	5:R:202:TRP:CE2	2.45	0.52
1:A:773:THR:HB	1:A:791:ASN:HB2	1.92	0.52
1:B:325:ILE:HG23	1:B:340:VAL:HG13	1.91	0.52
3:D:733:LEU:HD22	3:D:745:LEU:HD23	1.92	0.52
3:N:646:LYS:HE3	5:R:9:ASP:HA	1.91	0.52
6:U:145:ARG:O	6:U:152:VAL:N	2.43	0.52
6:V:113:LEU:HD11	6:V:275:PHE:HE2	1.73	0.52
1:A:834:GLY:N	1:A:839:MET:SD	2.83	0.52
1:B:320:PRO:HB3	1:B:350:PHE:CB	2.40	0.52
2:C:447:GLN:HG3	3:D:707:LEU:HD11	1.92	0.52
1:L:470:SER:HA	1:L:599:THR:HG21	1.92	0.52
5:R:82:LYS:HZ2	5:R:98:GLU:CD	2.18	0.52
1:T:193:LEU:HD12	1:T:199:LEU:HB3	1.92	0.52
1:T:408:GLN:NE2	1:T:410:TRP:HE1	2.07	0.52
6:U:268:ILE:HG12	6:U:269:GLY:H	1.74	0.52
1:A:402:TYR:OH	1:A:427:TRP:NE1	2.37	0.52
4:E:31:SER:OG	4:E:33:ASP:OD1	2.26	0.52
4:G:247:ILE:HB	4:G:272:ALA:HB3	1.92	0.52
4:O:284:VAL:HB	4:O:293:LEU:HD11	1.92	0.52
1:L:564:TYR:HB2	1:L:595:LEU:HD13	1.92	0.51
3:N:668:LEU:HG	3:N:747:MET:HE1	1.91	0.51
3:N:709:PRO:HB2	3:N:848:LYS:HD2	1.93	0.51
1:T:557:VAL:HG11	1:T:588:LEU:HD22	1.91	0.51
1:A:784:ARG:HA	1:A:791:ASN:HA	1.91	0.51
1:L:515:LEU:HD21	1:L:523:ARG:HH11	1.74	0.51
1:T:640:MET:HE1	1:T:645:ASN:HB3	1.91	0.51
6:V:43:SER:HB3	6:V:54:MET:HB2	1.92	0.51
4:E:197:VAL:HG21	4:E:240:ILE:HD12	1.93	0.51
1:T:584:ASN:OD1	1:T:585:ASN:N	2.44	0.51
1:B:825:THR:HG22	3:D:936:ASN:HD21	1.73	0.51
5:H:160:PRO:HG3	5:H:223:SER:H	1.74	0.51
3:N:550:LEU:HB2	3:N:652:ILE:HD13	1.93	0.51
4:Q:27:MET:HB3	4:Q:39:TRP:HB2	1.93	0.51
5:R:214:TRP:HB2	5:R:236:GLN:HB2	1.92	0.51
6:V:291:ALA:HB2	6:V:319:VAL:HG21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:66:ALA:HB3	4:Q:73:VAL:HB	1.93	0.51
6:V:273:LEU:N	6:V:302:ASN:OD1	2.43	0.51
1:B:112:HIS:O	1:B:114:ARG:NH1	2.43	0.51
4:F:27:MET:O	4:F:39:TRP:N	2.43	0.51
1:L:667:ASP:OD2	4:O:234:SER:OG	2.24	0.51
1:T:590:VAL:HG11	1:T:611:VAL:HG21	1.93	0.51
6:V:184:PHE:CZ	6:V:227:PHE:HB3	2.46	0.51
1:A:430:LEU:HD13	1:A:681:GLN:HG3	1.92	0.51
1:A:662:MET:HE3	1:A:662:MET:HA	1.93	0.51
5:R:59:PRO:HD2	5:R:79:TYR:HB3	1.93	0.51
2:C:414:ASP:OD2	2:C:418:ARG:NH2	2.44	0.51
6:U:269:GLY:O	6:U:303:PHE:HE1	1.93	0.51
2:C:421:LEU:HB3	2:C:658:ILE:HG21	1.93	0.50
4:F:16:HIS:N	4:F:30:CYS:O	2.39	0.50
6:U:3:LEU:HD12	6:U:81:VAL:HG22	1.93	0.50
6:U:113:LEU:HD11	6:U:273:LEU:HD11	1.92	0.50
4:G:277:HIS:ND1	4:G:281:VAL:HG22	2.26	0.50
4:P:81:ARG:HA	4:P:115:SER:HA	1.94	0.50
6:V:9:ARG:HB3	6:V:75:THR:HG21	1.93	0.50
3:D:871:TYR:HB2	3:D:879:ARG:HD2	1.94	0.50
4:E:287:ASN:ND2	4:E:292:VAL:HG12	2.26	0.50
1:T:411:ARG:HG3	1:T:414:ILE:HD12	1.92	0.50
1:B:338:MET:O	1:B:340:VAL:HG23	2.11	0.50
2:C:426:LEU:HD23	2:C:457:CYS:HB2	1.92	0.50
5:H:53:LEU:HD13	5:H:86:TRP:CD2	2.47	0.50
1:T:593:ALA:O	1:T:597:SER:OG	2.27	0.50
2:C:683:LEU:HD11	4:G:231:LEU:HD21	1.93	0.50
1:A:526:ALA:HA	1:A:591:MET:SD	2.52	0.50
2:M:415:THR:HG23	2:M:419:TYR:CZ	2.47	0.50
6:V:118:TYR:H	6:V:238:SER:HB2	1.77	0.50
1:A:626:ASP:HA	1:A:629:LEU:HB3	1.94	0.50
6:V:79:LEU:HB2	6:V:123:ILE:HB	1.94	0.50
1:B:84:ASN:ND2	1:B:86:ARG:H	2.08	0.50
1:B:456:ILE:HB	1:B:651:LEU:HD23	1.93	0.50
5:H:31:CYS:HB2	5:H:60:VAL:HB	1.94	0.50
1:A:690:ASP:OD2	1:A:692:ARG:NH2	2.41	0.50
3:N:927:CYS:HA	1:T:710:TRP:CD1	2.46	0.50
2:C:628:LEU:HG	3:D:691:ASP:HB2	1.92	0.49
1:A:669:THR:HG23	1:A:671:ASP:H	1.76	0.49
1:B:208:LEU:HD21	1:B:227:VAL:HA	1.94	0.49
3:D:659:HIS:HE1	3:D:689:ARG:HH11	1.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:31:SER:OG	4:G:32:SER:N	2.44	0.49
1:T:590:VAL:HB	1:T:605:VAL:HG23	1.94	0.49
1:B:121:TRP:CZ2	1:B:129:LEU:HD12	2.47	0.49
1:T:660:ASP:OD1	1:T:692:ARG:NH1	2.44	0.49
6:U:102:ILE:HD12	6:U:112:VAL:HG21	1.95	0.49
1:L:368:TRP:HZ3	1:L:377:CYS:HB2	1.77	0.49
4:G:107:THR:HG21	4:G:153:TRP:HD1	1.78	0.49
4:E:14:LEU:O	4:E:32:SER:N	2.46	0.49
1:L:787:LEU:HD12	1:L:838:HIS:HB3	1.94	0.49
6:V:3:LEU:HD11	6:V:79:LEU:HB3	1.92	0.49
1:A:637:THR:HG23	1:A:652:THR:HG22	1.95	0.49
1:B:606:LEU:HD11	1:B:624:LEU:HD21	1.95	0.49
4:E:134:SER:OG	4:E:138:ILE:O	2.28	0.49
4:G:128:LEU:HD23	4:G:144:ALA:HB3	1.94	0.49
1:L:662:MET:HE2	1:L:675:ALA:HA	1.95	0.49
3:N:884:LYS:NZ	1:T:851:VAL:O	2.45	0.49
1:B:705:ASP:OD1	1:B:713:ARG:NH1	2.45	0.49
5:R:213:ASP:HB3	5:R:236:GLN:HB3	1.93	0.49
1:L:785:CYS:HA	1:L:834:GLY:HA2	1.95	0.48
5:R:88:GLU:HB2	5:R:93:TRP:CD2	2.48	0.48
6:U:46:GLU:HG3	6:U:51:TYR:CE2	2.48	0.48
6:U:279:GLY:O	6:U:280:ILE:C	2.55	0.48
4:E:64:THR:HG21	4:E:120:LYS:HA	1.95	0.48
1:L:580:ARG:NH1	1:L:589:CYS:SG	2.86	0.48
5:R:83:VAL:HB	5:R:99:HIS:HB3	1.95	0.48
1:A:456:ILE:O	1:A:460:VAL:HG22	2.13	0.48
2:C:445:VAL:HG13	2:C:652:MET:SD	2.53	0.48
5:H:212:SER:OG	5:H:237:ASP:OD2	2.30	0.48
4:E:167:CYS:SG	4:E:168:ILE:N	2.86	0.48
5:R:118:LEU:HB3	5:R:134:TYR:HB3	1.95	0.48
6:U:182:ASN:HD21	6:U:225:ILE:HG22	1.77	0.48
6:U:187:LEU:HA	6:U:256:THR:HG21	1.96	0.48
1:B:665:TYR:HD1	1:B:668:ARG:HH12	1.62	0.48
3:N:674:GLN:NE2	3:N:700:THR:O	2.34	0.48
