



Full wwPDB EM Validation Report ⓘ

Jul 27, 2026 – 01:37 PM EDT

PDB ID : 10JC / pdb_000010jc
EMDB ID : EMD-75213
Title : CCAN dimer purified from budding yeast
Authors : Mengqiu, J.; Sue, B.
Deposited on : 2026-01-22
Resolution : 6.50 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:

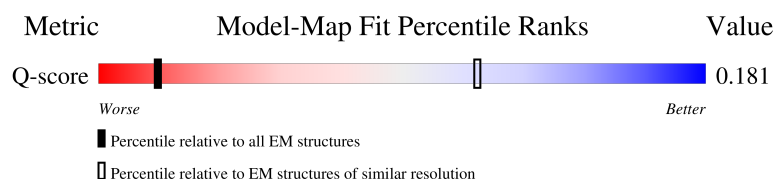
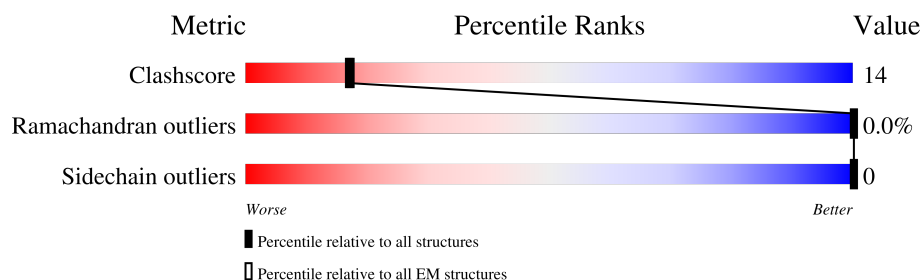
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 6.50 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	556 (6.00 - 7.00)

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 $\leq 5\%$. 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	181	12% 48% 27% 25%
1	B	181	55% 50% 25% 25%
1	H	181	12% 14% 6% 81%
2	C	733	9% 41% 19% 41%

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Mol	Chain	Length	Quality of chain
2	D	733	
2	I	733	
3	E	239	
3	F	239	
3	K	239	
4	T	361	
5	W	89	
6	G	245	
6	L	245	
7	J	458	
7	N	458	
8	M	368	
8	O	368	
9	P	369	
9	R	369	
10	Q	406	
10	S	406	
11	U	324	
11	V	324	
12	Y	238	
12	b	238	
13	Z	153	
13	c	153	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 94342 atoms, of which 47385 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 Inner kinetochore subunit MCM16.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	H	35	Total	C	H	N	O	S	0	0
			552	173	275	44	59	1		
1	A	136	Total	C	H	N	O	S	0	0
			2313	717	1178	203	214	1		
1	B	136	Total	C	H	N	O	S	0	0
			2313	717	1178	203	214	1		

- Molecule 2 is a protein called Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	I	243	Total	C	H	N	O	S	0	0
			3975	1263	2030	330	344	8		
2	C	436	Total	C	H	N	O	S	0	0
			7143	2296	3592	587	646	22		
2	D	436	Total	C	H	N	O	S	0	0
			7143	2296	3592	587	646	22		

- Molecule 3 is a protein called Inner kinetochore subunit MCM22.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	K	101	Total	C	H	N	O	S	0	0
			1661	521	840	140	158	2		
3	E	118	Total	C	H	N	O	S	0	0
			1899	592	958	164	182	3		
3	F	118	Total	C	H	N	O	S	0	0
			1899	592	958	164	182	3		

- Molecule 4 is a protein called Inner kinetochore subunit CNN1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	T	92	Total	C	H	N	O	S	0	0
			1543	488	782	125	144	4		

- Molecule 5 is a protein called Inner kinetochore subunit WIP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	W	69	Total	C	H	N	O	S	0	0
			1111	348	560	96	105	2		

- Molecule 6 is a protein called Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	241	Total	C	H	N	O	S	0	0
			3887	1244	1946	320	366	11		
6	G	241	Total	C	H	N	O	S	0	0
			3887	1244	1946	320	366	11		

- Molecule 7 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	N	391	Total	C	H	N	O	S	0	0
			6390	2053	3224	537	563	13		
7	J	391	Total	C	H	N	O	S	0	0
			6390	2053	3224	537	563	13		

- Molecule 8 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	O	241	Total	C	H	N	O	S	0	0
			3976	1277	1997	328	369	5		
8	M	241	Total	C	H	N	O	S	0	0
			3976	1277	1997	328	369	5		

- Molecule 9 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	P	257	Total	C	H	N	O	S	0	0
			4308	1358	2192	366	378	14		
9	R	257	Total	C	H	N	O	S	0	0
			4308	1358	2192	366	378	14		

- Molecule 10 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	Q	258	Total	C	H	N	O	S	0	0
			4339	1355	2195	375	405	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	S	258	Total	C	H	N	O	S	0	0
			4339	1355	2195	375	405	9		

- Molecule 11 is a protein called K7_Ame1p.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	U	184	Total	C	H	N	O	S	0	0
			2953	928	1468	255	299	3		
11	V	184	Total	C	H	N	O	S	0	0
			2953	928	1468	255	299	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	269	GLU	GLY	conflict	UNP G2W9L4
V	269	GLU	GLY	conflict	UNP G2W9L4

- Molecule 12 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Y	223	Total	C	H	N	O	S	0	0
			3253	1027	1590	281	349	6		
12	b	223	Total	C	H	N	O	S	0	0
			3253	1027	1590	281	349	6		

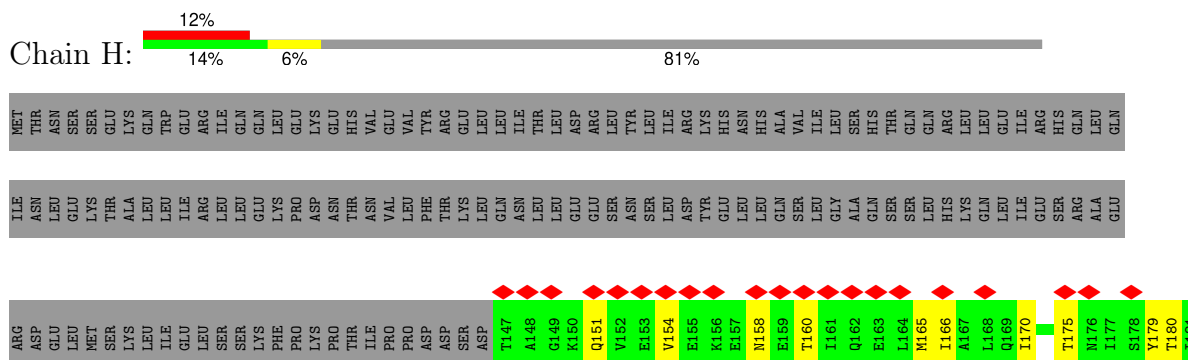
- Molecule 13 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Z	151	Total	C	H	N	O	S	0	0
			2289	740	1109	204	235	1		
13	c	151	Total	C	H	N	O	S	0	0
			2289	740	1109	204	235	1		

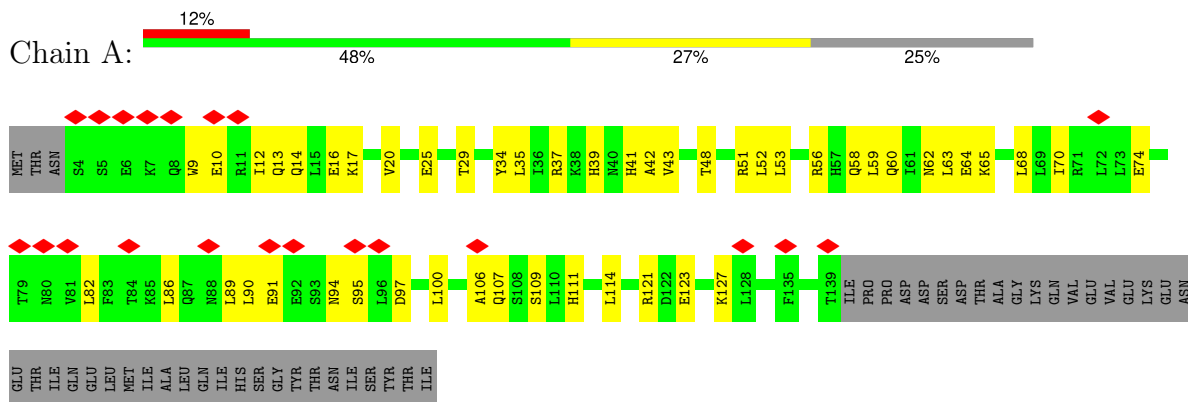
3 Residue-property plots

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

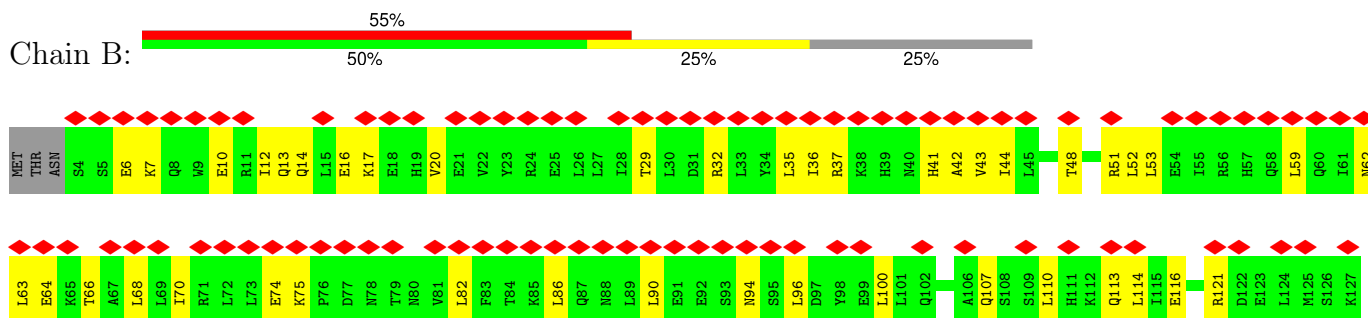
• Molecule 1: Inner kinetochore subunit MCM16

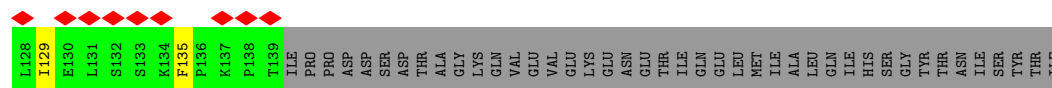


• Molecule 1: Inner kinetochore subunit MCM16

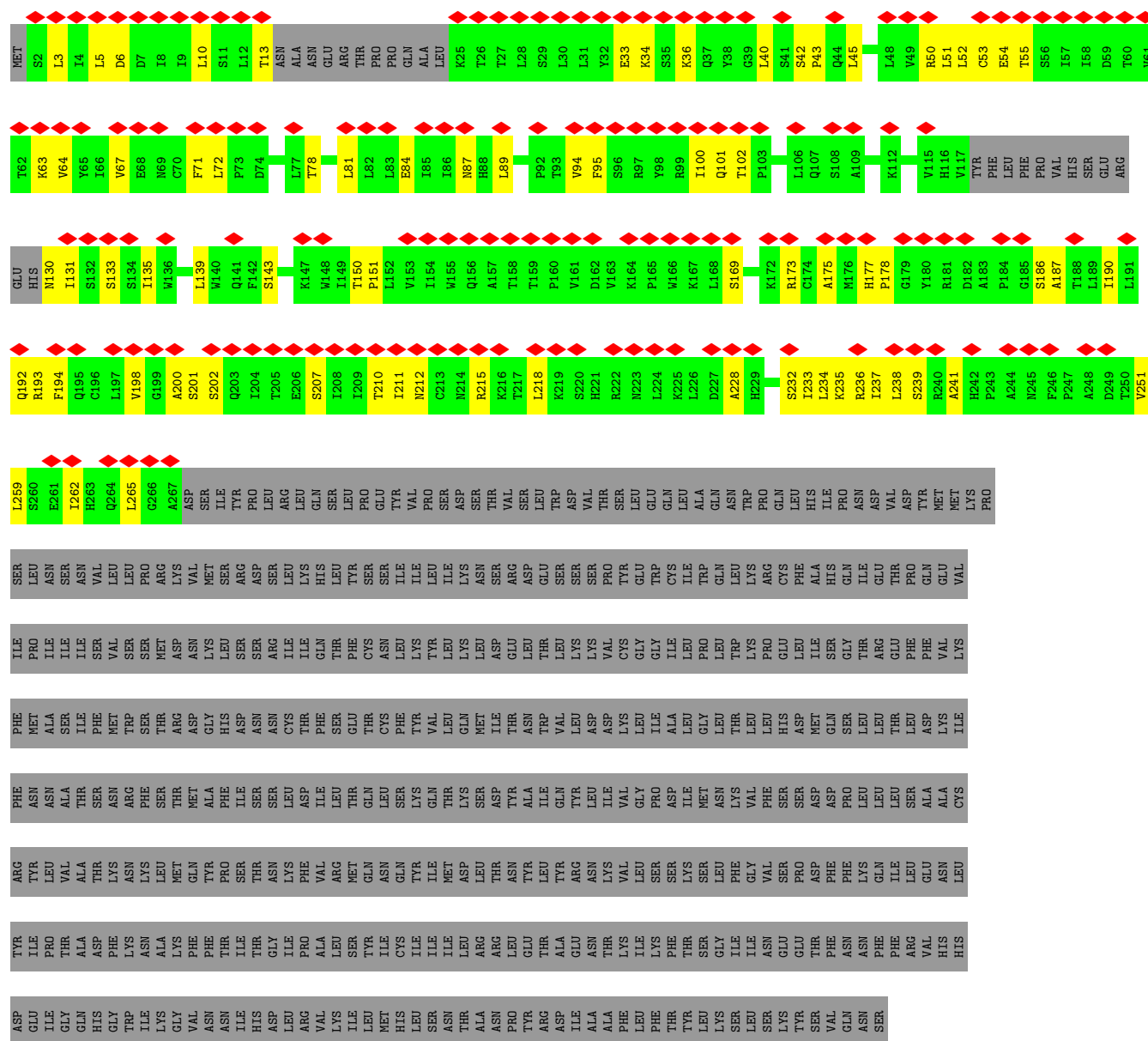


• Molecule 1: Inner kinetochore subunit MCM16

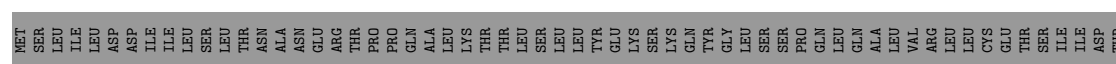


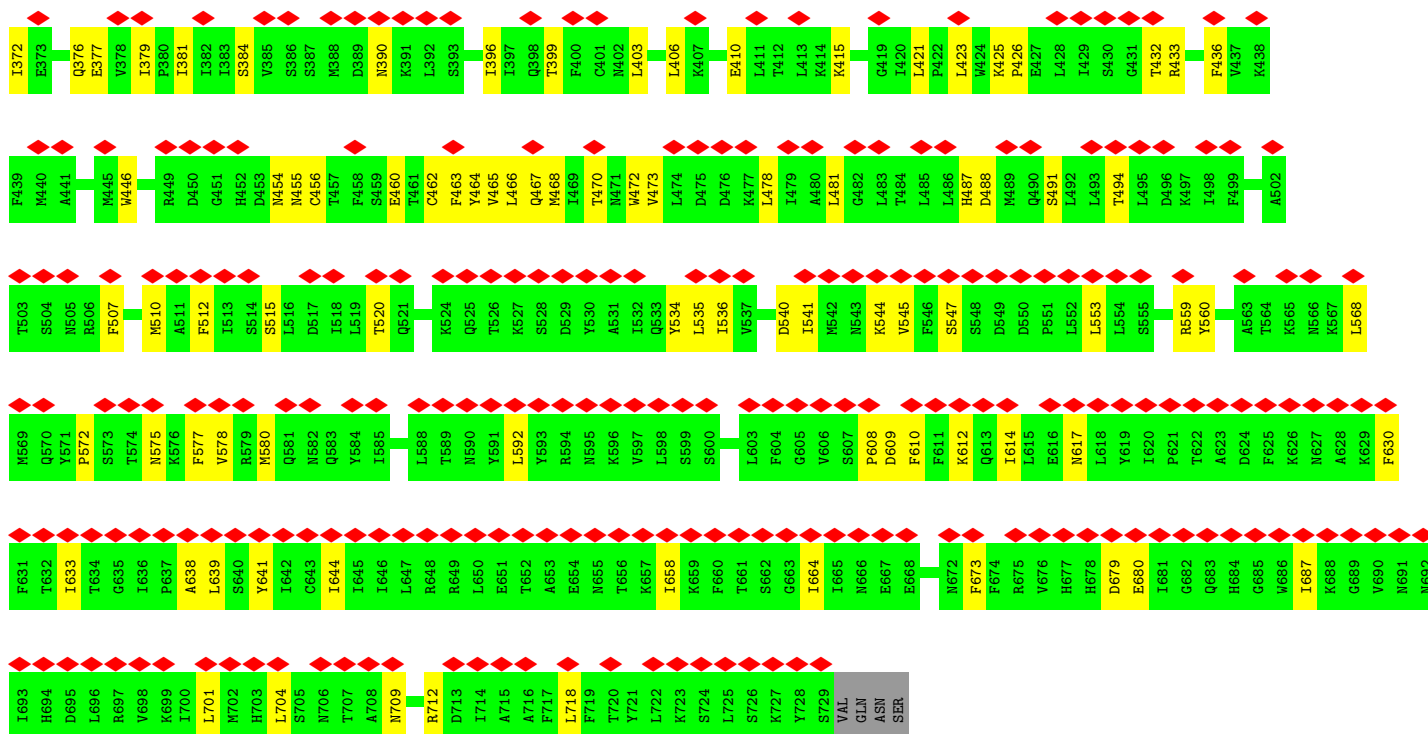


• Molecule 2: Inner kinetochore subunit CTF3

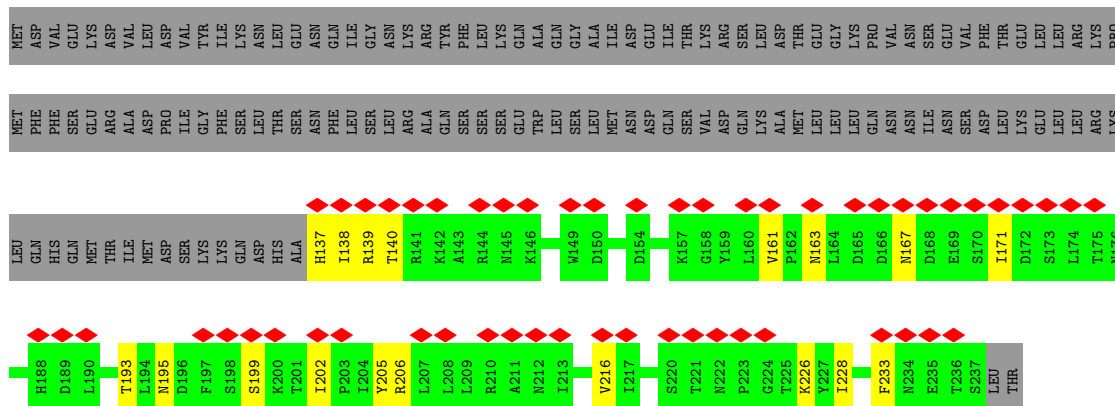
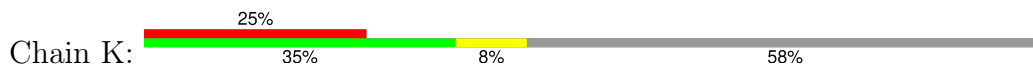


• Molecule 2: Inner kinetochore subunit CTF3

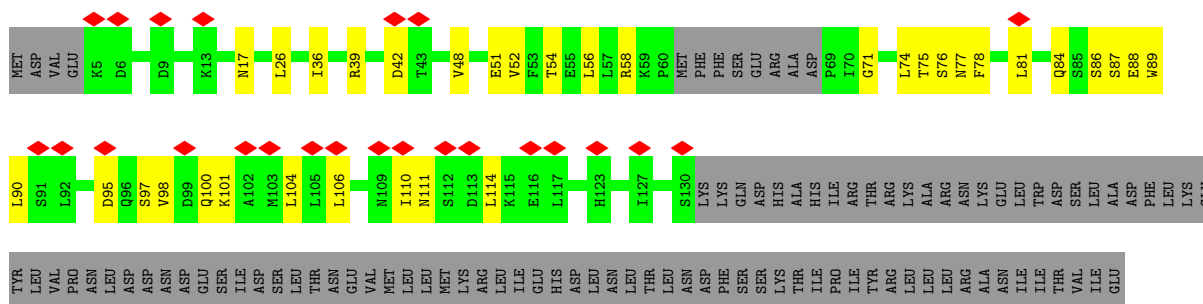
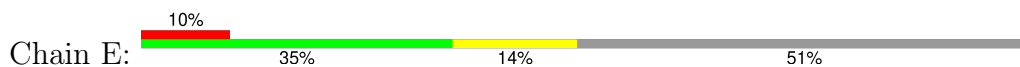




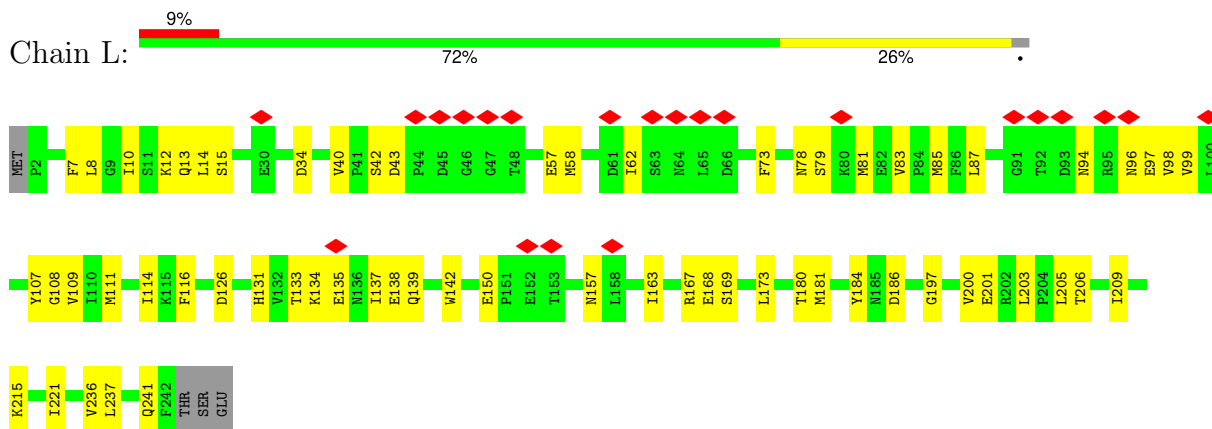
• Molecule 3: Inner kinetochore subunit MCM22



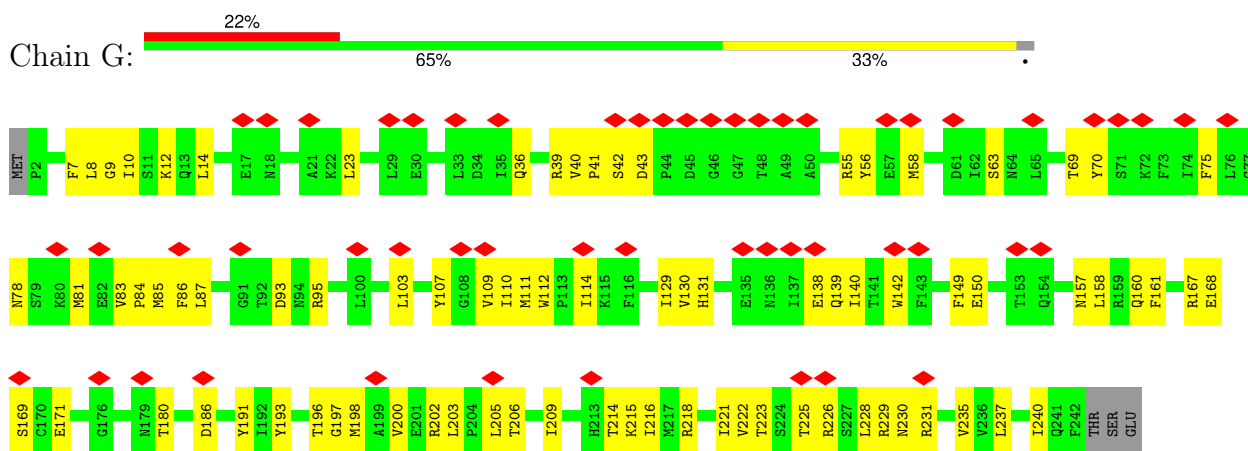
• Molecule 3: Inner kinetochore subunit MCM22



