Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 10:23 pm GMT

PDB ID	:	6TB4
EMDB ID	:	EMD-10438
Title	:	Structure of SAGA bound to TBP
Authors	:	Papai, G.; Frechard, A.; Kolesnikova, O.; Crucifix, C.; Schultz, P.; Ben-Shem, A.
Deposited on	:	2019-10-31
Resolution	:	3.80 Å(reported)

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

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

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

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

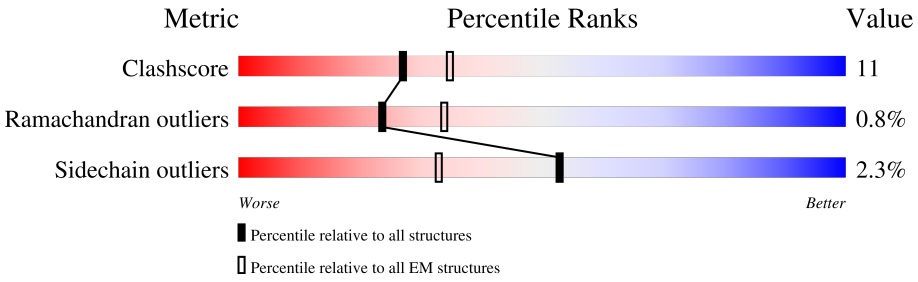
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	M	243	74% 37% 31% 6% 26%
2	A	448	28% 31% 7% 61%
3	C	698	9% 8% 91%
4	F	517	33% 33% 7% 59%
5	D	341	39% 37% 21% 39%
6	E	1191	6% 10% 87%
7	J	217	19% 36% 7% 56%
8	K	609	15% 17% 7% 75%

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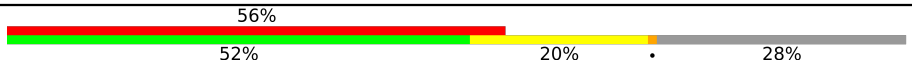
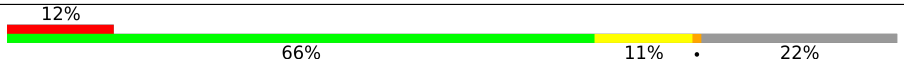
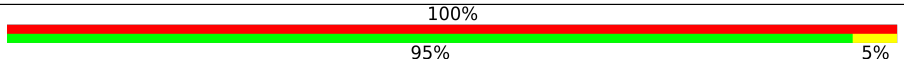
Mol	Chain	Length	Quality of chain
9	G	722	
10	H	485	
11	I	153	
12	L	3825	
13	B	76	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 40740 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 TATA-box Binding Protein (TBP).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	M	180	1415	921	242	246	6	0	0

- Molecule 2 is a protein called Transcriptional coactivator HFI1/ADA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	173	1300	816	228	250	6	0	0

- Molecule 3 is a protein called SAGA-associated factor 73 (Sgf73).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	65	518	331	94	90	3	0	0

- Molecule 4 is a protein called Spt20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	210	1682	1071	292	315	4	0	0

- Molecule 5 is a protein called Subunit of the SAGA and SAGA-like transcriptional regulatory complexes, interacts with Spt15p to act.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	209	1616	1016	298	295	7	0	0

- Molecule 6 is a protein called Subunit of the SAGA transcriptional regulatory complex, involved in proper assembly of the complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	154	Total	C	N	O	S	0	0
			1232	784	208	233	7		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	96	Total	C	N	O	S	0	0
			768	489	120	156	3		

- Molecule 8 is a protein called Subunit (61/68 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	154	Total	C	N	O	S	0	0
			1192	747	216	226	3		

- Molecule 9 is a protein called Subunit (90 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	522	Total	C	N	O	S	0	0
			4075	2581	719	756	19		

- Molecule 10 is a protein called Subunit (60 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	421	Total	C	N	O	S	0	0
			3263	2084	556	617	6		

- Molecule 11 is a protein called Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	123	Total	C	N	O	S	0	0
			981	632	169	178	2		

- Molecule 12 is a protein called Transcription-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	2968	Total	C	N	O	S	0	0
			22318	14296	3864	4071	87		

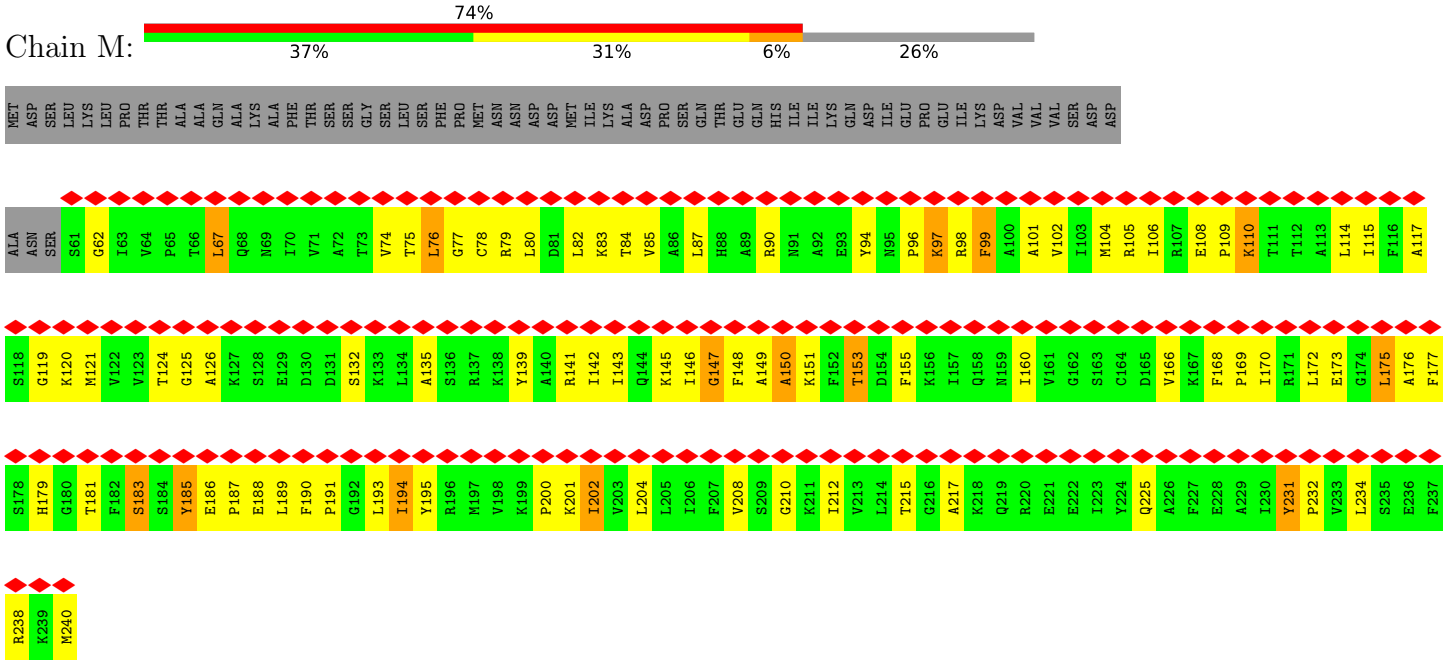
- Molecule 13 is a protein called Transcriptional adapter 3 (Ada3).

Mol	Chain	Residues	Atoms				AltConf	Trace
13	B	76	Total	C	N	O	0	0
			380	228	76	76		

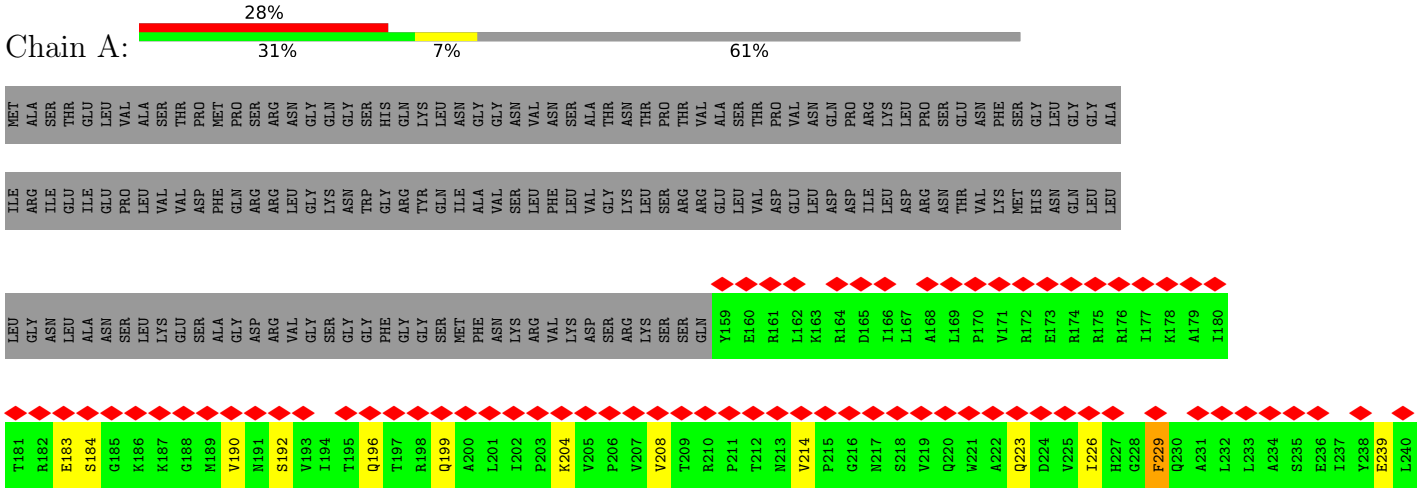
3 Residue-property plots (i)

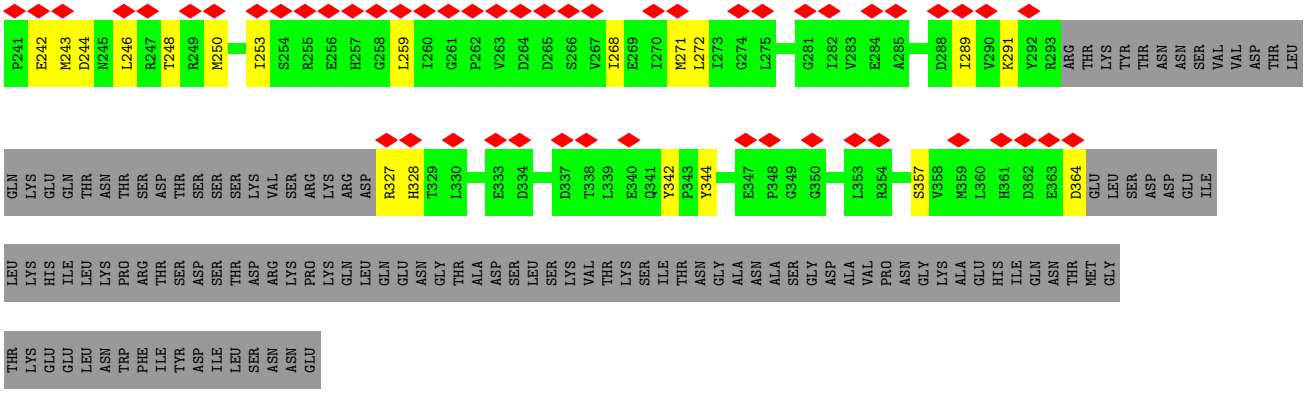
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