4:P:251:LYS:O	4:P:267:GLU:N	2.46	0.48
4:Q:31:SER:OG	4:Q:32:SER:N	2.46	0.48
5:H:160:PRO:HD2	5:H:220:TRP:CD1	2.49	0.48
6:V:288:LEU:HD13	6:V:316:VAL:HG23	1.95	0.48
1:T:43:LEU:N	1:T:51:ALA:O	2.47	0.48
1:A:429:THR:O	1:A:433:MET:HG3	2.14	0.48
1:B:543:GLU:O	1:B:546:SER:OG	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:MET:HE1	1:B:678:CYS:HB2	1.95	0.48
2:C:447:GLN:HG3	3:D:707:LEU:HD21	1.96	0.48
4:G:72:GLN:HB2	4:G:88:GLU:HB3	1.96	0.48
1:T:474:TRP:CD1	1:T:532:LEU:HB3	2.49	0.48
6:U:13:LEU:HD23	6:U:69:LEU:HD21	1.96	0.48
2:M:451:MET:HE1	3:N:728:LEU:HD22	1.96	0.48
3:N:694:GLN:O	3:N:698:LEU:HG	2.14	0.48
4:O:31:SER:OG	4:O:33:ASP:OD1	2.24	0.48
6:V:6:LEU:HB2	6:V:78:VAL:HB	1.96	0.48
1:B:709:PHE:HB3	1:B:712:LYS:HB2	1.95	0.47
4:E:197:VAL:HB	4:E:215:LEU:HB2	1.96	0.47
1:L:812:SER:HB3	2:M:790:SER:HB3	1.95	0.47
1:B:7:ASP:O	1:B:21:CYS:N	2.47	0.47
4:O:244:ASP:OD1	4:O:244:ASP:N	2.46	0.47
5:R:212:SER:OG	5:R:237:ASP:OD2	2.27	0.47
1:B:362:PRO:HB2	1:B:707:TRP:HD1	1.79	0.47
4:Q:161:CYS:O	4:Q:162:LYS:HG3	2.13	0.47
4:F:61:TRP:N	4:F:77:CYS:O	2.44	0.47
1:B:394:MET:HE1	1:B:672:VAL:H	1.79	0.47
1:B:457:LYS:O	1:B:461:LYS:HG2	2.15	0.47
2:C:669:ASP:OD1	2:C:669:ASP:N	2.47	0.47
1:L:422:GLN:HB3	1:L:646:LEU:HB2	1.97	0.47
1:L:781:PRO:HB3	4:Q:148:MET:HE3	1.95	0.47
3:N:931:VAL:HG21	3:N:945:GLY:HA2	1.96	0.47
5:R:258:LEU:HD21	5:R:289:TRP:CD2	2.49	0.47
6:V:97:ILE:HB	6:V:101:VAL:HG12	1.97	0.47
1:A:431:HIS:NE2	1:A:435:GLN:OE1	2.48	0.47
1:B:286:LEU:HD11	1:B:325:ILE:HG22	1.96	0.47
1:B:490:ARG:NH2	1:B:626:ASP:OD1	2.44	0.47
2:M:414:ASP:O	2:M:418:ARG:HG2	2.15	0.47
2:M:443:ASN:O	2:M:447:GLN:HG2	2.15	0.47
1:T:434:LYS:O	1:T:437:THR:OG1	2.30	0.47
2:C:455:ILE:HG13	3:D:698:LEU:HD21	1.96	0.47
4:E:181:MET:HE1	4:E:266:PHE:CZ	2.49	0.47
1:L:523:ARG:NE	1:L:615:ASP:OD2	2.43	0.47
5:R:70:TYR:OH	5:R:114:HIS:O	2.31	0.47
6:U:207:TYR:CE1	6:V:29:LYS:HB2	2.49	0.47
1:A:640:MET:CE	1:A:645:ASN:HB3	2.44	0.47
2:C:427:ALA:HA	2:C:453:ARG:HG3	1.96	0.47
5:H:38:LYS:HB2	5:H:49:LEU:HD11	1.97	0.47
5:H:264:VAL:O	5:H:282:GLY:N	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:36:ARG:HG2	6:V:36:ARG:HH11	1.80	0.47
1:A:616:ARG:HH21	1:A:636:LEU:HD11	1.80	0.46
1:L:732:GLN:O	2:M:720:SER:OG	2.26	0.46
5:R:265:VAL:HA	5:R:281:GLY:HA2	1.97	0.46
1:T:529:LEU:HD13	1:T:561:LEU:HD21	1.97	0.46
6:U:44:LEU:HD11	6:U:51:TYR:HD2	1.80	0.46
3:D:659:HIS:CE1	3:D:689:ARG:HH11	2.33	0.46
4:E:277:HIS:CD2	4:E:303:ARG:HD2	2.51	0.46
5:H:22:ASP:CG	5:H:27:ARG:H	2.23	0.46
1:L:713:ARG:NH2	2:M:745:VAL:O	2.42	0.46
2:M:660:LEU:HA	2:M:663:ARG:HH21	1.81	0.46
4:O:280:GLN:OE1	4:O:280:GLN:N	2.34	0.46
1:B:637:THR:HG23	1:B:652:THR:HG22	1.98	0.46
3:N:936:ASN:HD22	1:T:823:TRP:HB3	1.80	0.46
1:A:511:PHE:HE2	1:A:527:VAL:HG21	1.79	0.46
1:B:724:ASP:OD2	1:B:727:SER:OG	2.31	0.46
4:O:50:THR:O	4:O:101:SER:OG	2.33	0.46
4:O:195:ALA:HB2	4:O:216:MET:HA	1.95	0.46
5:R:10:THR:HB	5:R:12:HIS:HD2	1.80	0.46
5:R:151:ILE:HB	5:R:187:CYS:HB2	1.97	0.46
1:A:673:GLN:NE2	1:A:700:TYR:OH	2.48	0.46
3:D:552:TYR:HB2	5:H:286:VAL:HG21	1.97	0.46
4:O:196:LYS:NZ	4:O:219:THR:O	2.37	0.46
1:T:405:ASP:OD2	1:T:411:ARG:NH2	2.49	0.46
6:U:113:LEU:HD21	6:U:273:LEU:HD21	1.97	0.46
3:D:669:ASN:H	3:D:676:THR:HG21	1.80	0.46
3:D:677:CYS:HB3	3:D:700:THR:OG1	2.16	0.46
3:D:852:ASP:HB2	3:D:855:ASN:HB3	1.97	0.46
3:N:743:GLN:NE2	3:N:866:TYR:OH	2.49	0.46
1:B:84:ASN:HB3	6:U:255:LEU:HD22	1.98	0.46
4:G:107:THR:HG21	4:G:153:TRP:CD1	2.50	0.46
5:H:60:VAL:HA	5:H:78:SER:HA	1.98	0.46
5:H:132:LEU:HG	5:H:142:VAL:HG22	1.98	0.46
1:A:598:GLU:OE1	1:A:598:GLU:N	2.49	0.46
1:B:688:LEU:O	1:B:694:GLN:NE2	2.40	0.46
2:C:779:CYS:HB2	2:C:787:CYS:SG	2.56	0.46
1:L:608:GLU:O	1:L:616:ARG:NH1	2.49	0.46
4:O:197:VAL:HB	4:O:215:LEU:HB2	1.98	0.46
3:D:659:HIS:CE1	3:D:689:ARG:HD2	2.51	0.46
5:H:31:CYS:HB3	5:H:37:VAL:HG22	1.98	0.46
5:H:238:GLY:HA2	5:H:265:VAL:HG23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:430:LEU:HD13	1:L:681:GLN:HG3	1.97	0.46
2:M:339:ASN:ND2	4:Q:62:ARG:HH22	2.14	0.46
3:N:927:CYS:HA	1:T:710:TRP:CG	2.50	0.46
5:R:238:GLY:HA2	5:R:265:VAL:HG23	1.98	0.46
1:B:679:MET:HE3	1:B:679:MET:HA	1.97	0.45
2:C:415:THR:HB	2:C:419:TYR:CZ	2.50	0.45
1:L:523:ARG:NH2	1:L:615:ASP:OD1	2.44	0.45
1:L:580:ARG:HG3	1:L:581:LEU:HD12	1.98	0.45
1:T:688:LEU:HD21	1:T:724:ASP:HB2	1.98	0.45
2:C:675:HIS:CG	4:G:175:SER:HB2	2.50	0.45
4:Q:67:HIS:CG	4:Q:68:PRO:HD2	2.50	0.45
6:U:265:MET:HG3	6:U:266:VAL:H	1.81	0.45
6:V:316:VAL:HA	6:V:319:VAL:HG12	1.96	0.45
1:A:594:PHE:HB2	1:A:605:VAL:HG21	1.99	0.45
1:B:784:ARG:NH1	1:B:789:LEU:O	2.49	0.45
1:B:587:TYR:O	1:B:591:MET:HG3	2.17	0.45
1:B:703:LEU:HD12	4:F:288:ILE:HG13	1.97	0.45
2:C:743:CYS:HB3	2:C:748:HIS:H	1.81	0.45
1:A:399:LEU:HA	1:A:712:LYS:HE3	1.97	0.45
1:A:531:ASN:HA	1:A:622:LYS:HE2	1.97	0.45