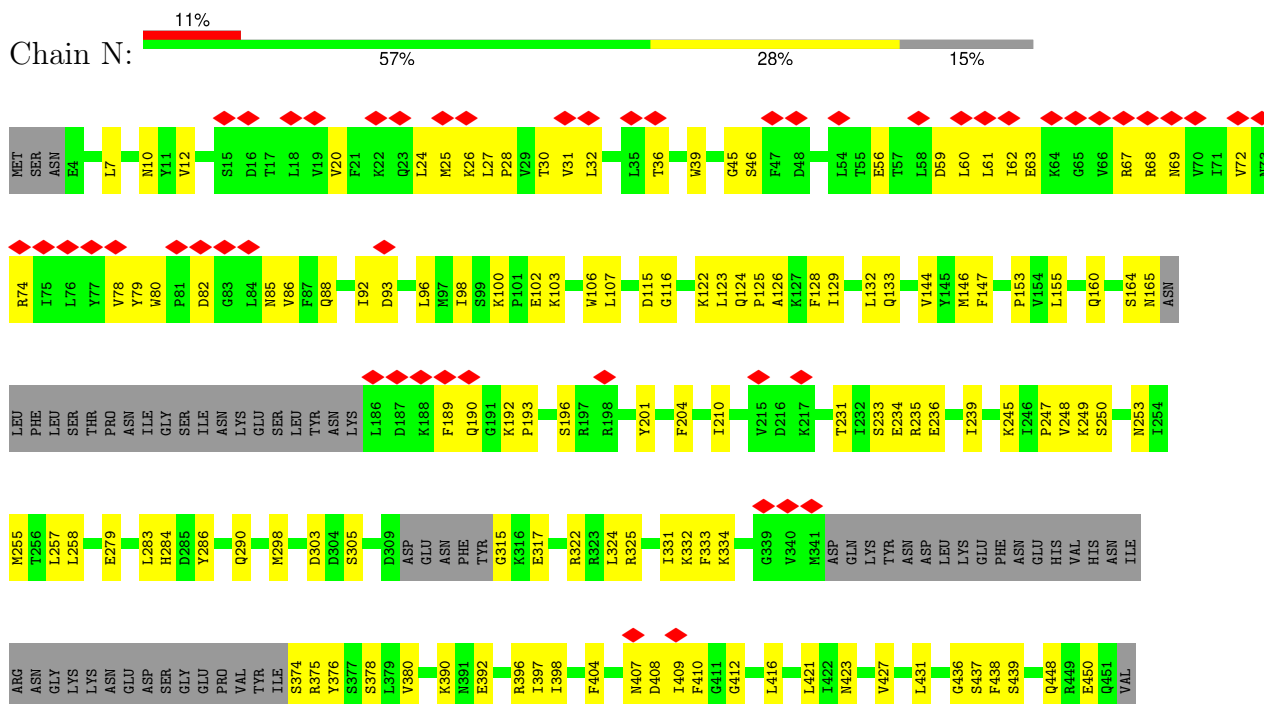
• Molecule 6: Inner kinetochore subunit IML3



• Molecule 6: Inner kinetochore subunit IML3



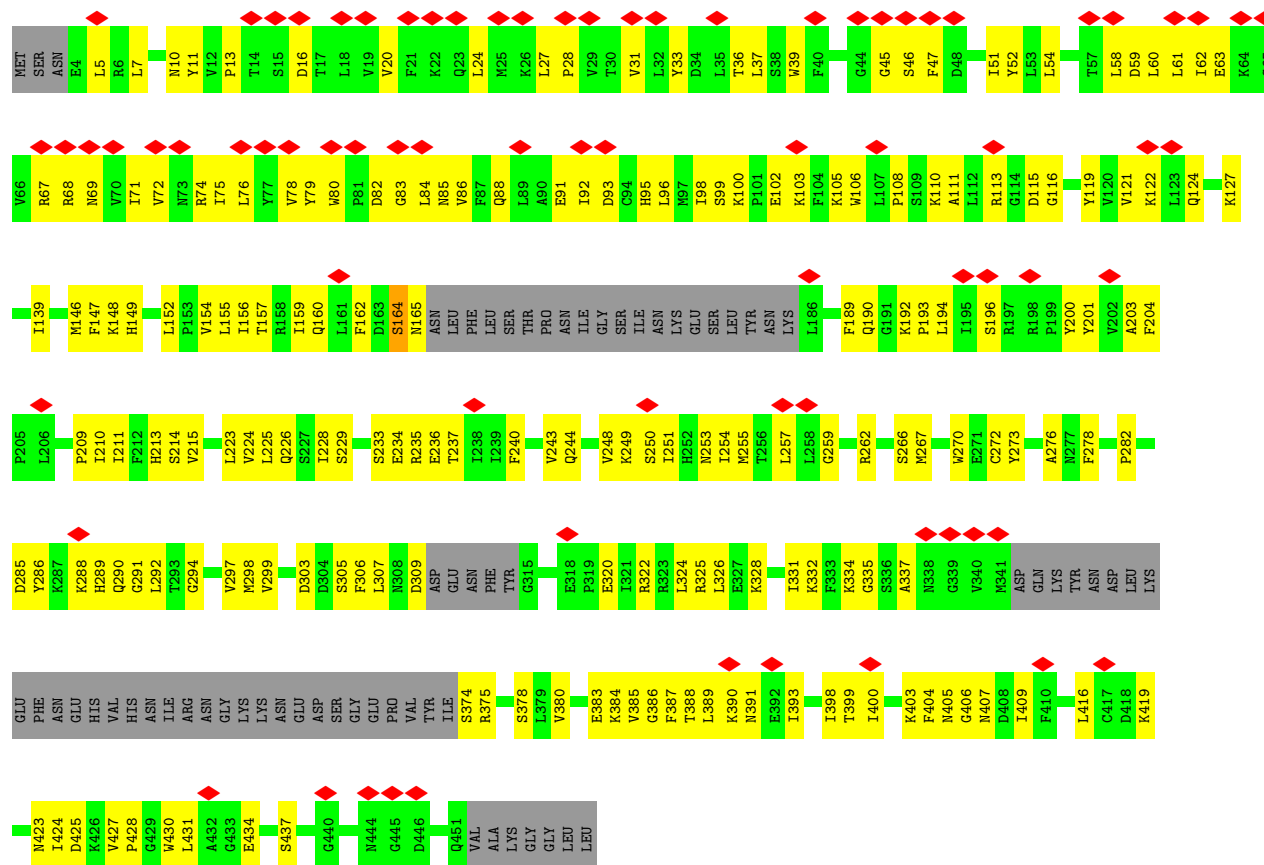
• Molecule 7: Inner kinetochore subunit CHL4



ALA
LYS
GLY
GLY
LEU
LEU

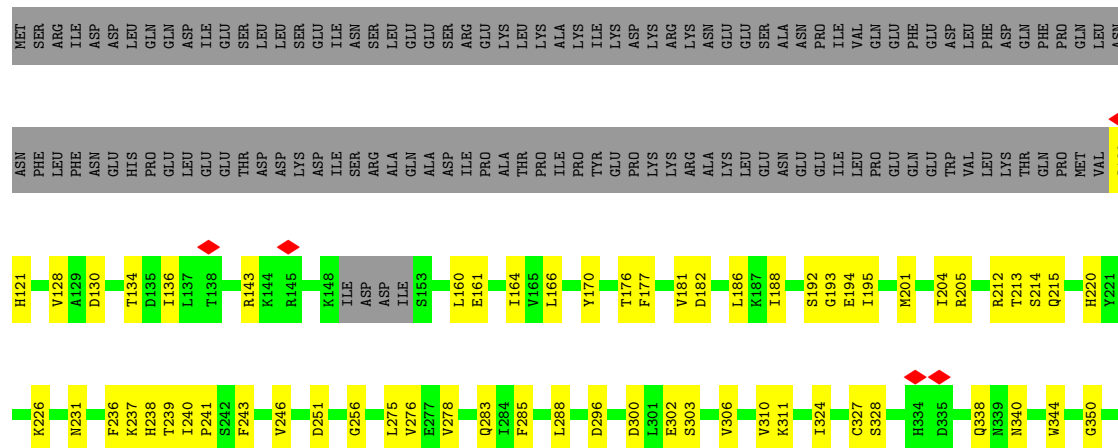
• Molecule 7: Inner kinetochore subunit CHL4

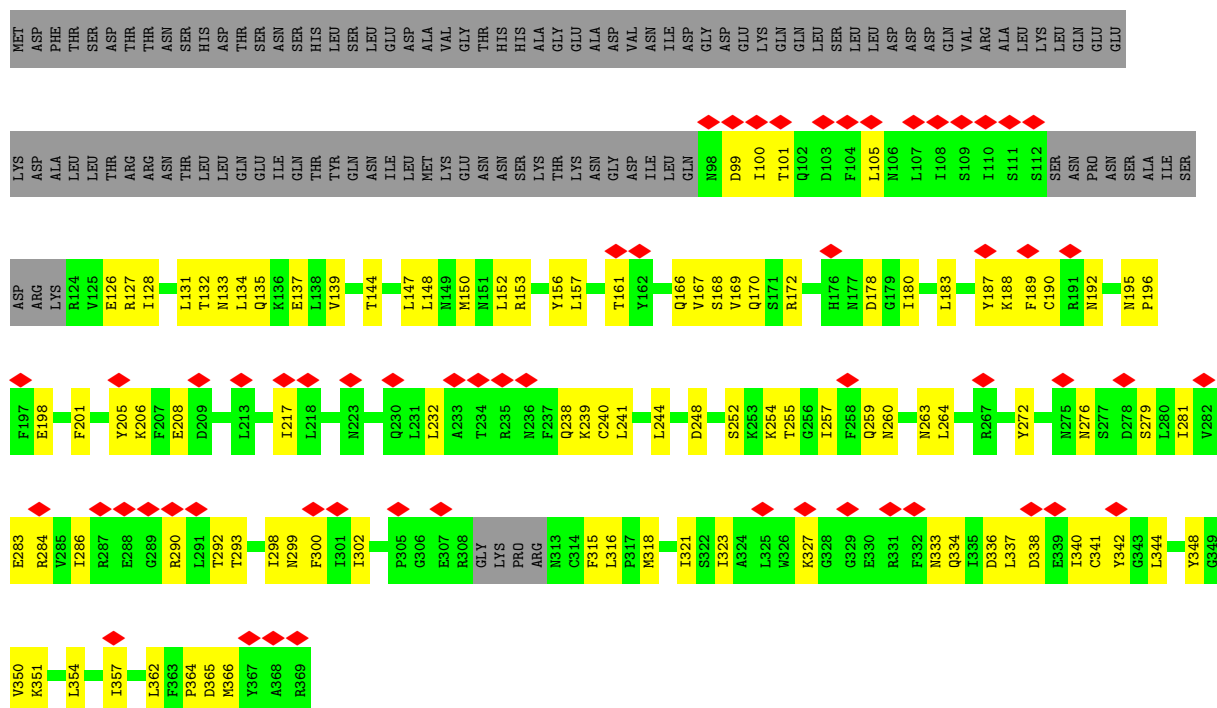
Chain J: 



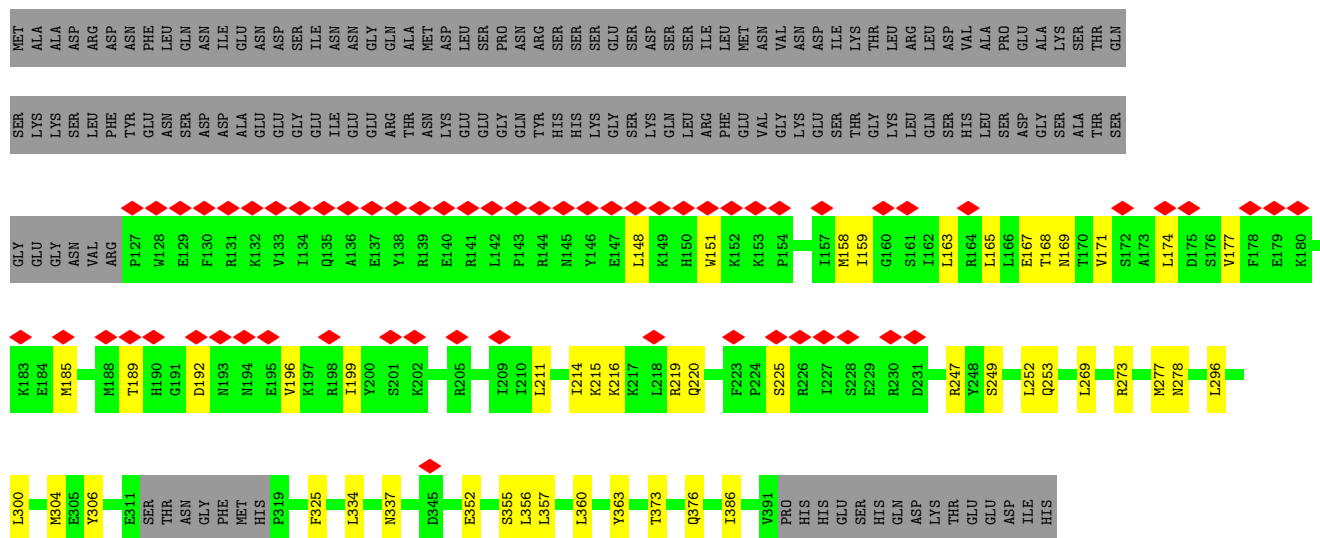
• Molecule 8: Inner kinetochore subunit MCM21

Chain O: 

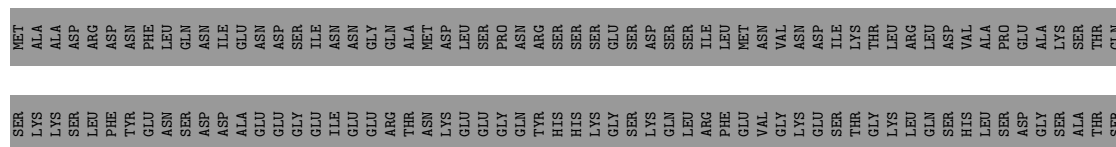
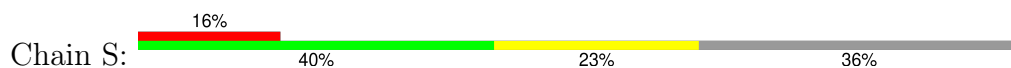




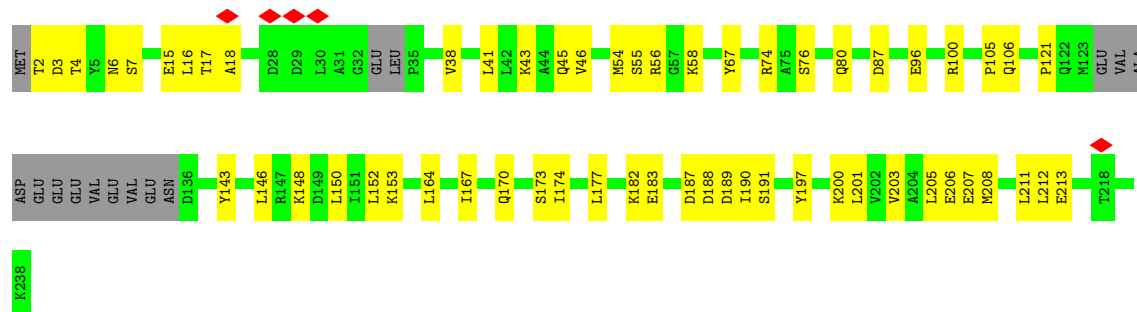
• Molecule 10: Inner kinetochore subunit OKP1



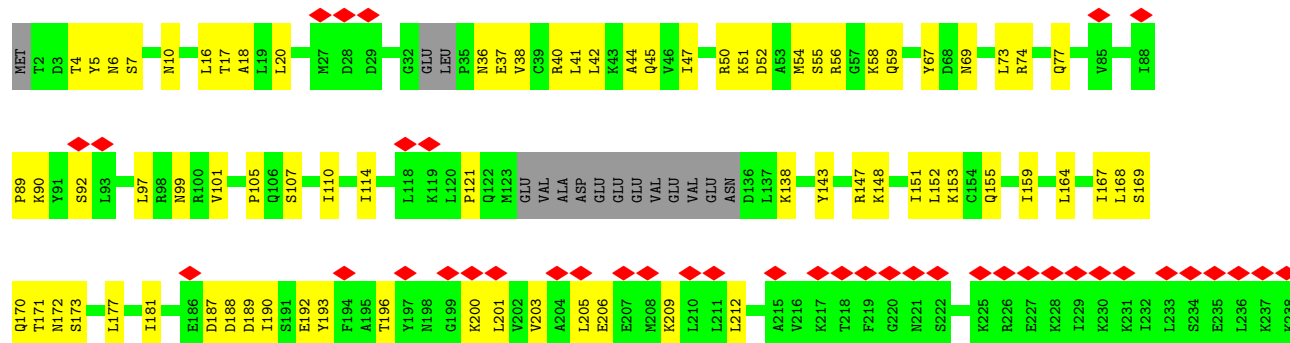
• Molecule 10: Inner kinetochore subunit OKP1



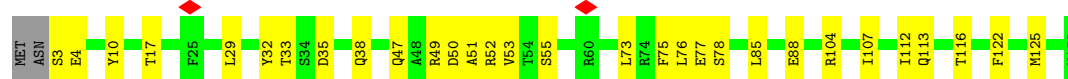
Chain Y: 69% 24% 6%



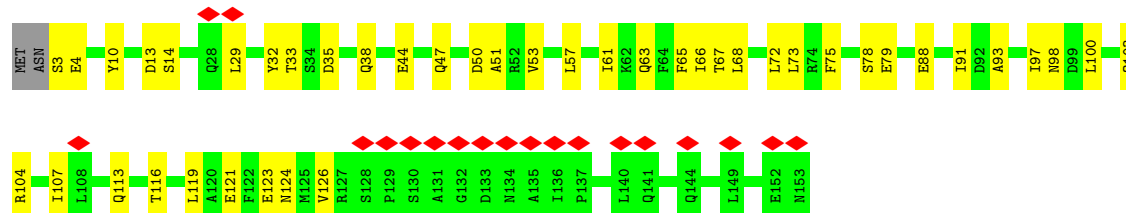
Chain b:



Chain Z: 79% 20%



Chain c:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.921	Depositor
Minimum map value	-1.182	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.394	Depositor
Map size (Å)	457.96002, 457.96002, 457.96002	wwPDB
Map dimensions	214, 214, 214	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.14, 2.14, 2.14	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/1150	0.37	0/1548
1	B	0.17	0/1150	0.40	0/1548
1	H	0.15	0/279	0.34	0/375
2	C	0.18	0/3632	0.35	1/4917 (0.0%)
2	D	0.15	0/3632	0.33	0/4917
2	I	0.15	0/1988	0.38	0/2706
3	E	0.18	0/951	0.33	0/1277
3	F	0.15	0/951	0.28	0/1277
3	K	0.13	0/833	0.33	0/1127
4	T	0.13	0/772	0.35	0/1040
5	W	0.13	0/557	0.33	0/748
6	G	0.20	0/1981	0.39	0/2684
6	L	0.21	0/1981	0.38	1/2684 (0.0%)
7	J	0.25	0/3239	0.41	0/4372
7	N	0.22	0/3239	0.37	0/4372
8	M	0.21	0/2017	0.38	0/2713
8	O	0.21	0/2017	0.33	0/2713
9	P	0.22	0/2149	0.36	0/2888
9	R	0.21	0/2149	0.36	0/2888
10	Q	0.20	0/2175	0.35	0/2913
10	S	0.22	0/2175	0.42	0/2913
11	U	0.22	0/1499	0.35	0/2018
11	V	0.21	0/1499	0.41	0/2018
12	Y	0.21	0/1672	0.38	0/2252
12	b	0.24	0/1672	0.44	0/2252
13	Z	0.20	0/1195	0.30	0/1616
13	c	0.23	0/1195	0.37	0/1616
All	All	0.20	0/47749	0.37	2/64392 (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
2	I	0	1
12	Y	0	1
12	b	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	498	ILE	N-CA-C	-5.50	107.50	112.12
6	L	62	ILE	N-CA-C	-5.20	107.51	111.62

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	201	SER	Peptide
12	Y	187	ASP	Peptide
12	b	187	ASP	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	1135	1178	1177	49	0
1	B	1135	1178	1177	51	0
1	H	277	275	274	8	0
2	C	3551	3592	3590	103	0
2	D	3551	3592	3590	86	0
2	I	1945	2030	2025	53	0
3	E	941	958	957	34	0
3	F	941	958	957	37	0
3	K	821	840	839	17	0
4	T	761	782	781	15	0
5	W	551	560	559	9	0
6	G	1941	1946	1946	74	0
6	L	1941	1946	1946	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	3166	3224	3220	170	0
7	N	3166	3224	3220	107	0
8	M	1979	1997	1995	67	0
8	O	1979	1997	1995	50	0
9	P	2116	2192	2189	53	0
9	R	2116	2192	2189	82	0
10	Q	2144	2195	2195	48	0
10	S	2144	2195	2195	88	0
11	U	1485	1468	1465	41	0
11	V	1485	1468	1465	78	0
12	Y	1663	1590	1588	44	0
12	b	1663	1590	1588	70	0
13	Z	1180	1109	1108	22	0
13	c	1180	1109	1108	35	0
All	All	46957	47385	47338	1298	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 14.