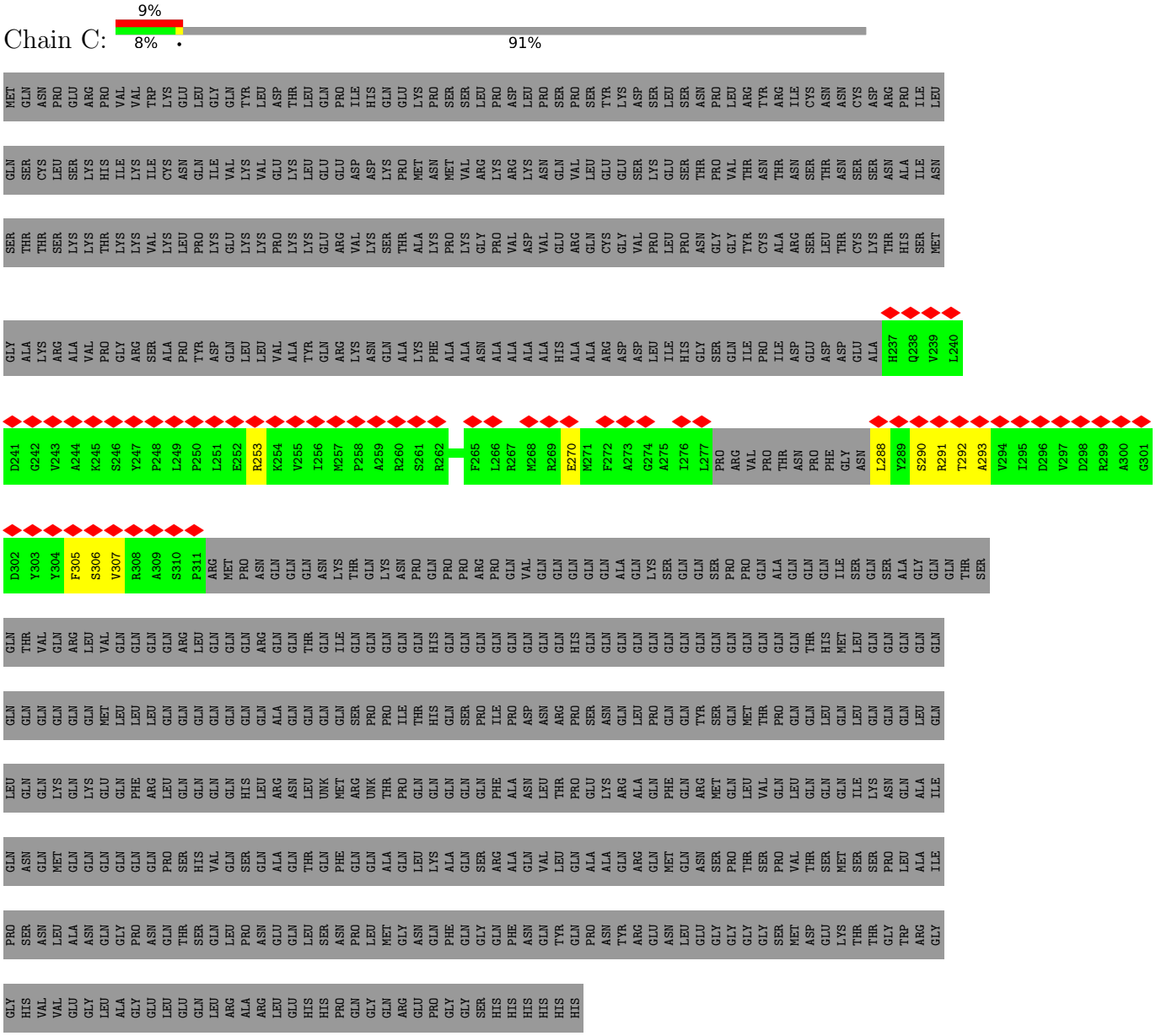


• Molecule 2: Transcriptional coactivator HFI1/ADA1

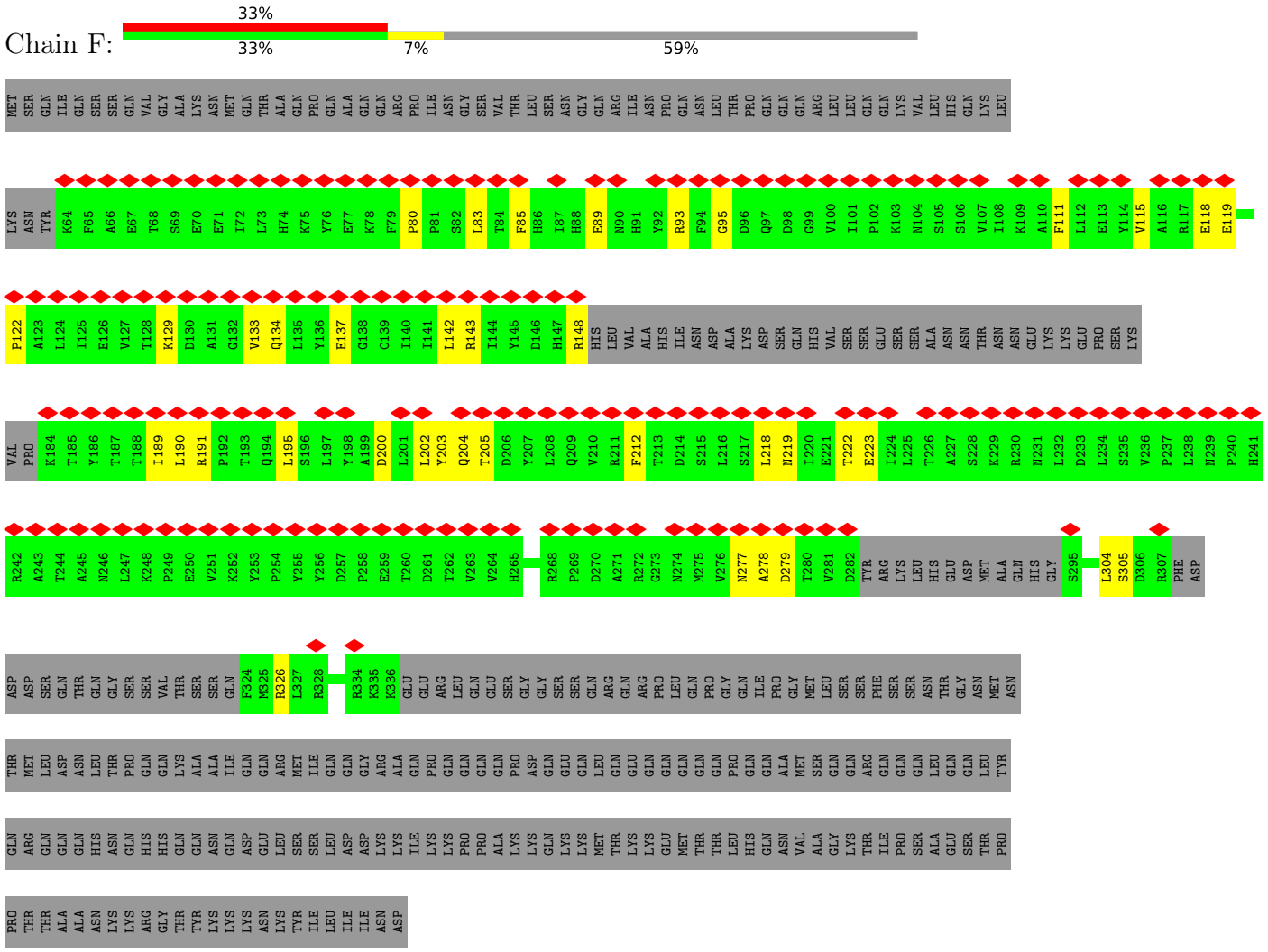




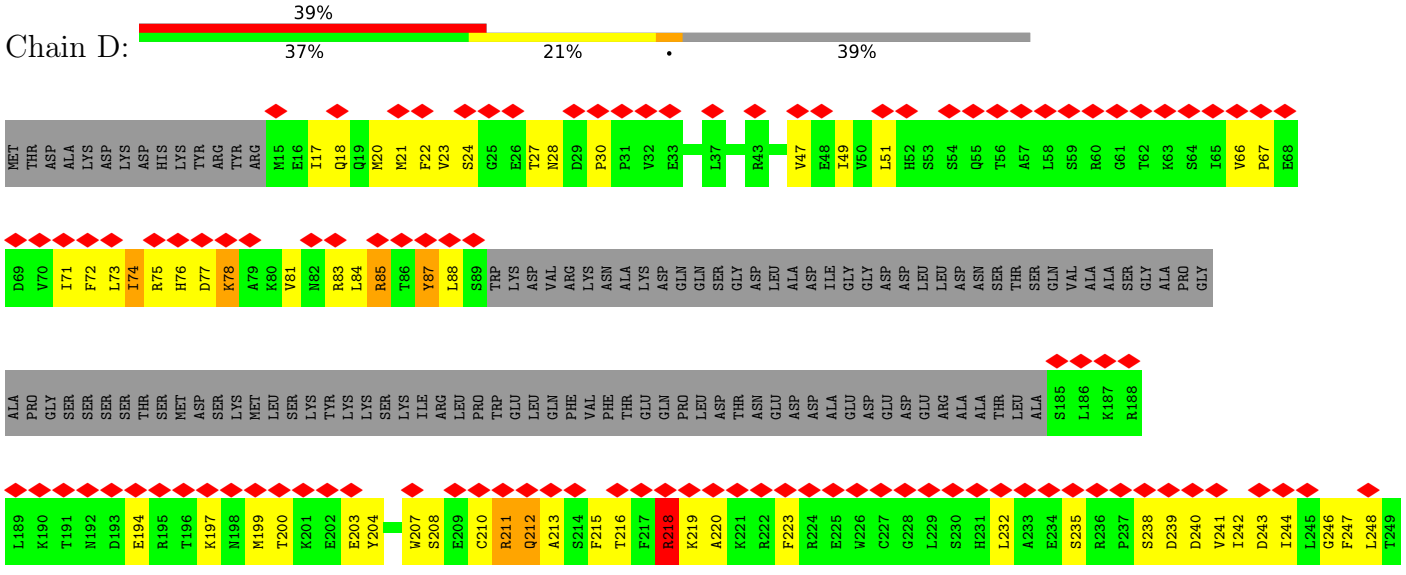
• Molecule 3: SAGA-associated factor 73 (Sgf73)

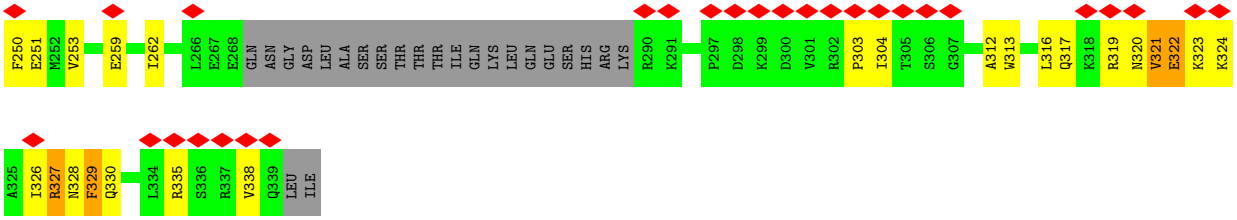


• Molecule 4: Spt20

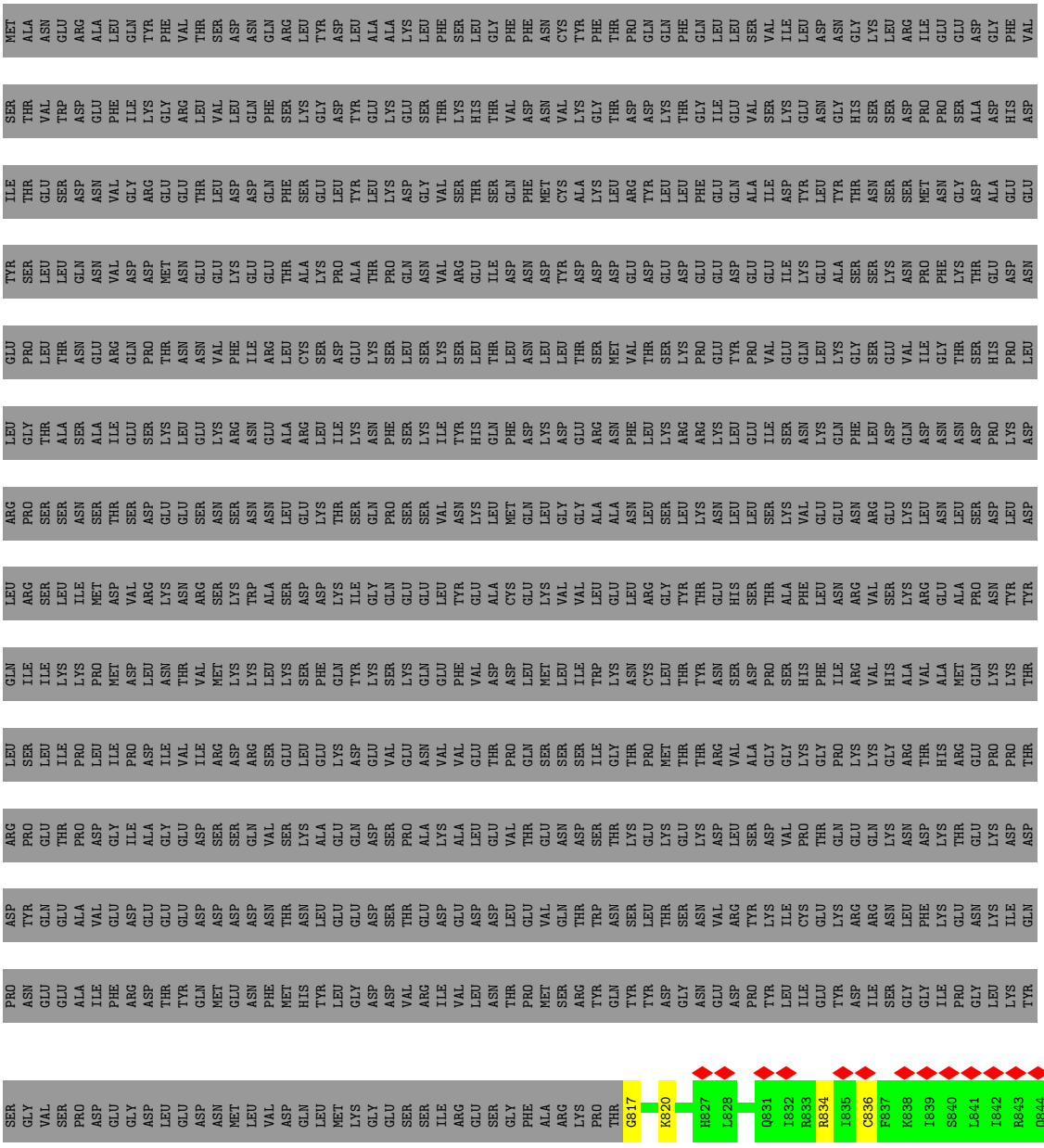


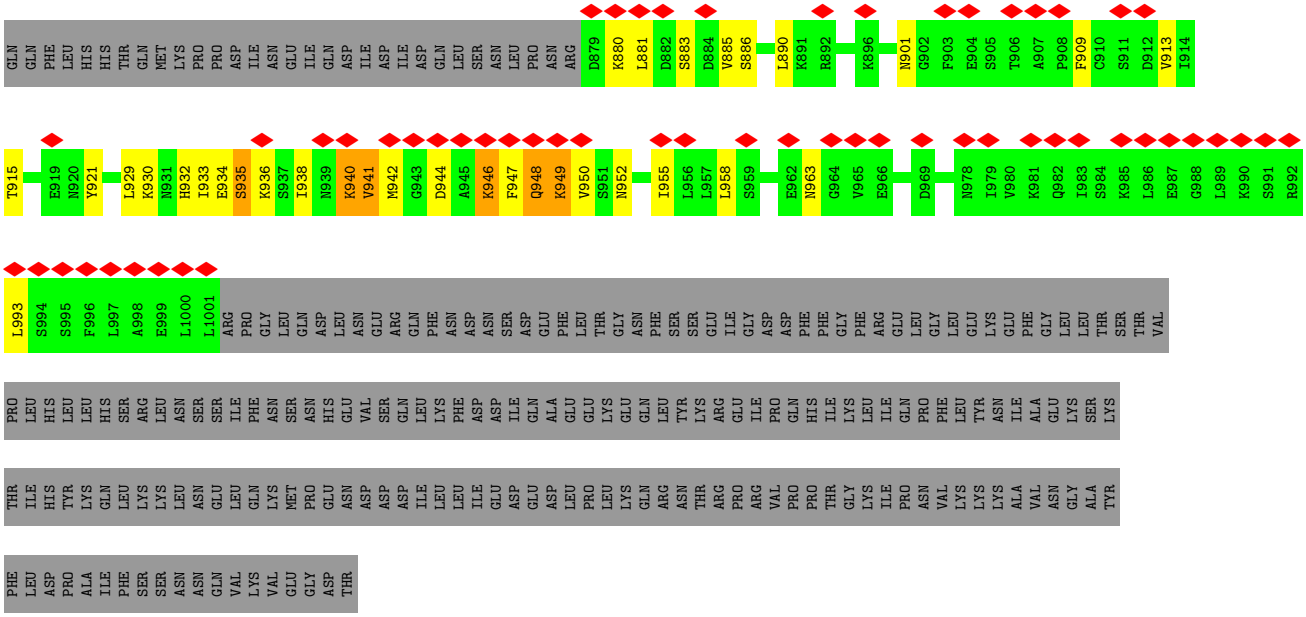
• Molecule 5: Subunit of the SAGA and SAGA-like transcriptional regulatory complexes, interacts with Spt15p to act