1:A:788:CYS:SG	1:A:790:ILE:HG22	2.56	0.45
5:H:106:VAL:HG22	5:H:124:SER:HB2	1.98	0.45
3:N:934:SER:OG	1:T:859:MET:SD	2.69	0.45
6:U:118:TYR:CD2	6:U:188:THR:HB	2.51	0.45
1:B:190:LEU:HD22	1:B:200:LEU:HD12	1.98	0.45
1:B:362:PRO:HB2	1:B:707:TRP:CD1	2.52	0.45
1:B:534:ILE:O	1:B:538:ILE:HG12	2.15	0.45
3:D:944:GLY:HA2	3:D:950:MET:HE2	1.99	0.45
1:L:626:ASP:OD1	1:L:626:ASP:N	2.47	0.45
1:A:559:MET:HB2	1:T:576:CYS:SG	2.56	0.45
1:A:559:MET:O	1:A:562:SER:OG	2.32	0.45
1:B:823:TRP:HZ2	3:D:968:CYS:HB3	1.82	0.45
3:N:662:LEU:HD22	3:N:666:TYR:CE1	2.51	0.45
3:N:936:ASN:HB3	1:T:823:TRP:CE3	2.52	0.45
4:O:245:VAL:HG23	4:O:281:VAL:HG21	1.98	0.45
4:O:320:LYS:HE2	4:O:326:VAL:HG21	1.99	0.45
1:B:851:VAL:O	3:D:884:LYS:NZ	2.50	0.45
1:L:833:GLY:HA3	2:M:715:LEU:HD13	1.98	0.45
2:M:426:LEU:HD22	2:M:663:ARG:HH12	1.81	0.45
4:O:11:HIS:CD2	4:O:37:LYS:HD2	2.52	0.45
3:D:658:VAL:HG12	3:D:743:GLN:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:367:MET:HE2	4:O:7:ILE:HG13	1.99	0.45
6:U:29:LYS:HB2	6:V:207:TYR:CE1	2.52	0.45
1:A:457:LYS:HZ2	1:A:634:GLU:HA	1.82	0.45
2:M:426:LEU:HD23	2:M:457:CYS:HB2	1.99	0.45
3:D:704:ASP:OD1	3:D:705:LEU:N	2.50	0.44
1:L:557:VAL:HG11	1:L:588:LEU:HD22	1.99	0.44
6:U:184:PHE:CE1	6:U:227:PHE:HB3	2.53	0.44
6:V:184:PHE:N	6:V:263:TRP:O	2.41	0.44
1:B:426:LEU:HD22	1:B:646:LEU:HD22	1.99	0.44
4:F:14:LEU:O	4:F:32:SER:N	2.50	0.44
1:T:787:LEU:HD21	1:T:842:TRP:HB2	1.98	0.44
1:B:426:LEU:HD21	1:B:678:CYS:SG	2.58	0.44
2:M:427:ALA:HB2	2:M:457:CYS:SG	2.57	0.44
4:Q:81:ARG:HG2	4:Q:114:THR:C	2.42	0.44
5:R:21:MET:HA	5:R:28:LEU:HA	2.00	0.44
6:V:105:LEU:HD23	6:V:105:LEU:HA	1.89	0.44
1:A:695:TYR:OH	4:E:230:ASN:ND2	2.41	0.44
1:B:229:GLY:HA3	1:B:243:PHE:CE1	2.53	0.44
2:C:636:LEU:HD21	3:D:728:LEU:HB2	1.99	0.44
4:E:107:THR:HG21	4:E:153:TRP:CD1	2.52	0.44
4:E:198:GLN:HB3	4:E:211:LYS:HE3	2.00	0.44
4:O:204:GLU:O	4:O:207:ARG:NH1	2.50	0.44
4:Q:231:LEU:HD22	4:Q:289:THR:HA	2.00	0.44
1:T:464:LEU:H	1:T:487:ASN:HD22	1.65	0.44
6:U:118:TYR:CE1	6:U:256:THR:HG22	2.53	0.44
6:U:241:MET:HE3	6:U:246:GLN:HA	1.99	0.44
1:A:850:PRO:O	2:C:709:ASN:ND2	2.50	0.44
3:N:696:TRP:HZ3	3:N:751:VAL:HG21	1.83	0.44
1:L:420:ASP:HB3	1:L:423:LEU:HB2	1.99	0.44
3:N:659:HIS:HB2	3:N:662:LEU:HB2	1.99	0.44
3:N:926:ILE:O	1:T:713:ARG:NH2	2.51	0.44
1:B:77:LEU:HD21	1:B:89:LEU:HD23	1.99	0.44
2:C:442:ARG:CZ	2:C:445:VAL:HG21	2.48	0.44
2:C:450:THR:O	2:C:454:ILE:HG12	2.17	0.44
4:Q:180:PRO:HB2	4:Q:202:TYR:HB3	1.99	0.44
4:Q:241:ALA:HB2	4:Q:284:VAL:HG13	1.98	0.44
1:T:362:PRO:HB3	1:T:706:ALA:HB1	1.99	0.44
1:A:624:LEU:HD23	1:A:629:LEU:HA	1.99	0.44
1:L:547:SER:OG	1:L:548:GLU:N	2.51	0.44
1:T:410:TRP:HB3	1:T:431:HIS:CG	2.53	0.44
1:T:516:VAL:HG21	1:T:540:ILE:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:HD13	1:B:92:LEU:HB3	1.98	0.44
1:B:362:PRO:O	1:B:707:TRP:NE1	2.49	0.44
1:T:401:ARG:NH2	1:T:712:LYS:HE2	2.33	0.44
1:T:408:GLN:OE1	1:T:411:ARG:NH1	2.50	0.44
1:A:360:TRP:HE1	4:E:294:ALA:HB2	1.82	0.43
1:B:84:ASN:ND2	1:B:86:ARG:HB2	2.33	0.43
1:L:617:VAL:HG21	1:L:651:LEU:HD21	2.00	0.43
3:N:950:MET:HB3	1:T:820:PHE:CE1	2.53	0.43
4:P:4:ALA:HA	1:T:377:CYS:HA	1.99	0.43
5:R:106:VAL:HA	5:R:124:SER:HA	2.00	0.43
1:T:792:MET:HA	1:T:824:PHE:HE2	1.83	0.43
3:D:544:PHE:HE1	5:H:278:ALA:HB2	1.84	0.43
5:H:291:GLU:OE2	5:H:296:GLN:N	2.51	0.43
1:L:531:ASN:OD1	1:L:622:LYS:NZ	2.51	0.43
1:L:732:GLN:NE2	2:M:742:MET:O	2.50	0.43
4:O:233:ARG:NH2	4:O:289:THR:O	2.50	0.43
5:R:22:ASP:OD1	5:R:26:THR:N	2.49	0.43
2:C:673:GLN:OE1	2:C:701:THR:OG1	2.35	0.43
3:D:868:GLU:OE2	5:H:23:TYR:OH	2.24	0.43
4:O:161:CYS:SG	4:O:198:GLN:NE2	2.91	0.43
6:V:27:LEU:HD23	6:V:27:LEU:HA	1.91	0.43
6:V:42:PHE:HD1	6:V:55:VAL:HG12	1.83	0.43
3:N:954:PHE:HB3	3:N:969:LEU:HD11	2.01	0.43
6:U:241:MET:HE1	6:U:249:PHE:CD1	2.54	0.43
1:B:409:VAL:HG11	1:B:681:GLN:HE22	1.82	0.43
1:T:401:ARG:HE	1:T:401:ARG:HB2	1.60	0.43
6:U:229:ALA:HB3	6:U:240:VAL:HB	2.01	0.43
4:E:78:SER:OG	4:E:79:PHE:N	2.51	0.43
4:G:129:MET:HE3	4:G:129:MET:HB2	1.84	0.43
5:R:12:HIS:CE1	5:R:38:LYS:HG3	2.53	0.43
1:A:666:VAL:O	1:A:670:GLY:N	2.50	0.43
1:A:699:ASN:HB3	4:E:231:LEU:HD12	2.00	0.43
1:B:701:ARG:HH21	3:D:928:HIS:HE1	1.66	0.43
3:D:743:GLN:HG3	3:D:866:TYR:CZ	2.53	0.43
4:E:122:ALA:HB1	4:E:126:MET:HE3	2.00	0.43
2:C:427:ALA:HB2	2:C:457:CYS:SG	2.59	0.43
4:E:123:PRO:HG2	4:E:126:MET:HE2	2.01	0.43
5:H:12:HIS:ND1	5:H:32:SER:HB3	2.34	0.43
1:L:744:ILE:HG13	2:M:758:GLN:HE21	1.84	0.43
4:O:241:ALA:HB2	4:O:284:VAL:HG13	2.00	0.43
6:U:269:GLY:O	6:U:303:PHE:CE1	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:TRP:HB3	3:D:936:ASN:ND2	2.34	0.43
1:T:199:LEU:HD23	1:T:199:LEU:HA	1.94	0.43
6:V:105:LEU:HD21	6:V:133:VAL:HA	2.01	0.43
6:V:189:LEU:HD21	6:V:254:LEU:CD2	2.38	0.43
1:B:229:GLY:HA3	1:B:243:PHE:HE1	1.84	0.43