All (1298) 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)
10:S:141:ARG:O	10:S:141:ARG:NE	1.97	0.97
8:M:247:GLN:NE2	8:M:251:ASP:OD2	1.98	0.96
10:Q:185:MET:HE1	10:Q:199:ILE:HD12	1.47	0.94
8:M:300:ASP:OD1	8:M:303:SER:N	2.02	0.92
7:J:244:GLN:NE2	7:J:437:SER:O	2.03	0.92
1:A:37:ARG:NH2	8:O:130:ASP:OD2	2.04	0.90
13:c:75:PHE:O	13:c:78:SER:OG	1.89	0.90
6:G:55:ARG:NH2	6:G:228:LEU:O	2.05	0.90
10:Q:249:SER:OG	12:Y:6:ASN:OD1	1.90	0.88
9:P:235:ARG:O	9:P:239:LYS:NZ	2.07	0.87
10:S:183:LYS:NZ	10:S:184:GLU:OE2	2.09	0.86
7:J:233:SER:OG	7:J:236:GLU:O	1.91	0.86
10:S:187:GLN:NE2	10:S:188:MET:SD	2.48	0.86
11:U:302:TYR:OH	12:Y:183:GLU:OE2	1.95	0.84
2:D:415:LYS:NZ	3:F:99:ASP:OD2	2.11	0.84
12:Y:121:PRO:O	12:Y:143:TYR:OH	1.96	0.84
7:N:233:SER:OG	7:N:236:GLU:O	1.96	0.82
2:I:192:GLN:NE2	2:I:265:LEU:O	2.13	0.82
7:N:93:ASP:OD2	7:N:201:TYR:OH	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:LEU:O	2:I:13:THR:OG1	1.97	0.81
10:S:283:ASN:OD1	11:V:243:GLN:NE2	2.14	0.81
7:N:439:SER:OG	7:N:450:GLU:OE2	1.96	0.81
7:N:122:LYS:NZ	8:O:302:GLU:OE2	2.13	0.80
7:J:122:LYS:NZ	8:M:302:GLU:OE2	2.15	0.80
7:J:282:PRO:O	8:M:168:ASN:ND2	2.15	0.80
10:Q:253:GLN:OE1	12:Y:2:THR:OG1	2.00	0.80
6:L:10:ILE:HD12	6:L:85:MET:HG2	1.62	0.79
11:V:288:ASN:OD1	11:V:289:ILE:N	2.14	0.79
12:b:6:ASN:OD1	12:b:10:ASN:ND2	2.16	0.79
1:B:68:LEU:HD21	3:F:71:GLY:HA3	1.64	0.78
6:G:191:TYR:OH	7:J:391:ASN:OD1	2.00	0.78
7:J:165:ASN:ND2	7:J:193:PRO:O	2.15	0.78
2:D:377:GLU:N	2:D:377:GLU:OE1	2.15	0.78
1:B:100:LEU:HD23	2:D:510:MET:CE	2.13	0.78
7:J:85:ASN:OD1	7:J:86:VAL:N	2.18	0.77
2:I:33:GLU:OE2	2:I:34:LYS:NZ	2.17	0.77
1:A:91:GLU:O	1:A:95:SER:OG	2.03	0.77
7:N:315:GLY:N	7:N:317:GLU:OE2	2.19	0.76
2:I:50:ARG:NH1	2:I:84:GLU:OE2	2.19	0.76
2:C:511:ALA:O	2:C:514:SER:OG	2.04	0.75
4:T:298:TRP:CE3	4:T:301:ILE:HD11	2.21	0.74
2:C:294:THR:N	2:C:298:GLN:OE1	2.17	0.74
9:R:279:SER:OG	9:R:299:ASN:OD1	2.00	0.74
13:c:32:TYR:HD1	13:c:33:THR:HG23	1.51	0.74
9:P:177:ASN:OD1	9:P:178:ASP:N	2.20	0.73
4:T:337:VAL:HG23	4:T:340:MET:HE2	1.71	0.73
6:L:78:ASN:HB3	6:L:81:MET:HE2	1.69	0.73
6:G:149:PHE:HE1	6:G:205:LEU:HD13	1.53	0.73
2:D:709:ASN:O	2:D:712:ARG:NE	2.21	0.72
12:b:153:LYS:NZ	13:c:98:ASN:OD1	2.21	0.72
6:G:93:ASP:OD2	6:G:95:ARG:NH2	2.23	0.71
11:U:146:PHE:HD1	11:U:150:LEU:HD12	1.55	0.71
1:B:107:GLN:OE1	2:D:467:GLN:NE2	2.22	0.71
2:D:403:LEU:HD12	2:D:406:LEU:HD23	1.72	0.71
7:N:378:SER:OG	7:N:408:ASP:OD2	2.02	0.71
7:N:85:ASN:OD1	7:N:86:VAL:N	2.23	0.71
13:c:75:PHE:O	13:c:79:GLU:OE1	2.09	0.71
9:P:166:GLN:NE2	9:P:190:CYS:SG	2.63	0.71
6:G:197:GLY:O	7:J:423:ASN:N	2.24	0.71
8:O:192:SER:OG	8:O:194:GLU:OE2	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:155:LEU:O	7:J:204:PHE:N	2.21	0.70
13:c:4:GLU:OE2	13:c:4:GLU:N	2.24	0.70
7:N:124:GLN:N	7:N:124:GLN:OE1	2.24	0.70
1:A:68:LEU:HD21	3:E:71:GLY:HA3	1.71	0.70
2:D:381:ILE:O	2:D:384:SER:OG	2.08	0.70
2:I:36:LYS:O	2:I:237:ILE:HD11	1.92	0.69
11:V:186:THR:OG1	11:V:187:ARG:NH1	2.25	0.69
7:N:46:SER:N	7:N:79:TYR:O	2.25	0.69
7:N:427:VAL:HG23	7:N:431:LEU:HD23	1.72	0.69
1:A:90:LEU:HD13	2:C:641:TYR:CD1	2.27	0.69
1:B:42:ALA:HB1	3:F:48:VAL:HG22	1.75	0.69
6:G:149:PHE:HZ	6:G:200:VAL:HG23	1.56	0.69
11:V:288:ASN:O	11:V:292:ILE:HD12	1.93	0.69
12:b:167:ILE:HD11	13:c:119:LEU:HD11	1.74	0.69
2:I:207:SER:O	2:I:210:THR:OG1	2.07	0.68
1:A:121:ARG:HH22	3:E:110:ILE:HG23	1.58	0.68
7:N:7:LEU:O	7:N:133:GLN:NE2	2.26	0.68
13:Z:88:GLU:N	13:Z:88:GLU:OE1	2.27	0.68
7:J:389:LEU:HD21	7:J:391:ASN:OD1	1.93	0.68
2:D:535:LEU:O	2:D:560:TYR:OH	2.10	0.68
10:S:235:GLU:OE1	10:S:235:GLU:N	2.25	0.68
6:G:7:PHE:HB3	6:G:114:ILE:HD12	1.76	0.68
3:E:100:GLN:O	3:E:104:LEU:HD23	1.92	0.68
10:Q:252:LEU:HD22	12:Y:67:TYR:HE2	1.57	0.68
10:S:363:TYR:CE1	12:b:167:ILE:HD13	2.29	0.68
2:C:679:ASP:OD1	2:C:680:GLU:N	2.27	0.68
9:R:284:ARG:NH2	9:R:365:ASP:OD1	2.27	0.68
2:I:51:LEU:O	2:I:55:THR:HG22	1.94	0.67
3:E:84:GLN:O	3:E:87:SER:OG	2.12	0.67
1:B:100:LEU:HB3	2:D:510:MET:HE1	1.77	0.67
2:I:239:SER:OG	10:S:144:ARG:NH1	2.23	0.67
7:N:160:GLN:NE2	7:N:196:SER:OG	2.28	0.67
1:B:64:GLU:O	1:B:68:LEU:HD23	1.94	0.67
10:S:188:MET:HE3	11:V:169:LEU:HD13	1.76	0.67
9:R:327:LYS:HD3	11:V:263:LEU:HD12	1.77	0.67
2:D:421:LEU:HD21	2:D:465:VAL:HG12	1.77	0.67
10:S:208:GLU:O	10:S:212:THR:HG23	1.95	0.67
2:I:236:ARG:CZ	10:S:144:ARG:HE	2.08	0.67
9:P:141:LYS:NZ	9:P:145:LEU:O	2.27	0.67
3:F:17:ASN:O	8:M:143:ARG:NH1	2.28	0.67
8:O:300:ASP:OD1	8:O:303:SER:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:7:PHE:C	6:G:8:LEU:HD12	2.21	0.66
6:G:81:MET:HE1	6:G:237:LEU:HD21	1.77	0.66
12:b:73:LEU:O	12:b:77:GLN:NE2	2.28	0.66
2:C:512:PHE:O	2:C:515:SER:OG	2.13	0.66
7:J:299:VAL:HG23	9:R:126:GLU:OE2	1.95	0.66
8:M:283:GLN:NE2	8:M:287:ASP:OD2	2.29	0.66
2:D:312:VAL:HG21	2:D:355:SER:HB2	1.76	0.66
6:L:126:ASP:OD1	6:L:184:TYR:N	2.27	0.66
10:Q:269:LEU:HD13	11:U:226:GLU:OE1	1.95	0.66
2:C:351:ASP:OD2	2:C:353:SER:OG	2.13	0.65
13:c:50:ASP:OD1	13:c:51:ALA:N	2.29	0.65
2:I:194:PHE:O	2:I:198:VAL:HG12	1.95	0.65
13:c:93:ALA:O	13:c:97:ILE:HD12	1.96	0.65
8:M:220:HIS:ND1	8:M:239:THR:O	2.27	0.65
11:U:275:SER:OG	11:U:276:GLN:N	2.29	0.65
6:L:81:MET:HE1	6:L:237:LEU:HD21	1.77	0.65
6:G:157:ASN:O	7:J:407:ASN:N	2.30	0.65
7:J:255:MET:O	7:J:259:GLY:N	2.28	0.64
11:V:194:ASP:OD2	12:b:56:ARG:N	2.30	0.64
4:T:274:GLN:NE2	4:T:277:ASP:OD2	2.30	0.64
2:D:313:ASP:OD2	2:D:314:TYR:N	2.30	0.64
1:A:107:GLN:OE1	2:C:467:GLN:NE2	2.31	0.64
8:O:195:ILE:HD13	9:P:139:VAL:HG22	1.80	0.64
8:O:310:VAL:HG13	8:O:311:LYS:H	1.62	0.64
7:J:200:TYR:OH	7:J:213:HIS:ND1	2.31	0.64
10:S:175:ASP:OD1	10:S:176:SER:N	2.31	0.64
13:Z:50:ASP:OD1	13:Z:51:ALA:N	2.31	0.64
7:J:111:ALA:N	7:J:209:PRO:O	2.31	0.64
11:V:135:ILE:HD12	11:V:135:ILE:H	1.63	0.64
9:P:364:PRO:HB2	11:U:264:LEU:HD13	1.79	0.64
6:G:149:PHE:CE1	6:G:205:LEU:HD13	2.32	0.64
12:Y:76:SER:O	12:Y:80:GLN:NE2	2.31	0.64
10:Q:185:MET:HE3	10:Q:189:THR:HG21	1.80	0.63
8:O:188:ILE:HG22	8:O:195:ILE:HG13	1.79	0.63
8:M:164:ILE:HG13	9:R:150:MET:HE1	1.80	0.63
1:A:25:GLU:OE2	3:E:26:LEU:HD22	1.98	0.63
1:A:42:ALA:HB1	3:E:48:VAL:HG22	1.81	0.63
1:A:106:ALA:O	1:A:109:SER:OG	2.16	0.63
7:N:392:GLU:OE1	7:N:397:ILE:HD13	1.98	0.63
12:b:155:GLN:O	12:b:159:ILE:HD12	1.97	0.63
12:b:188:ASP:OD1	12:b:189:ASP:N	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:609:ASP:OD1	2:C:610:PHE:N	2.32	0.63
3:E:17:ASN:O	8:O:143:ARG:NH1	2.31	0.63
2:D:299:LEU:HD13	3:F:117:LEU:HD21	1.81	0.63
12:Y:191:SER:N	13:Z:125:MET:HE3	2.14	0.63
1:B:75:LYS:HE3	1:B:75:LYS:HA	1.80	0.63
7:J:164:SER:OG	10:S:247:ARG:NH2	2.31	0.63
11:V:299:MET:SD	12:b:177:LEU:HD21	2.38	0.62
1:A:68:LEU:HD21	3:E:71:GLY:CA	2.29	0.62
2:C:416:VAL:O	2:C:420:ILE:HG22	1.99	0.62
1:B:68:LEU:HD21	3:F:71:GLY:CA	2.29	0.62
10:S:287:LEU:HD12	10:S:291:LEU:HD11	1.80	0.62
6:G:149:PHE:CZ	6:G:200:VAL:HG23	2.34	0.62
3:F:86:SER:O	3:F:90:LEU:HD23	1.99	0.62
13:Z:75:PHE:O	13:Z:78:SER:OG	2.17	0.62
8:M:310:VAL:HG23	8:M:311:LYS:H	1.65	0.62
9:R:365:ASP:OD2	9:R:366:MET:N	2.33	0.62
7:N:250:SER:O	7:N:253:ASN:N	2.33	0.62
10:Q:356:LEU:HD21	12:Y:153:LYS:HD3	1.82	0.62
1:B:6:GLU:O	1:B:10:GLU:OE1	2.17	0.62
7:J:427:VAL:HG23	7:J:431:LEU:HD23	1.81	0.62
11:U:242:GLU:O	11:U:246:LEU:HD23	2.00	0.61
2:D:421:LEU:HD23	2:D:464:TYR:HB3	1.83	0.61
1:A:64:GLU:O	1:A:68:LEU:HD23	2.00	0.61
1:B:12:ILE:HD11	3:F:15:LEU:HD12	1.81	0.61
8:M:290:ALA:O	8:M:292:LYS:NZ	2.32	0.61
7:N:27:LEU:HD21	7:N:96:LEU:HD12	1.82	0.61
1:B:110:LEU:O	1:B:114:LEU:HD23	2.00	0.61
3:K:216:VAL:HG13	3:K:226:LYS:HE3	1.82	0.61
2:C:512:PHE:CE2	2:C:545:VAL:HG11	2.36	0.61
13:Z:32:TYR:HD1	13:Z:33:THR:HG23	1.66	0.61
1:B:90:LEU:O	1:B:94:ASN:ND2	2.34	0.61
10:S:148:LEU:HD22	10:S:151:TRP:CH2	2.36	0.61
10:S:340:ILE:HG21	10:S:348:LEU:HD11	1.82	0.61
9:R:152:LEU:HD11	9:R:156:TYR:CZ	2.36	0.60
1:A:90:LEU:O	1:A:94:ASN:ND2	2.34	0.60
2:C:293:VAL:HG13	2:C:298:GLN:HB2	1.84	0.60
1:B:37:ARG:HH12	8:M:128:VAL:HG12	1.66	0.60
2:D:421:LEU:HD21	2:D:465:VAL:CG1	2.31	0.60
12:b:201:LEU:O	12:b:205:LEU:HD23	2.01	0.60
12:Y:208:MET:SD	12:Y:212:LEU:HD23	2.40	0.60
9:R:283:GLU:OE2	9:R:293:THR:OG1	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:494:THR:HG21	2:C:541:ILE:HG23	1.84	0.60
2:D:494:THR:HG21	2:D:541:ILE:HG23	1.84	0.60
2:D:641:TYR:HA	2:D:644:ILE:HD12	1.84	0.60
7:J:257:LEU:HD11	7:J:380:VAL:HG11	1.83	0.60
9:P:99:ASP:OD1	9:P:100:ILE:N	2.33	0.60
10:Q:185:MET:HE2	10:Q:196:VAL:HA	1.83	0.60
3:F:71:GLY:HA2	3:F:74:LEU:HD12	1.84	0.60
7:J:59:ASP:O	7:J:63:GLU:OE1	2.20	0.60
11:V:185:MET:O	11:V:188:ASP:OD1	2.19	0.60
2:I:5:LEU:HD13	2:I:40:LEU:HG	1.84	0.60
10:Q:158:MET:HE1	10:Q:225:SER:HA	1.83	0.60
10:S:377:MET:HE2	11:V:295:PHE:CE1	2.36	0.59
5:W:75:PRO:O	5:W:79:GLU:OE1	2.20	0.59
10:Q:219:ARG:O	10:Q:219:ARG:NH1	2.35	0.59
7:J:115:ASP:OD1	7:J:116:GLY:N	2.35	0.59
9:R:198:GLU:OE1	9:R:198:GLU:N	2.35	0.59
11:V:179:GLN:NE2	12:b:36:ASN:OD1	2.36	0.59
2:C:709:ASN:O	2:C:712:ARG:NE	2.35	0.59
11:V:296:VAL:HG12	12:b:177:LEU:HD22	1.82	0.59
13:c:32:TYR:CD1	13:c:33:THR:HG23	2.35	0.59
6:L:7:PHE:HB3	6:L:114:ILE:HD12	1.82	0.59
2:D:454:ASN:OD1	2:D:455:ASN:N	2.36	0.59
6:G:214:THR:OG1	6:G:222:VAL:O	2.18	0.59
8:M:327:CYS:SG	8:M:328:SER:N	2.75	0.59
13:c:35:ASP:OD2	13:c:38:GLN:N	2.32	0.59
3:K:205:TYR:HE1	3:K:228:ILE:HG21	1.66	0.59
11:V:161:SER:OG	11:V:168:LYS:N	2.35	0.59
7:N:102:GLU:N	7:N:102:GLU:OE1	2.36	0.59
1:A:41:HIS:NE2	3:E:42:ASP:OD1	2.36	0.59
11:U:288:ASN:OD1	11:U:289:ILE:N	2.36	0.59
2:I:150:THR:HG21	2:I:186:SER:HB2	1.83	0.59
7:N:25:MET:O	7:N:68:ARG:NH1	2.34	0.59
7:N:165:ASN:ND2	7:N:193:PRO:O	2.33	0.59
13:c:68:LEU:HD23	13:c:72:LEU:HD23	1.84	0.59
6:G:150:GLU:HB2	6:G:206:THR:HG21	1.85	0.59
7:J:58:LEU:HD13	7:J:61:LEU:HD12	1.84	0.59
7:J:102:GLU:OE1	7:J:102:GLU:N	2.30	0.59
1:A:82:LEU:O	1:A:86:LEU:HD23	2.03	0.59
2:D:432:THR:OG1	2:D:481:LEU:HD21	2.03	0.58
10:Q:216:LYS:HE3	10:Q:216:LYS:HA	1.85	0.58
12:Y:4:THR:O	12:Y:7:SER:OG	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:257:ILE:HD11	9:R:354:LEU:HD12	1.84	0.58
1:A:51:ARG:HH21	2:C:495:LEU:HD23	1.68	0.58
10:Q:386:ILE:HD11	11:U:305:LEU:HD21	1.85	0.58
2:D:580:MET:HE3	2:D:580:MET:HA	1.84	0.58
7:J:306:PHE:CE2	7:J:307:LEU:HG	2.38	0.58
1:B:36:ILE:HG22	3:F:36:ILE:HD13	1.86	0.58
1:B:114:LEU:HB3	2:D:423:LEU:HD11	1.85	0.58
7:J:155:LEU:N	7:J:204:PHE:O	2.33	0.58
7:J:334:LYS:HZ2	7:J:378:SER:HA	1.69	0.58
2:C:489:MET:N	2:C:489:MET:HE2	2.19	0.58
6:G:78:ASN:HB3	6:G:81:MET:HE2	1.85	0.58
10:S:203:LYS:HE3	11:V:173:LEU:HD11	1.86	0.58
2:D:512:PHE:O	2:D:515:SER:OG	2.18	0.58
2:D:520:THR:HG21	2:D:559:ARG:HG3	1.86	0.58
9:R:334:GLN:N	9:R:334:GLN:OE1	2.35	0.58
2:C:658:ILE:HD11	2:C:680:GLU:HB3	1.84	0.58
6:G:70:TYR:CG	6:G:70:TYR:O	2.57	0.58
10:S:172:SER:O	10:S:175:ASP:OD1	2.22	0.58
7:J:85:ASN:HB3	7:J:88:GLN:OE1	2.03	0.57
7:N:106:TRP:C	7:N:107:LEU:HD12	2.29	0.57
13:Z:73:LEU:O	13:Z:77:GLU:OE1	2.22	0.57
8:M:316:GLU:C	8:M:317:LEU:HD22	2.29	0.57
11:V:275:SER:OG	11:V:276:GLN:N	2.33	0.57
12:b:4:THR:O	12:b:7:SER:OG	2.19	0.57
7:J:192:LYS:O	7:J:192:LYS:HG3	2.04	0.57
11:V:275:SER:OG	11:V:276:GLN:OE1	2.08	0.57
2:I:232:SER:HB3	10:S:145:ASN:N	2.20	0.57
11:U:285:ASP:OD1	11:U:286:ASP:N	2.38	0.57
7:J:374:SER:OG	7:J:375:ARG:NH1	2.38	0.57
1:A:59:LEU:HD12	1:A:60:GLN:N	2.19	0.57
3:F:100:GLN:O	3:F:104:LEU:HD23	2.05	0.57
10:Q:159:ILE:O	10:Q:163:LEU:HD23	2.04	0.57
7:J:154:VAL:C	7:J:155:LEU:HD22	2.30	0.57
9:R:272:TYR:OH	9:R:281:ILE:HG21	2.05	0.57
11:V:285:ASP:OD1	11:V:286:ASP:N	2.38	0.57
1:B:110:LEU:O	1:B:113:GLN:HG2	2.04	0.57
2:D:390:ASN:ND2	2:D:425:LYS:O	2.29	0.57
7:J:424:ILE:O	7:J:427:VAL:HG12	2.05	0.57
9:R:135:GLN:O	9:R:139:VAL:HG23	2.05	0.57
2:D:679:ASP:OD1	2:D:680:GLU:N	2.38	0.56
7:N:164:SER:OG	10:Q:247:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:170:GLN:NE2	9:P:186:ASN:OD1	2.30	0.56
6:L:81:MET:SD	6:L:241:GLN:NE2	2.78	0.56
7:N:85:ASN:HB3	7:N:88:GLN:OE1	2.05	0.56
10:S:188:MET:CE	11:V:169:LEU:HD13	2.36	0.56
10:S:198:ARG:O	10:S:201:SER:OG	2.17	0.56
3:K:139:ARG:NH1	3:K:140:THR:OG1	2.37	0.56
2:C:481:LEU:O	2:C:484:THR:OG1	2.22	0.56
2:C:520:THR:HG21	2:C:559:ARG:HG3	1.87	0.56
7:N:68:ARG:NE	10:S:171:VAL:HG21	2.20	0.56
9:R:217:ILE:HG12	9:R:232:LEU:HD13	1.87	0.56
2:I:238:LEU:O	2:I:241:ALA:HB3	2.06	0.56
1:B:100:LEU:CD1	3:F:90:LEU:HD21	2.35	0.56
9:R:137:GLU:OE2	9:R:148:LEU:N	2.33	0.56
7:N:132:LEU:HD22	7:N:231:THR:HG21	1.88	0.56
2:D:312:VAL:HA	2:D:315:MET:HE2	1.87	0.56
7:J:391:ASN:O	7:J:398:ILE:N	2.33	0.56
13:Z:3:SER:OG	13:Z:4:GLU:N	2.38	0.56
10:S:269:LEU:HB2	11:V:227:ILE:HD11	1.87	0.56
11:U:155:LEU:N	11:U:175:LEU:HD21	2.21	0.56
6:L:138:GLU:N	6:L:138:GLU:OE1	2.39	0.55
7:N:283:LEU:O	9:P:210:SER:OG	2.21	0.55
7:J:146:MET:SD	7:J:157:THR:HG22	2.46	0.55
9:R:169:VAL:HG22	9:R:172:ARG:HH11	1.71	0.55
11:V:176:ARG:NH2	11:V:179:GLN:OE1	2.40	0.55
4:T:334:ILE:HD13	4:T:340:MET:HG2	1.89	0.55
7:N:59:ASP:O	7:N:63:GLU:OE1	2.25	0.55
6:L:87:LEU:HD21	6:L:111:MET:HE2	1.87	0.55
8:O:170:TYR:CE1	9:P:167:VAL:HG11	2.41	0.55
12:Y:96:GLU:OE1	12:Y:100:ARG:NH2	2.39	0.55
1:B:100:LEU:HD23	2:D:510:MET:HE2	1.88	0.55
7:J:27:LEU:HD21	7:J:96:LEU:HD12	1.87	0.55
9:R:340:ILE:HG23	11:V:256:LEU:HD21	1.89	0.55
9:R:364:PRO:HG3	11:V:263:LEU:HD23	1.87	0.55
3:E:71:GLY:HA2	3:E:74:LEU:HD12	1.87	0.55
3:E:86:SER:O	3:E:90:LEU:HD23	2.06	0.55
7:J:93:ASP:OD2	7:J:201:TYR:OH	2.24	0.55
11:V:275:SER:HG	11:V:276:GLN:H	1.55	0.55
9:R:128:ILE:HD12	9:R:132:THR:HG21	1.88	0.55
2:C:429:ILE:HG23	2:C:481:LEU:HD22	1.89	0.55
2:C:638:ALA:C	2:C:639:LEU:HD22	2.31	0.55
9:R:298:ILE:CD1	9:R:323:ILE:HG22	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:269:LEU:HD22	11:V:226:GLU:OE2	2.05	0.55
11:V:286:ASP:O	11:V:289:ILE:HG12	2.06	0.55
9:R:166:GLN:NE2	9:R:190:CYS:SG	2.77	0.55
11:V:185:MET:O	11:V:189:LEU:HG	2.07	0.55
10:Q:185:MET:CE	10:Q:199:ILE:HD12	2.30	0.55
2:C:331:MET:N	2:C:331:MET:HE2	2.22	0.55
2:C:391:LYS:O	2:C:394:SER:OG	2.18	0.55
11:U:142:PHE:CB	11:U:185:MET:HE2	2.37	0.55
7:J:46:SER:N	7:J:79:TYR:O	2.37	0.55
7:J:237:THR:HG21	11:V:231:LYS:HB2	1.89	0.55
2:C:476:ASP:OD1	2:C:477:LYS:N	2.40	0.55
2:D:376:GLN:OE1	2:D:376:GLN:N	2.40	0.55
8:O:220:HIS:ND1	8:O:239:THR:O	2.40	0.54
10:S:269:LEU:HD11	10:S:273:ARG:NH2	2.21	0.54
12:b:121:PRO:O	12:b:143:TYR:OH	2.23	0.54
7:N:126:ALA:O	7:N:129:ILE:HG22	2.06	0.54
6:G:70:TYR:OH	6:G:226:ARG:O	2.25	0.54
7:J:226:GLN:O	7:J:229:SER:OG	2.22	0.54
7:J:299:VAL:HG23	9:R:126:GLU:CD	2.31	0.54
8:M:321:GLN:O	8:M:323:GLU:OE1	2.24	0.54
13:Z:47:GLN:O	13:Z:50:ASP:OD1	2.24	0.54
2:D:406:LEU:HD21	2:D:446:TRP:CD1	2.43	0.54
7:J:20:VAL:O	7:J:24:LEU:HD23	2.07	0.54
10:S:382:HIS:ND1	10:S:385:GLU:OE2	2.40	0.54
7:N:26:LYS:NZ	10:S:208:GLU:OE2	2.40	0.54
7:J:189:PHE:CG	7:J:190:GLN:N	2.75	0.54
1:A:121:ARG:NH2	3:E:111:ASN:OD1	2.41	0.54
7:J:322:ARG:O	7:J:326:LEU:HD23	2.08	0.54
11:V:299:MET:SD	11:V:299:MET:O	2.66	0.54
1:B:63:LEU:HD23	2:D:614:ILE:HG21	1.90	0.54
1:B:100:LEU:HD12	3:F:90:LEU:HD21	1.88	0.54
3:F:89:TRP:HE3	3:F:90:LEU:HD22	1.73	0.54
8:M:307:SER:HA	8:M:316:GLU:HA	1.89	0.54
8:O:195:ILE:N	9:P:135:GLN:OE1	2.40	0.54
2:C:646:ILE:HD12	2:C:703:HIS:ND1	2.23	0.54
9:P:350:VAL:O	9:P:354:LEU:HD23	2.07	0.54
10:S:321:GLY:O	10:S:324:THR:OG1	2.19	0.54
11:V:187:ARG:NE	11:V:187:ARG:HA	2.22	0.54
7:N:115:ASP:OD1	7:N:116:GLY:N	2.41	0.54
11:U:163:ASP:OD1	11:U:164:ASP:N	2.41	0.54
7:J:106:TRP:CE2	7:J:251:ILE:HD13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:84:GLN:O	3:E:88:GLU:OE1	2.26	0.53
10:Q:304:MET:HE2	10:Q:304:MET:HA	1.89	0.53
7:J:328:LYS:HE3	7:J:424:ILE:HG21	1.89	0.53
8:M:165:VAL:O	8:M:169:VAL:HG23	2.07	0.53
2:I:89:LEU:HD22	2:I:139:LEU:HD22	1.89	0.53
3:K:216:VAL:HG13	3:K:226:LYS:CE	2.38	0.53
7:N:334:LYS:NZ	7:N:376:TYR:O	2.41	0.53
9:P:192:ASN:ND2	9:P:195:ASN:OD1	2.41	0.53
1:B:53:LEU:HD21	3:F:56:LEU:HD21	1.91	0.53
6:G:223:THR:HG22	6:G:225:THR:H	1.73	0.53
7:J:320:GLU:O	7:J:324:LEU:HD23	2.09	0.53
11:U:286:ASP:O	11:U:289:ILE:HG22	2.09	0.53
7:J:74:ARG:O	7:J:78:VAL:HG12	2.07	0.53
9:R:276:ASN:ND2	11:V:297:ASP:OD2	2.41	0.53
4:T:337:VAL:HG22	4:T:341:PHE:CE1	2.43	0.53
6:G:39:ARG:O	6:G:39:ARG:HG2	2.07	0.53
10:S:257:ARG:HE	10:S:258:LEU:HD23	1.73	0.53
13:c:121:GLU:O	13:c:124:ASN:OD1	2.26	0.53
2:C:462:CYS:O	2:C:466:LEU:HD23	2.08	0.53
9:R:170:GLN:N	9:R:170:GLN:OE1	2.42	0.53
6:L:116:PHE:HE2	6:L:221:ILE:HD11	1.73	0.53
6:L:131:HIS:N	6:L:139:GLN:O	2.35	0.53
11:V:183:ASP:OD2	12:b:40:ARG:NH2	2.41	0.53
13:c:13:ASP:OD1	13:c:14:SER:N	2.41	0.53
9:R:299:ASN:O	9:R:321:ILE:HA	2.09	0.53
11:V:166:PHE:CE2	11:V:170:LEU:HD11	2.43	0.53
12:b:200:LYS:HA	12:b:203:VAL:HG12	1.91	0.53
13:c:53:VAL:O	13:c:57:LEU:HD23	2.09	0.53
7:N:128:PHE:CE1	7:N:132:LEU:HD21	2.44	0.53
10:Q:163:LEU:HD21	10:Q:215:LYS:HG2	1.92	0.53
8:M:177:PHE:CD1	8:M:204:ILE:HG22	2.43	0.53
10:Q:185:MET:HE1	10:Q:199:ILE:CD1	2.31	0.52
2:C:569:MET:SD	2:C:570:GLN:N	2.83	0.52
3:E:89:TRP:HE3	3:E:90:LEU:HD22	1.74	0.52
7:N:74:ARG:O	7:N:78:VAL:HG12	2.10	0.52
11:U:150:LEU:HD13	11:U:178:PHE:CE1	2.45	0.52
1:B:114:LEU:CD2	3:F:104:LEU:HD21	2.39	0.52
10:S:142:LEU:HD13	10:S:146:TYR:CD2	2.45	0.52
12:b:17:THR:HG23	12:b:18:ALA:N	2.25	0.52
12:b:181:ILE:HG23	12:b:190:ILE:HD12	1.92	0.52
2:I:45:LEU:HD22	2:I:71:PHE:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:239:SER:HG	10:S:144:ARG:NH1	2.04	0.52
2:C:330:VAL:C	2:C:331:MET:HE2	2.35	0.52
7:J:278:PHE:O	7:J:290:GLN:NE2	2.43	0.52
12:b:51:LYS:O	12:b:52:ASP:OD1	2.27	0.52
2:D:425:LYS:HD3	2:D:426:PRO:HD2	1.91	0.52
7:J:16:ASP:O	7:J:20:VAL:HG23	2.10	0.52
7:J:192:LYS:O	7:J:192:LYS:CG	2.58	0.52
9:R:350:VAL:HG13	9:R:351:LYS:N	2.25	0.52
12:b:170:GLN:O	12:b:173:SER:OG	2.26	0.52
12:b:188:ASP:O	12:b:189:ASP:C	2.52	0.52
6:L:96:ASN:O	6:L:99:VAL:HG12	2.09	0.52
7:N:68:ARG:HE	10:S:171:VAL:HG21	1.75	0.52
7:N:374:SER:OG	7:N:375:ARG:N	2.42	0.52
1:B:51:ARG:HD2	2:D:540:ASP:HB2	1.90	0.52
12:b:50:ARG:HE	12:b:54:MET:CE	2.23	0.52
2:C:381:ILE:O	2:C:384:SER:OG	2.27	0.52
7:N:107:LEU:HD11	7:N:247:PRO:HG3	1.91	0.52
12:Y:190:ILE:HB	13:Z:125:MET:HE2	1.92	0.52
6:G:75:PHE:CD2	6:G:87:LEU:HB3	2.45	0.52
7:J:124:GLN:OE1	7:J:127:LYS:N	2.37	0.52
7:J:322:ARG:O	7:J:325:ARG:HG3	2.10	0.52
1:A:20:VAL:HG21	3:E:77:ASN:HD22	1.74	0.52
7:N:100:LYS:HZ2	7:N:103:LYS:HG3	1.75	0.52
9:P:170:GLN:N	9:P:170:GLN:OE1	2.43	0.52
4:T:325:VAL:HG23	4:T:340:MET:SD	2.50	0.51
8:O:310:VAL:HG13	8:O:311:LYS:N	2.26	0.51
1:B:70:ILE:HD13	2:D:664:ILE:HD13	1.91	0.51
2:D:701:LEU:HD11	2:D:718:LEU:HD23	1.92	0.51
10:S:389:VAL:HG23	10:S:390:PHE:CD1	2.45	0.51
2:I:94:VAL:HG11	4:T:357:GLU:HG3	1.91	0.51
7:N:448:GLN:N	7:N:448:GLN:OE1	2.44	0.51
8:O:285:PHE:HD1	8:O:288:LEU:HD12	1.74	0.51
2:D:462:CYS:O	2:D:465:VAL:HG22	2.10	0.51
7:J:253:ASN:HB3	7:J:380:VAL:HG13	1.92	0.51
2:I:215:ARG:HA	2:I:218:LEU:HD21	1.91	0.51
2:C:632:THR:OG1	2:C:633:ILE:N	2.44	0.51
7:N:279:GLU:OE2	8:O:205:ARG:NH2	2.44	0.51
6:L:81:MET:HE1	6:L:237:LEU:CD2	2.41	0.51
7:N:61:LEU:HD11	7:N:74:ARG:NH1	2.25	0.51
10:Q:167:GLU:O	10:Q:171:VAL:HG23	2.09	0.51
10:S:297:HIS:ND1	10:S:299:VAL:HG22	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:232:SER:HB3	10:S:145:ASN:HB3	1.93	0.51
2:I:232:SER:O	2:I:233:ILE:C	2.51	0.51
2:C:393:SER:HA	2:C:420:ILE:HD11	1.92	0.51
7:J:285:ASP:OD2	7:J:288:LYS:N	2.35	0.51
10:S:303:ALA:HA	10:S:306:TYR:CE1	2.46	0.51
1:A:70:ILE:HD13	2:C:664:ILE:HD13	1.91	0.51
2:C:420:ILE:HG23	2:C:421:LEU:N	2.24	0.51
6:G:158:LEU:HD21	6:G:161:PHE:CE1	2.46	0.51
10:Q:253:GLN:OE1	12:Y:3:ASP:N	2.39	0.51
2:D:433:ARG:NH2	2:D:488:ASP:OD1	2.44	0.51
7:J:428:PRO:HG3	7:J:430:TRP:CZ2	2.46	0.51
10:S:302:LYS:O	10:S:305:GLU:HG3	2.11	0.51
2:C:413:LEU:HA	2:C:416:VAL:HG12	1.93	0.51
10:Q:357:LEU:HB3	10:Q:360:LEU:HD23	1.91	0.51
1:B:96:LEU:O	1:B:100:LEU:HD13	2.10	0.51
2:D:468:MET:HE3	2:D:472:TRP:CE2	2.46	0.51
6:G:10:ILE:HD12	6:G:85:MET:HG3	1.92	0.51
7:J:95:HIS:HA	7:J:98:ILE:HG12	1.93	0.51
7:J:297:VAL:O	9:R:126:GLU:N	2.38	0.51
2:I:259:LEU:O	2:I:262:ILE:HG22	2.11	0.51
2:C:328:ARG:NH2	2:C:332:SER:OG	2.37	0.51
6:L:34:ASP:HB3	6:L:57:GLU:HB2	1.93	0.51
10:Q:199:ILE:HD11	11:U:166:PHE:CZ	2.46	0.51
7:J:251:ILE:HD12	7:J:254:ILE:CG2	2.41	0.51
8:M:207:GLU:O	9:R:238:GLN:NE2	2.40	0.51
11:V:288:ASN:OD1	11:V:289:ILE:HG23	2.10	0.51
1:A:17:LYS:O	1:A:20:VAL:HG22	2.11	0.51
1:A:97:ASP:OD2	2:C:711:TYR:OH	2.29	0.51
7:N:258:LEU:HD11	7:N:438:PHE:HZ	1.76	0.51
12:Y:174:ILE:HD12	13:Z:122:PHE:CE1	2.46	0.51
13:Z:113:GLN:O	13:Z:116:THR:OG1	2.25	0.51
9:R:166:GLN:N	9:R:166:GLN:OE1	2.44	0.51
12:b:40:ARG:CZ	12:b:40:ARG:HA	2.41	0.51
13:c:61:ILE:HB	13:c:65:PHE:CZ	2.46	0.51
2:C:589:THR:OG1	2:C:594:ARG:NH2	2.43	0.50
6:L:180:THR:OG1	6:L:186:ASP:OD2	2.28	0.50
7:N:412:GLY:O	7:N:416:LEU:HD23	2.11	0.50
12:Y:41:LEU:O	12:Y:45:GLN:OE1	2.29	0.50
13:c:61:ILE:O	13:c:65:PHE:CD2	2.64	0.50
1:H:154:VAL:O	1:H:158:ASN:ND2	2.36	0.50
3:K:205:TYR:CE1	3:K:228:ILE:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:537:VAL:HG22	2:C:537:VAL:O	2.11	0.50
7:N:436:GLY:O	7:N:437:SER:OG	2.20	0.50
11:U:178:PHE:O	11:U:181:ILE:HG22	2.11	0.50
12:Y:188:ASP:O	12:Y:189:ASP:C	2.55	0.50
9:R:169:VAL:HG22	9:R:172:ARG:NH1	2.26	0.50
11:V:289:ILE:HG22	12:b:170:GLN:CG	2.42	0.50
2:C:543:ASN:OD1	2:C:544:LYS:N	2.45	0.50
7:N:100:LYS:HZ2	7:N:103:LYS:CG	2.25	0.50
7:N:233:SER:O	7:N:234:GLU:HG2	2.11	0.50
7:J:273:TYR:OH	9:R:144:THR:O	2.08	0.50
1:A:48:THR:O	1:A:52:LEU:HD23	2.12	0.50
2:C:388:MET:SD	2:C:388:MET:N	2.74	0.50
2:C:677:HIS:ND1	2:C:680:GLU:OE1	2.44	0.50
12:Y:55:SER:OG	12:Y:58:LYS:HG2	2.12	0.50
10:S:352:GLU:O	10:S:355:SER:OG	2.27	0.50
2:D:575:ASN:HB2	2:D:578:VAL:HG23	1.93	0.50
10:S:302:LYS:O	10:S:306:TYR:CD1	2.64	0.50
7:N:82:ASP:OD1	7:N:82:ASP:N	2.43	0.50
10:Q:177:VAL:HG22	11:U:176:ARG:HG2	1.94	0.50
10:S:370:LEU:HD21	13:c:123:GLU:HB2	1.94	0.50
1:A:39:HIS:CE1	3:E:52:VAL:HG21	2.46	0.50
7:N:56:GLU:O	7:N:60:LEU:HD23	2.12	0.50
12:Y:17:THR:HG23	12:Y:18:ALA:N	2.26	0.50
13:Z:17:THR:OG1	13:Z:50:ASP:OD2	2.23	0.50
1:B:13:GLN:O	1:B:16:GLU:HG2	2.11	0.50
6:G:130:VAL:O	6:G:229:ARG:NH1	2.45	0.50
6:G:203:LEU:CD2	7:J:416:LEU:HD22	2.41	0.50
9:R:153:ARG:O	9:R:157:LEU:HD23	2.12	0.50
9:R:201:PHE:CE2	9:R:241:LEU:HD21	2.46	0.50
2:I:235:LYS:CG	10:S:144:ARG:HD2	2.42	0.50
10:Q:373:THR:O	10:Q:376:GLN:NE2	2.45	0.50
1:A:13:GLN:O	1:A:16:GLU:HG2	2.12	0.50
2:C:539:PRO:HD3	2:C:580:MET:HE1	1.93	0.50
3:E:110:ILE:O	3:E:114:LEU:HD23	2.12	0.50
11:U:188:ASP:O	11:U:192:ILE:HG12	2.12	0.50
4:T:348:LEU:CD2	5:W:44:LEU:HD11	2.42	0.49
6:L:131:HIS:O	6:L:139:GLN:N	2.41	0.49
6:L:209:ILE:HG23	6:L:215:LYS:HB3	1.94	0.49
8:O:324:ILE:HD12	8:O:350:GLY:O	2.11	0.49
7:J:82:ASP:OD1	7:J:83:GLY:N	2.45	0.49
12:b:50:ARG:O	12:b:50:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:104:ARG:O	13:c:107:ILE:HG22	2.12	0.49
12:Y:15:GLU:C	12:Y:16:LEU:HD22	2.36	0.49
13:c:88:GLU:N	13:c:88:GLU:OE1	2.45	0.49
4:T:337:VAL:HG22	4:T:341:PHE:CD1	2.48	0.49
3:E:51:GLU:OE2	3:E:52:VAL:HG23	2.12	0.49
8:O:177:PHE:CD1	8:O:204:ILE:HG22	2.48	0.49
9:P:217:ILE:HG12	9:P:232:LEU:HD13	1.94	0.49
7:J:262:ARG:CZ	8:M:218:LYS:HZ2	2.24	0.49
9:R:259:GLN:NE2	9:R:263:ASN:OD1	2.44	0.49
11:V:223:VAL:O	11:V:226:GLU:HG3	2.12	0.49
1:B:48:THR:O	1:B:52:LEU:HD23	2.12	0.49
1:A:43:VAL:HG22	1:A:43:VAL:O	2.13	0.49
6:L:15:SER:O	6:L:107:TYR:OH	2.07	0.49
7:N:303:ASP:OD1	7:N:305:SER:OG	2.23	0.49
1:B:10:GLU:O	1:B:14:GLN:OE1	2.31	0.49
2:D:364:LEU:HD11	2:D:368:PHE:CZ	2.48	0.49
9:R:183:LEU:HD22	9:R:205:TYR:OH	2.12	0.49
10:S:269:LEU:HD13	11:V:226:GLU:OE1	2.12	0.49
1:A:10:GLU:O	1:A:14:GLN:OE1	2.31	0.49
1:B:43:VAL:HG22	1:B:43:VAL:O	2.13	0.49
2:D:608:PRO:O	2:D:612:LYS:N	2.45	0.49
10:S:152:LYS:O	10:S:223:PHE:N	2.39	0.49
10:Q:177:VAL:HG22	11:U:176:ARG:CG	2.43	0.49
7:J:10:ASN:HA	7:J:85:ASN:ND2	2.28	0.49
13:c:113:GLN:O	13:c:116:THR:OG1	2.26	0.49
11:U:142:PHE:HB3	11:U:185:MET:HE2	1.94	0.49
7:N:189:PHE:O	7:N:190:GLN:HG3	2.13	0.49
12:Y:200:LYS:HA	12:Y:203:VAL:HG12	1.95	0.49
7:J:257:LEU:HD23	7:J:267:MET:HE2	1.95	0.49
7:J:276:ALA:HB3	8:M:218:LYS:HE2	1.95	0.49
8:M:200:GLU:OE2	8:M:226:LYS:HG3	2.13	0.49
10:S:272:THR:HG22	11:V:236:TRP:CH2	2.48	0.49
10:S:276:CYS:HB2	11:V:236:TRP:CZ3	2.48	0.49
2:C:540:ASP:N	2:C:540:ASP:OD1	2.44	0.49
9:P:212:LEU:HD22	9:P:237:PHE:HE2	1.77	0.49
2:D:462:CYS:O	2:D:466:LEU:HD23	2.13	0.49
12:b:41:LEU:O	12:b:45:GLN:OE1	2.30	0.49
1:H:160:THR:HG22	3:K:233:PHE:HB2	1.94	0.48
1:H:170:ILE:HD11	2:I:135:ILE:HD13	1.95	0.48
2:I:6:ASP:O	2:I:10:LEU:HD13	2.13	0.48
2:D:638:ALA:C	2:D:639:LEU:HD22	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:183:ASP:O	11:V:186:THR:OG1	2.31	0.48
6:L:10:ILE:HG21	6:L:14:LEU:HD23	1.94	0.48
2:D:568:LEU:HD22	2:D:578:VAL:HG22	1.95	0.48
3:F:93:MET:SD	3:F:97:SER:OG	2.71	0.48
11:V:236:TRP:O	11:V:240:GLN:OE1	2.31	0.48
12:b:37:GLU:OE2	13:c:32:TYR:HB2	2.13	0.48
12:b:167:ILE:O	12:b:171:THR:HG23	2.13	0.48
7:N:128:PHE:O	7:N:132:LEU:HD23	2.13	0.48
6:G:55:ARG:NH1	6:G:230:ASN:OD1	2.46	0.48
7:J:47:PHE:CE2	7:J:54:LEU:HD13	2.48	0.48
8:M:122:GLN:O	8:M:122:GLN:CD	2.56	0.48
8:M:310:VAL:HG23	8:M:311:LYS:N	2.28	0.48
11:V:292:ILE:HD12	11:V:292:ILE:H	1.78	0.48
2:I:143:SER:OG	4:T:351:GLU:OE2	2.30	0.48
2:C:666:ASN:OD1	2:C:669:THR:OG1	2.29	0.48
7:N:322:ARG:O	7:N:325:ARG:HG3	2.12	0.48
7:J:298:MET:HA	9:R:126:GLU:OE1	2.14	0.48
11:V:299:MET:SD	12:b:177:LEU:HD11	2.54	0.48
13:c:47:GLN:O	13:c:50:ASP:OD1	2.32	0.48
10:Q:352:GLU:O	10:Q:355:SER:OG	2.29	0.48
2:I:52:LEU:O	2:I:63:LYS:NZ	2.47	0.48
2:I:211:ILE:HG22	2:I:212:ASN:H	1.78	0.48
8:O:251:ASP:O	8:O:256:GLY:N	2.47	0.48
8:O:338:GLN:N	8:O:338:GLN:OE1	2.46	0.48
9:P:201:PHE:CE2	9:P:241:LEU:HD21	2.49	0.48
1:B:121:ARG:NH2	3:F:111:ASN:OD1	2.46	0.48
7:J:331:ILE:HG13	7:J:337:ALA:HA	1.96	0.48
6:L:150:GLU:HB3	6:L:206:THR:HG21	1.96	0.48
8:O:136:ILE:HG23	8:O:143:ARG:HB2	1.96	0.48
9:R:348:TYR:OH	10:S:303:ALA:N	2.41	0.48
11:V:155:LEU:N	11:V:175:LEU:HD21	2.28	0.48
2:C:489:MET:HE2	2:C:489:MET:CA	2.44	0.48
6:L:203:LEU:HD23	7:N:421:LEU:HB3	1.96	0.48
9:P:252:SER:O	9:P:255:THR:OG1	2.29	0.48
2:D:288:VAL:HG13	2:D:306:LEU:HD12	1.96	0.48
2:D:367:CYS:SG	2:D:379:ILE:HD11	2.54	0.48
7:J:189:PHE:O	7:J:190:GLN:HG3	2.14	0.48
8:M:160:LEU:HD12	9:R:131:LEU:HG	1.95	0.48
11:V:276:GLN:N	11:V:276:GLN:OE1	2.46	0.48
3:K:139:ARG:NH1	3:K:140:THR:CB	2.77	0.48
11:V:306:LEU:O	11:V:309:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:692:ASN:OD1	2:C:695:ASP:N	2.37	0.47
7:N:25:MET:HE3	7:N:72:VAL:HG11	1.96	0.47
7:N:98:ILE:HD11	7:N:147:PHE:HE2	1.78	0.47
11:U:194:ASP:OD2	12:Y:56:ARG:N	2.41	0.47
2:D:658:ILE:HG22	2:D:673:PHE:HZ	1.79	0.47
9:R:133:ASN:OD1	9:R:134:LEU:N	2.47	0.47
10:S:228:SER:N	10:S:231:ASP:OD2	2.39	0.47
11:V:174:ASP:O	11:V:178:PHE:CD2	2.66	0.47
1:H:165:MET:HE2	1:H:180:THR:CG2	2.44	0.47
2:C:364:LEU:CD2	2:C:382:ILE:HD13	2.44	0.47
7:N:45:GLY:HA2	7:N:80:TRP:NE1	2.29	0.47
7:N:85:ASN:OD1	7:N:86:VAL:HG22	2.14	0.47
11:U:143:ILE:HG13	11:U:185:MET:HE1	1.96	0.47
2:D:470:THR:HA	2:D:473:VAL:HG22	1.95	0.47
3:F:33:ILE:HA	3:F:36:ILE:HG22	1.96	0.47
9:R:290:ARG:HG2	9:R:290:ARG:O	2.13	0.47
10:S:252:LEU:HD22	12:b:67:TYR:HE2	1.78	0.47
2:C:592:LEU:O	2:C:633:ILE:N	2.47	0.47
7:N:404:PHE:HB3	7:N:409:ILE:HD12	1.96	0.47
8:O:327:CYS:SG	8:O:328:SER:N	2.87	0.47
12:Y:208:MET:SD	12:Y:208:MET:C	2.97	0.47
7:J:155:LEU:O	7:J:204:PHE:HB2	2.14	0.47
8:M:163:TYR:HB3	9:R:150:MET:HE2	1.96	0.47
11:V:280:ASP:OD1	11:V:281:ASP:N	2.47	0.47
12:b:44:ALA:O	12:b:47:ILE:HG22	2.13	0.47
2:I:101:GLN:NE2	2:I:102:THR:O	2.47	0.47
6:L:157:ASN:OD1	7:N:408:ASP:HB3	2.14	0.47
7:N:290:GLN:HG3	9:P:148:LEU:HD21	1.96	0.47
9:P:336:ASP:OD1	9:P:337:LEU:N	2.47	0.47
1:B:135:PHE:CZ	3:F:121:LEU:HD11	2.50	0.47
7:J:33:TYR:O	7:J:36:THR:OG1	2.29	0.47
8:M:188:ILE:HG22	8:M:195:ILE:HG13	1.96	0.47
8:M:212:ARG:HB2	8:M:283:GLN:HG2	1.95	0.47
11:V:187:ARG:CZ	12:b:47:ILE:HD11	2.45	0.47
6:L:87:LEU:HD12	6:L:87:LEU:C	2.39	0.47
11:U:296:VAL:HG22	12:Y:177:LEU:HD22	1.96	0.47
12:Y:55:SER:O	12:Y:58:LYS:N	2.48	0.47
1:B:135:PHE:CE2	3:F:121:LEU:HD11	2.49	0.47
2:D:460:GLU:O	2:D:463:PHE:CD1	2.67	0.47
2:D:609:ASP:OD1	2:D:610:PHE:N	2.43	0.47
6:G:161:PHE:HB2	7:J:403:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:200:GLU:OE2	8:M:233:TRP:CH2	2.68	0.47
9:R:338:ASP:OD2	10:S:337:ASN:ND2	2.41	0.47
10:S:232:LEU:O	10:S:232:LEU:HG	2.15	0.47
10:S:341:LYS:NZ	10:S:342:SER:O	2.47	0.47
13:c:3:SER:OG	13:c:4:GLU:N	2.43	0.47
2:I:130:ASN:O	2:I:133:SER:OG	2.28	0.47
1:A:25:GLU:O	1:A:29:THR:HG23	2.13	0.47
10:Q:165:LEU:O	10:Q:169:ASN:ND2	2.47	0.47
12:Y:188:ASP:O	12:Y:189:ASP:OD1	2.32	0.47
8:M:158:SER:O	8:M:161:GLU:HG3	2.15	0.47
2:C:537:VAL:HG22	2:C:541:ILE:HD12	1.97	0.47
8:O:181:VAL:CG1	8:O:186:LEU:HD21	2.44	0.47
1:B:114:LEU:HD21	3:F:104:LEU:HD21	1.95	0.47
2:D:545:VAL:HB	2:D:553:LEU:HD21	1.97	0.47
6:G:83:VAL:HG13	6:G:83:VAL:O	2.13	0.47
7:J:251:ILE:HD12	7:J:254:ILE:HG21	1.96	0.47
8:M:134:THR:HG22	8:M:134:THR:O	2.15	0.47
9:R:167:VAL:HG23	9:R:187:TYR:CE1	2.50	0.47
9:R:336:ASP:OD1	9:R:337:LEU:N	2.48	0.47
11:V:300:ASP:HB3	11:V:304:GLY:H	1.80	0.47
2:I:78:THR:HG23	2:I:81:LEU:H	1.79	0.47
3:K:167:ASN:ND2	3:K:167:ASN:O	2.48	0.47
5:W:75:PRO:C	5:W:79:GLU:OE1	2.57	0.47
6:L:197:GLY:O	7:N:423:ASN:N	2.43	0.47
10:Q:174:LEU:HA	11:U:177:LEU:HD21	1.97	0.47
10:Q:277:MET:SD	10:Q:278:ASN:N	2.88	0.47
6:G:150:GLU:CG	6:G:206:THR:HG21	2.45	0.47
6:G:223:THR:HG22	6:G:225:THR:N	2.29	0.47
7:J:215:VAL:O	7:J:215:VAL:HG23	2.15	0.47
7:J:332:LYS:HG2	7:J:424:ILE:HD11	1.96	0.47