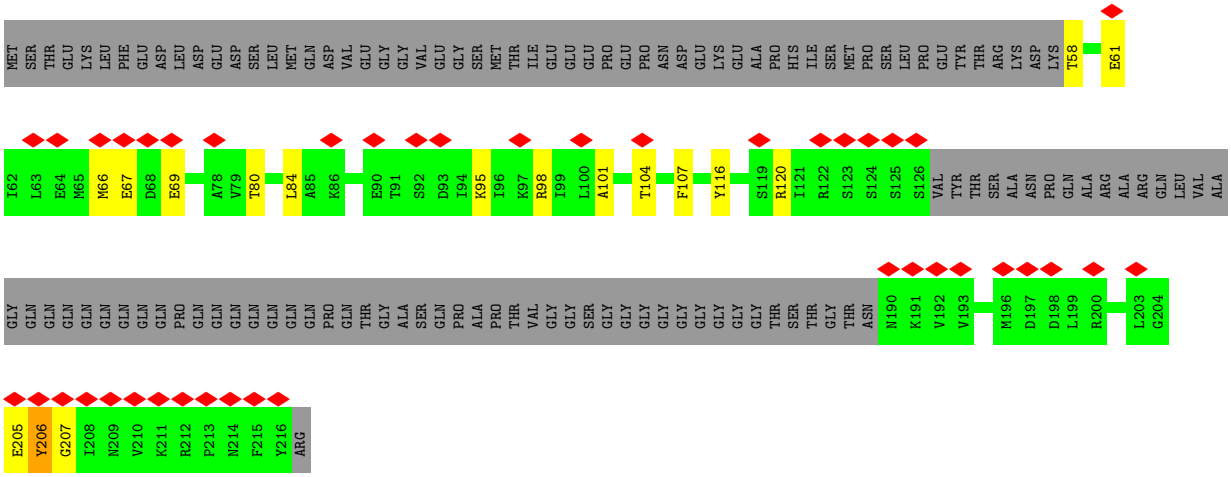
• Molecule 6: Subunit of the SAGA transcriptional regulatory complex, involved in proper assembly of the complex





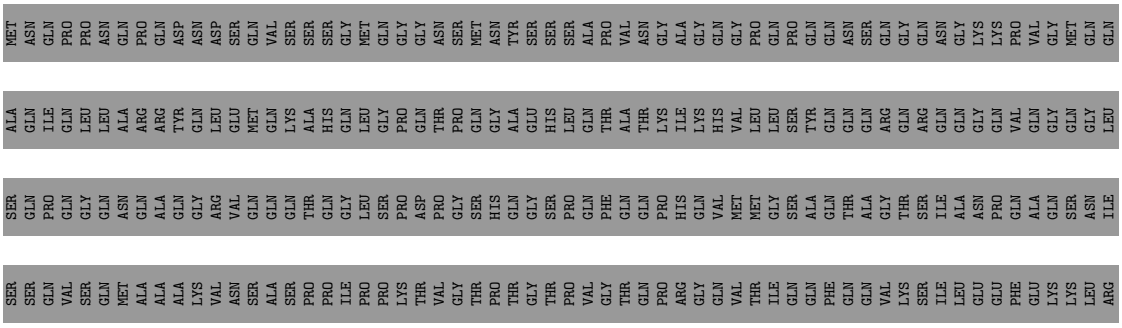
• Molecule 7: Transcription initiation factor TFIID subunit 10

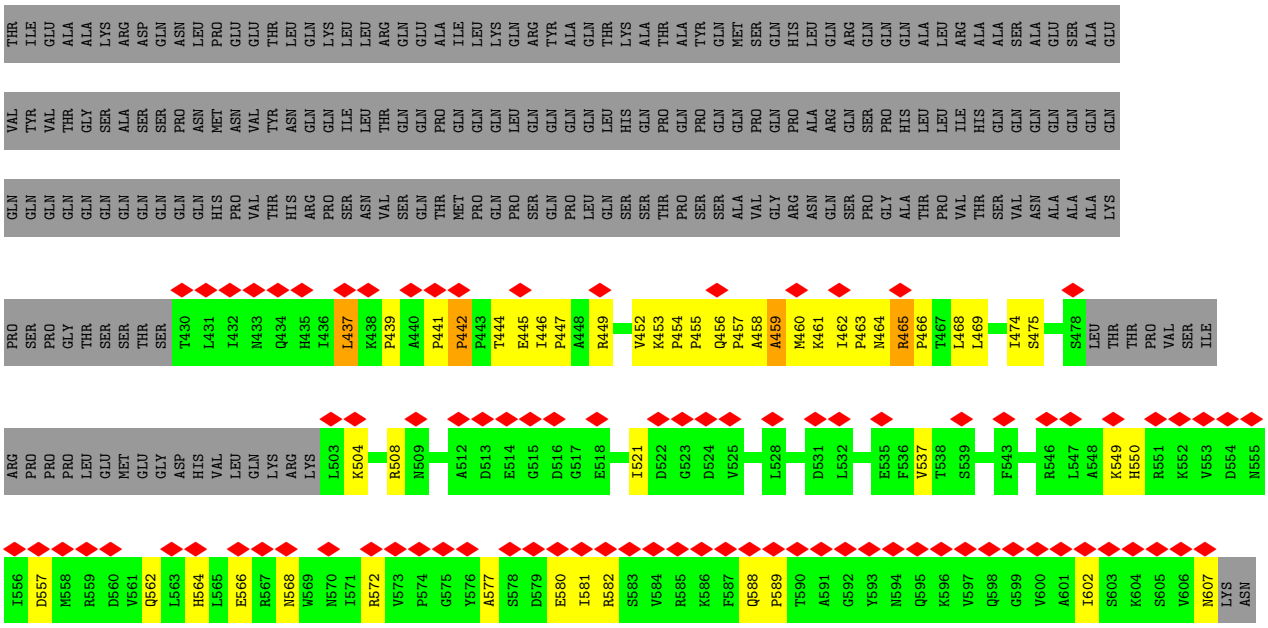
Chain J:



• Molecule 8: Subunit (61/68 kDa) of TFIID and SAGA complexes

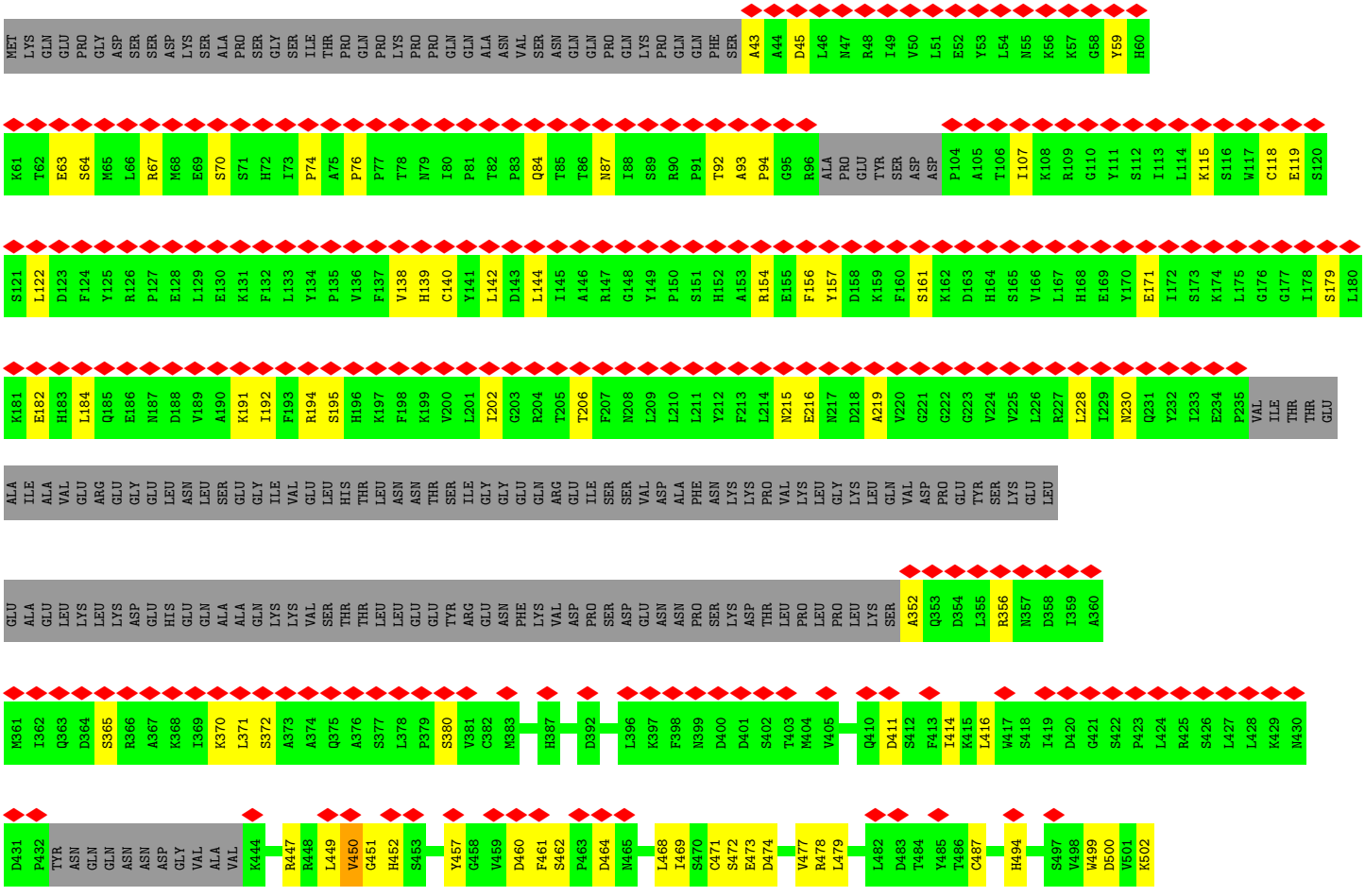
Chain K:

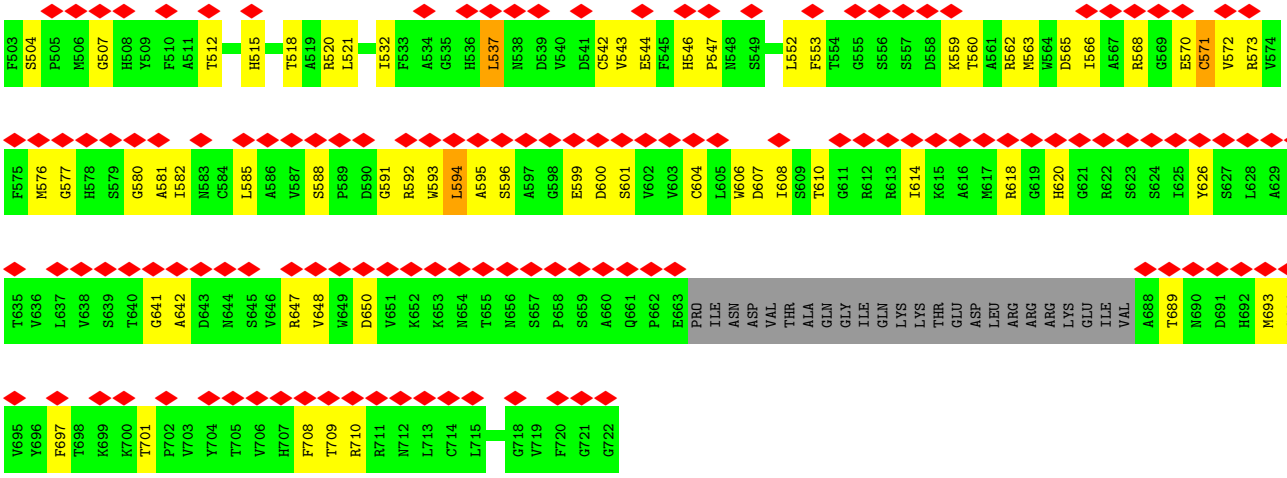




• Molecule 9: Subunit (90 kDa) of TFIID and SAGA complexes

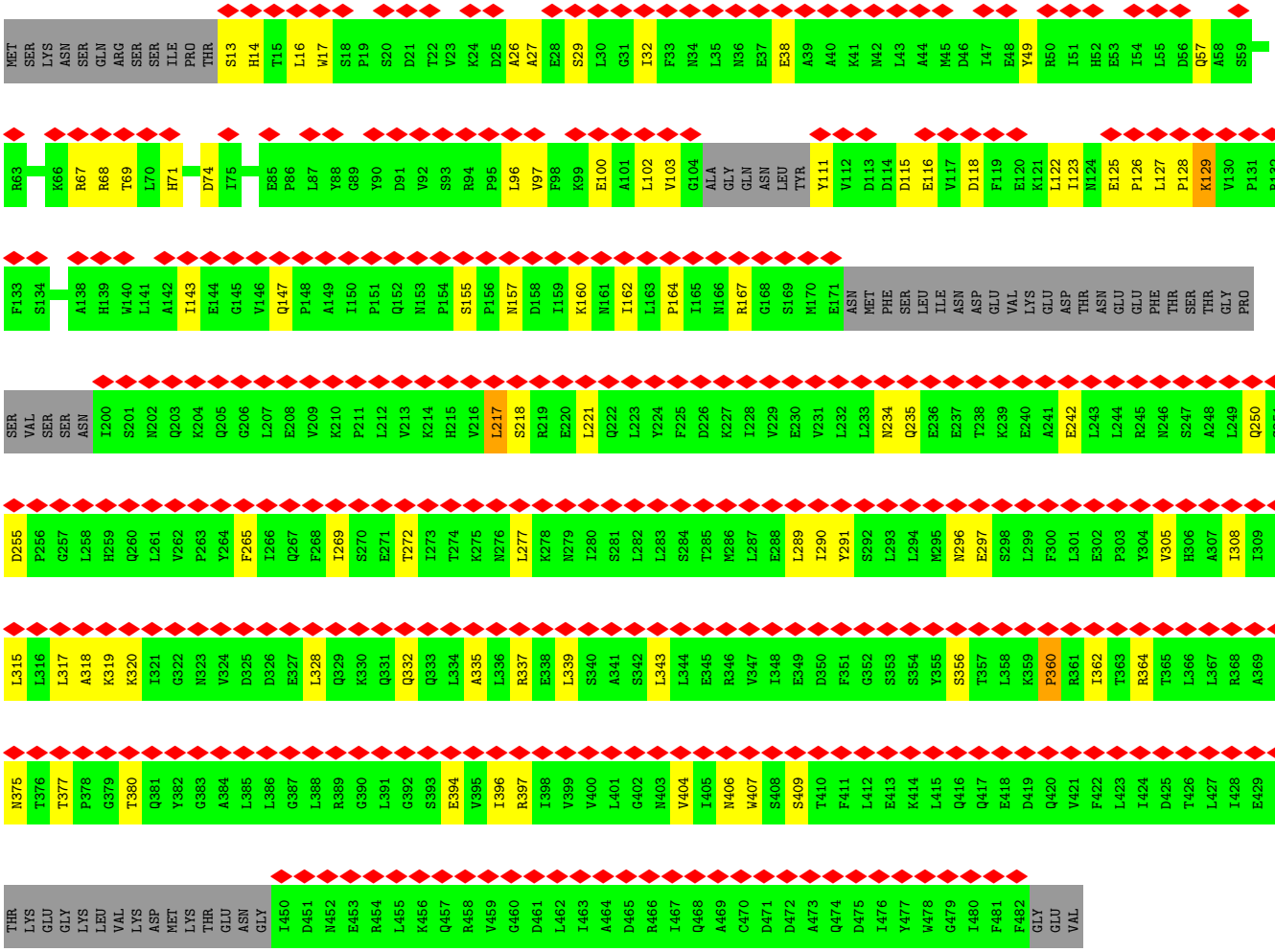
Chain G:





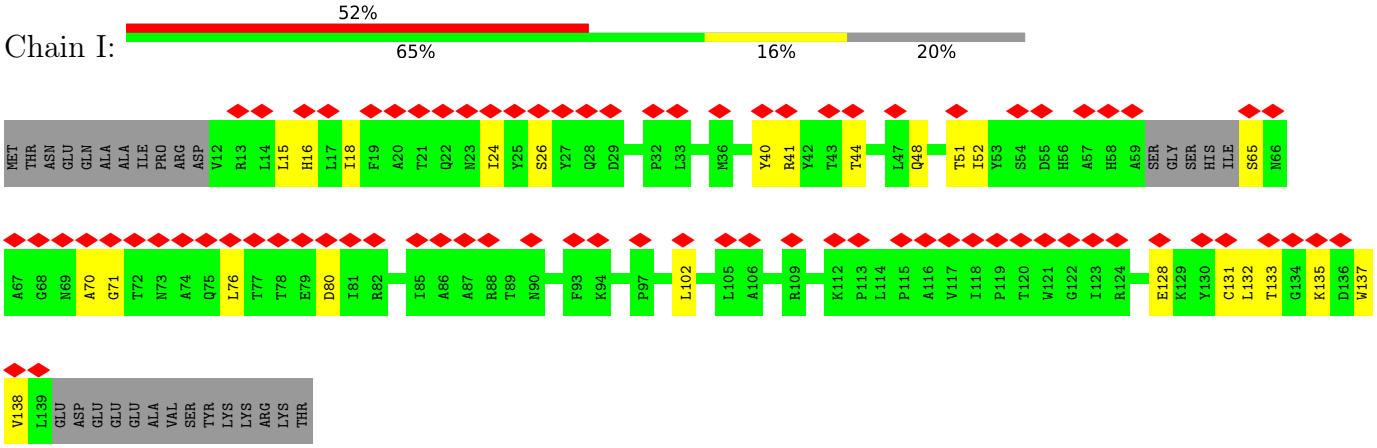
• Molecule 10: Subunit (60 kDa) of TFIID and SAGA complexes

Chain H:



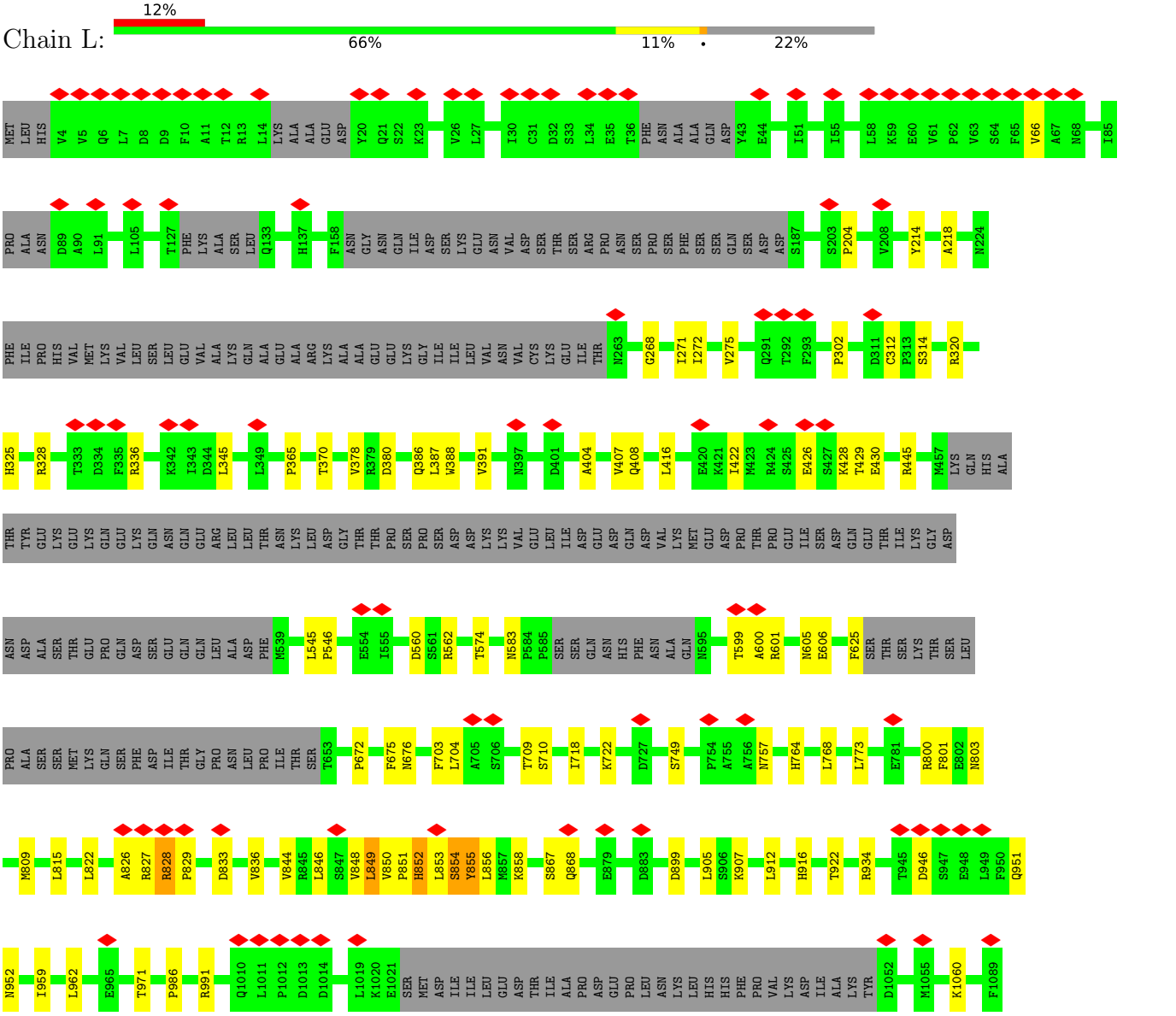
• Molecule 11: Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation

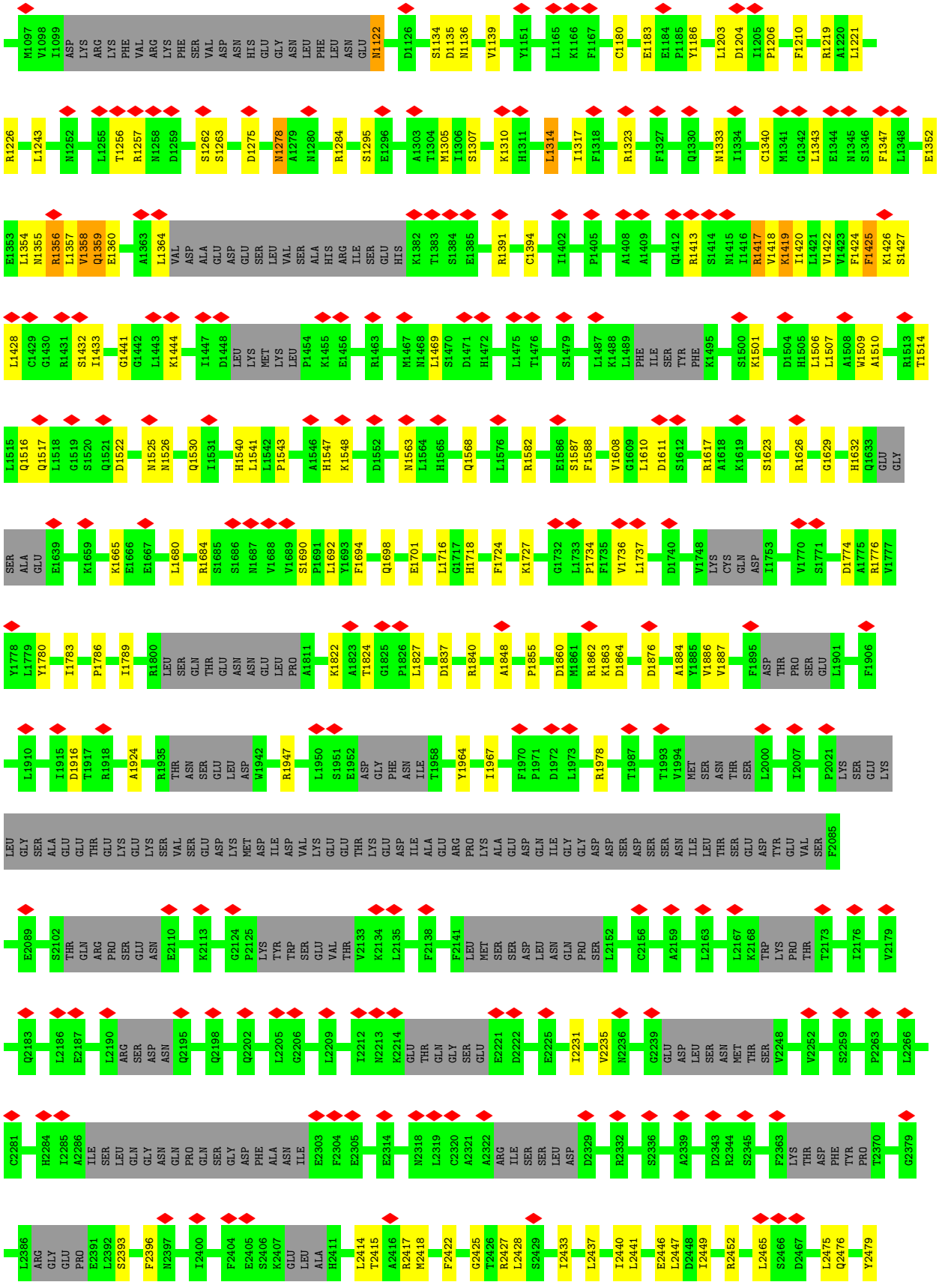
Chain I:



• Molecule 12: Transcription-associated protein

Chain L:

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D1126
S1134 D1135 N1136
V1139
Y1151
L1165 K1166 F1167
C1180
E1183
E1184 P1185 Y1186
L1203 D1204 I1205 P1206
F1210
R1219 A1220 L1221
R1226
L1243
N1252
L1255 T1256 R1257 N1258 D1259
S1262 S1263
D1275
N1278 A1279 N1280
R1284
S1295 E1296
A1303 T1304 M1305 T1306 S1307
K1310 H1311
L1314
I1317 F1318
R1323
F1327
Q1330
N1333 I1334
C1340 M1341 G1342 L1343 E1344 N1345 S1346 F1347 L1348
E1352
E1353 L1354 N1355 R1356 L1357 V1358 Q1359 E1360
A1363 L1364 VAL ASP ALA GLU ASP GLU SER LEU VAL SER ALA HIS ARG ILE SER GLU HIS K1382 T1383 S1384 E1385
R1391
C1394
I1402
P1405
A1408 A1409
Q1412 R1413 S1414 N1415 I1416 R1417 V1418 K1419 I1420 L1421 V1422 V1423 F1424 F1425 K1426 S1427
L1428 C1429 G1430 R1431 S1432 I1433
G1441 G1442 L1443 K1444
I1447 D1448 LEU LYS MET LYS LEU P1454 K1455 E1456
R1463
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L1475 T1476
S1479
L1487 K1488 L1489 PHE ILE SER TYR PHE K1495
S1500 K1501
D1504 H1505 L1506 L1507 A1508 W1509 A1510
R1513 T1514
L1515 Q1516 Q1517 L1518 G1519 S1520 Q1521 D1522
N1525 N1526
Q1530 I1531
H1540 L1541 L1542 P1543
A1546 H1547 K1548
D1552
N1563 L1564 H1565
Q1568
L1576
R1582
E1586 S1587 F1588
V1608 G1609 L1610 D1611 S1612
R1617 A1618 K1619
S1623
R1626
G1629
H1632 Q1633 GLU GLY
SER ALA GLU E1639
K1659
K1665 E1666 E1667
L1680
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Q1698
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D1740
V1748 LYS CYS GLN ASP I1753
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Y1778 L1779 Y1780
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P1786
I1789
R1800 LEU SER GLN THR GLU ASN ASN GLU LEU PRO A1811
K1822 A1823 T1824 G1825 P1826 L1827
D1837
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A1848
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D1876
A1884 Y1885 V1886 V1887
F1895 ASP THR PRO SER GLU L1901
F1906
L1910
T1915 D1916 T1917 R1918
A1924
R1935 THR ASN SER GLU LEU ASP W1942
R1947
L1950 S1951 E1952 ASP GLY PHE ASN ILE T1958
Y1964
I1967
F1970 P1971 D1972 L1973
R1978
T1987
T1993 V1994 MET SER ASN THR SER L2000
I2007
P2021 LYS SER GLU LYS
LEU GLY SER ALA GLU GLU THR GLU LYS GLU LYS SER VAL SER GLU ASP LYS MET ASP ILE ASP VAL LYS GLU GLU THR LYS GLU ASP ILE ALA GLU ARG PRO LYS ALA GLU ASP GLN ILE GLY GLY ASP ASP SER ASP SER SER ASN ILE LEU THR SER GLU ASP TYR GLU VAL SER F2085
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F2138
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Q2202
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L2209
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E2225
I2231
V2235
N2236
G2239 GLU ASP LEU SER ASN MET THR SER V2248
V2252
S2259
P2263
L2266
C2281
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E2314
N2318 L2319 C2320 A2321 A2322 ARG ILE SER SER LEU ASP D2329
R2332
S2336
A2339
D2343 R2344 S2345
F2363 LYS THR ASP PHE TYR PRO T2370
G2379
L2386 ARG GLY GLU PRO
E2391 L2392 S2393
F2396
N2397
I2400
F2404 E2405 S2406 K2407 GLU LEU ALA H2411
L2414 T2415 A2416 R2417 M2418
F2422
G2425 T2426 R2427 L2428 S2429
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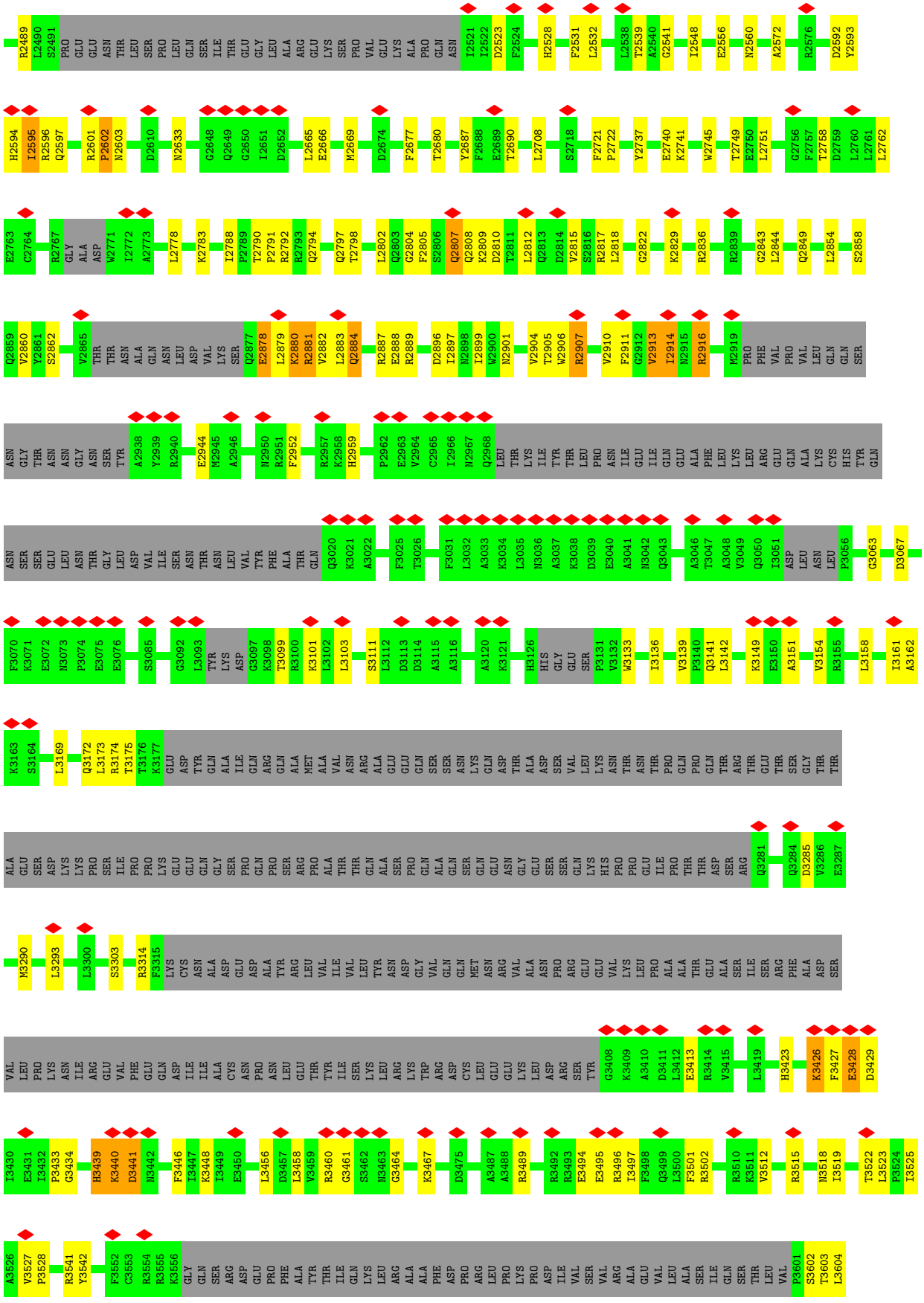
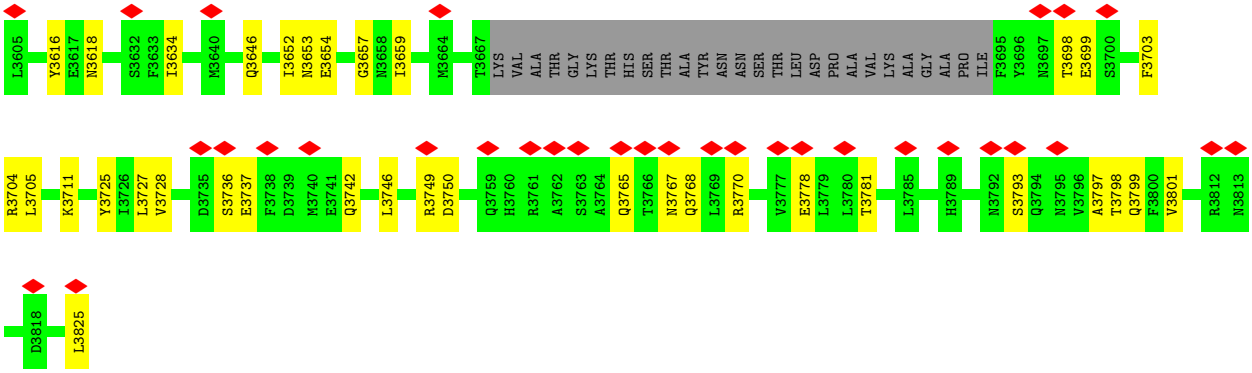
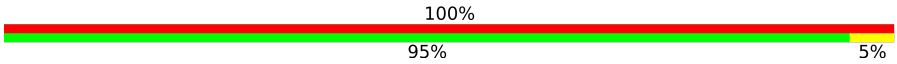
L2475 Q2476
Y2479

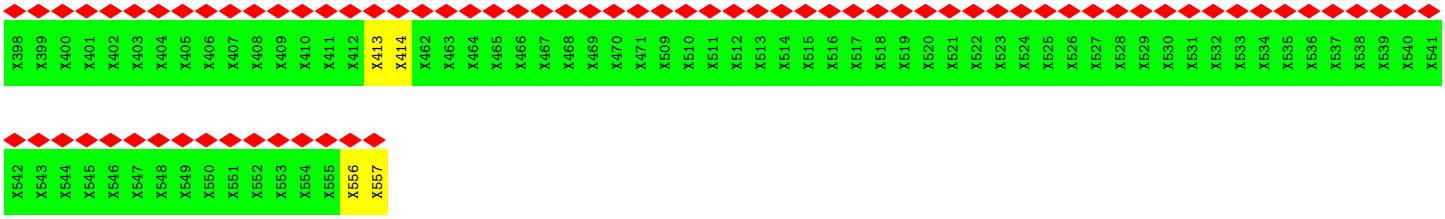




• Molecule 13: Transcriptional adapter 3 (Ada3)

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	354104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.8	Depositor
Minimum defocus (nm)	0.8	Depositor
Maximum defocus (nm)	4.5	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.125	Depositor
Minimum map value	-1.547	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	558.08, 558.08, 558.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	M	0.88	2/1442 (0.1%)	0.78	2/1942 (0.1%)
2	A	0.44	0/1319	0.60	0/1794
3	C	0.35	0/528	0.61	0/710
4	F	0.34	0/1718	0.58	0/2335
5	D	0.51	0/1641	0.65	0/2213
6	E	0.45	0/1246	0.62	0/1667
7	J	0.47	0/779	0.60	0/1051
8	K	0.42	0/1213	0.66	0/1647
9	G	0.52	0/4177	0.60	0/5661
10	H	0.38	0/3315	0.60	0/4500
11	I	0.44	0/1006	0.63	0/1374
12	L	0.33	0/22712	0.54	0/30825
All	All	0.41	2/41096 (0.0%)	0.58	2/55719 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	194	ILE	C-N	27.38	1.97	1.34
1	M	183	SER	C-N	6.38	1.48	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	62	GLY	N-CA-C	6.94	130.46	113.10
1	M	194	ILE	CA-C-N	-6.13	103.71	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	183	SER	Mainchain