4:E:241:ALA:HB2	4:E:284:VAL:HG13	2.00	0.43
4:G:215:LEU:HD22	4:G:268:ILE:HG21	2.01	0.43
5:H:69:MET:HE2	5:H:69:MET:HB3	1.97	0.43
1:L:660:ASP:OD1	1:L:692:ARG:NH1	2.51	0.43
1:L:703:LEU:HD11	4:O:231:LEU:HD11	2.01	0.43
4:O:72:GLN:HB2	4:O:88:GLU:HB3	2.00	0.43
5:R:88:GLU:HB2	5:R:93:TRP:CE2	2.54	0.43
1:T:637:THR:HG23	1:T:652:THR:HG22	2.01	0.43
6:U:43:SER:HB3	6:U:54:MET:HB2	2.01	0.43
1:A:712:LYS:HA	1:A:715:GLU:HG2	2.01	0.42
3:D:707:LEU:HD23	3:D:719:TRP:CD2	2.54	0.42
1:T:401:ARG:HH12	1:T:715:GLU:CD	2.27	0.42
2:C:685:GLN:HG2	2:C:690:TRP:HZ3	1.84	0.42
4:F:202:TYR:HA	4:F:209:TYR:HA	2.01	0.42
1:L:456:ILE:HG12	1:L:650:LEU:O	2.19	0.42
4:O:154:SER:OG	4:O:156:GLN:NE2	2.44	0.42
1:A:362:PRO:O	1:A:707:TRP:NE1	2.41	0.42
4:F:125:HIS:NE2	4:F:173:SER:O	2.52	0.42
4:F:293:LEU:HB3	4:F:305:TRP:HB2	2.01	0.42
4:G:18:VAL:HG22	4:G:29:THR:HG22	2.02	0.42
5:H:78:SER:OG	5:H:79:TYR:N	2.52	0.42
5:R:214:TRP:O	5:R:236:GLN:N	2.47	0.42
6:V:229:ALA:HB3	6:V:240:VAL:HB	2.00	0.42
1:B:8:ILE:O	1:B:329:ALA:HB2	2.20	0.42
4:G:226:ALA:O	4:G:286:TRP:NE1	2.49	0.42
5:H:221:ALA:HB1	5:H:274:ALA:HB1	2.02	0.42
5:R:236:GLN:HA	5:R:264:VAL:HG23	1.99	0.42
6:U:105:LEU:HG	6:U:137:LEU:HD11	2.01	0.42
6:V:118:TYR:CD2	6:V:188:THR:HB	2.55	0.42
4:G:277:HIS:CD2	4:G:303:ARG:HH21	2.37	0.42
5:H:191:ILE:HB	5:H:208:LEU:HB2	2.00	0.42
5:R:66:ALA:HB3	5:R:73:ILE:HB	2.01	0.42
6:V:201:LEU:HD21	6:V:230:PHE:CE2	2.54	0.42
1:A:581:LEU:H	1:A:581:LEU:HD23	1.84	0.42
1:B:663:GLU:OE1	1:B:692:ARG:NH1	2.48	0.42
2:C:750:VAL:HG22	2:C:765:HIS:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:154:ASN:H	5:H:186:GLY:HA2	1.84	0.42
5:H:214:TRP:O	5:H:236:GLN:N	2.46	0.42
5:H:235:SER:OG	5:H:236:GLN:N	2.52	0.42
1:L:625:SER:O	1:L:629:LEU:N	2.42	0.42
3:N:953:TRP:CH2	3:N:957:GLN:HG3	2.54	0.42
3:N:968:CYS:O	3:N:972:SER:HB3	2.19	0.42
5:R:41:ASP:HB3	5:R:48:ILE:HB	2.02	0.42
1:A:436:TYR:CE2	1:A:492:LEU:HD13	2.55	0.42
3:D:545:CYS:CB	5:H:21:MET:HB2	2.50	0.42
4:E:121:PHE:CE1	4:E:130:LEU:HD12	2.55	0.42
2:M:356:LYS:HA	4:Q:14:LEU:HD22	2.01	0.42
4:Q:299:ASP:OD1	4:Q:299:ASP:N	2.53	0.42
1:T:640:MET:CE	1:T:645:ASN:HB3	2.50	0.42
1:B:199:LEU:HD23	1:B:212:ASP:HA	2.00	0.42
4:Q:247:ILE:HB	4:Q:272:ALA:HB3	2.01	0.42
1:A:732:GLN:O	2:C:720:SER:OG	2.25	0.42
4:F:206:THR:HG23	4:F:208:LYS:H	1.85	0.42
5:H:265:VAL:HA	5:H:281:GLY:HA2	2.02	0.42
1:L:710:TRP:CG	2:M:746:CYS:HA	2.55	0.42
1:T:404:LEU:HD23	1:T:404:LEU:HA	1.88	0.42
1:T:465:GLY:N	1:T:626:ASP:OD2	2.51	0.42
3:D:924:CYS:SG	3:D:945:GLY:HA3	2.60	0.42
5:H:32:SER:OG	5:H:33:SER:N	2.52	0.42
5:H:221:ALA:HB3	5:H:230:THR:HB	2.02	0.42
6:U:112:VAL:HG12	6:U:125:VAL:HG12	2.02	0.42
4:E:281:VAL:HA	4:E:297:GLY:HA2	2.02	0.41
4:F:166:SER:N	4:F:185:GLY:O	2.52	0.41
4:F:229:PRO:O	4:F:233:ARG:NH1	2.53	0.41
4:G:244:ASP:OD1	4:G:244:ASP:N	2.52	0.41
5:R:53:LEU:HB3	5:R:86:TRP:CZ3	2.55	0.41
1:T:204:MET:N	1:T:207:ASN:O	2.53	0.41
1:T:821:ASN:HA	1:T:836:ALA:HB3	2.01	0.41
1:A:487:ASN:HB3	1:A:489:GLU:HG2	2.00	0.41
4:Q:195:ALA:HB2	4:Q:216:MET:HA	2.01	0.41
1:T:338:MET:O	1:T:350:PHE:N	2.53	0.41
1:B:690:ASP:HB3	1:B:693:VAL:HG22	2.01	0.41
4:G:139:VAL:HG21	4:G:184:VAL:HG21	2.03	0.41
6:U:225:ILE:HD13	6:U:267:ARG:HD3	2.02	0.41
6:V:126:ARG:H	6:V:126:ARG:HG3	1.59	0.41
1:L:456:ILE:HB	1:L:651:LEU:HD23	2.03	0.41
4:Q:237:ILE:HG12	4:Q:249:THR:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:307:ALA:HB2	4:Q:313:TRP:CE2	2.55	0.41
1:B:116:CYS:HA	1:B:133:LEU:HD23	2.03	0.41
1:B:393:LYS:O	1:B:396:LEU:HG	2.20	0.41
2:C:726:MET:HE2	2:C:726:MET:HB3	1.97	0.41
5:R:108:SER:HB3	5:R:155:ALA:HA	2.02	0.41
1:T:847:ALA:O	1:T:857:LYS:HG2	2.20	0.41
1:A:390:ILE:HG13	1:A:394:MET:SD	2.60	0.41
1:B:84:ASN:HD22	1:B:84:ASN:C	2.29	0.41
1:B:410:TRP:HB2	1:B:428:TYR:CE1	2.55	0.41
1:B:695:TYR:HD1	1:B:699:ASN:HD21	1.67	0.41
4:G:276:ASN:OD1	4:G:303:ARG:NH1	2.52	0.41
2:M:669:ASP:OD1	2:M:669:ASP:N	2.51	0.41
3:N:536:PHE:O	5:R:216:ARG:NH1	2.50	0.41
4:O:66:ALA:HB3	4:O:73:VAL:HB	2.01	0.41
1:B:660:ASP:OD1	1:B:692:ARG:NH1	2.47	0.41
4:P:245:VAL:N	4:P:274:PHE:O	2.53	0.41
1:T:662:MET:HE2	1:T:662:MET:HB2	1.69	0.41
6:U:270:GLY:CA	6:U:303:PHE:CE1	2.97	0.41
1:B:515:LEU:HD11	1:B:523:ARG:NH1	2.33	0.41
4:E:26:ARG:H	4:E:26:ARG:HG2	1.67	0.41
4:G:67:HIS:CG	4:G:68:PRO:HD2	2.56	0.41
5:H:18:ASP:OD1	5:H:19:ALA:N	2.54	0.41
1:L:734:PHE:CZ	2:M:718:ASN:HB2	2.56	0.41
2:M:345:TYR:OH	4:Q:304:LEU:HD22	2.19	0.41
4:O:126:MET:HE1	4:O:170:TRP:CZ3	2.56	0.41
1:A:573:ARG:HE	1:A:573:ARG:HB3	1.58	0.41
1:A:839:MET:HE3	1:A:839:MET:HB3	1.87	0.41
1:B:8:ILE:C	1:B:9:LEU:HD12	2.45	0.41
1:B:352:VAL:HG13	1:B:353:PHE:N	2.35	0.41
4:E:173:SER:OG	4:E:178:HIS:ND1	2.46	0.41
4:G:126:MET:HE1	4:G:170:TRP:CZ3	2.55	0.41
4:G:307:ALA:HB2	4:G:313:TRP:CD2	2.56	0.41
5:H:70:TYR:CD2	5:H:118:LEU:HB2	2.56	0.41
1:L:606:LEU:HB3	1:L:632:TYR:CE1	2.55	0.41