11:V:234:LYS:HD2	11:V:235:ASP:N	2.29	0.47
1:A:59:LEU:O	1:A:62:ASN:OD1	2.32	0.47
6:L:157:ASN:O	7:N:407:ASN:N	2.46	0.47
11:U:155:LEU:HA	11:U:175:LEU:HD11	1.97	0.47
7:J:404:PHE:HB3	7:J:409:ILE:HD12	1.95	0.47
7:J:428:PRO:HG2	7:J:431:LEU:HB2	1.97	0.47
9:R:99:ASP:OD1	9:R:100:ILE:N	2.48	0.47
12:b:55:SER:OG	12:b:58:LYS:HD3	2.15	0.47
12:b:89:PRO:O	12:b:92:SER:OG	2.33	0.47
3:K:193:THR:HG23	3:K:195:ASN:H	1.80	0.47
1:A:90:LEU:HB3	2:C:641:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:383:ILE:HD11	2:C:416:VAL:HA	1.97	0.47
6:L:12:LYS:HB2	6:L:109:VAL:HG12	1.97	0.47
10:Q:171:VAL:HG11	7:J:68:ARG:HE	1.80	0.47
12:Y:205:LEU:O	12:Y:205:LEU:HD23	2.15	0.47
6:G:161:PHE:CB	7:J:404:PHE:HA	2.45	0.47
7:J:159:ILE:CD1	7:J:224:VAL:HG13	2.46	0.47
8:M:164:ILE:CG1	9:R:150:MET:HE1	2.44	0.47
6:L:7:PHE:C	6:L:8:LEU:HD12	2.40	0.46
1:B:62:ASN:OD1	1:B:63:LEU:N	2.48	0.46
2:D:456:CYS:O	2:D:460:GLU:N	2.36	0.46
6:G:87:LEU:HD12	6:G:87:LEU:C	2.40	0.46
7:J:393:ILE:HG12	7:J:398:ILE:HD12	1.97	0.46
10:S:165:LEU:O	10:S:169:ASN:OD1	2.33	0.46
10:S:370:LEU:HD11	13:c:119:LEU:HB3	1.97	0.46
12:b:168:LEU:HD23	12:b:172:ASN:OD1	2.16	0.46
1:H:175:THR:O	2:I:87:ASN:ND2	2.48	0.46
2:C:456:CYS:O	2:C:459:SER:OG	2.28	0.46
6:L:58:MET:HB3	6:L:73:PHE:CB	2.46	0.46
8:O:170:TYR:HD2	9:P:157:LEU:HD13	1.79	0.46
11:U:239:LEU:O	11:U:242:GLU:HG2	2.15	0.46
10:S:259:GLU:OE1	12:b:74:ARG:NH2	2.48	0.46
10:S:373:THR:O	10:S:376:GLN:NE2	2.48	0.46
12:b:143:TYR:HB2	13:c:91:ILE:HD11	1.98	0.46
12:Y:203:VAL:O	12:Y:206:GLU:HG3	2.16	0.46
6:G:160:GLN:O	7:J:405:ASN:N	2.48	0.46
7:J:384:LYS:O	7:J:385:VAL:HG13	2.15	0.46
9:R:341:CYS:HA	9:R:357:ILE:HD11	1.97	0.46
1:A:62:ASN:OD1	1:A:63:LEU:N	2.48	0.46
6:L:40:VAL:O	6:L:42:SER:N	2.45	0.46
1:B:35:LEU:HG	3:F:56:LEU:HD22	1.97	0.46
7:J:108:PRO:HB2	7:J:210:ILE:HD11	1.98	0.46
7:N:10:ASN:HA	7:N:85:ASN:ND2	2.30	0.46
7:N:123:LEU:HD11	7:N:204:PHE:CG	2.51	0.46
10:Q:296:LEU:HD11	10:Q:300:LEU:HB2	1.97	0.46
6:G:202:ARG:NH2	7:J:306:PHE:O	2.48	0.46
7:J:148:LYS:NZ	7:J:152:LEU:O	2.37	0.46
7:J:292:LEU:C	7:J:292:LEU:HD23	2.40	0.46
8:M:162:ASP:O	8:M:165:VAL:HG22	2.15	0.46
13:c:75:PHE:CZ	13:c:79:GLU:OE2	2.69	0.46
2:I:150:THR:OG1	2:I:151:PRO:HD3	2.15	0.46
2:C:592:LEU:HD23	2:C:718:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:142:PHE:HB2	11:U:185:MET:HE2	1.98	0.46
2:D:293:VAL:HG13	2:D:298:GLN:HB2	1.97	0.46
10:S:292:ILE:HD12	10:S:304:MET:HE1	1.96	0.46
12:b:203:VAL:O	12:b:206:GLU:HG3	2.15	0.46
13:c:50:ASP:HA	13:c:53:VAL:HG22	1.97	0.46
2:C:618:LEU:O	2:C:626:LYS:NZ	2.36	0.46
9:P:161:THR:HG23	9:P:162:TYR:N	2.31	0.46
2:D:403:LEU:CD1	2:D:406:LEU:HD23	2.45	0.46
7:J:33:TYR:O	7:J:37:LEU:HD13	2.15	0.46
7:J:374:SER:OG	7:J:375:ARG:N	2.48	0.46
8:M:348:LEU:HD12	8:M:358:LYS:HD2	1.97	0.46
12:b:17:THR:HG23	12:b:18:ALA:H	1.79	0.46
2:C:410:GLU:HG3	2:C:411:LEU:HD22	1.98	0.46
11:U:165:GLN:O	11:U:169:LEU:HD23	2.15	0.46
12:b:50:ARG:HE	12:b:54:MET:HE2	1.80	0.46
7:J:113:ARG:NE	7:J:236:GLU:OE2	2.48	0.46
7:J:154:VAL:HG22	7:J:155:LEU:N	2.31	0.46
8:M:136:ILE:HG23	8:M:143:ARG:HB2	1.96	0.46
7:N:128:PHE:CZ	7:N:132:LEU:HD21	2.50	0.46
2:D:701:LEU:CD1	2:D:718:LEU:HD23	2.46	0.46
9:R:178:ASP:OD2	9:R:180:ILE:HD12	2.16	0.46
6:G:36:GLN:HE21	6:G:55:ARG:HD3	1.81	0.45
7:J:110:LYS:O	7:J:240:PHE:HA	2.16	0.45
10:S:276:CYS:HB2	11:V:236:TRP:CH2	2.52	0.45
1:A:90:LEU:HD13	2:C:641:TYR:CG	2.50	0.45
11:U:146:PHE:CD1	11:U:150:LEU:HD12	2.43	0.45
7:J:243:VAL:HG22	7:J:243:VAL:O	2.16	0.45
9:R:341:CYS:SG	9:R:342:TYR:N	2.89	0.45
10:S:174:LEU:HD12	10:S:175:ASP:N	2.31	0.45
2:C:707:THR:HA	2:C:712:ARG:CZ	2.46	0.45
6:L:43:ASP:N	6:L:43:ASP:OD1	2.47	0.45
7:N:20:VAL:O	7:N:24:LEU:HD23	2.17	0.45
9:P:104:PHE:CE1	9:P:108:ILE:HD11	2.51	0.45
9:P:199:ILE:HG22	9:P:200:GLN:N	2.31	0.45
9:P:199:ILE:CD1	9:P:220:ILE:HG23	2.46	0.45
1:B:66:THR:HG21	2:D:630:PHE:HB2	1.97	0.45
2:D:488:ASP:O	2:D:491:SER:OG	2.24	0.45
2:D:507:PHE:HE1	3:F:92:LEU:HD21	1.81	0.45
2:D:572:PRO:O	2:D:578:VAL:HG21	2.17	0.45
11:V:166:PHE:O	11:V:169:LEU:HD23	2.17	0.45
2:C:586:MET:HE1	2:C:594:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:687:ILE:HD12	2:C:687:ILE:H	1.81	0.45
7:J:250:SER:O	7:J:253:ASN:N	2.48	0.45
2:I:198:VAL:HG13	2:I:200:ALA:H	1.81	0.45
7:N:132:LEU:CD2	7:N:231:THR:HG21	2.46	0.45
7:N:153:PRO:HD2	7:N:255:MET:HE1	1.99	0.45
11:U:166:PHE:O	11:U:169:LEU:HD23	2.16	0.45
12:Y:38:VAL:HG22	13:Z:29:LEU:HD12	1.98	0.45
2:D:299:LEU:HD22	3:F:117:LEU:HD11	1.98	0.45
7:J:102:GLU:O	7:J:249:LYS:HD3	2.17	0.45
7:J:255:MET:O	7:J:259:GLY:CA	2.64	0.45
8:M:338:GLN:O	8:M:341:LYS:HG2	2.17	0.45
9:R:192:ASN:ND2	9:R:195:ASN:OD1	2.48	0.45
12:b:54:MET:SD	13:c:10:TYR:OH	2.66	0.45
2:I:3:LEU:O	2:I:6:ASP:OD1	2.35	0.45
7:N:284:HIS:HA	9:P:210:SER:OG	2.17	0.45
9:P:269:THR:HG22	9:P:284:ARG:HB2	1.98	0.45
2:D:544:LYS:O	2:D:547:SER:OG	2.28	0.45
6:G:40:VAL:HB	6:G:41:PRO:HD3	1.98	0.45
9:R:298:ILE:CG1	9:R:321:ILE:HD11	2.47	0.45
10:S:389:VAL:HG23	10:S:390:PHE:HD1	1.82	0.45
1:A:74:GLU:OE1	1:A:74:GLU:HA	2.17	0.45
6:L:12:LYS:NZ	6:L:108:GLY:O	2.41	0.45
2:D:704:LEU:O	2:D:709:ASN:ND2	2.47	0.45
7:J:51:ILE:HG13	7:J:52:TYR:N	2.31	0.45
2:I:169:SER:OG	2:I:173:ARG:NH2	2.49	0.45
5:W:36:SER:OG	5:W:37:SER:N	2.49	0.45
2:C:367:CYS:SG	2:C:379:ILE:HD11	2.57	0.45
7:N:67:ARG:HE	10:S:168:THR:HB	1.80	0.45
7:N:283:LEU:HB3	9:P:210:SER:HB3	1.98	0.45
2:D:379:ILE:HG21	2:D:415:LYS:HG2	1.99	0.45
12:b:188:ASP:O	12:b:189:ASP:OD1	2.35	0.45
2:I:218:LEU:HD23	2:I:218:LEU:H	1.82	0.45
2:D:687:ILE:H	2:D:687:ILE:HD12	1.82	0.45
7:J:386:GLY:O	7:J:387:PHE:HD1	1.99	0.45
9:R:300:PHE:HZ	10:S:332:LEU:HD13	1.82	0.45
11:V:160:LYS:O	11:V:162:ASP:N	2.48	0.45
11:V:227:ILE:O	11:V:231:LYS:HG2	2.17	0.45
1:A:111:HIS:HA	1:A:114:LEU:HD12	1.99	0.45
2:C:416:VAL:HG13	2:C:417:CYS:N	2.32	0.45
7:N:25:MET:CE	7:N:72:VAL:HG11	2.47	0.45
8:O:134:THR:O	8:O:134:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:299:MET:O	11:U:299:MET:HG2	2.17	0.45
12:Y:146:LEU:O	12:Y:150:LEU:HD23	2.17	0.45
2:D:536:ILE:HD13	2:D:577:PHE:CD1	2.52	0.45
6:G:9:GLY:O	6:G:111:MET:HG3	2.17	0.45
6:G:216:ILE:HG22	6:G:221:ILE:HG23	1.98	0.45
9:R:189:PHE:HB3	9:R:248:ASP:OD2	2.16	0.45
12:b:99:ASN:HB3	12:b:105:PRO:HD3	1.98	0.45
12:b:148:LYS:O	12:b:152:LEU:HD23	2.17	0.45
12:b:189:ASP:O	12:b:192:GLU:HG3	2.16	0.45
2:I:235:LYS:HE3	2:I:251:VAL:HB	1.99	0.44
2:C:315:MET:HE3	2:C:344:ILE:CD1	2.47	0.44
2:C:568:LEU:HD22	2:C:578:VAL:HG22	1.98	0.44
6:L:83:VAL:O	6:L:83:VAL:HG13	2.17	0.44
9:P:234:THR:OG1	9:P:239:LYS:NZ	2.50	0.44
1:B:82:LEU:O	1:B:86:LEU:HD23	2.17	0.44
6:G:63:SER:O	6:G:69:THR:OG1	2.35	0.44
11:V:167:ARG:HG3	11:V:171:TYR:CE2	2.51	0.44
2:C:351:ASP:CG	2:C:353:SER:HG	2.24	0.44
6:L:7:PHE:CD2	6:L:236:VAL:HG11	2.52	0.44
2:D:297:GLU:OE1	2:D:297:GLU:N	2.34	0.44
6:G:81:MET:HE3	6:G:84:PRO:HA	1.99	0.44
7:J:7:LEU:N	7:J:7:LEU:HD12	2.33	0.44
13:c:66:ILE:HG13	13:c:67:THR:N	2.33	0.44
4:T:315:LYS:HE2	4:T:331:MET:HE1	1.99	0.44
6:L:205:LEU:C	6:L:205:LEU:HD23	2.42	0.44
7:N:324:LEU:HD12	9:P:125:VAL:HG22	1.99	0.44
8:O:226:LYS:NZ	8:O:231:ASN:OD1	2.21	0.44
10:Q:171:VAL:HG21	7:J:68:ARG:CZ	2.47	0.44
11:U:280:ASP:OD1	11:U:281:ASP:N	2.51	0.44
1:B:17:LYS:O	1:B:20:VAL:HG22	2.18	0.44
7:J:124:GLN:OE1	7:J:127:LYS:HB3	2.17	0.44
8:M:300:ASP:OD1	8:M:303:SER:CA	2.65	0.44
9:R:334:GLN:O	11:V:284:ARG:NH2	2.51	0.44
13:c:63:GLN:HA	13:c:66:ILE:HG12	1.99	0.44
2:C:544:LYS:O	2:C:547:SER:OG	2.29	0.44
3:E:106:LEU:O	3:E:110:ILE:HG22	2.18	0.44
7:N:59:ASP:O	7:N:62:ILE:HG12	2.18	0.44
8:O:120:GLN:OE1	8:O:121:HIS:N	2.50	0.44
1:B:129:ILE:HG21	2:D:350:ARG:NH1	2.32	0.44
7:J:28:PRO:O	7:J:31:VAL:HG22	2.18	0.44
7:J:61:LEU:CD1	7:J:71:ILE:HD13	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:423:ASN:OD1	7:J:425:ASP:N	2.50	0.44
11:U:295:PHE:O	11:U:299:MET:SD	2.76	0.44
2:D:592:LEU:O	2:D:633:ILE:N	2.51	0.44
6:G:158:LEU:HD21	6:G:161:PHE:CD1	2.53	0.44
6:G:180:THR:OG1	6:G:186:ASP:OD2	2.33	0.44
6:G:196:THR:HB	6:G:198:MET:HE2	1.99	0.44
7:J:61:LEU:HD11	7:J:74:ARG:NH1	2.31	0.44
9:R:298:ILE:HG13	9:R:321:ILE:HD11	1.99	0.44
10:S:171:VAL:O	10:S:174:LEU:HG	2.17	0.44
11:V:178:PHE:O	11:V:181:ILE:HG22	2.18	0.44
11:V:230:LEU:HD11	11:V:236:TRP:HZ3	1.82	0.44
11:V:246:LEU:O	11:V:250:VAL:HG23	2.18	0.44
1:H:151:GLN:OE1	3:K:138:ILE:HG22	2.18	0.44
2:I:150:THR:HB	2:I:190:ILE:HD11	1.99	0.44
2:I:228:ALA:HB1	10:S:145:ASN:O	2.17	0.44
4:T:282:THR:O	4:T:286:LEU:HG	2.18	0.44
2:C:312:VAL:HG12	2:C:316:MET:HE1	1.98	0.44
7:N:155:LEU:N	7:N:204:PHE:O	2.47	0.44
7:N:233:SER:C	7:N:235:ARG:H	2.26	0.44
7:N:245:LYS:O	7:N:245:LYS:HD3	2.18	0.44
8:O:296:ASP:OD1	8:O:296:ASP:N	2.50	0.44
12:Y:43:LYS:HA	12:Y:46:VAL:HG12	2.00	0.44
2:D:351:ASP:N	2:D:351:ASP:OD1	2.50	0.44
2:D:366:ARG:NH1	6:G:112:TRP:CD1	2.86	0.44
2:D:658:ILE:HG22	2:D:673:PHE:CZ	2.53	0.44
2:I:72:LEU:HD22	2:I:234:LEU:HA	2.00	0.44
1:A:25:GLU:CD	3:E:26:LEU:HD22	2.42	0.44
8:O:275:LEU:O	8:O:278:VAL:HG12	2.18	0.44
7:N:210:ILE:HG21	7:N:258:LEU:HB3	1.99	0.44
7:N:298:MET:SD	7:N:298:MET:C	3.01	0.44
7:N:333:PHE:CE1	7:N:410:PHE:HB3	2.53	0.44
11:U:150:LEU:HD13	11:U:178:PHE:HE1	1.80	0.44
6:G:231:ARG:O	6:G:235:VAL:HG23	2.18	0.44
9:R:206:LYS:HG3	9:R:208:GLU:O	2.18	0.44
10:S:151:TRP:CD2	10:S:222:LYS:HD3	2.52	0.44
10:S:328:ASP:HA	10:S:331:GLU:OE2	2.18	0.44
2:I:175:ALA:HB2	2:I:187:ALA:CB	2.48	0.44
7:N:390:LYS:HA	7:N:398:ILE:O	2.18	0.44
13:Z:104:ARG:HD2	13:Z:107:ILE:HD11	1.99	0.44
6:G:10:ILE:HD11	6:G:87:LEU:HD23	1.98	0.44
8:M:227:ARG:N	8:M:232:SER:O	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:180:ILE:HG12	9:R:205:TYR:O	2.18	0.44
1:A:53:LEU:O	1:A:56:ARG:HG2	2.18	0.43
3:E:95:ASP:O	3:E:98:VAL:HG12	2.18	0.43
7:N:286:TYR:CE1	8:O:161:GLU:OE2	2.71	0.43
8:O:164:ILE:HG12	9:P:150:MET:HE2	2.00	0.43
9:P:175:VAL:HG12	9:P:177:ASN:OD1	2.18	0.43
9:P:257:ILE:O	9:P:261:LEU:HD23	2.18	0.43
11:U:300:ASP:HB3	11:U:304:GLY:H	1.82	0.43
2:D:396:ILE:HA	2:D:399:THR:HG22	1.99	0.43
6:G:205:LEU:O	6:G:218:ARG:HD3	2.17	0.43
7:J:108:PRO:HA	7:J:211:ILE:O	2.17	0.43
7:J:147:PHE:CZ	7:J:156:ILE:HB	2.53	0.43
7:J:286:TYR:HB2	8:M:164:ILE:HG21	1.99	0.43
10:S:296:LEU:CD1	10:S:304:MET:HE3	2.48	0.43
12:b:147:ARG:O	12:b:151:ILE:HG12	2.17	0.43
2:C:580:MET:HE2	2:C:584:TYR:OH	2.18	0.43
6:L:94:ASN:O	6:L:97:GLU:HG3	2.18	0.43
6:L:142:TRP:HB3	6:L:167:ARG:HG2	2.00	0.43
7:N:67:ARG:HB2	7:N:69:ASN:OD1	2.18	0.43
8:O:130:ASP:OD1	8:O:130:ASP:N	2.50	0.43
8:O:181:VAL:HG11	8:O:186:LEU:HD21	1.98	0.43
10:Q:171:VAL:O	10:Q:174:LEU:HG	2.18	0.43
7:J:162:PHE:HD1	7:J:196:SER:HA	1.83	0.43
9:R:240:CYS:O	9:R:244:LEU:HG	2.18	0.43
9:R:284:ARG:NE	9:R:362:LEU:O	2.44	0.43
2:I:211:ILE:HG22	2:I:212:ASN:N	2.34	0.43
7:N:12:VAL:HG13	7:N:12:VAL:O	2.18	0.43
9:P:128:ILE:HG22	9:P:132:THR:HG21	2.01	0.43
12:Y:164:LEU:HB2	13:Z:112:ILE:HD11	2.00	0.43
6:G:142:TRP:HB3	6:G:167:ARG:HG2	1.99	0.43
7:J:203:ALA:O	7:J:211:ILE:HD12	2.17	0.43
7:J:233:SER:O	7:J:234:GLU:HG2	2.17	0.43
7:J:405:ASN:OD1	7:J:406:GLY:N	2.51	0.43
8:M:179:PRO:CD	9:R:153:ARG:HG2	2.49	0.43
9:R:180:ILE:HG23	9:R:205:TYR:O	2.19	0.43
9:R:316:LEU:O	9:R:318:MET:SD	2.76	0.43
12:b:164:LEU:HA	12:b:167:ILE:HG22	2.00	0.43
2:C:489:MET:HE2	2:C:489:MET:HA	2.00	0.43
7:N:239:ILE:CD1	11:U:232:ALA:HB3	2.49	0.43
9:P:135:GLN:O	9:P:139:VAL:HG23	2.18	0.43
9:P:227:LYS:HB3	9:P:304:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:432:THR:HB	2:D:436:PHE:CE1	2.53	0.43
7:J:61:LEU:HD13	7:J:71:ILE:HD13	1.98	0.43
7:J:67:ARG:HB2	7:J:69:ASN:OD1	2.19	0.43
7:J:100:LYS:CG	7:J:103:LYS:HG2	2.48	0.43
7:J:225:LEU:HA	7:J:228:ILE:HD12	2.00	0.43
9:R:188:LYS:HD2	9:R:196:PRO:HB2	2.00	0.43
3:K:139:ARG:NH1	3:K:140:THR:HB	2.33	0.43
1:A:51:ARG:NH2	2:C:495:LEU:HD23	2.31	0.43
1:A:70:ILE:O	1:A:74:GLU:HG2	2.18	0.43
9:P:173:ASP:N	9:P:173:ASP:OD1	2.49	0.43
1:B:68:LEU:HD11	3:F:72:PHE:H	1.84	0.43
3:F:97:SER:HB3	3:F:101:LYS:HZ3	1.84	0.43
7:J:160:GLN:HG2	7:J:162:PHE:CE1	2.54	0.43
7:J:192:LYS:N	7:J:193:PRO:HD3	2.34	0.43
10:S:302:LYS:HA	10:S:305:GLU:HG3	1.99	0.43
5:W:79:GLU:HA	5:W:82:THR:HG22	2.01	0.43
1:A:89:LEU:HD13	3:E:76:SER:HA	2.00	0.43
2:C:421:LEU:N	2:C:422:PRO:HD2	2.31	0.43
2:C:539:PRO:CD	2:C:580:MET:HE1	2.48	0.43
6:L:173:LEU:HD21	7:N:398:ILE:HG21	1.99	0.43
7:N:392:GLU:OE2	7:N:396:ARG:N	2.52	0.43
10:Q:220:GLN:CD	10:Q:220:GLN:O	2.61	0.43
1:B:74:GLU:HA	2:D:664:ILE:HD12	2.00	0.43
8:M:163:TYR:CB	9:R:150:MET:HE2	2.48	0.43
8:M:238:HIS:CD2	8:M:246:VAL:HG21	2.54	0.43
10:S:223:PHE:CZ	11:V:138:LEU:HG	2.54	0.43
11:V:288:ASN:O	11:V:291:ASP:N	2.51	0.43
2:I:53:CYS:SG	2:I:54:GLU:N	2.91	0.43
2:D:559:ARG:NE	2:D:559:ARG:HA	2.33	0.43
8:M:241:PRO:HB2	8:M:243:PHE:CE2	2.54	0.43
12:b:38:VAL:HG22	13:c:29:LEU:HD22	1.99	0.43
2:C:575:ASN:O	2:C:579:ARG:NE	2.51	0.43
7:N:248:VAL:HG22	7:N:249:LYS:N	2.34	0.43
9:P:341:CYS:O	9:P:345:ILE:HG12	2.18	0.43
10:Q:148:LEU:HB3	10:Q:151:TRP:CZ2	2.54	0.43
1:B:135:PHE:HE1	3:F:125:MET:HE2	1.84	0.43
7:J:28:PRO:HA	7:J:68:ARG:NH2	2.32	0.43
7:J:294:GLY:C	9:R:127:ARG:HE	2.27	0.43
12:b:38:VAL:HG12	12:b:42:LEU:HD23	2.00	0.43
2:I:193:ARG:HD2	2:I:265:LEU:HD21	2.01	0.43
2:C:477:LYS:O	2:C:478:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:317:GLU:OE1	7:N:317:GLU:N	2.51	0.43
7:N:416:LEU:HD13	7:N:421:LEU:HD12	2.01	0.43
7:N:439:SER:HG	7:N:450:GLU:CD	2.26	0.43
8:O:340:ASN:OD1	8:O:344:TRP:NE1	2.52	0.43
10:Q:171:VAL:HG21	7:J:68:ARG:NE	2.34	0.43
2:D:339:LEU:HD21	3:F:113:ASP:HB3	2.01	0.43
7:J:390:LYS:HD3	7:J:399:THR:HG22	2.00	0.43
9:R:323:ILE:HD13	9:R:341:CYS:HB3	2.00	0.43
12:b:90:LYS:C	12:b:92:SER:H	2.26	0.43
12:b:110:ILE:O	12:b:114:ILE:HG12	2.18	0.43
2:I:64:VAL:HA	2:I:67:VAL:HG22	1.99	0.43
3:K:202:ILE:O	3:K:206:ARG:HG2	2.19	0.43
6:L:168:GLU:HG2	6:L:169:SER:N	2.33	0.43
7:N:28:PRO:O	7:N:31:VAL:HG22	2.18	0.43
7:N:30:THR:HG23	7:N:31:VAL:N	2.34	0.43
7:N:92:ILE:HG13	7:N:93:ASP:N	2.34	0.43
7:N:164:SER:OG	7:N:165:ASN:N	2.50	0.43
8:O:193:GLY:O	8:O:195:ILE:HD12	2.18	0.43
12:Y:148:LYS:O	12:Y:152:LEU:HD23	2.19	0.43
12:Y:205:LEU:HD23	12:Y:205:LEU:C	2.44	0.43
1:B:6:GLU:HG2	1:B:7:LYS:N	2.34	0.43
3:F:25:PHE:CE2	8:M:123:MET:HE1	2.54	0.43
9:R:157:LEU:HA	9:R:161:THR:HG22	2.01	0.43
3:K:199:SER:HA	3:K:202:ILE:HD12	2.00	0.42
1:A:100:LEU:HD22	2:C:506:ARG:HH21	1.84	0.42
2:C:561:LEU:HA	2:C:564:THR:HG22	2.00	0.42
6:L:97:GLU:OE2	6:L:98:VAL:HG23	2.18	0.42
7:N:192:LYS:N	7:N:193:PRO:HD3	2.34	0.42
9:P:366:MET:O	9:P:369:ARG:NH2	2.52	0.42
8:M:160:LEU:C	8:M:160:LEU:HD23	2.44	0.42
10:S:167:GLU:O	10:S:171:VAL:HG23	2.19	0.42
10:S:373:THR:O	10:S:376:GLN:HG3	2.18	0.42
11:V:235:ASP:N	11:V:235:ASP:OD1	2.52	0.42
11:V:255:ARG:NH1	11:V:255:ARG:HG2	2.34	0.42
5:W:6:LEU:HD23	5:W:47:ALA:HB1	2.01	0.42
7:N:257:LEU:HD21	7:N:380:VAL:HG11	2.02	0.42
8:O:240:ILE:HB	8:O:246:VAL:HG11	2.01	0.42
8:O:276:VAL:HG11	9:P:315:PHE:CE1	2.54	0.42
9:P:331:ARG:NH2	9:P:334:GLN:OE1	2.52	0.42
12:Y:188:ASP:OD1	12:Y:188:ASP:N	2.52	0.42
6:G:196:THR:CB	6:G:198:MET:HE2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:98:ILE:HG13	7:J:99:SER:N	2.34	0.42
11:V:189:LEU:O	11:V:192:ILE:HG12	2.19	0.42
12:b:193:TYR:HA	12:b:196:THR:OG1	2.18	0.42
1:H:179:TYR:HA	2:I:131:ILE:HD13	2.01	0.42
4:T:349:PRO:O	4:T:353:GLN:HG2	2.18	0.42
1:A:65:LYS:HD2	3:E:75:THR:N	2.35	0.42
2:C:516:LEU:HA	2:C:519:LEU:HD12	2.01	0.42
7:N:28:PRO:HA	7:N:68:ARG:NH2	2.35	0.42
8:O:212:ARG:HB2	8:O:283:GLN:HG2	1.99	0.42
9:P:346:LYS:HD3	10:Q:325:PHE:CE1	2.54	0.42
12:Y:207:GLU:O	12:Y:211:LEU:HD23	2.19	0.42
1:B:44:ILE:HG23	1:B:44:ILE:O	2.19	0.42
1:B:90:LEU:HD13	2:D:641:TYR:CG	2.54	0.42
7:J:430:TRP:CZ3	7:J:431:LEU:HD13	2.54	0.42
8:M:236:PHE:O	8:M:237:LYS:HD2	2.19	0.42
10:S:223:PHE:CZ	11:V:137:VAL:HG23	2.54	0.42
10:S:356:LEU:C	10:S:357:LEU:HD22	2.44	0.42
11:V:206:LEU:HA	11:V:209:VAL:HG22	2.01	0.42
1:A:123:GLU:CD	1:A:127:LYS:HZ3	2.26	0.42
2:C:494:THR:HA	2:C:499:PHE:HD2	1.84	0.42
2:C:504:SER:HB2	3:E:78:PHE:CE1	2.54	0.42
7:N:129:ILE:HD11	7:N:144:VAL:HG22	2.01	0.42
7:N:331:ILE:HG23	7:N:332:LYS:N	2.35	0.42
10:Q:192:ASP:O	10:Q:196:VAL:HG23	2.19	0.42
1:B:59:LEU:O	1:B:62:ASN:OD1	2.36	0.42
6:G:23:LEU:HD21	6:G:58:MET:HE1	2.02	0.42
6:G:103:LEU:HD12	6:G:107:TYR:CE2	2.55	0.42
7:J:13:PRO:HD2	7:J:84:LEU:O	2.19	0.42
9:R:101:THR:O	9:R:105:LEU:HG	2.19	0.42
9:R:252:SER:O	9:R:255:THR:OG1	2.33	0.42
9:R:298:ILE:HD13	9:R:323:ILE:HG22	2.00	0.42
12:b:37:GLU:OE2	12:b:38:VAL:HG23	2.19	0.42
1:A:35:LEU:HG	3:E:56:LEU:HD22	2.00	0.42
7:N:416:LEU:CD1	7:N:421:LEU:HD12	2.49	0.42
9:P:321:ILE:HG13	10:Q:334:LEU:HD11	2.01	0.42
12:Y:197:TYR:O	12:Y:201:LEU:HG	2.18	0.42
2:D:358:GLU:OE1	6:G:110:ILE:HD11	2.20	0.42
6:G:87:LEU:HD21	6:G:111:MET:CE	2.50	0.42
6:G:150:GLU:CB	6:G:206:THR:HG21	2.48	0.42
7:J:146:MET:HE3	7:J:147:PHE:O	2.19	0.42
7:J:383:GLU:OE1	7:J:407:ASN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:179:PRO:HB2	9:R:147:LEU:HB2	2.01	0.42
10:S:268:LEU:CD2	11:V:227:ILE:HD12	2.49	0.42
2:C:609:ASP:OD2	3:E:58:ARG:HD3	2.20	0.42
6:L:181:MET:O	6:L:181:MET:HG3	2.20	0.42
7:N:125:PRO:HB3	7:N:146:MET:HE3	2.02	0.42
10:Q:211:LEU:HD23	10:Q:215:LYS:HD3	2.02	0.42
10:Q:363:TYR:CE2	12:Y:167:ILE:HG12	2.54	0.42
1:B:20:VAL:HG21	3:F:77:ASN:HD22	1.84	0.42
3:F:52:VAL:O	3:F:55:GLU:HG2	2.20	0.42
3:F:54:THR:O	3:F:58:ARG:HG2	2.19	0.42
6:G:86:PHE:HD1	6:G:237:LEU:HD13	1.84	0.42
7:J:39:TRP:CE2	7:J:88:GLN:HG3	2.55	0.42
7:J:95:HIS:O	7:J:98:ILE:HG12	2.19	0.42
7:J:233:SER:C	7:J:235:ARG:H	2.27	0.42
7:J:390:LYS:HA	7:J:398:ILE:O	2.20	0.42
8:M:156:ASP:O	8:M:159:GLU:HG2	2.20	0.42
8:M:324:ILE:HD12	8:M:324:ILE:H	1.84	0.42
8:M:348:LEU:HA	8:M:358:LYS:HD2	2.01	0.42
10:S:192:ASP:O	10:S:196:VAL:HG23	2.18	0.42
11:V:165:GLN:O	11:V:169:LEU:HD23	2.19	0.42
1:A:58:GLN:HG3	2:C:501:ASN:ND2	2.35	0.42
2:C:590:ASN:HA	2:C:594:ARG:HB2	2.01	0.42
2:C:700:ILE:HG22	2:C:704:LEU:HD23	2.02	0.42
7:N:39:TRP:CE2	7:N:88:GLN:HG3	2.54	0.42
7:J:139:ILE:HG21	7:J:223:LEU:HD21	2.02	0.42
7:J:272:CYS:HB3	7:J:335:GLY:O	2.20	0.42
8:M:266:LEU:HD23	8:M:266:LEU:C	2.43	0.42
12:b:97:LEU:O	12:b:101:VAL:HG23	2.20	0.42
13:c:44:GLU:HA	13:c:47:GLN:OE1	2.20	0.42
3:E:54:THR:O	3:E:58:ARG:HG2	2.20	0.42
3:E:81:LEU:HA	3:E:84:GLN:HG3	2.01	0.42
2:D:617:ASN:ND2	8:M:122:GLN:O	2.53	0.42
7:J:124:GLN:OE1	7:J:127:LYS:CB	2.68	0.42
7:J:200:TYR:CE1	7:J:214:SER:HB3	2.55	0.42
8:M:130:ASP:OD1	8:M:130:ASP:N	2.52	0.42
10:S:284:LYS:O	10:S:288:THR:HG23	2.20	0.42
10:S:343:THR:O	10:S:346:VAL:HG23	2.20	0.42
12:b:16:LEU:O	12:b:20:LEU:HB2	2.20	0.42
12:b:138:LYS:HD2	12:b:138:LYS:N	2.35	0.42
2:I:177:HIS:ND1	2:I:178:PRO:O	2.45	0.42
5:W:75:PRO:O	5:W:78:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TRP:HE3	1:A:12:ILE:HD11	1.84	0.42
2:D:406:LEU:HD12	2:D:410:GLU:HG3	2.02	0.42
7:J:331:ILE:CG1	7:J:337:ALA:HA	2.49	0.42
7:J:427:VAL:O	7:J:427:VAL:HG13	2.20	0.42
8:M:251:ASP:O	8:M:256:GLY:N	2.53	0.42
9:R:239:LYS:HB3	9:R:315:PHE:CD2	2.55	0.42
2:C:296:LEU:N	2:C:296:LEU:HD23	2.35	0.42
2:C:510:MET:HE2	3:E:89:TRP:HE1	1.85	0.42
8:O:176:THR:HB	9:P:157:LEU:HD21	2.01	0.42
12:Y:54:MET:SD	13:Z:10:TYR:OH	2.73	0.42
12:Y:74:ARG:NE	13:Z:76:LEU:HD11	2.35	0.42
6:G:129:ILE:HD12	6:G:140:ILE:HG23	2.02	0.42
6:G:168:GLU:HG2	6:G:169:SER:N	2.35	0.42
8:M:223:LEU:C	8:M:224:LEU:HD22	2.44	0.42
8:M:240:ILE:HB	8:M:246:VAL:HG11	2.02	0.42
9:R:344:LEU:HD22	11:V:252:LEU:HD21	2.01	0.42
10:S:148:LEU:HD22	10:S:151:TRP:CZ2	2.55	0.42
4:T:300:THR:HG23	5:W:79:GLU:OE2	2.20	0.41
6:L:116:PHE:CE2	6:L:221:ILE:HD11	2.53	0.41
8:O:182:ASP:HB2	8:O:201:MET:HE2	2.01	0.41
9:P:226:LEU:HD23	9:P:226:LEU:C	2.45	0.41
10:Q:165:LEU:O	10:Q:169:ASN:CG	2.63	0.41
1:B:37:ARG:NH1	8:M:128:VAL:HG12	2.34	0.41
2:D:299:LEU:HD21	2:D:303:TRP:CE3	2.54	0.41
6:G:138:GLU:OE1	6:G:138:GLU:N	2.53	0.41
6:G:150:GLU:OE1	6:G:160:GLN:HB3	2.20	0.41
6:G:209:ILE:HG23	6:G:215:LYS:HE3	2.02	0.41
7:J:92:ILE:HG13	7:J:93:ASP:N	2.34	0.41
7:J:154:VAL:O	7:J:155:LEU:HD22	2.20	0.41
8:M:241:PRO:HB2	8:M:243:PHE:CZ	2.55	0.41
12:b:55:SER:O	12:b:59:GLN:OE1	2.38	0.41
6:L:13:GLN:OE1	6:L:79:SER:HA	2.20	0.41
7:N:69:ASN:HB3	10:S:168:THR:HG21	2.01	0.41
8:O:213:THR:HG23	8:O:215:GLN:HB2	2.02	0.41
9:P:287:ARG:O	9:P:287:ARG:NE	2.50	0.41
13:Z:49:ARG:O	13:Z:53:VAL:HG22	2.20	0.41
6:G:237:LEU:O	6:G:240:ILE:HG12	2.20	0.41
7:J:424:ILE:HG23	7:J:425:ASP:N	2.35	0.41
8:M:309:PHE:HD1	8:M:314:LYS:HA	1.84	0.41
8:M:316:GLU:OE1	8:M:316:GLU:N	2.53	0.41
10:S:215:LYS:O	10:S:218:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:363:TYR:HE1	12:b:167:ILE:HD13	1.79	0.41
3:K:167:ASN:C	3:K:167:ASN:HD22	2.27	0.41
2:C:622:THR:HG21	2:C:668:GLU:OE2	2.21	0.41
2:C:633:ILE:HG23	2:C:634:THR:N	2.35	0.41
7:N:32:LEU:O	7:N:36:THR:HG23	2.20	0.41
8:O:170:TYR:CD2	9:P:157:LEU:HB3	2.55	0.41
10:Q:168:THR:C	7:J:67:ARG:HH21	2.29	0.41
3:F:52:VAL:HA	3:F:55:GLU:HG2	2.02	0.41
6:G:14:LEU:HB2	6:G:107:TYR:CD1	2.55	0.41
6:G:191:TYR:HE2	7:J:400:ILE:HG13	1.85	0.41
7:J:309:ASP:OD1	7:J:309:ASP:N	2.51	0.41
8:M:328:SER:HG	12:b:107:SER:HA	1.85	0.41
10:S:240:LYS:O	10:S:244:ILE:HG12	2.21	0.41
12:b:4:THR:HG23	12:b:5:TYR:N	2.35	0.41
2:C:400:PHE:O	2:C:402:ASN:N	2.54	0.41
2:C:440:MET:O	2:C:443:ILE:HG22	2.21	0.41
8:O:355:LEU:C	8:O:355:LEU:HD23	2.45	0.41
11:U:198:SER:O	11:U:201:GLU:HG3	2.20	0.41
6:G:157:ASN:HA	7:J:407:ASN:HB2	2.02	0.41
7:J:105:LYS:HA	7:J:248:VAL:O	2.21	0.41
9:R:254:LYS:HD3	9:R:302:ILE:HD11	2.01	0.41
10:S:158:MET:HE1	10:S:225:SER:HA	2.02	0.41
10:S:222:LYS:O	10:S:222:LYS:HG3	2.20	0.41
12:b:209:LYS:O	12:b:212:LEU:HG	2.20	0.41
2:I:95:PHE:O	3:K:163:ASN:ND2	2.47	0.41
1:A:70:ILE:HA	2:C:664:ILE:CD1	2.49	0.41
2:C:589:THR:HB	2:C:594:ARG:HE	1.85	0.41
8:O:241:PRO:HB2	8:O:243:PHE:CE2	2.54	0.41
8:O:300:ASP:OD1	8:O:303:SER:CA	2.68	0.41
13:Z:35:ASP:OD2	13:Z:38:GLN:N	2.38	0.41
6:G:209:ILE:HG23	6:G:215:LYS:HB3	2.02	0.41
7:J:72:VAL:HA	7:J:75:ILE:HG12	2.01	0.41
8:M:324:ILE:HD12	8:M:350:GLY:O	2.19	0.41
12:b:42:LEU:HA	12:b:45:GLN:CD	2.45	0.41
13:c:100:LEU:HA	13:c:103:GLN:OE1	2.20	0.41
1:A:34:TYR:HD1	8:O:128:VAL:HG13	1.85	0.41
8:O:236:PHE:O	8:O:237:LYS:HD2	2.20	0.41
10:Q:269:LEU:HD11	10:Q:273:ARG:NH2	2.36	0.41
13:Z:50:ASP:HA	13:Z:53:VAL:HG22	2.02	0.41
6:G:43:ASP:N	6:G:43:ASP:OD1	2.53	0.41
6:G:168:GLU:O	6:G:171:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:262:ARG:O	7:J:266:SER:OG	2.38	0.41
7:J:388:THR:HA	7:J:400:ILE:O	2.20	0.41
9:R:260:ASN:O	9:R:264:LEU:HD23	2.20	0.41
6:L:200:VAL:HG23	6:L:201:GLU:N	2.35	0.41
7:N:239:ILE:HD11	11:U:232:ALA:HB3	2.02	0.41
8:O:166:LEU:HD11	9:P:167:VAL:CG1	2.51	0.41
7:J:75:ILE:HG13	7:J:76:LEU:N	2.35	0.41
7:J:434:GLU:OE2	8:M:237:LYS:HD3	2.21	0.41
9:R:333:ASN:O	9:R:336:ASP:OD1	2.39	0.41
10:S:163:LEU:HD22	10:S:211:LEU:HD21	2.03	0.41
10:S:292:ILE:HD12	10:S:304:MET:CE	2.51	0.41
13:c:123:GLU:HA	13:c:126:VAL:HG12	2.02	0.41
3:K:161:VAL:HG12	3:K:171:ILE:HG22	2.01	0.41
1:A:114:LEU:HD11	3:E:100:GLN:HE22	1.86	0.41
2:C:443:ILE:HG23	2:C:458:PHE:HD1	1.86	0.41
2:C:470:THR:HA	2:C:473:VAL:HG22	2.03	0.41
3:E:97:SER:HB3	3:E:101:LYS:NZ	2.36	0.41
6:L:135:GLU:HG2	6:L:137:ILE:HG22	2.03	0.41
12:Y:182:LYS:HD2	12:Y:188:ASP:HB3	2.02	0.41
1:B:29:THR:HA	1:B:32:ARG:HG2	2.03	0.41
1:B:41:HIS:ND1	3:F:40:SER:OG	2.52	0.41
6:G:12:LYS:HB2	6:G:109:VAL:HG12	2.03	0.41
6:G:40:VAL:O	6:G:42:SER:N	2.49	0.41
6:G:149:PHE:CD1	6:G:205:LEU:HA	2.55	0.41
7:J:5:LEU:O	7:J:7:LEU:HD12	2.21	0.41
7:J:51:ILE:HG13	7:J:52:TYR:H	1.86	0.41
7:J:119:TYR:CE2	7:J:121:VAL:HA	2.56	0.41
7:J:419:LYS:HE2	7:J:419:LYS:HA	2.03	0.41
11:V:188:ASP:OD1	11:V:189:LEU:N	2.54	0.41
4:T:348:LEU:HD22	5:W:44:LEU:HD11	2.03	0.41
2:C:496:ASP:OD1	2:C:499:PHE:O	2.38	0.41
2:C:646:ILE:HG21	2:C:700:ILE:HG23	2.02	0.41
6:L:133:THR:HG22	6:L:134:LYS:N	2.36	0.41
6:L:150:GLU:CB	6:L:206:THR:HG21	2.50	0.41
7:N:68:ARG:O	7:N:72:VAL:HG23	2.21	0.41
8:O:214:SER:OG	9:P:212:LEU:O	2.35	0.41
9:P:157:LEU:HA	9:P:161:THR:HG22	2.03	0.41
11:U:170:LEU:O	11:U:173:LEU:HG	2.21	0.41
13:Z:52:ARG:O	13:Z:55:SER:OG	2.34	0.41
2:D:366:ARG:HH12	2:D:372:ILE:HA	1.86	0.41
3:F:95:ASP:O	3:F:98:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:59:ASP:O	7:J:60:LEU:C	2.64	0.41
7:J:200:TYR:CD1	7:J:214:SER:HB3	2.56	0.41
9:R:167:VAL:HG22	9:R:168:SER:N	2.36	0.41
9:R:187:TYR:O	9:R:198:GLU:HA	2.20	0.41
12:b:55:SER:O	12:b:58:LYS:N	2.54	0.41
1:H:166:ILE:HD11	2:I:131:ILE:HD11	2.03	0.41
1:A:25:GLU:OE1	3:E:26:LEU:HD13	2.21	0.41
2:C:483:LEU:HD21	2:C:522:LEU:HD13	2.03	0.41
2:C:545:VAL:HB	2:C:553:LEU:HD21	2.02	0.41
7:N:102:GLU:HG3	7:N:250:SER:HB3	2.03	0.41
1:B:113:GLN:O	1:B:116:GLU:HG3	2.21	0.41
7:J:33:TYR:CD1	7:J:37:LEU:HD13	2.56	0.41
9:R:188:LYS:NZ	9:R:198:GLU:OE1	2.50	0.41
11:V:230:LEU:HD11	11:V:236:TRP:CZ3	2.55	0.41
11:V:292:ILE:HB	12:b:170:GLN:OE1	2.21	0.41
11:V:292:ILE:HD13	12:b:170:GLN:OE1	2.20	0.41
1:A:70:ILE:HA	2:C:664:ILE:HD13	2.03	0.40
2:C:291:TRP:CH2	2:C:309:PRO:CB	3.04	0.40
2:C:598:LEU:HA	2:C:608:PRO:HB3	2.02	0.40
6:L:14:LEU:HB2	6:L:107:TYR:CD1	2.57	0.40
7:N:27:LEU:HD21	7:N:96:LEU:CD1	2.51	0.40
9:P:290:ARG:CD	9:P:290:ARG:O	2.69	0.40
10:Q:211:LEU:HA	10:Q:214:ILE:HG12	2.02	0.40
10:Q:306:TYR:CD1	10:Q:306:TYR:C	2.99	0.40
12:Y:212:LEU:HD12	12:Y:213:GLU:N	2.35	0.40
6:G:56:TYR:HB2	6:G:75:PHE:HB2	2.03	0.40
6:G:193:TYR:CZ	7:J:306:PHE:CE2	3.09	0.40
7:J:45:GLY:HA2	7:J:80:TRP:NE1	2.36	0.40
7:J:194:LEU:HD23	7:J:194:LEU:HA	1.90	0.40
7:J:289:HIS:CE1	7:J:291:GLY:H	2.38	0.40
10:S:185:MET:HE2	10:S:196:VAL:HA	2.02	0.40
11:V:255:ARG:NH2	11:V:258:ASP:OD2	2.54	0.40
12:b:69:ASN:O	12:b:73:LEU:HD23	2.20	0.40
12:b:169:SER:HA	12:b:172:ASN:OD1	2.21	0.40
2:I:42:SER:HB3	2:I:43:PRO:HD3	2.02	0.40
3:E:36:ILE:O	3:E:39:ARG:HG2	2.22	0.40
2:D:299:LEU:CD1	3:F:117:LEU:HD21	2.50	0.40
7:J:39:TRP:CD2	7:J:88:GLN:HG3	2.56	0.40
7:J:91:GLU:OE2	7:J:95:HIS:ND1	2.53	0.40
7:J:303:ASP:OD1	7:J:305:SER:OG	2.31	0.40
7:J:386:GLY:C	7:J:387:PHE:CD1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:209:PHE:CZ	8:M:214:SER:HA	2.56	0.40
9:R:152:LEU:HD11	9:R:156:TYR:OH	2.22	0.40
13:c:72:LEU:HD12	13:c:73:LEU:N	2.35	0.40
2:I:130:ASN:OD1	2:I:131:ILE:N	2.54	0.40
2:C:342:SER:O	2:C:346:ILE:HG13	2.21	0.40
7:N:25:MET:HE2	7:N:72:VAL:HG21	2.03	0.40
12:Y:170:GLN:O	12:Y:173:SER:OG	2.34	0.40
2:D:311:ASP:OD1	2:D:313:ASP:OD2	2.39	0.40
6:G:9:GLY:O	6:G:111:MET:HA	2.20	0.40
6:G:193:TYR:CE2	7:J:306:PHE:CZ	3.10	0.40
7:J:270:TRP:CD1	8:M:237:LYS:HE2	2.56	0.40
7:J:390:LYS:CD	7:J:399:THR:HG22	2.50	0.40
8:M:171:ARG:HA	8:M:176:THR:HG21	2.03	0.40
8:M:291:LYS:HB2	8:M:293:ILE:CD1	2.50	0.40
10:S:174:LEU:HA	10:S:177:VAL:HG12	2.04	0.40
10:S:386:ILE:HD11	11:V:305:LEU:HD21	2.03	0.40
11:V:161:SER:OG	11:V:168:LYS:CA	2.69	0.40
11:V:165:GLN:O	11:V:165:GLN:OE1	2.40	0.40
2:I:100:ILE:HG22	2:I:101:GLN:N	2.37	0.40
2:C:432:THR:HG21	2:C:472:TRP:HH2	1.86	0.40
2:C:641:TYR:HA	2:C:644:ILE:HD12	2.03	0.40
6:L:163:ILE:HD12	6:L:163:ILE:N	2.37	0.40
8:O:160:LEU:HD11	9:P:150:MET:HG3	2.04	0.40
8:O:222:VAL:HG22	8:O:238:HIS:HB2	2.03	0.40
8:O:285:PHE:CE2	8:O:306:VAL:HG21	2.57	0.40
9:P:254:LYS:HB2	9:P:300:PHE:CE2	2.56	0.40
10:Q:337:ASN:OD1	11:U:284:ARG:NH2	2.47	0.40
11:U:150:LEU:HB3	11:U:178:PHE:CE1	2.56	0.40
12:Y:87:ASP:HB2	13:Z:85:LEU:O	2.22	0.40
12:Y:105:PRO:O	12:Y:106:GLN:HB2	2.22	0.40
2:D:487:HIS:NE2	2:D:534:TYR:O	2.55	0.40
7:J:11:TYR:O	7:J:86:VAL:HG23	2.22	0.40
7:J:59:ASP:O	7:J:62:ILE:HG12	2.20	0.40
7:J:148:LYS:HD2	7:J:149:HIS:N	2.36	0.40
9:R:286:ILE:CG1	9:R:292:THR:HG23	2.51	0.40
12:b:20:LEU:HD23	12:b:20:LEU:C	2.46	0.40
12:b:38:VAL:O	12:b:42:LEU:HD23	2.21	0.40
12:b:52:ASP:O	12:b:58:LYS:HE2	2.22	0.40
3:K:137:HIS:CG	3:K:138:ILE:H	2.39	0.40
2:C:379:ILE:HB	2:C:380:PRO:HD3	2.04	0.40
2:C:501:ASN:O	3:E:78:PHE:CD1	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:58:MET:HB3	6:L:73:PHE:HB2	2.04	0.40
10:Q:269:LEU:HD12	10:Q:269:LEU:O	2.21	0.40
2:D:299:LEU:C	2:D:299:LEU:HD23	2.47	0.40
2:D:478:LEU:HD12	2:D:478:LEU:O	2.21	0.40
6:G:131:HIS:N	6:G:139:GLN:O	2.45	0.40
7:J:164:SER:OG	7:J:165:ASN:N	2.52	0.40
8:M:330:LEU:C	8:M:330:LEU:HD23	2.47	0.40
9:R:157:LEU:HD13	9:R:161:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	134/181 (74%)	129 (96%)	5 (4%)	0	100	100
1	B	134/181 (74%)	132 (98%)	2 (2%)	0	100	100
1	H	33/181 (18%)	33 (100%)	0	0	100	100
2	C	432/733 (59%)	411 (95%)	21 (5%)	0	100	100
2	D	432/733 (59%)	412 (95%)	20 (5%)	0	100	100
2	I	237/733 (32%)	222 (94%)	14 (6%)	1 (0%)	30	67
3	E	114/239 (48%)	114 (100%)	0	0	100	100
3	F	114/239 (48%)	114 (100%)	0	0	100	100
3	K	99/239 (41%)	96 (97%)	3 (3%)	0	100	100
4	T	90/361 (25%)	86 (96%)	4 (4%)	0	100	100
5	W	65/89 (73%)	64 (98%)	1 (2%)	0	100	100
6	G	239/245 (98%)	227 (95%)	12 (5%)	0	100	100
6	L	239/245 (98%)	227 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	J	383/458 (84%)	357 (93%)	25 (6%)	1 (0%)	36	72
7	N	383/458 (84%)	354 (92%)	29 (8%)	0	100	100
8	M	237/368 (64%)	223 (94%)	14 (6%)	0	100	100
8	O	237/368 (64%)	222 (94%)	15 (6%)	0	100	100
9	P	251/369 (68%)	238 (95%)	13 (5%)	0	100	100
9	R	251/369 (68%)	237 (94%)	14 (6%)	0	100	100
10	Q	254/406 (63%)	247 (97%)	7 (3%)	0	100	100
10	S	254/406 (63%)	243 (96%)	11 (4%)	0	100	100
11	U	180/324 (56%)	172 (96%)	8 (4%)	0	100	100
11	V	180/324 (56%)	171 (95%)	9 (5%)	0	100	100
12	Y	217/238 (91%)	209 (96%)	8 (4%)	0	100	100
12	b	217/238 (91%)	202 (93%)	15 (7%)	0	100	100
13	Z	149/153 (97%)	148 (99%)	1 (1%)	0	100	100
13	c	149/153 (97%)	146 (98%)	3 (2%)	0	100	100
All	All	5704/9031 (63%)	5436 (95%)	266 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	202	SER
7	J	164	SER