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	M	1415	0	1492	88	0
2	A	1300	0	1254	30	0
3	C	518	0	528	9	0
4	F	1682	0	1622	30	0
5	D	1616	0	1558	122	0
6	E	1232	0	1276	40	0
7	J	768	0	754	11	0
8	K	1192	0	1214	89	0
9	G	4075	0	3934	102	0
10	H	3263	0	3258	69	0
11	I	981	0	982	18	0
12	L	22318	0	20960	376	0
13	B	380	0	85	2	0
All	All	40740	0	38917	865	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (865) 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)
8:K:469:LEU:HD13	12:L:2788:ILE:CG2	1.31	1.51
8:K:469:LEU:CD1	12:L:2788:ILE:HG21	1.57	1.34
12:L:828:ARG:H	12:L:829:PRO:HD3	1.06	1.20
1:M:194:ILE:HG22	1:M:195:TYR:N	1.57	1.19
1:M:194:ILE:C	1:M:195:TYR:N	1.97	1.17
5:D:212:GLN:HE21	5:D:212:GLN:HA	1.12	1.11
1:M:191:PRO:HA	5:D:211:ARG:HD2	1.25	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:466:PRO:HA	12:L:2791:PRO:HG2	1.33	1.08
8:K:469:LEU:CD1	12:L:2788:ILE:CG2	2.22	1.07
8:K:468:LEU:HB3	12:L:2829:LYS:HZ1	1.05	1.07
8:K:469:LEU:HD13	12:L:2788:ILE:HG22	1.30	1.07
5:D:78:LYS:HE3	5:D:78:LYS:HA	1.38	1.05
8:K:468:LEU:HB3	12:L:2829:LYS:NZ	1.70	1.04
5:D:66:VAL:HG12	5:D:67:PRO:HD2	1.44	0.99
1:M:173:GLU:HG2	5:D:197:LYS:HA	1.44	0.97
8:K:465:ARG:HH21	12:L:2843:GLY:H	1.10	0.96
12:L:849:LEU:HD12	12:L:849:LEU:H	1.31	0.95
5:D:66:VAL:CG1	5:D:67:PRO:HD2	1.99	0.93
5:D:212:GLN:HA	5:D:212:GLN:NE2	1.81	0.93
12:L:828:ARG:H	12:L:829:PRO:CD	1.82	0.92
8:K:441:PRO:HA	12:L:912:LEU:HD21	1.51	0.92
1:M:99:PHE:CE2	1:M:101:ALA:HB3	2.05	0.91
1:M:172:LEU:HB3	1:M:193:LEU:HD13	1.50	0.91
12:L:828:ARG:N	12:L:829:PRO:HD3	1.83	0.91
12:L:2916:ARG:NH2	12:L:2916:ARG:HB2	1.84	0.91
9:G:546:HIS:CD2	9:G:547:PRO:HD2	2.06	0.90
8:K:468:LEU:CB	12:L:2829:LYS:HZ1	1.87	0.88
9:G:543:VAL:HG22	9:G:552:LEU:HD11	1.55	0.88
1:M:194:ILE:CG2	1:M:195:TYR:N	2.36	0.88
1:M:188:GLU:OE1	5:D:85:ARG:NH2	2.07	0.87
6:E:938:ILE:HD12	6:E:938:ILE:H	1.38	0.87
5:D:216:THR:CG2	5:D:246:GLY:HA3	2.06	0.86
8:K:462:ILE:HB	12:L:2737:TYR:HE1	1.38	0.86
5:D:78:LYS:HE3	5:D:78:LYS:CA	2.06	0.86
12:L:2854:LEU:HD13	12:L:2906:TRP:CH2	2.11	0.85
8:K:474:ILE:HD13	12:L:2592:ASP:HB3	1.59	0.85
8:K:469:LEU:HD13	12:L:2788:ILE:HG21	0.88	0.85
8:K:442:PRO:HD2	12:L:912:LEU:HD22	1.58	0.85
12:L:1425:PHE:O	12:L:1428:LEU:N	2.10	0.83
9:G:546:HIS:CD2	9:G:547:PRO:CD	2.62	0.82
10:H:27:ALA:HB1	10:H:32:ILE:HD11	1.62	0.82
1:M:189:LEU:HA	5:D:85:ARG:HG2	1.61	0.81
8:K:454:PRO:N	8:K:455:PRO:HD2	1.95	0.81
1:M:82:LEU:HD13	1:M:101:ALA:HA	1.61	0.81
9:G:537:LEU:HD12	9:G:537:LEU:H	1.46	0.81
2:A:246:LEU:HD11	8:K:537:VAL:HG21	1.62	0.81
12:L:1203:LEU:O	12:L:1203:LEU:HD23	1.81	0.80
9:G:478:ARG:NH1	9:G:487:CYS:SG	2.55	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:173:GLU:CG	5:D:197:LYS:HA	2.13	0.79
5:D:303:PRO:HB2	5:D:304:ILE:HG12	1.66	0.78
1:M:176:ALA:HB2	1:M:193:LEU:HD11	1.65	0.78
1:M:191:PRO:CA	5:D:211:ARG:HD2	2.09	0.78
8:K:465:ARG:HH21	12:L:2843:GLY:N	1.82	0.78
1:M:191:PRO:HA	5:D:211:ARG:CD	2.12	0.78
6:E:938:ILE:HD12	6:E:938:ILE:N	1.99	0.78
10:H:127:LEU:O	10:H:127:LEU:HD12	1.84	0.77
1:M:108:GLU:HA	1:M:110:LYS:N	1.99	0.77
12:L:2593:TYR:H	12:L:2596:ARG:HG2	1.48	0.77
12:L:1122:ASN:HD22	12:L:1122:ASN:N	1.82	0.76
12:L:1354:LEU:HA	12:L:1357:LEU:HD22	1.68	0.76
1:M:101:ALA:HB1	1:M:115:ILE:O	1.85	0.76
12:L:2854:LEU:HD13	12:L:2906:TRP:HH2	1.49	0.76
2:A:239:GLU:N	2:A:239:GLU:OE1	2.18	0.76
5:D:323:LYS:HE2	7:J:107:PHE:HD1	1.51	0.76
12:L:2916:ARG:HB2	12:L:2916:ARG:CZ	2.16	0.76
12:L:2907:ARG:HH11	12:L:2907:ARG:HG2	1.51	0.76
12:L:2884:GLN:HA	12:L:2884:GLN:NE2	2.00	0.75
12:L:844:VAL:HB	12:L:849:LEU:HD22	1.68	0.75
12:L:2601:ARG:HB3	12:L:2602:PRO:HD2	1.68	0.75
8:K:462:ILE:HB	12:L:2737:TYR:CE1	2.20	0.75
2:A:327:ARG:NH1	2:A:328:HIS:O	2.20	0.74
10:H:129:LYS:HZ2	10:H:129:LYS:HA	1.52	0.74
5:D:322:GLU:OE2	5:D:322:GLU:HA	1.87	0.74
12:L:428:LYS:HE2	12:L:430:GLU:HG3	1.68	0.74
5:D:72:PHE:O	5:D:75:ARG:HB2	1.87	0.74
8:K:441:PRO:HA	12:L:912:LEU:CD2	2.17	0.74
9:G:414:ILE:HB	9:G:449:LEU:HB2	1.68	0.73
12:L:1417:ARG:HA	12:L:1420:ILE:HD12	1.70	0.73
8:K:453:LYS:C	8:K:455:PRO:HD2	2.08	0.73
9:G:537:LEU:HD12	9:G:537:LEU:N	2.04	0.73
9:G:568:ARG:HG2	9:G:570:GLU:HG2	1.69	0.73
9:G:546:HIS:HB2	9:G:553:PHE:HE1	1.54	0.72
5:D:78:LYS:HA	5:D:78:LYS:CE	2.17	0.72
9:G:67:ARG:O	9:G:70:SER:OG	2.07	0.72
4:F:115:VAL:HG22	4:F:190:LEU:HD21	1.71	0.72
12:L:849:LEU:HD12	12:L:849:LEU:N	2.03	0.72
8:K:453:LYS:HG2	8:K:455:PRO:HD2	1.71	0.72
5:D:73:LEU:HD23	5:D:73:LEU:O	1.89	0.72
5:D:317:GLN:C	5:D:319:ARG:H	1.93	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:188:GLU:CG	5:D:247:PHE:HA	2.20	0.72
5:D:216:THR:HB	5:D:243:ASP:HA	1.70	0.71
7:J:66:MET:O	7:J:98:ARG:NH1	2.24	0.71
8:K:468:LEU:O	12:L:2829:LYS:NZ	2.18	0.70
9:G:457:TYR:HE2	9:G:473:GLU:HB3	1.57	0.70
1:M:188:GLU:HG2	5:D:247:PHE:HA	1.72	0.70
8:K:474:ILE:CD1	12:L:2592:ASP:HB3	2.21	0.70
12:L:846:LEU:HG	12:L:850:VAL:HG11	1.74	0.70
5:D:21:MET:CE	5:D:250:PHE:HA	2.21	0.70
8:K:466:PRO:CA	12:L:2791:PRO:HG2	2.19	0.69
8:K:550:HIS:NE2	11:I:80:ASP:OD1	2.25	0.69
8:K:580:GLU:O	11:I:65:SER:N	2.25	0.69
6:E:948:GLN:HA	6:E:948:GLN:OE1	1.93	0.69
4:F:202:LEU:O	4:F:205:THR:OG1	2.08	0.69
5:D:20:MET:SD	5:D:213:ALA:HB3	2.34	0.68
8:K:456:GLN:HA	12:L:2669:MET:HG3	1.74	0.68
9:G:581:ALA:HB3	9:G:599:GLU:HG2	1.75	0.68
5:D:20:MET:SD	5:D:210:CYS:HA	2.34	0.68
9:G:118:CYS:SG	9:G:119:GLU:N	2.67	0.68
9:G:620:HIS:CE1	9:G:641:GLY:HA3	2.29	0.68
5:D:320:ASN:C	5:D:322:GLU:H	1.95	0.67
12:L:846:LEU:HA	12:L:850:VAL:HB	1.77	0.67
6:E:817:GLY:N	7:J:69:GLU:OE2	2.26	0.67
12:L:849:LEU:H	12:L:849:LEU:CD1	2.06	0.67
9:G:594:LEU:HG	9:G:606:TRP:HB2	1.75	0.67
5:D:21:MET:HE2	5:D:253:VAL:HG21	1.77	0.67
5:D:66:VAL:HG12	5:D:67:PRO:CD	2.22	0.67
8:K:447:PRO:HG3	12:L:2788:ILE:HG23	1.77	0.67
11:I:48:GLN:O	11:I:51:THR:OG1	2.11	0.67
8:K:453:LYS:HG2	8:K:455:PRO:CD	2.26	0.66
9:G:157:TYR:O	9:G:161:SER:N	2.28	0.66
5:D:241:VAL:HA	5:D:244:ILE:HD12	1.78	0.66
6:E:938:ILE:H	6:E:938:ILE:CD1	2.08	0.66
9:G:520:ARG:HG3	9:G:532:ILE:HG12	1.78	0.66
10:H:129:LYS:HA	10:H:129:LYS:NZ	2.11	0.66
10:H:404:VAL:HG12	10:H:407:TRP:CZ2	2.31	0.66
6:E:946:LYS:HE2	6:E:946:LYS:HA	1.78	0.66
9:G:43:ALA:N	9:G:45:ASP:OD1	2.28	0.65
12:L:2802:LEU:HD12	12:L:2815:VAL:HG11	1.77	0.65
12:L:2849:GLN:NE2	12:L:2889:ARG:O	2.29	0.65
8:K:454:PRO:N	8:K:455:PRO:CD	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:278:ALA:HB3	8:K:521:ILE:HG12	1.79	0.65
11:I:128:GLU:N	11:I:128:GLU:OE1	2.28	0.64
1:M:82:LEU:HB3	1:M:94:TYR:HE2	1.60	0.64
5:D:71:ILE:O	5:D:74:ILE:HG12	1.97	0.64
6:E:952:ASN:ND2	11:I:138:VAL:O	2.30	0.64
8:K:469:LEU:HD12	12:L:2788:ILE:HG21	1.72	0.64
5:D:326:ILE:O	5:D:328:ASN:N	2.30	0.64
8:K:582:ARG:NH2	11:I:70:ALA:O	2.30	0.64
9:G:154:ARG:NH2	9:G:179:SER:OG	2.31	0.64
12:L:1425:PHE:O	12:L:1427:SER:N	2.31	0.64
12:L:3303:SER:HB3	12:L:3427:PHE:HD2	1.61	0.64
5:D:259:GLU:HG3	5:D:316:LEU:HD21	1.80	0.64
7:J:67:GLU:OE1	7:J:95:LYS:NZ	2.30	0.64
12:L:328:ARG:HD3	12:L:370:THR:HG22	1.79	0.64
1:M:169:PRO:HA	1:M:208:VAL:O	1.99	0.63
5:D:248:LEU:O	5:D:251:GLU:HG2	1.98	0.63
9:G:494:HIS:NE2	9:G:520:ARG:HD3	2.14	0.63
10:H:375:ASN:ND2	10:H:377:THR:O	2.31	0.63
5:D:73:LEU:HD23	5:D:73:LEU:C	2.19	0.63
8:K:468:LEU:C	12:L:2829:LYS:HZ3	2.01	0.63
12:L:2878:GLU:HA	12:L:2881:ARG:HD3	1.79	0.63
12:L:365:PRO:HB3	12:L:407:VAL:HG11	1.81	0.63
12:L:2854:LEU:HD13	12:L:2906:TRP:CZ2	2.33	0.62
9:G:647:ARG:NH2	10:H:167:ARG:O	2.32	0.62
1:M:177:PHE:HB2	5:D:194:GLU:HA	1.80	0.62
12:L:846:LEU:HA	12:L:850:VAL:CG2	2.29	0.62
5:D:17:ILE:N	5:D:17:ILE:HD12	2.14	0.62
12:L:2880:LYS:H	12:L:2880:LYS:HD2	1.64	0.62
9:G:462:SER:OG	9:G:464:ASP:OD1	2.04	0.62
8:K:439:PRO:HB3	12:L:916:HIS:CE1	2.34	0.62
10:H:217:LEU:HD12	10:H:218:SER:H	1.65	0.62
12:L:1122:ASN:N	12:L:1122:ASN:ND2	2.44	0.62
9:G:546:HIS:CD2	9:G:547:PRO:HD3	2.35	0.61
12:L:3501:PHE:HB2	12:L:3523:LEU:HD21	1.81	0.61
1:M:189:LEU:HB3	5:D:84:LEU:HD22	1.81	0.61
5:D:49:ILE:HG23	5:D:73:LEU:HD13	1.82	0.61
10:H:317:LEU:O	10:H:380:THR:HG22	2.00	0.61
1:M:115:ILE:HD13	1:M:121:MET:SD	2.40	0.61
10:H:265:PHE:CE2	10:H:289:LEU:HD11	2.36	0.61
12:L:1611:ASP:HA	12:L:1617:ARG:HH12	1.65	0.61
9:G:87:ASN:ND2	9:G:219:ALA:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:450:VAL:HG22	9:G:451:GLY:H	1.65	0.61
12:L:2812:LEU:O	12:L:2815:VAL:HG22	1.99	0.61
1:M:204:LEU:HD23	1:M:212:ILE:HD12	1.83	0.61
5:D:78:LYS:O	5:D:78:LYS:HD3	2.01	0.61
5:D:320:ASN:C	5:D:322:GLU:N	2.53	0.61
2:A:289:ILE:O	6:E:958:LEU:HD21	2.01	0.60
5:D:21:MET:HE1	5:D:250:PHE:HA	1.82	0.60
5:D:320:ASN:CB	5:D:324:LYS:HB2	2.32	0.60
6:E:946:LYS:HA	6:E:946:LYS:CE	2.32	0.60
5:D:216:THR:HG23	5:D:246:GLY:HA3	1.83	0.60
12:L:428:LYS:HG3	12:L:430:GLU:HG2	1.84	0.60
6:E:890:LEU:HD22	6:E:915:THR:HG23	1.83	0.60
12:L:2907:ARG:HG2	12:L:2907:ARG:NH1	2.10	0.60
5:D:76:HIS:C	5:D:78:LYS:N	2.53	0.60
9:G:620:HIS:HA	9:G:647:ARG:HE	1.67	0.60
12:L:704:LEU:HD13	12:L:749:SER:HB2	1.82	0.60
5:D:76:HIS:C	5:D:78:LYS:H	2.04	0.60
9:G:518:THR:HG21	11:I:102:LEU:HD22	1.82	0.60
10:H:277:LEU:O	10:H:320:LYS:NZ	2.34	0.60
12:L:853:LEU:O	12:L:855:TYR:N	2.35	0.60
12:L:1837:ASP:OD1	12:L:1840:ARG:NH1	2.35	0.60
12:L:3652:ILE:HG22	12:L:3659:ILE:HG12	1.82	0.60
1:M:188:GLU:HA	1:M:188:GLU:OE2	2.02	0.60
1:M:185:TYR:OH	5:D:211:ARG:HD3	2.02	0.59