2:M:410:ARG:HD2	2:M:410:ARG:HA	1.81	0.41
2:M:426:LEU:HD13	2:M:663:ARG:HH22	1.86	0.41
2:M:430:CYS:CB	2:M:453:ARG:HB2	2.51	0.41
3:N:696:TRP:CH2	3:N:747:MET:HB3	2.56	0.41
3:N:870:LEU:HD23	3:N:873:TRP:CE3	2.55	0.41
4:O:13:ASP:HB3	4:O:32:SER:HB3	2.03	0.41
4:Q:307:ALA:HB2	4:Q:313:TRP:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:196:GLU:HA	5:R:202:TRP:HA	2.02	0.41
1:T:101:LYS:O	1:T:103:LEU:N	2.53	0.41
1:T:464:LEU:H	1:T:487:ASN:ND2	2.19	0.41
1:T:823:TRP:O	1:T:835:HIS:HA	2.21	0.41
6:U:113:LEU:HD11	6:U:273:LEU:CD1	2.51	0.41
6:U:281:VAL:O	6:U:282:ALA:C	2.61	0.41
1:A:625:SER:O	1:A:629:LEU:N	2.45	0.41
2:C:345:TYR:OH	2:C:349:GLY:HA2	2.21	0.41
2:C:636:LEU:HD11	3:D:723:PRO:O	2.20	0.41
5:H:258:LEU:HD21	5:H:289:TRP:CD2	2.56	0.41
6:V:284:ILE:HD12	6:V:306:ALA:HB2	2.02	0.41
1:A:522:GLU:HG2	1:A:523:ARG:N	2.36	0.40
4:G:275:ASP:OD1	4:G:275:ASP:N	2.54	0.40
2:M:683:LEU:HD11	4:Q:231:LEU:HD21	2.02	0.40
3:N:855:ASN:ND2	3:N:858:GLN:OE1	2.52	0.40
3:N:960:CYS:SG	3:N:962:THR:HG22	2.61	0.40
6:V:14:SER:HB2	6:V:301:PHE:CG	2.56	0.40
6:V:113:LEU:HD11	6:V:275:PHE:CE2	2.54	0.40
1:B:9:LEU:HB3	1:B:68:TRP:HE1	1.86	0.40
4:F:167:CYS:O	4:F:185:GLY:N	2.41	0.40
1:L:456:ILE:O	1:L:460:VAL:HG22	2.21	0.40
1:L:487:ASN:HB3	1:L:490:ARG:HG3	2.03	0.40
1:L:541:LEU:HB2	1:L:558:ALA:HB2	2.03	0.40
1:L:638:ASN:O	1:L:642:GLU:HG2	2.21	0.40
3:N:538:ARG:O	5:R:17:HIS:ND1	2.54	0.40
5:R:72:ASN:HB2	5:R:88:GLU:HB3	2.03	0.40
6:U:14:SER:HB2	6:U:301:PHE:CG	2.55	0.40
6:U:187:LEU:HA	6:U:256:THR:CG2	2.51	0.40
4:O:134:SER:OG	4:O:136:ASP:OD1	2.34	0.40
2:C:681:ILE:HD13	2:C:681:ILE:HA	1.91	0.40
5:H:109:VAL:HB	5:H:120:LEU:HD11	2.02	0.40
4:Q:240:ILE:HG22	4:Q:242:THR:HG23	2.04	0.40
6:V:13:LEU:HD23	6:V:71:VAL:HG22	2.03	0.40
1:A:679:MET:O	1:A:683:SER:OG	2.38	0.40
1:A:783:PRO:O	1:A:792:MET:HG2	2.21	0.40
1:B:784:ARG:HA	1:B:791:ASN:HA	2.04	0.40
1:L:433:MET:HE3	1:L:453:TYR:CD1	2.57	0.40
4:Q:41:LYS:HD2	4:Q:47:TRP:CZ2	2.55	0.40
4:Q:284:VAL:HB	4:Q:293:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	420/875 (48%)	412 (98%)	8 (2%)	0	100 100
1	B	661/875 (76%)	628 (95%)	32 (5%)	1 (0%)	44 75
1	L	440/875 (50%)	438 (100%)	2 (0%)	0	100 100
1	T	675/875 (77%)	655 (97%)	20 (3%)	0	100 100
2	C	223/790 (28%)	216 (97%)	7 (3%)	0	100 100
2	M	235/790 (30%)	229 (97%)	6 (3%)	0	100 100
3	D	233/974 (24%)	231 (99%)	1 (0%)	1 (0%)	30 64
3	N	240/974 (25%)	238 (99%)	2 (1%)	0	100 100
4	E	277/360 (77%)	273 (99%)	4 (1%)	0	100 100
4	F	231/360 (64%)	219 (95%)	12 (5%)	0	100 100
4	G	272/360 (76%)	264 (97%)	8 (3%)	0	100 100
4	O	299/360 (83%)	289 (97%)	10 (3%)	0	100 100
4	P	276/360 (77%)	269 (98%)	7 (2%)	0	100 100
4	Q	298/360 (83%)	289 (97%)	9 (3%)	0	100 100
5	H	270/322 (84%)	263 (97%)	7 (3%)	0	100 100
5	R	281/322 (87%)	275 (98%)	6 (2%)	0	100 100
6	U	262/329 (80%)	251 (96%)	6 (2%)	5 (2%)	6 34
6	V	256/329 (78%)	249 (97%)	7 (3%)	0	100 100
All	All	5849/10490 (56%)	5688 (97%)	154 (3%)	7 (0%)	50 79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	U	268	ILE
6	U	279	GLY
6	U	267	ARG
6	U	271	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	U	280	ILE
1	B	353	PHE
3	D	973	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/771 (41%)	317 (100%)	0	100	100
1	B	379/771 (49%)	377 (100%)	2 (0%)	86	93
1	L	363/771 (47%)	363 (100%)	0	100	100
1	T	360/771 (47%)	360 (100%)	0	100	100
2	C	153/677 (23%)	153 (100%)	0	100	100
2	M	198/677 (29%)	198 (100%)	0	100	100
3	D	142/858 (17%)	142 (100%)	0	100	100
3	N	196/858 (23%)	196 (100%)	0	100	100
4	E	178/310 (57%)	178 (100%)	0	100	100
4	F	49/310 (16%)	49 (100%)	0	100	100
4	G	204/310 (66%)	204 (100%)	0	100	100
4	O	251/310 (81%)	251 (100%)	0	100	100
4	P	53/310 (17%)	53 (100%)	0	100	100
4	Q	252/310 (81%)	252 (100%)	0	100	100
5	H	183/272 (67%)	182 (100%)	1 (0%)	86	93
5	R	223/272 (82%)	223 (100%)	0	100	100
6	U	184/284 (65%)	180 (98%)	4 (2%)	47	70
6	V	188/284 (66%)	188 (100%)	0	100	100
All	All	3873/9126 (42%)	3866 (100%)	7 (0%)	91	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ASN
1	B	351	THR
5	H	6	ASN
6	U	267	ARG
6	U	268	ILE
6	U	280	ILE
6	U	281	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	542	ASN
1	A	702	ASN
1	A	821	ASN
1	B	82	GLN
1	B	84	ASN
1	B	542	ASN
1	B	555	ASN
1	B	638	ASN
2	C	785	HIS
3	D	659	HIS
3	D	855	ASN
3	D	936	ASN
4	E	72	GLN
4	E	157	HIS
4	E	198	GLN
4	E	223	HIS
4	F	23	HIS
5	H	62	GLN
1	L	484	GLN
2	M	339	ASN
2	M	647	GLN
2	M	691	ASN
3	N	743	GLN
3	N	843	GLN
3	N	847	ASN
3	N	936	ASN
4	O	102	HIS
4	O	125	HIS
4	O	152	GLN
4	O	198	GLN
4	O	236	HIS
4	P	236	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Q	23	HIS
4	Q	157	HIS
5	R	6	ASN
1	T	431	HIS
1	T	513	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 29 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.