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	131/172 (76%)	131 (100%)	0	100	100
1	B	131/172 (76%)	131 (100%)	0	100	100
1	H	31/172 (18%)	31 (100%)	0	100	100
2	C	407/683 (60%)	407 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	407/683 (60%)	407 (100%)	0	100	100
2	I	224/683 (33%)	224 (100%)	0	100	100
3	E	107/223 (48%)	107 (100%)	0	100	100
3	F	107/223 (48%)	107 (100%)	0	100	100
3	K	95/223 (43%)	95 (100%)	0	100	100
4	T	89/339 (26%)	89 (100%)	0	100	100
5	W	57/76 (75%)	57 (100%)	0	100	100
6	G	217/221 (98%)	217 (100%)	0	100	100
6	L	217/221 (98%)	217 (100%)	0	100	100
7	J	353/416 (85%)	353 (100%)	0	100	100
7	N	353/416 (85%)	353 (100%)	0	100	100
8	M	226/347 (65%)	226 (100%)	0	100	100
8	O	226/347 (65%)	226 (100%)	0	100	100
9	P	241/344 (70%)	241 (100%)	0	100	100
9	R	241/344 (70%)	241 (100%)	0	100	100
10	Q	242/378 (64%)	242 (100%)	0	100	100
10	S	242/378 (64%)	242 (100%)	0	100	100
11	U	168/309 (54%)	168 (100%)	0	100	100
11	V	168/309 (54%)	168 (100%)	0	100	100
12	Y	175/219 (80%)	175 (100%)	0	100	100
12	b	175/219 (80%)	175 (100%)	0	100	100
13	Z	121/143 (85%)	121 (100%)	0	100	100
13	c	121/143 (85%)	121 (100%)	0	100	100
All	All	5272/8403 (63%)	5272 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	169	GLN
2	I	87	ASN
2	I	88	HIS
2	I	116	HIS