5:D:21:MET:HE3	5:D:250:PHE:HA	1.84	0.59
10:H:269:ILE:O	10:H:272:THR:OG1	2.16	0.59
12:L:3736:SER:OG	12:L:3737:GLU:N	2.35	0.59
1:M:202:ILE:HD11	1:M:217:ALA:HB2	1.84	0.59
5:D:317:GLN:C	5:D:319:ARG:N	2.55	0.59
8:K:437:LEU:H	8:K:437:LEU:HD23	1.67	0.59
4:F:119:GLU:OE1	4:F:119:GLU:N	2.36	0.59
8:K:469:LEU:CD1	12:L:2788:ILE:HG22	2.14	0.59
12:L:848:VAL:C	12:L:851:PRO:HD2	2.23	0.59
12:L:1352:GLU:HA	12:L:1355:ASN:HB2	1.83	0.59
2:A:226:ILE:HA	2:A:229:PHE:CE2	2.37	0.59
12:L:3440:LYS:HG3	12:L:3446:PHE:CE1	2.38	0.59
12:L:3704:ARG:NH2	12:L:3825:LEU:O	2.36	0.59
12:L:3767:ASN:OD1	12:L:3770:ARG:NH2	2.35	0.59
6:E:952:ASN:OD1	11:I:137:TRP:NE1	2.35	0.59
12:L:3169:LEU:HG	12:L:3173:LEU:HD23	1.85	0.59
12:L:2805:PHE:CZ	12:L:2812:LEU:HG	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:556:UNK:O	13:B:557:UNK:C	2.50	0.58
6:E:921:TYR:HD1	7:J:104:THR:HG22	1.68	0.58
8:K:446:ILE:HG13	12:L:2595:ILE:HG12	1.84	0.58
10:H:100:GLU:OE2	10:H:111:TYR:N	2.35	0.58
12:L:2913:VAL:HG12	12:L:2914:ILE:HD13	1.84	0.58
5:D:84:LEU:HD23	5:D:84:LEU:O	2.02	0.58
12:L:2593:TYR:HB2	12:L:2596:ARG:HA	1.86	0.58
1:M:190:PHE:HB3	5:D:88:LEU:HG	1.84	0.58
10:H:38:GLU:N	10:H:38:GLU:OE1	2.36	0.58
10:H:162:ILE:HG22	10:H:164:PRO:HD2	1.86	0.58
4:F:223:GLU:HG2	9:G:576:MET:HB2	1.85	0.58
10:H:296:ASN:OD1	10:H:297:GLU:N	2.36	0.58
1:M:168:PHE:CD1	1:M:238:ARG:HG3	2.39	0.58
4:F:83:LEU:O	4:F:142:LEU:HD13	2.03	0.58
6:E:946:LYS:HD2	6:E:946:LYS:N	2.17	0.58
12:L:2601:ARG:N	12:L:2601:ARG:HE	2.02	0.58
12:L:2428:LEU:HD11	12:L:2433:ILE:HD11	1.85	0.58
2:A:229:PHE:HZ	3:C:270:GLU:HG2	1.69	0.58
12:L:850:VAL:O	12:L:853:LEU:HB3	2.03	0.58
1:M:82:LEU:CB	1:M:94:TYR:HE2	2.18	0.57
5:D:87:TYR:CD1	5:D:87:TYR:C	2.77	0.57
12:L:905:LEU:HD22	12:L:922:THR:HG23	1.85	0.57
12:L:1355:ASN:O	12:L:1358:VAL:HG13	2.04	0.57
12:L:2836:ARG:NH2	12:L:3618:ASN:OD1	2.37	0.57
10:H:125:GLU:N	10:H:126:PRO:HD3	2.18	0.57
6:E:921:TYR:CD1	7:J:104:THR:HG22	2.39	0.57
10:H:250:GLN:OE1	10:H:253:ARG:NE	2.33	0.57
11:I:41:ARG:O	11:I:44:THR:OG1	2.19	0.57
12:L:851:PRO:O	12:L:852:HIS:HB3	2.03	0.57
10:H:129:LYS:HZ3	10:H:129:LYS:HB2	1.70	0.57
4:F:89:GLU:OE2	4:F:148:ARG:NH1	2.37	0.57
9:G:500:ASP:HB2	9:G:502:LYS:HE2	1.85	0.57
12:L:378:VAL:HG12	12:L:380:ASP:H	1.70	0.57
12:L:2860:VAL:HG13	12:L:2879:LEU:HD11	1.86	0.57
12:L:3458:LEU:H	12:L:3458:LEU:HD23	1.69	0.57
1:M:108:GLU:HA	1:M:110:LYS:H	1.70	0.57
9:G:620:HIS:NE2	9:G:641:GLY:HA3	2.20	0.57
12:L:3727:LEU:HD22	12:L:3798:THR:HG22	1.85	0.57
1:M:87:LEU:O	1:M:90:ARG:HG2	2.04	0.57
10:H:102:LEU:HD23	10:H:103:VAL:N	2.20	0.57
12:L:1355:ASN:HA	12:L:1358:VAL:CG1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:191:PRO:HB3	5:D:212:GLN:CG	2.34	0.56
9:G:572:VAL:HG12	9:G:573:ARG:HG2	1.87	0.56
12:L:2880:LYS:N	12:L:2880:LYS:CD	2.67	0.56
3:C:288:LEU:HD21	3:C:292:THR:HG21	1.87	0.56
9:G:546:HIS:HB2	9:G:553:PHE:CE1	2.35	0.56
12:L:853:LEU:O	12:L:856:LEU:N	2.37	0.56
12:L:2880:LYS:HD2	12:L:2880:LYS:N	2.20	0.56
12:L:2880:LYS:CA	12:L:2880:LYS:HE3	2.35	0.56
4:F:111:PHE:CE1	4:F:115:VAL:HG21	2.41	0.56
6:E:885:VAL:HA	10:H:128:PRO:CG	2.35	0.56
12:L:3433:PRO:HB2	12:L:3527:VAL:HG11	1.86	0.56
1:M:74:VAL:HG23	1:M:155:PHE:HA	1.87	0.56
8:K:456:GLN:HG3	12:L:2677:PHE:CE2	2.41	0.56
6:E:932:HIS:O	6:E:935:SER:HB2	2.04	0.56
8:K:460:MET:SD	8:K:460:MET:N	2.76	0.56
12:L:302:PRO:HD3	12:L:336:ARG:HH22	1.71	0.56
12:L:3174:ARG:NH1	12:L:3290:MET:SD	2.79	0.56
12:L:2896:ASP:HB3	12:L:2899:ILE:HG12	1.86	0.56
10:H:356:SER:O	10:H:360:PRO:HG2	2.05	0.56
12:L:827:ARG:O	12:L:828:ARG:HB2	2.05	0.56
5:D:320:ASN:HB3	5:D:324:LYS:HB2	1.89	0.55
12:L:946:ASP:O	12:L:951:GLN:NE2	2.39	0.55
12:L:3439:HIS:C	12:L:3440:LYS:HG2	2.27	0.55
12:L:583:ASN:ND2	12:L:600:ALA:O	2.39	0.55
8:K:455:PRO:HB2	8:K:457:PRO:HD2	1.88	0.55
12:L:2414:LEU:O	12:L:2417:ARG:NH1	2.40	0.55
1:M:139:TYR:O	1:M:143:ILE:HG12	2.06	0.55
5:D:88:LEU:C	5:D:88:LEU:HD13	2.27	0.55
5:D:326:ILE:HD12	5:D:327:ARG:N	2.21	0.55
10:H:265:PHE:HE2	10:H:289:LEU:HD11	1.70	0.55
9:G:546:HIS:CG	9:G:547:PRO:HD2	2.42	0.55
12:L:3698:THR:OG1	12:L:3699:GLU:N	2.39	0.55
1:M:143:ILE:O	1:M:150:ALA:HB2	2.06	0.55
1:M:189:LEU:HD21	5:D:81:VAL:HG12	1.87	0.55
5:D:212:GLN:HE21	5:D:212:GLN:CA	2.02	0.55
1:M:83:LYS:O	1:M:87:LEU:HG	2.07	0.54
1:M:187:PRO:CB	5:D:211:ARG:HB2	2.37	0.54
5:D:238:SER:OG	5:D:240:ASP:OD1	2.11	0.54
5:D:317:GLN:O	5:D:319:ARG:N	2.35	0.54
10:H:218:SER:OG	10:H:221:LEU:N	2.38	0.54
12:L:3429:ASP:HB2	12:L:3448:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:99:PHE:CZ	1:M:114:LEU:HD12	2.43	0.54
2:A:208:VAL:HG21	2:A:214:VAL:HG11	1.88	0.54
1:M:115:ILE:CD1	1:M:121:MET:SD	2.95	0.54
1:M:189:LEU:HD13	5:D:84:LEU:HD13	1.89	0.54
5:D:22:PHE:CE2	5:D:30:PRO:HD3	2.43	0.54
12:L:822:LEU:HD22	12:L:1186:TYR:H	1.72	0.54
12:L:3458:LEU:HD23	12:L:3458:LEU:N	2.22	0.54
5:D:259:GLU:HB2	5:D:312:ALA:HB1	1.88	0.54
9:G:593:TRP:HE1	9:G:614:ILE:HD12	1.72	0.54
9:G:631:SER:OG	9:G:634:GLY:N	2.39	0.54
12:L:1822:LYS:NZ	12:L:1864:ASP:OD2	2.41	0.54
1:M:173:GLU:HB2	5:D:204:TYR:CD1	2.43	0.54
4:F:212:PHE:HE2	4:F:218:LEU:HD21	1.72	0.54
5:D:199:MET:HA	5:D:203:GLU:CB	2.37	0.54
10:H:394:GLU:N	10:H:394:GLU:OE1	2.40	0.54
12:L:2916:ARG:HB2	12:L:2916:ARG:HH21	1.71	0.54
8:K:464:ASN:OD1	12:L:2669:MET:SD	2.65	0.54
10:H:115:ASP:OD1	10:H:116:GLU:N	2.41	0.54
11:I:40:TYR:O	11:I:44:THR:HG23	2.07	0.54
5:D:216:THR:CG2	5:D:243:ASP:HA	2.38	0.54
5:D:17:ILE:HD12	5:D:17:ILE:H	1.72	0.54
12:L:3428:GLU:HG2	12:L:3429:ASP:H	1.73	0.54
12:L:846:LEU:O	12:L:850:VAL:HB	2.08	0.53
5:D:216:THR:CB	5:D:243:ASP:HA	2.38	0.53
12:L:2911:PHE:CE2	12:L:2944:GLU:HG3	2.44	0.53
12:L:1522:ASP:OD1	12:L:1522:ASP:N	2.41	0.53
5:D:66:VAL:HG13	5:D:67:PRO:HD2	1.87	0.53
5:D:317:GLN:HA	5:D:317:GLN:NE2	2.22	0.53
8:K:468:LEU:C	12:L:2829:LYS:NZ	2.61	0.53
13:B:413:UNK:O	13:B:414:UNK:C	2.56	0.53
4:F:93:ARG:NH2	4:F:95:GLY:O	2.41	0.53
10:H:332:GLN:N	10:H:332:GLN:OE1	2.42	0.53
12:L:1727:LYS:HG3	12:L:1776:ARG:HH21	1.73	0.53
12:L:3136:ILE:HG22	12:L:3161:ILE:HD13	1.89	0.53
4:F:277:ASN:OD1	4:F:278:ALA:N	2.42	0.53
9:G:411:ASP:N	9:G:411:ASP:OD1	2.42	0.53
9:G:537:LEU:H	9:G:537:LEU:CD1	2.20	0.53
12:L:1219:ARG:NH1	12:L:3413:GLU:OE2	2.41	0.53
10:H:13:SER:OG	10:H:14:HIS:N	2.41	0.53
9:G:521:LEU:HD23	9:G:521:LEU:O	2.08	0.53
12:L:959:ILE:HG21	12:L:2449:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:84:LEU:HD23	5:D:84:LEU:C	2.29	0.53
10:H:406:ASN:O	10:H:409:SER:OG	2.15	0.53
12:L:345:LEU:O	12:L:386:GLN:NE2	2.42	0.53
12:L:1278:ASN:O	12:L:1284:ARG:NH2	2.42	0.53
1:M:173:GLU:HG2	5:D:197:LYS:CA	2.29	0.53
1:M:188:GLU:OE1	5:D:85:ARG:CZ	2.57	0.53
5:D:313:TRP:O	5:D:317:GLN:HG2	2.08	0.53
5:D:323:LYS:HG3	5:D:323:LYS:O	2.08	0.53
10:H:217:LEU:HD12	10:H:218:SER:O	2.08	0.53
12:L:416:LEU:HD11	12:L:574:THR:HB	1.91	0.53
12:L:3101:LYS:O	12:L:3742:GLN:NE2	2.42	0.53
1:M:84:THR:HA	1:M:87:LEU:HD12	1.90	0.52
9:G:76:PRO:O	9:G:592:ARG:NH1	2.42	0.52
9:G:546:HIS:CG	9:G:547:PRO:CD	2.92	0.52
8:K:469:LEU:HD23	12:L:2790:THR:CG2	2.39	0.52
12:L:1526:ASN:O	12:L:1530:GLN:NE2	2.43	0.52
12:L:2528:HIS:O	12:L:2531:PHE:N	2.42	0.52
5:D:21:MET:HE2	5:D:253:VAL:CG2	2.38	0.52
7:J:80:THR:O	7:J:84:LEU:HD23	2.09	0.52
12:L:1886:VAL:HG22	12:L:1924:ALA:HB2	1.91	0.52
1:M:149:ALA:O	1:M:151:LYS:N	2.42	0.52
9:G:521:LEU:HD23	9:G:521:LEU:C	2.30	0.52
9:G:544:GLU:O	9:G:552:LEU:HD12	2.09	0.52
9:G:562:ARG:HB3	9:G:571:CYS:SG	2.49	0.52
5:D:326:ILE:HD12	5:D:326:ILE:C	2.30	0.52
12:L:852:HIS:CG	12:L:852:HIS:O	2.62	0.52
12:L:1355:ASN:HA	12:L:1358:VAL:HG12	1.91	0.52
12:L:3515:ARG:NH1	12:L:3518:ASN:OD1	2.43	0.52
2:A:223:GLN:OE1	2:A:223:GLN:HA	2.09	0.52
2:A:226:ILE:HA	2:A:229:PHE:CD2	2.44	0.52
8:K:442:PRO:CD	12:L:912:LEU:HD22	2.36	0.52
12:L:846:LEU:HA	12:L:850:VAL:CB	2.39	0.52
12:L:1307:SER:HA	12:L:1310:LYS:HD2	1.91	0.52
12:L:2884:GLN:NE2	12:L:2884:GLN:CA	2.72	0.52
5:D:218:ARG:C	5:D:220:ALA:H	2.12	0.52
8:K:468:LEU:CB	12:L:2829:LYS:NZ	2.58	0.52
8:K:602:ILE:O	8:K:607:ASN:N	2.43	0.52
1:M:185:TYR:C	1:M:185:TYR:HD1	2.13	0.52
8:K:460:MET:HG3	12:L:2758:THR:HG22	1.92	0.52
12:L:710:SER:O	12:L:757:ASN:ND2	2.43	0.52
1:M:102:VAL:HG12	1:M:115:ILE:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:84:GLN:OE1	9:G:215:ASN:O	2.28	0.51
9:G:202:ILE:HD11	9:G:206:THR:HG21	1.92	0.51
10:H:27:ALA:HB1	10:H:32:ILE:CD1	2.35	0.51
9:G:607:ASP:HB2	9:G:614:ILE:HG13	1.92	0.51
12:L:672:PRO:HA	12:L:675:PHE:HB3	1.93	0.51
12:L:1419:LYS:O	12:L:1422:VAL:HG22	2.11	0.51
12:L:1947:ARG:NH2	12:L:1964:TYR:OH	2.43	0.51
12:L:3141:GLN:NE2	12:L:3750:ASP:OD2	2.42	0.51
12:L:3495:GLU:HG3	12:L:3496:ARG:HD2	1.91	0.51
6:E:940:LYS:O	6:E:941:VAL:HB	2.09	0.51
12:L:1221:LEU:HD21	12:L:1243:LEU:HB3	1.92	0.51
6:E:947:PHE:HD1	6:E:947:PHE:O	1.94	0.51
12:L:899:ASP:N	12:L:899:ASP:OD1	2.41	0.51
12:L:2805:PHE:CE1	12:L:2812:LEU:HG	2.46	0.51
5:D:232:LEU:HD22	5:D:235:SER:OG	2.11	0.51
10:H:255:ASP:OD1	10:H:255:ASP:N	2.43	0.51
12:L:986:PRO:O	12:L:991:ARG:NH2	2.44	0.51
12:L:2601:ARG:O	12:L:2603:ASN:N	2.43	0.51
2:A:364:ASP:N	2:A:364:ASP:OD1	2.42	0.51
4:F:200:ASP:HA	4:F:203:TYR:HE2	1.75	0.51
6:E:935:SER:OG	6:E:940:LYS:HB2	2.11	0.51
10:H:362:ILE:N	10:H:362:ILE:HD13	2.24	0.51
12:L:3423:HIS:HA	12:L:3426:LYS:HB2	1.93	0.51