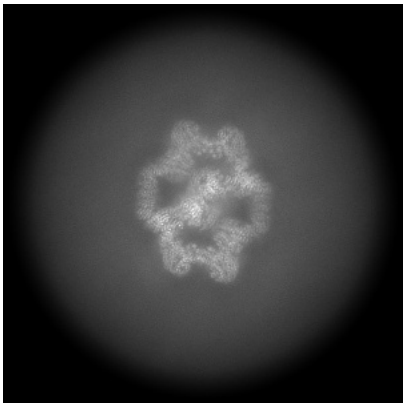
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70833. These allow visual inspection of the internal detail of the map and identification of artifacts.

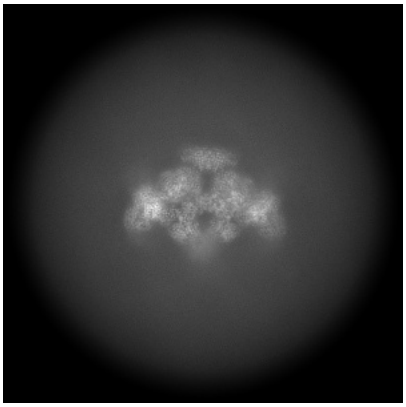
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

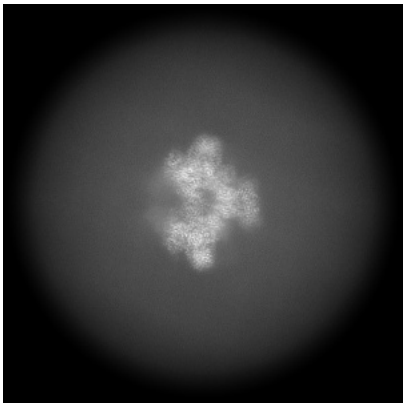
6.1.1 Primary map



X



Y

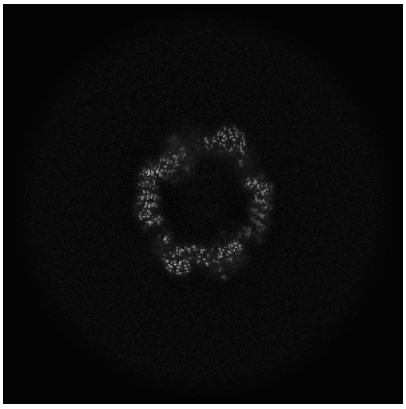


Z

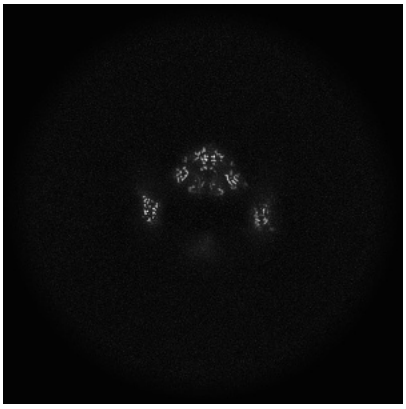
The images above show the map projected in three orthogonal directions.

6.2 Central slices

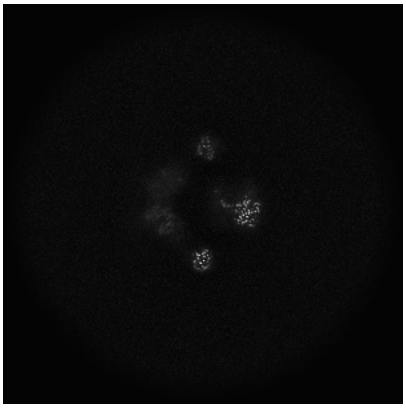
6.2.1 Primary map



X Index: 280



Y Index: 280

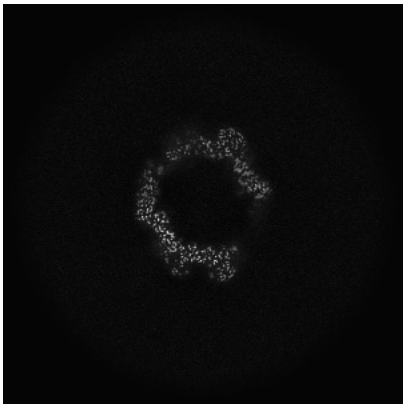


Z Index: 280

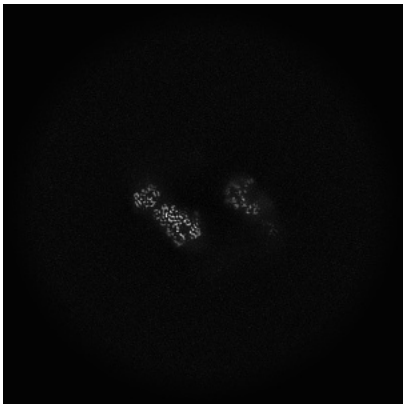
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

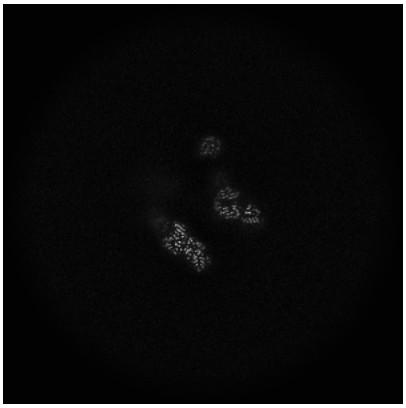
6.3.1 Primary map



X Index: 271



Y Index: 234

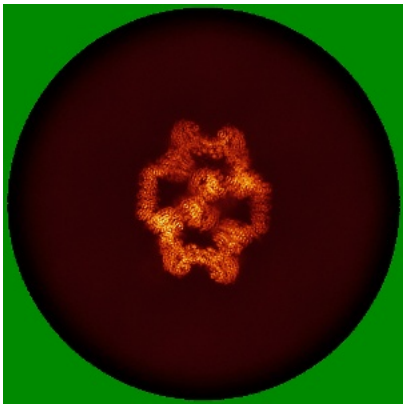


Z Index: 261

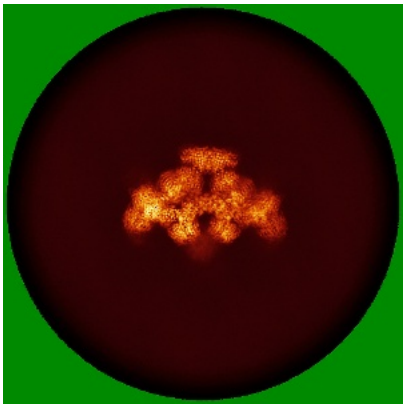
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

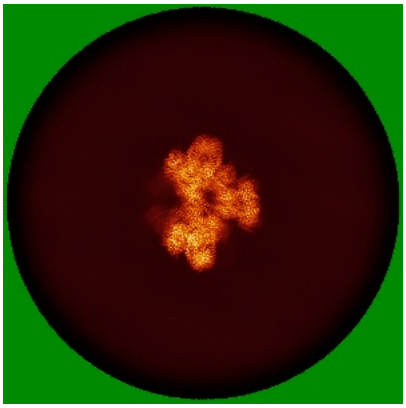
6.4.1 Primary map



X



Y

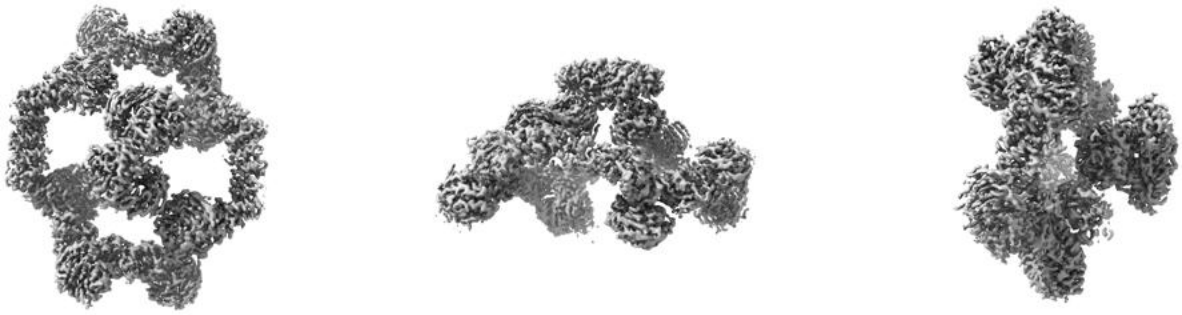


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

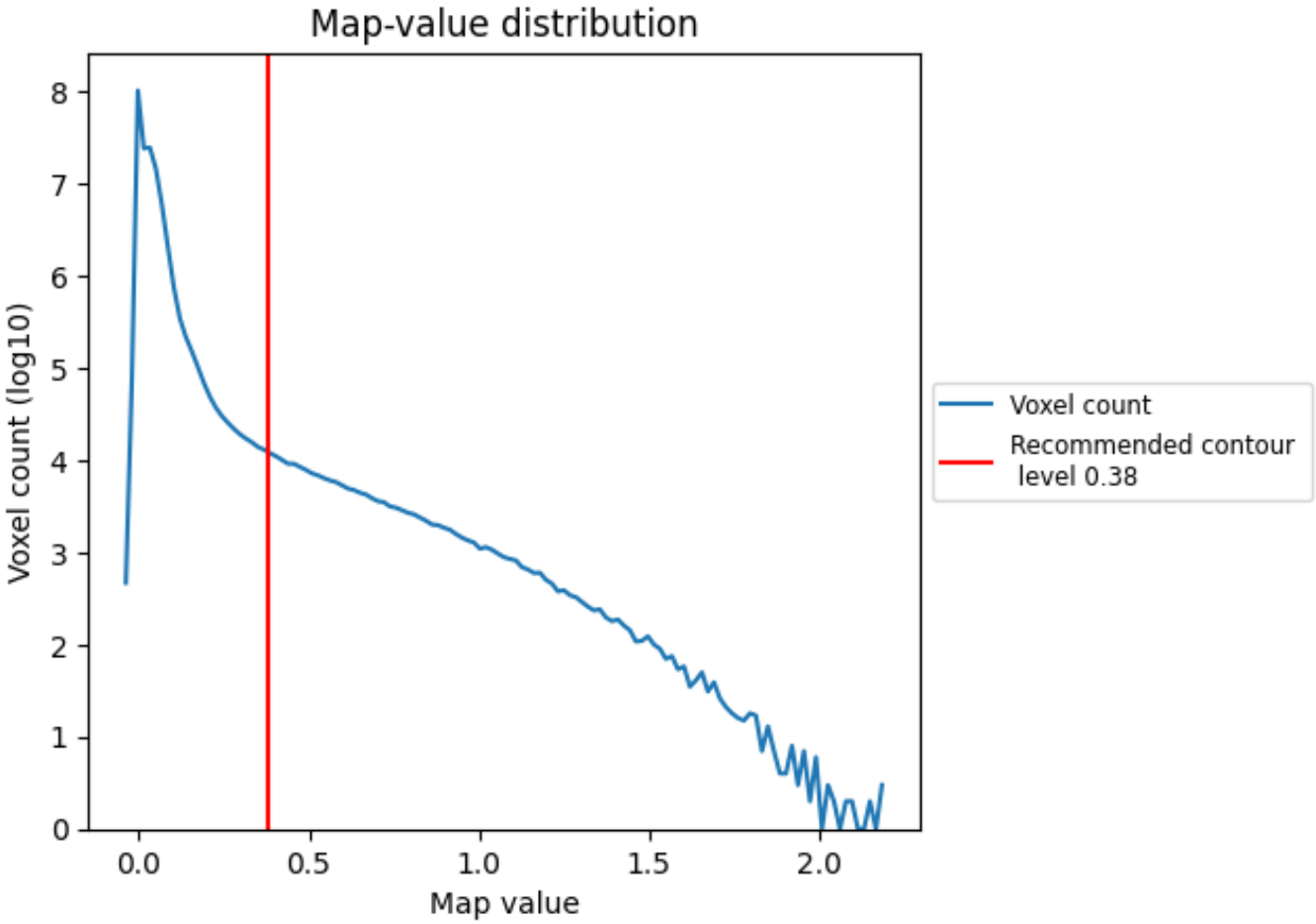
6.6 Mask visualisation (i)