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Mol	Chain	Res	Type
2	I	242	HIS
3	K	195	ASN
4	T	274	GLN
4	T	284	GLN
1	A	8	GLN
1	A	50	GLN
1	A	111	HIS
3	E	77	ASN
3	E	100	GLN
6	L	179	ASN
7	N	407	ASN
7	N	435	ASN
9	P	166	GLN
9	P	192	ASN
10	Q	150	HIS
10	Q	190	HIS
10	Q	330	HIS
10	Q	333	ASN
11	U	219	GLN
12	Y	106	GLN
13	Z	40	GLN
1	B	19	HIS
1	B	50	GLN
1	B	107	GLN
1	B	113	GLN
2	D	467	GLN
6	G	64	ASN
7	J	284	HIS
7	J	289	HIS
7	J	329	ASN
8	M	283	GLN
9	R	106	ASN
9	R	149	ASN
9	R	164	HIS
9	R	192	ASN
9	R	260	ASN
9	R	359	ASN
10	S	150	HIS
10	S	187	GLN
10	S	327	ASN
10	S	333	ASN
11	V	184	GLN

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Mol	Chain	Res	Type
11	V	199	ASN
11	V	217	ASN
11	V	219	GLN
11	V	243	GLN
11	V	294	HIS
12	b	77	GLN
13	c	23	GLN
13	c	28	GLN
13	c	80	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

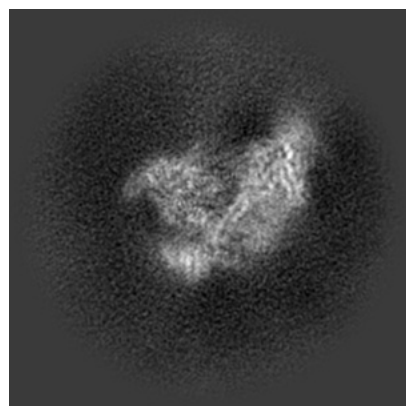
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75213. These allow visual inspection of the internal detail of the map and identification of artifacts.

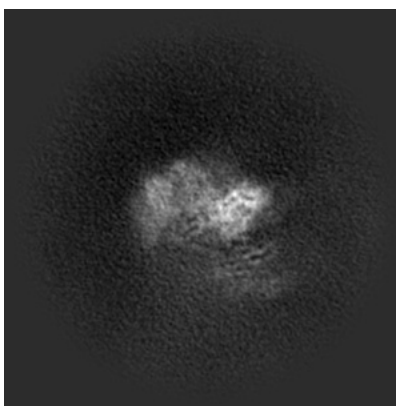
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

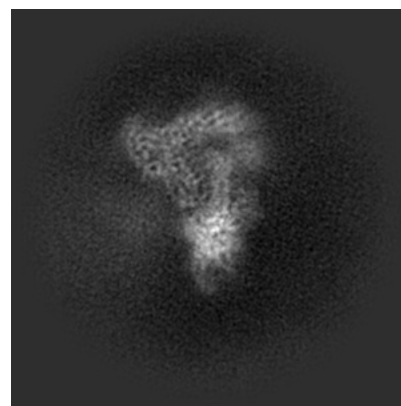
6.1.1 Primary map



X

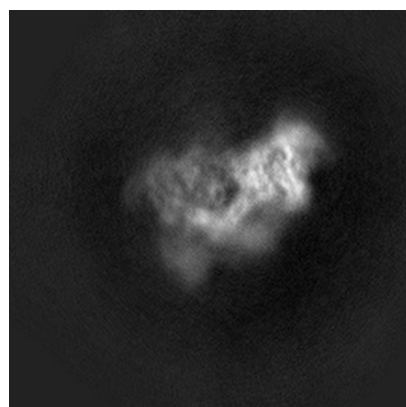


Y

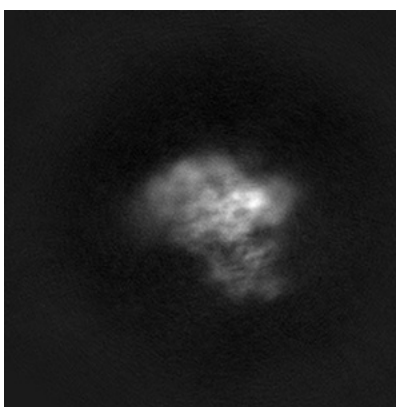


Z

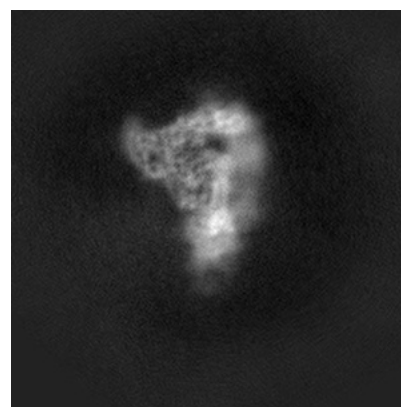
6.1.2 Raw map



X



Y

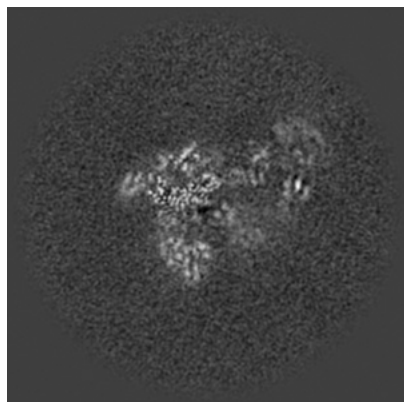


Z

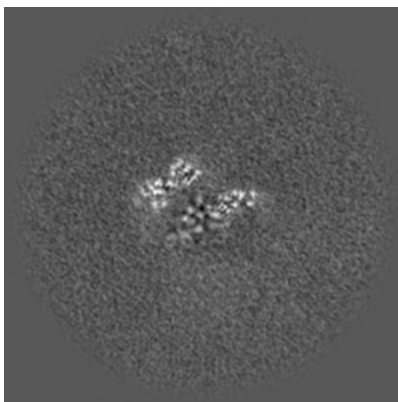
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

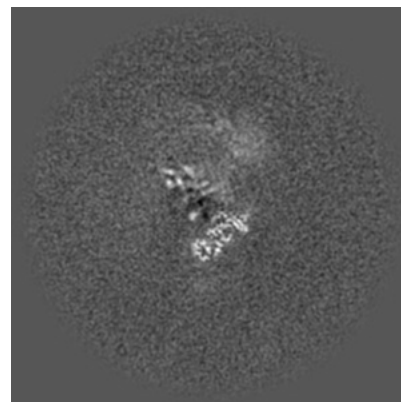
6.2.1 Primary map



X Index: 107

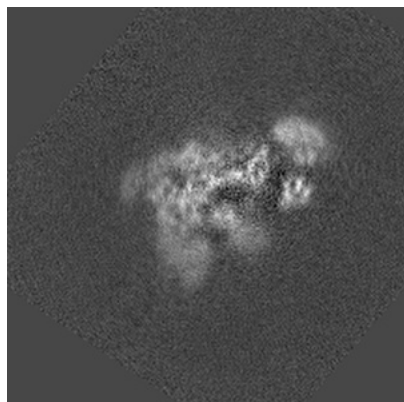


Y Index: 107

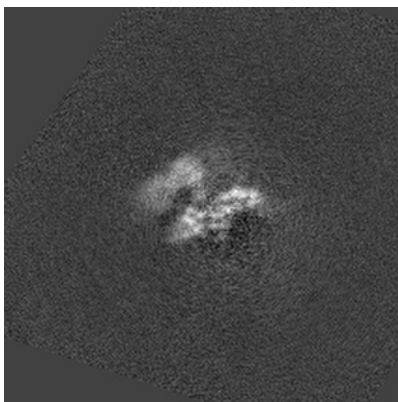


Z Index: 107

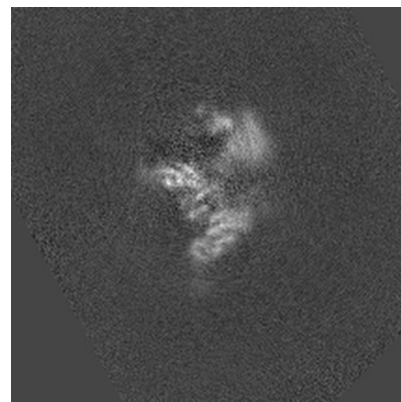
6.2.2 Raw map



X Index: 107



Y Index: 107

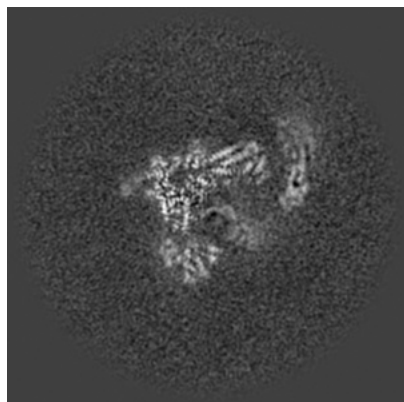


Z Index: 107

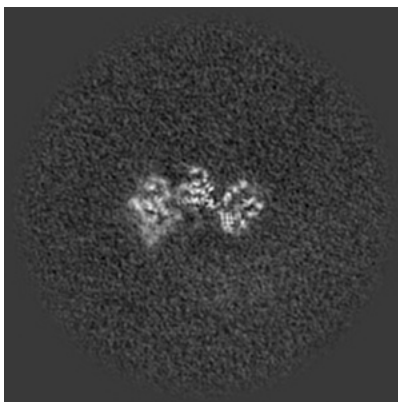
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

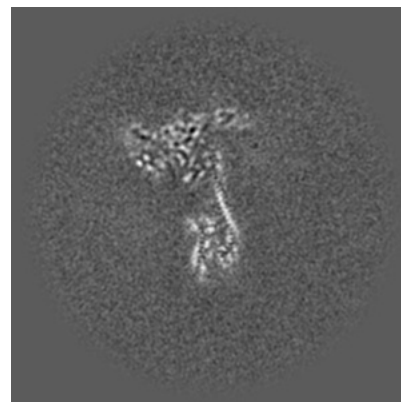
6.3.1 Primary map



X Index: 110

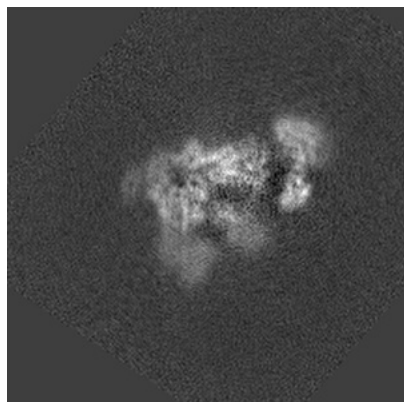


Y Index: 96

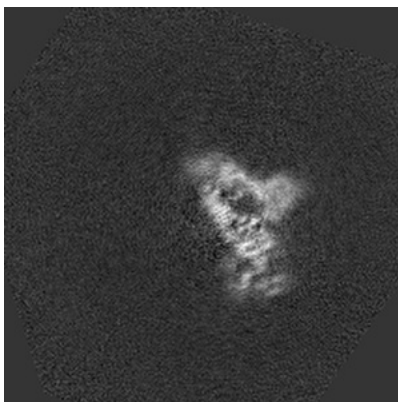


Z Index: 127

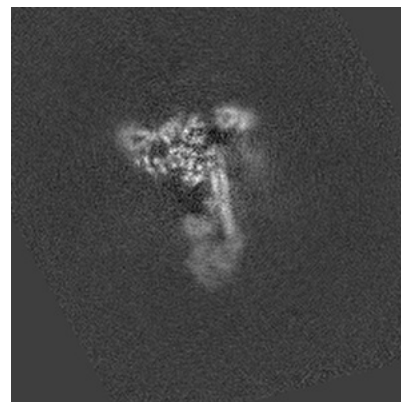
6.3.2 Raw map



X Index: 109



Y Index: 149

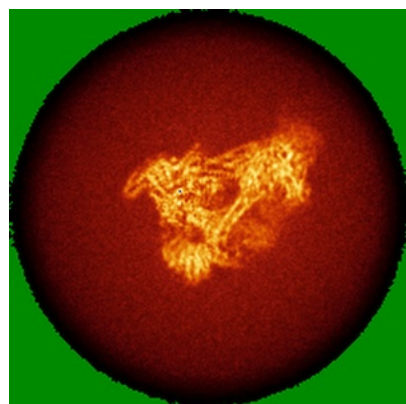


Z Index: 125

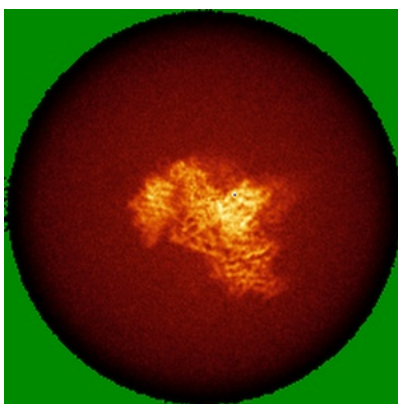
The images above show the largest variance slices of the map in three orthogonal directions.

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

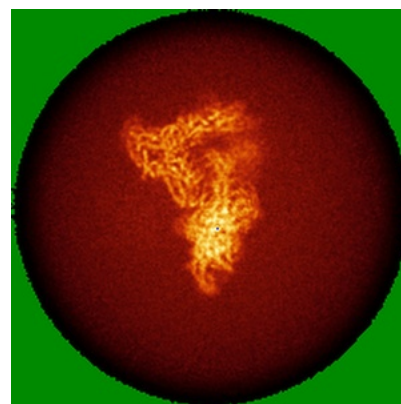
6.4.1 Primary map



X

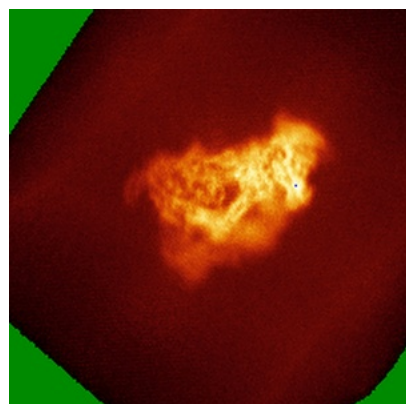


Y

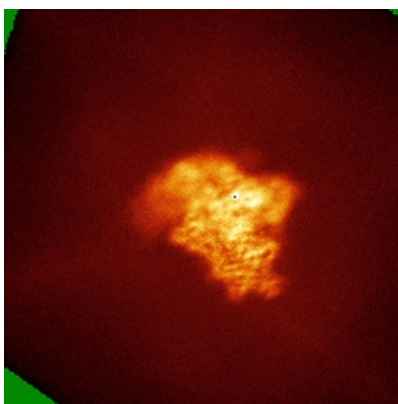


Z

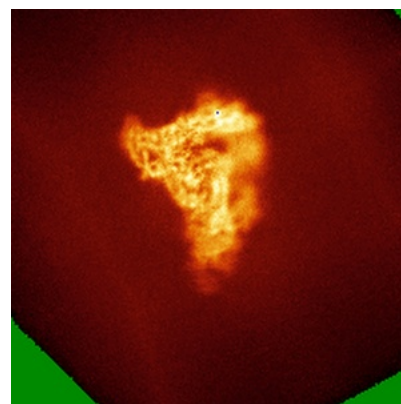
6.4.2 Raw map



X



Y

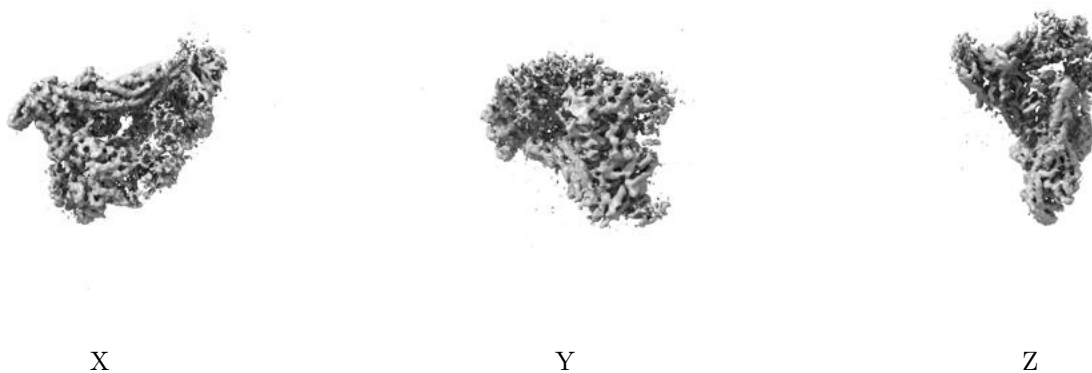


Z

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 0.394. 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.