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

7 Map analysis

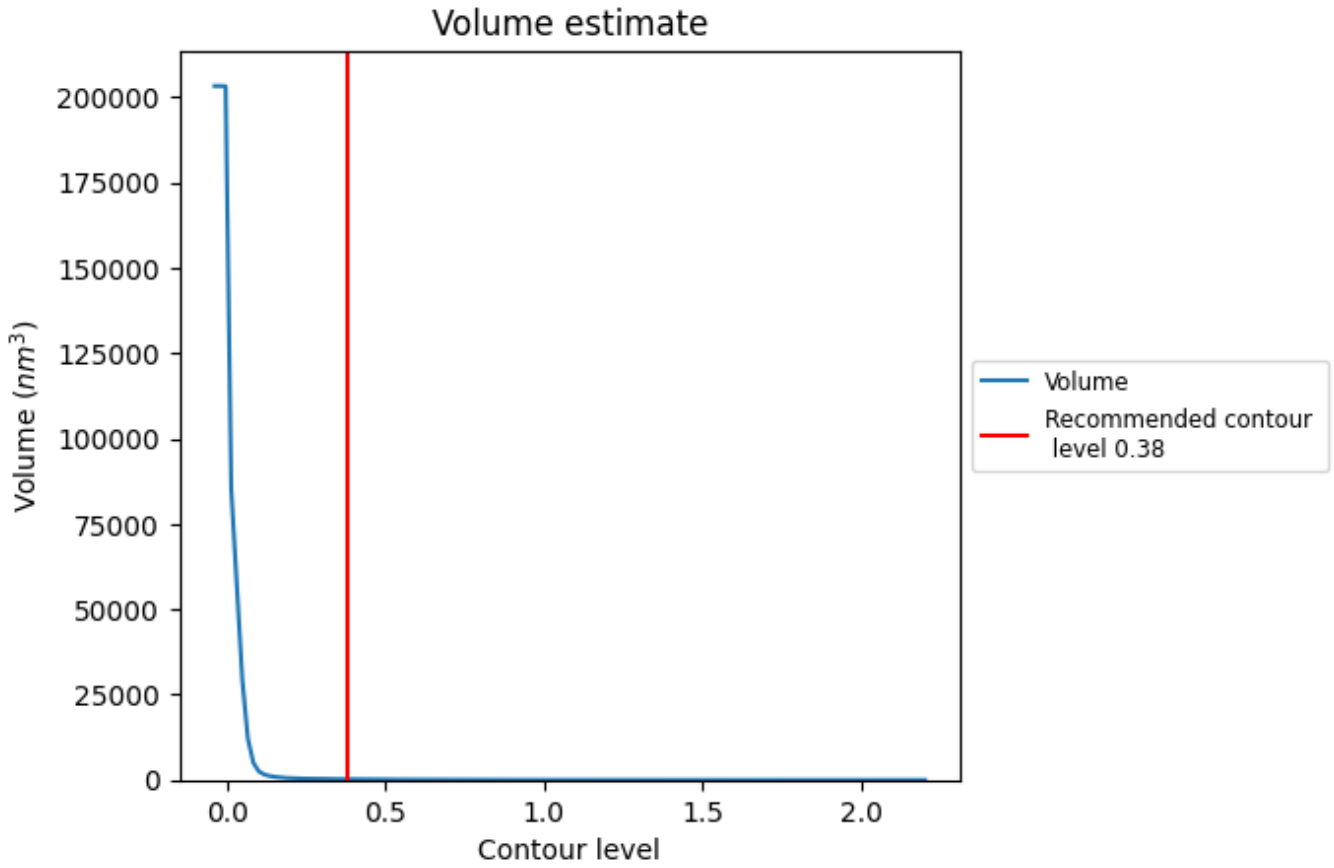
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

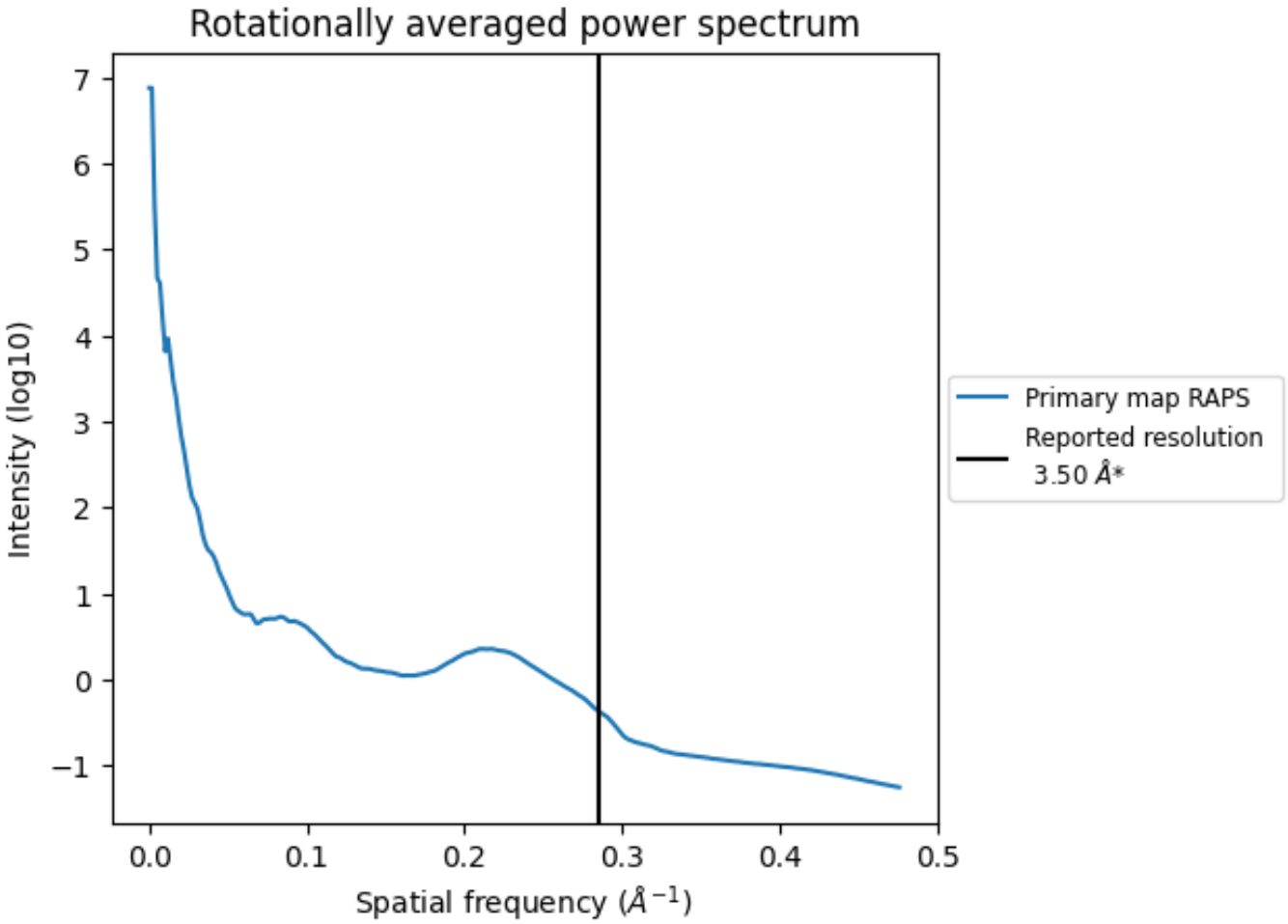
7.2 Volume estimate



The volume at the recommended contour level is 215 nm^3; this corresponds to an approximate mass of 194 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

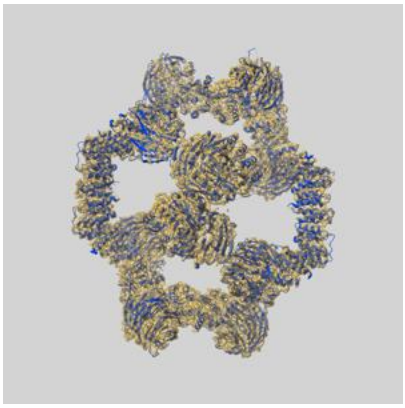
8 Fourier-Shell correlation

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

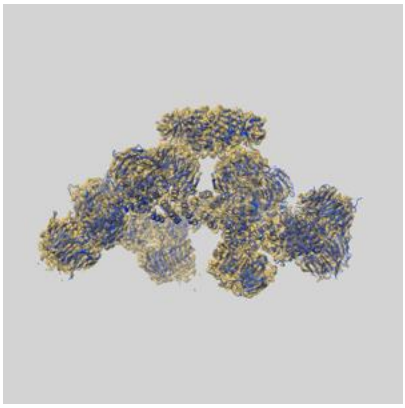
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70833 and PDB model 9OTI. Per-residue inclusion information can be found in section 3 on page 7.