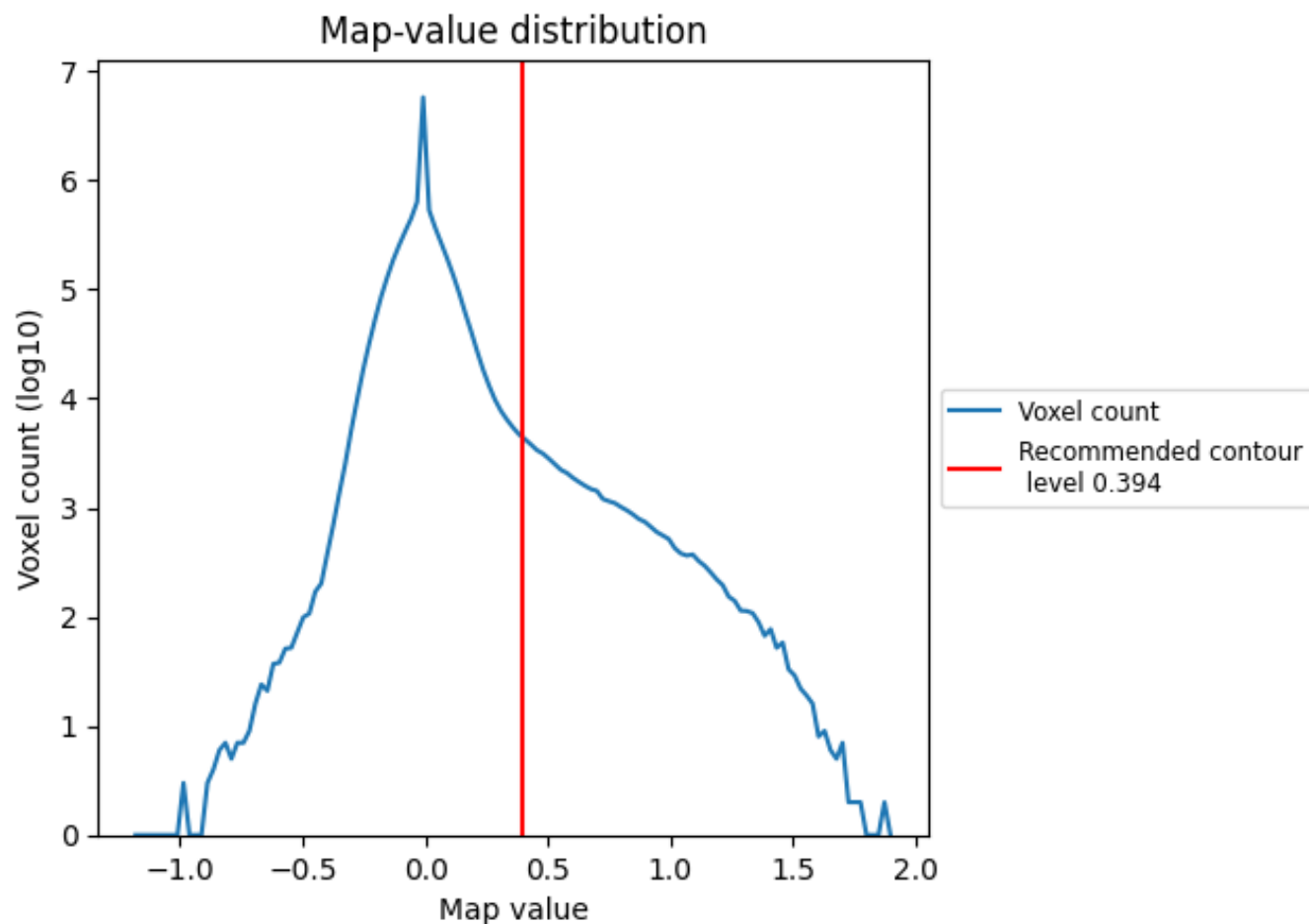
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

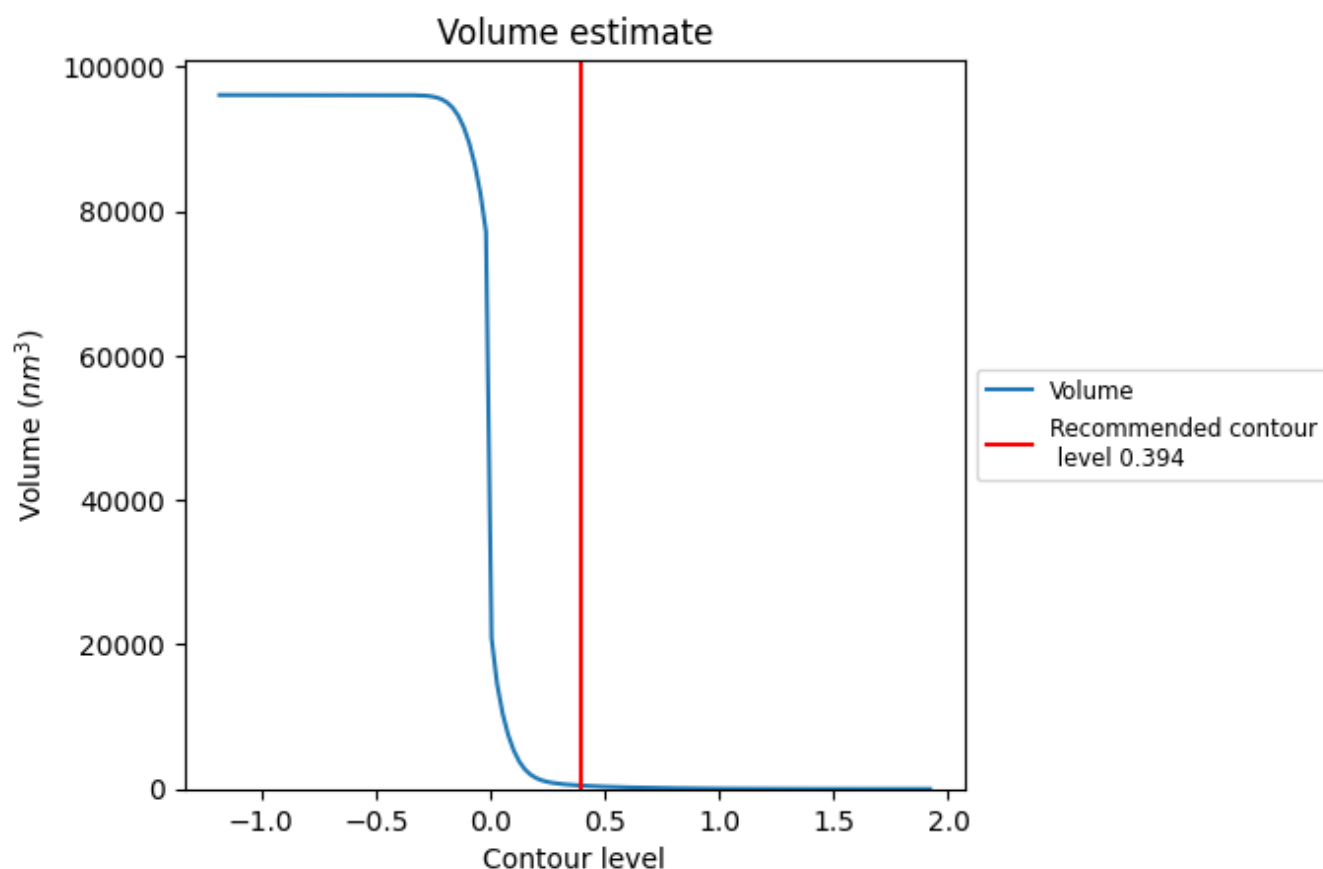
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

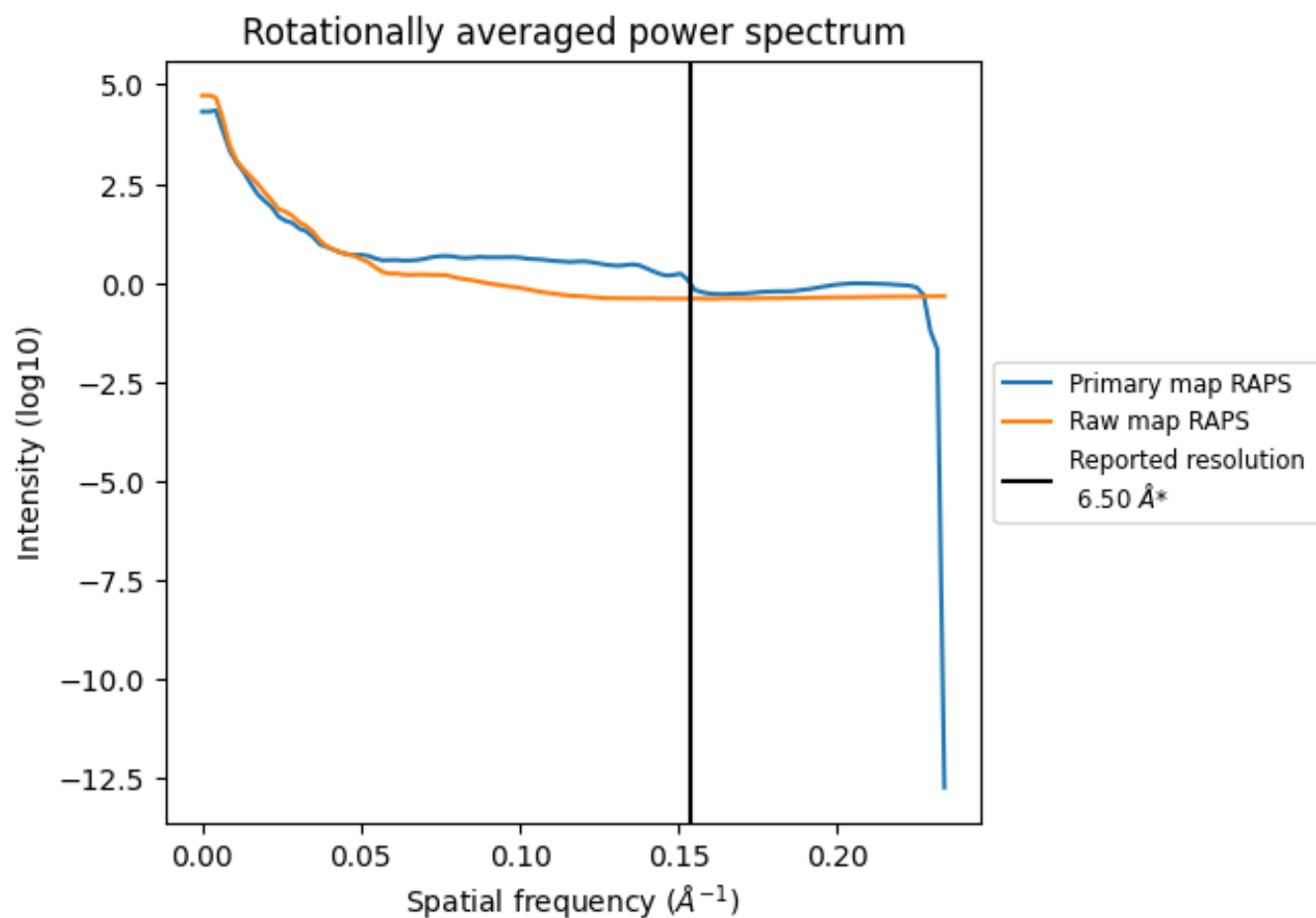
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 476 nm³; this corresponds to an approximate mass of 430 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 ⓘ

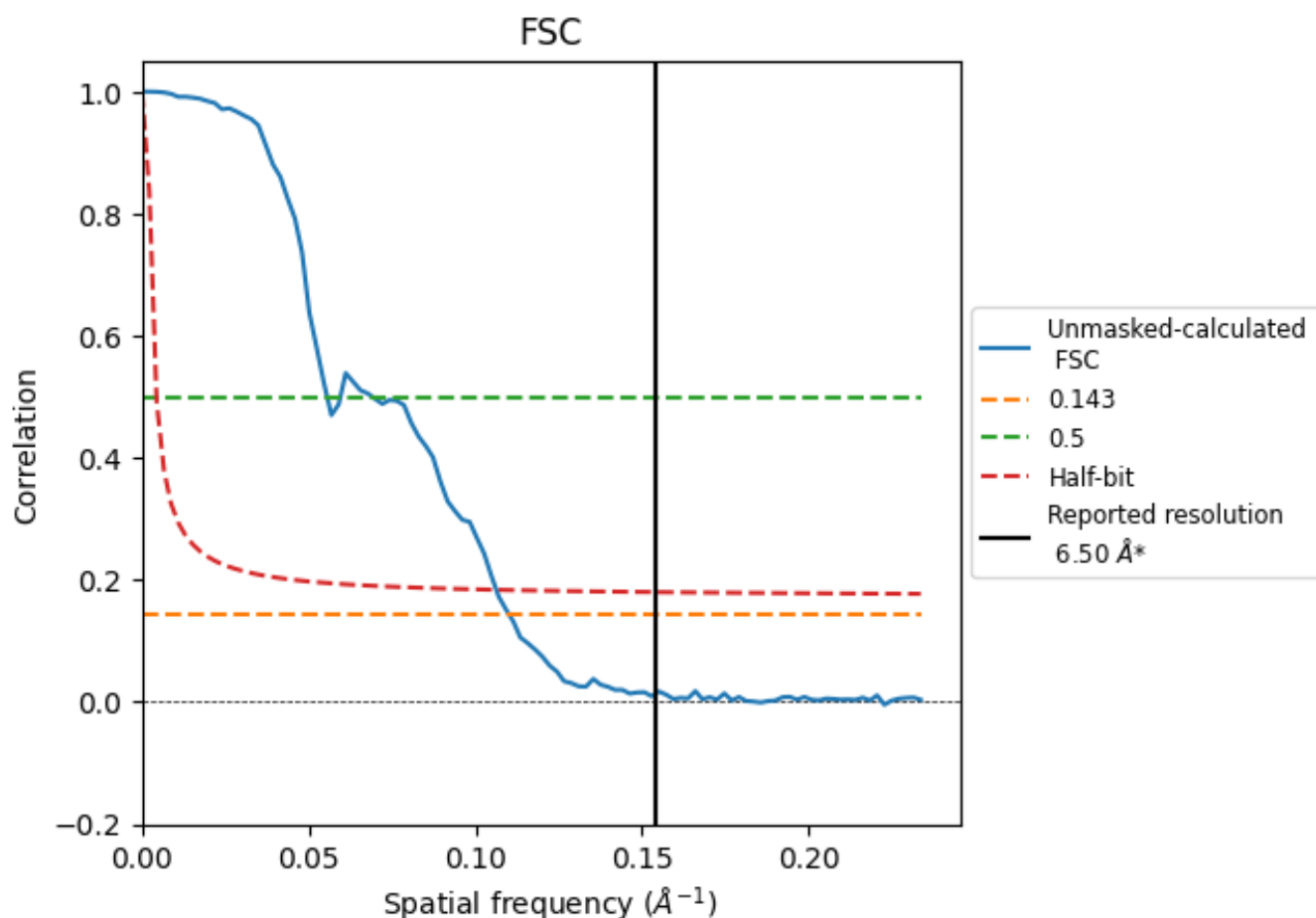


*Reported resolution corresponds to spatial frequency of 0.154 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.154 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

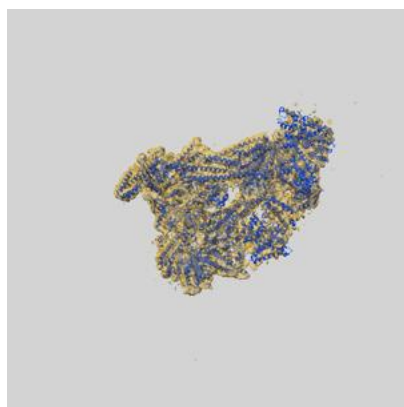
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.08	18.02	9.41

*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 9.08 differs from the reported value 6.5 by more than 10 %

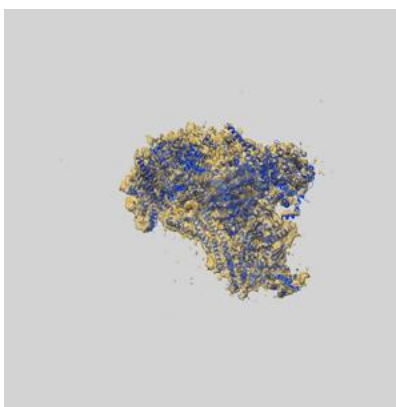
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75213 and PDB model 10JC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

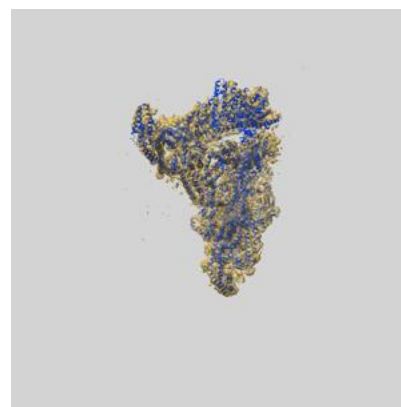
9.1 Map-model overlay [i](#)



X



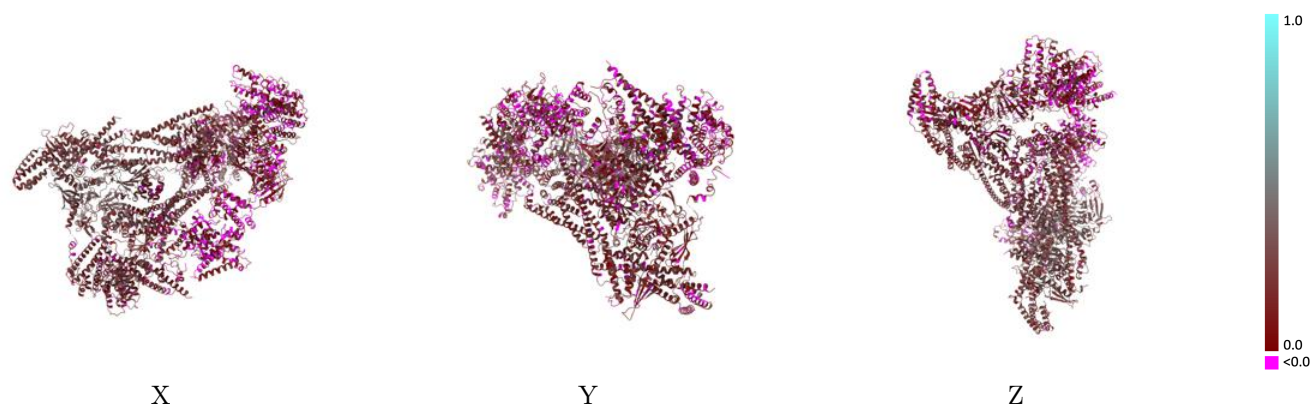
Y



Z

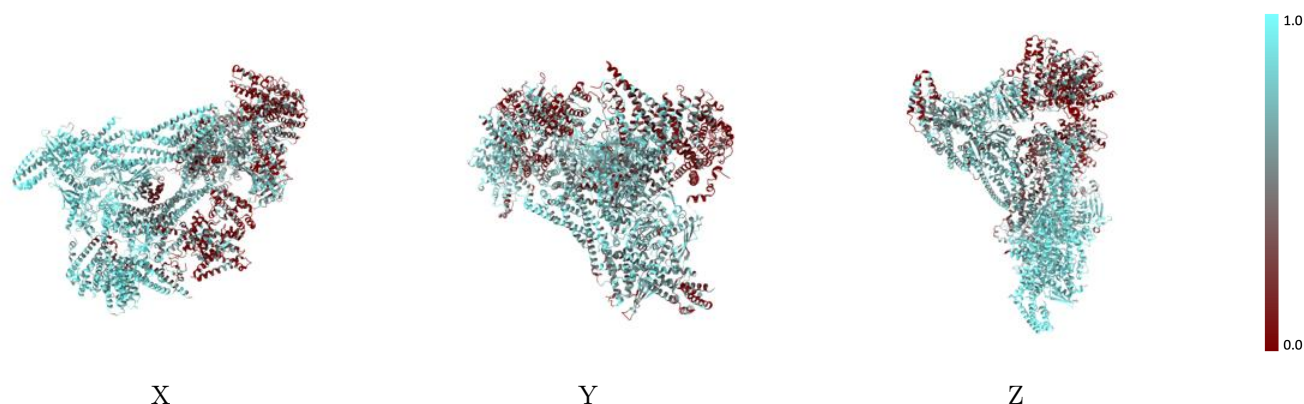
The images above show the 3D surface view of the map at the recommended contour level 0.394 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



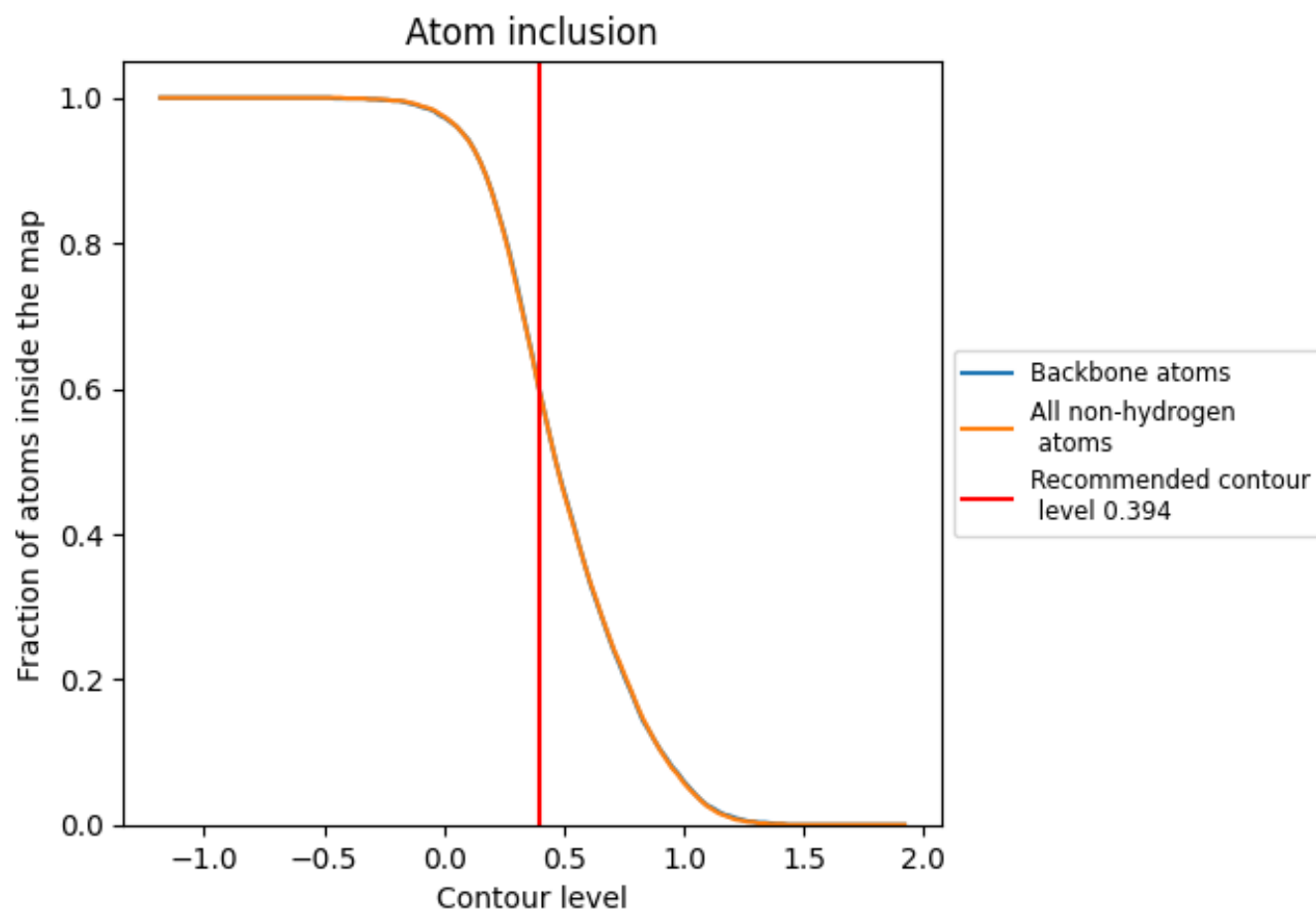
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.394).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 60% 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 (0.394) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6030	 0.1810
A	 0.7410	 0.1630
B	 0.2480	 0.0940
C	 0.7360	 0.1750
D	 0.3270	 0.0940
E	 0.7080	 0.1600
F	 0.2030	 0.1030
G	 0.6300	 0.1380
H	 0.3380	 0.0840
I	 0.2990	 0.0630
J	 0.6400	 0.1800
K	 0.3400	 0.0990
L	 0.7570	 0.2590
M	 0.5770	 0.1600
N	 0.7260	 0.2900
O	 0.8390	 0.2940
P	 0.8610	 0.2950
Q	 0.6030	 0.2100
R	 0.5990	 0.1620
S	 0.5520	 0.1600
T	 0.1750	 0.0310
U	 0.7470	 0.2330
V	 0.6190	 0.1770
W	 0.2610	 0.0540
Y	 0.8540	 0.2510
Z	 0.8400	 0.2490
b	 0.6400	 0.1740
c	 0.6890	 0.1800