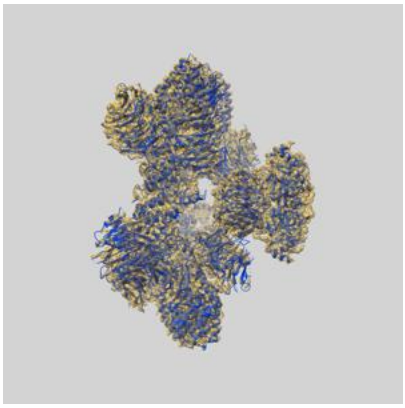
9.1 Map-model overlay



X



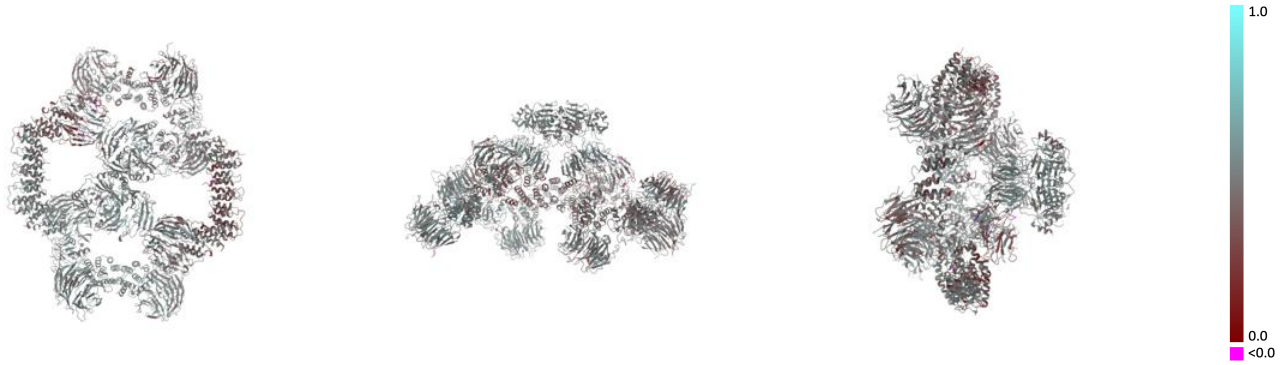
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.38 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.

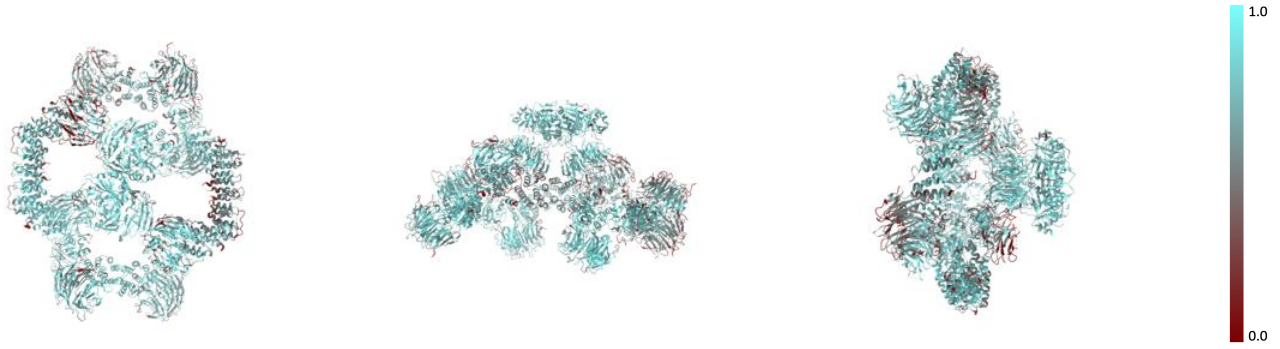
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

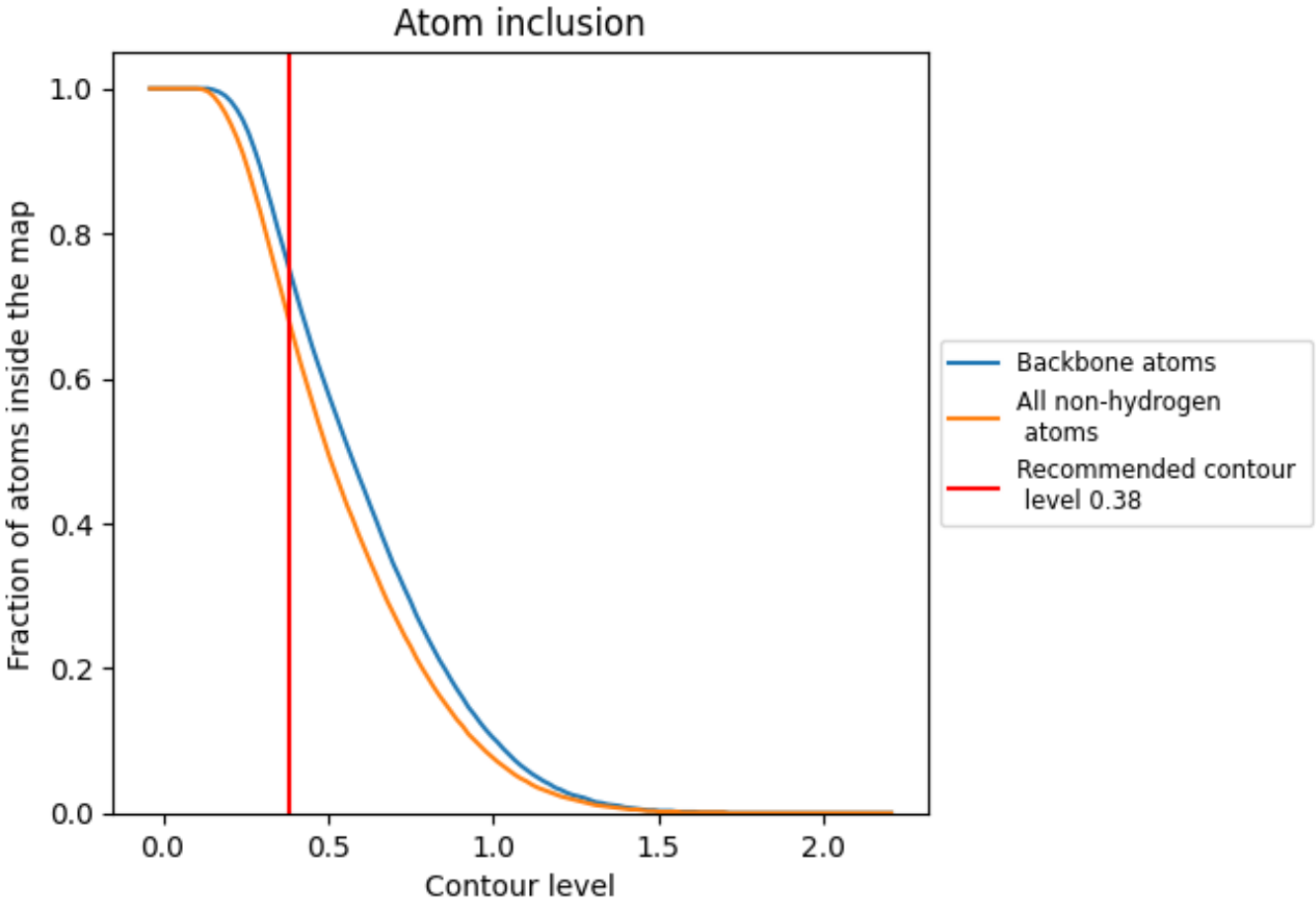
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.38).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6820	0.4730
A	0.6400	0.4340
B	0.6880	0.4600
C	0.6650	0.4670
D	0.6370	0.4590
E	0.7520	0.4720
F	0.4030	0.3860
G	0.5870	0.4540
H	0.4320	0.4300
L	0.7670	0.5030
M	0.7820	0.5210
N	0.7810	0.5100
O	0.7650	0.5060
P	0.6470	0.4480
Q	0.7210	0.5190
R	0.6940	0.4920
T	0.6690	0.4580
U	0.7460	0.4970
V	0.7780	0.4970