12:L:809:MET:HE1	12:L:844:VAL:HG21	1.92	0.51
12:L:1203:LEU:O	12:L:1206:PRO:HD2	2.10	0.51
12:L:1203:LEU:HD23	12:L:1206:PRO:HD2	1.93	0.51
1:M:105:ARG:O	1:M:106:ILE:HG23	2.10	0.51
5:D:74:ILE:HG13	5:D:78:LYS:HB3	1.92	0.51
8:K:461:LYS:HZ1	12:L:2792:ARG:NH2	2.09	0.51
9:G:650:ASP:HB3	9:G:693:MET:HE2	1.93	0.51
12:L:3456:LEU:HD12	12:L:3467:LYS:HB3	1.93	0.51
4:F:212:PHE:CE2	4:F:218:LEU:HD21	2.46	0.51
9:G:471:CYS:SG	9:G:499:TRP:O	2.69	0.51
10:H:328:LEU:O	10:H:332:GLN:NE2	2.43	0.51
12:L:562:ARG:NH1	12:L:625:PHE:O	2.44	0.51
12:L:2802:LEU:HD11	12:L:2858:SER:HB2	1.93	0.51
2:A:246:LEU:O	2:A:250:MET:HG3	2.11	0.51
9:G:494:HIS:CE1	9:G:520:ARG:HD3	2.45	0.51
2:A:192:SER:O	2:A:196:GLN:NE2	2.44	0.50
12:L:1314:LEU:O	12:L:1317:ILE:HG22	2.10	0.50
4:F:326:ARG:HG2	12:L:2751:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:836:CYS:SG	6:E:993:LEU:HD13	2.51	0.50
12:L:1698:GLN:HA	12:L:1701:GLU:HG2	1.93	0.50
12:L:2415:THR:HA	12:L:2418:MET:HE3	1.93	0.50
1:M:170:ILE:HD13	1:M:234:LEU:HD22	1.93	0.50
9:G:565:ASP:HB3	9:G:568:ARG:HB3	1.93	0.50
12:L:703:PHE:O	12:L:709:THR:OG1	2.29	0.50
12:L:1860:ASP:OD1	12:L:1860:ASP:N	2.45	0.50
12:L:2556:GLU:O	12:L:2560:ASN:ND2	2.44	0.50
12:L:2802:LEU:HD22	12:L:2854:LEU:HD12	1.92	0.50
1:M:185:TYR:C	1:M:185:TYR:CD1	2.84	0.50
9:G:380:SER:OG	10:H:143:ILE:O	2.20	0.50
12:L:1314:LEU:HG	12:L:1347:PHE:CZ	2.47	0.50
2:A:246:LEU:HG	2:A:250:MET:HE2	1.93	0.50
5:D:78:LYS:HE3	5:D:78:LYS:C	2.31	0.50
12:L:1507:LEU:HA	12:L:1510:ALA:HB3	1.92	0.50
12:L:2916:ARG:CZ	12:L:2916:ARG:CB	2.88	0.50
12:L:3746:LEU:HA	12:L:3749:ARG:HG2	1.93	0.50
1:M:67:LEU:HD13	1:M:160:ILE:HG23	1.94	0.50
1:M:142:ILE:HA	1:M:145:LYS:HE3	1.94	0.50
4:F:122:PRO:HG3	4:F:195:LEU:HD23	1.93	0.50
12:L:2880:LYS:HE3	12:L:2880:LYS:HA	1.94	0.50
12:L:3440:LYS:HG3	12:L:3446:PHE:HE1	1.75	0.50
10:H:290:ILE:HG22	10:H:343:LEU:HD11	1.93	0.50
12:L:1516:GLN:NE2	12:L:1563:ASN:O	2.45	0.50
6:E:948:GLN:HG3	6:E:950:VAL:O	2.11	0.49
9:G:122:LEU:HD21	10:H:291:TYR:CD1	2.46	0.49
9:G:469:ILE:HD11	9:G:479:LEU:HD12	1.93	0.49
12:L:1947:ARG:NH1	12:L:1978:ARG:O	2.45	0.49
4:F:219:ASN:O	4:F:222:THR:OG1	2.31	0.49
12:L:2880:LYS:H	12:L:2880:LYS:CD	2.23	0.49
1:M:80:LEU:HD21	1:M:143:ILE:HD12	1.93	0.49
12:L:2797:GLN:HG2	12:L:2818:LEU:HD21	1.93	0.49
10:H:96:LEU:HD23	10:H:97:VAL:N	2.27	0.49
4:F:200:ASP:HA	4:F:203:TYR:CE2	2.48	0.49
5:D:67:PRO:O	5:D:71:ILE:HG22	2.12	0.49
12:L:428:LYS:HG3	12:L:430:GLU:CG	2.42	0.49
12:L:2465:LEU:HB3	12:L:2593:TYR:HB3	1.95	0.49
12:L:3653:ASN:HB3	12:L:3657:GLY:H	1.78	0.49
2:A:208:VAL:CG2	2:A:214:VAL:HG11	2.42	0.49
12:L:1432:SER:OG	12:L:1433:ILE:N	2.45	0.49
12:L:2906:TRP:O	12:L:2910:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:279:ASP:O	8:K:521:ILE:HD11	2.12	0.49
5:D:329:PHE:N	5:D:329:PHE:CD1	2.80	0.49
1:M:82:LEU:CD1	1:M:101:ALA:HA	2.37	0.49
3:C:306:SER:OG	3:C:307:VAL:N	2.45	0.49
5:D:319:ARG:HG3	5:D:320:ASN:H	1.77	0.49
12:L:3175:THR:HG21	12:L:3528:PRO:HB2	1.94	0.49
1:M:108:GLU:HA	1:M:109:PRO:C	2.31	0.49
6:E:885:VAL:HA	10:H:128:PRO:HG3	1.95	0.49
12:L:1354:LEU:O	12:L:1358:VAL:HG12	2.13	0.49
12:L:1364:LEU:O	12:L:1391:ARG:NH1	2.45	0.49
1:M:175:LEU:O	1:M:179:HIS:HB2	2.13	0.49
2:A:190:VAL:HG22	2:A:192:SER:H	1.77	0.49
6:E:946:LYS:CE	6:E:946:LYS:CA	2.91	0.49
12:L:2475:LEU:O	12:L:2479:TYR:N	2.44	0.49
4:F:223:GLU:OE1	4:F:223:GLU:N	2.46	0.48
5:D:78:LYS:O	5:D:78:LYS:CD	2.61	0.48
11:I:133:THR:O	11:I:135:LYS:N	2.44	0.48
12:L:2665:LEU:HD21	12:L:2680:THR:HB	1.95	0.48
4:F:129:LYS:HG2	4:F:203:TYR:CE1	2.47	0.48
8:K:454:PRO:CD	8:K:455:PRO:CD	2.92	0.48
12:L:1256:THR:OG1	12:L:1257:ARG:N	2.47	0.48
12:L:1358:VAL:HG23	12:L:1394:CYS:HB3	1.95	0.48
8:K:564:HIS:ND1	8:K:568:ASN:OD1	2.44	0.48
9:G:139:HIS:ND1	9:G:228:LEU:HD22	2.29	0.48
12:L:545:LEU:HD12	12:L:546:PRO:HD2	1.94	0.48
8:K:439:PRO:HB3	12:L:916:HIS:HE1	1.75	0.48
6:E:885:VAL:HG22	10:H:128:PRO:HB2	1.95	0.48
10:H:26:ALA:O	10:H:29:SER:OG	2.22	0.48
12:L:599:THR:O	12:L:601:ARG:NH1	2.46	0.48
12:L:426:GLU:HG3	12:L:428:LYS:HD3	1.94	0.48
10:H:118:ASP:OD1	10:H:118:ASP:N	2.46	0.48
12:L:605:ASN:OD1	12:L:1568:GLN:NE2	2.46	0.48
12:L:387:LEU:HD21	12:L:422:ILE:HG12	1.95	0.48
6:E:909:PHE:O	6:E:913:VAL:HG23	2.14	0.48
9:G:171:GLU:OE1	9:G:171:GLU:N	2.45	0.48
10:H:317:LEU:HD12	10:H:319:LYS:H	1.78	0.48
12:L:2807:GLN:CB	12:L:2809:LYS:HE3	2.44	0.48
1:M:96:PRO:O	1:M:98:ARG:N	2.47	0.48
5:D:23:VAL:HA	5:D:27:THR:O	2.14	0.48
6:E:834:ARG:NH2	6:E:901:ASN:O	2.47	0.48
12:L:1514:THR:O	12:L:1517:GLN:NE2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:1724:PHE:HB3	12:L:1776:ARG:HD2	1.96	0.48
12:L:2528:HIS:CD2	12:L:2532:LEU:HD23	2.49	0.48
1:M:194:ILE:CA	1:M:195:TYR:N	2.76	0.47
4:F:115:VAL:HG13	4:F:190:LEU:HD11	1.96	0.47
8:K:458:ALA:O	8:K:459:ALA:HB2	2.14	0.47
9:G:94:PRO:HB3	9:G:566:ILE:HD11	1.96	0.47
9:G:184:LEU:O	9:G:191:LYS:NZ	2.41	0.47
11:I:131:CYS:SG	11:I:132:LEU:N	2.87	0.47
12:L:1180:CYS:HA	12:L:1183:GLU:HG2	1.96	0.47
12:L:2878:GLU:O	12:L:2882:VAL:HG13	2.14	0.47
12:L:2879:LEU:O	12:L:2882:VAL:HG22	2.14	0.47
9:G:650:ASP:HB3	9:G:693:MET:CE	2.43	0.47
2:A:229:PHE:CZ	3:C:270:GLU:HG2	2.50	0.47
5:D:84:LEU:HA	5:D:87:TYR:HD2	1.79	0.47
8:K:468:LEU:O	12:L:2790:THR:HG22	2.14	0.47
12:L:853:LEU:HD23	12:L:853:LEU:N	2.28	0.47
12:L:1262:SER:OG	12:L:1263:SER:N	2.47	0.47
12:L:1855:PRO:HA	12:L:1862:ARG:HH22	1.79	0.47
5:D:319:ARG:HH12	5:D:335:ARG:HG2	1.79	0.47
8:K:469:LEU:HB3	12:L:2788:ILE:CG2	2.44	0.47
12:L:2904:VAL:HG21	12:L:2952:PHE:HB2	1.95	0.47
12:L:3519:ILE:O	12:L:3519:ILE:HG13	2.13	0.47
5:D:17:ILE:H	5:D:17:ILE:CD1	2.26	0.47
5:D:208:SER:HB3	5:D:211:ARG:CZ	2.44	0.47
9:G:559:LYS:HG2	9:G:580:GLY:O	2.14	0.47
1:M:191:PRO:HB3	5:D:212:GLN:HG2	1.96	0.47
5:D:47:VAL:O	5:D:51:LEU:HD23	2.14	0.47
5:D:73:LEU:C	5:D:73:LEU:CD2	2.82	0.47
5:D:328:ASN:ND2	6:E:963:ASN:OD1	2.48	0.47
10:H:305:VAL:HA	10:H:308:ILE:HG22	1.97	0.47
12:L:1469:LEU:O	12:L:1501:LYS:NZ	2.47	0.47
12:L:1824:THR:H	12:L:1827:LEU:HD21	1.79	0.47
12:L:2914:ILE:HD13	12:L:2914:ILE:N	2.28	0.47
12:L:3162:ALA:HB2	12:L:3169:LEU:HD23	1.95	0.47
2:A:246:LEU:HG	2:A:250:MET:CE	2.45	0.47
4:F:118:GLU:O	4:F:191:ARG:N	2.45	0.47
4:F:189:ILE:C	4:F:190:LEU:HD12	2.35	0.47
4:F:304:LEU:CD2	8:K:475:SER:HB2	2.45	0.47
6:E:947:PHE:CD1	6:E:947:PHE:C	2.88	0.47
8:K:566:GLU:O	8:K:572:ARG:NH1	2.46	0.47
9:G:472:SER:OG	9:G:474:ASP:OD1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:854:SER:C	12:L:856:LEU:H	2.18	0.47
12:L:867:SER:OG	12:L:868:GLN:N	2.48	0.47
12:L:1417:ARG:HG2	12:L:1418:VAL:N	2.29	0.47
12:L:1684:ARG:HH12	12:L:1692:LEU:HD13	1.80	0.47
1:M:82:LEU:HG	1:M:117:ALA:HB2	1.97	0.47
9:G:626:TYR:CE2	9:G:642:ALA:HB2	2.50	0.47
12:L:1716:LEU:HG	12:L:1718:HIS:H	1.79	0.47
12:L:3798:THR:OG1	12:L:3799:GLN:N	2.44	0.47
9:G:546:HIS:NE2	9:G:547:PRO:HD2	2.29	0.47
10:H:157:ASN:HD22	10:H:160:LYS:HZ3	1.62	0.47
12:L:1134:SER:OG	12:L:1135:ASP:N	2.47	0.47
12:L:2808:GLN:HA	12:L:2808:GLN:OE1	2.14	0.47
2:A:244:ASP:O	2:A:248:THR:HG23	2.15	0.47
10:H:16:LEU:HD22	11:I:18:ILE:HG12	1.97	0.47
12:L:312:CYS:O	12:L:320:ARG:NH2	2.47	0.47
12:L:1203:LEU:HD22	12:L:1210:PHE:CE2	2.50	0.47
12:L:1848:ALA:HB2	12:L:1887:VAL:HG23	1.97	0.47
1:M:151:LYS:O	1:M:153:THR:HG22	2.15	0.46
2:A:271:MET:SD	8:K:537:VAL:HG23	2.55	0.46
8:K:441:PRO:CA	12:L:912:LEU:HD21	2.33	0.46
8:K:504:LYS:O	8:K:508:ARG:NH1	2.48	0.46
12:L:853:LEU:O	12:L:854:SER:C	2.54	0.46
9:G:576:MET:SD	9:G:577:GLY:N	2.88	0.46
12:L:952:ASN:OD1	12:L:952:ASN:N	2.48	0.46
4:F:137:GLU:O	9:G:59:TYR:N	2.45	0.46
5:D:75:ARG:O	5:D:75:ARG:HG2	2.16	0.46
8:K:444:THR:OG1	8:K:445:GLU:N	2.48	0.46
12:L:1441:GLY:HA2	12:L:1444:LYS:HG2	1.98	0.46
12:L:2601:ARG:O	12:L:2602:PRO:C	2.53	0.46
12:L:2959:HIS:HA	12:L:3512:VAL:HG11	1.96	0.46
1:M:75:THR:HB	1:M:120:LYS:HG2	1.97	0.46
2:A:357:SER:O	2:A:357:SER:OG	2.34	0.46
9:G:477:VAL:HG21	9:G:512:THR:HG21	1.97	0.46
12:L:1354:LEU:CA	12:L:1357:LEU:HD22	2.43	0.46
12:L:2425:GLY:HA2	12:L:2428:LEU:HD23	1.98	0.46
12:L:2812:LEU:HD11	12:L:2862:SER:HB2	1.97	0.46
8:K:465:ARG:O	12:L:2829:LYS:HE2	2.16	0.46
8:K:588:GLN:NE2	8:K:589:PRO:O	2.45	0.46
12:L:853:LEU:HD23	12:L:853:LEU:H	1.80	0.46
12:L:934:ARG:H	12:L:934:ARG:HG2	1.55	0.46
12:L:606:GLU:HB2	12:L:1694:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:78:LYS:CE	5:D:78:LYS:O	2.64	0.46
10:H:234:ASN:OD1	10:H:235:GLN:NE2	2.49	0.46
12:L:3434:GLY:HA3	12:L:3525:ILE:HD12	1.97	0.46
12:L:3602:SER:OG	12:L:3603:THR:N	2.48	0.46
1:M:117:ALA:C	1:M:119:GLY:H	2.19	0.46
9:G:642:ALA:O	10:H:68:ARG:NH2	2.49	0.46
10:H:69:THR:O	10:H:71:HIS:ND1	2.47	0.46
12:L:2901:ASN:O	12:L:2905:THR:HG22	2.16	0.46
5:D:66:VAL:CG1	5:D:67:PRO:CD	2.84	0.46
8:K:469:LEU:HB3	12:L:2788:ILE:HG22	1.97	0.46
12:L:2807:GLN:HB3	12:L:2809:LYS:HE3	1.98	0.46
1:M:172:LEU:HB2	5:D:204:TYR:CE2	2.52	0.45
5:D:17:ILE:N	5:D:17:ILE:CD1	2.79	0.45
7:J:58:THR:N	7:J:61:GLU:OE2	2.49	0.45
9:G:709:THR:HG22	9:G:710:ARG:H	1.80	0.45
12:L:828:ARG:N	12:L:829:PRO:CD	2.57	0.45
12:L:1608:VAL:O	12:L:1617:ARG:NH2	2.49	0.45
3:C:290:SER:OG	3:C:291:ARG:N	2.49	0.45
12:L:2807:GLN:HB3	12:L:2809:LYS:HG3	1.97	0.45
12:L:3458:LEU:H	12:L:3458:LEU:CD2	2.28	0.45
5:D:76:HIS:O	5:D:78:LYS:N	2.49	0.45
7:J:98:ARG:O	7:J:101:ALA:HB3	2.16	0.45
12:L:827:ARG:HH21	12:L:829:PRO:HB3	1.80	0.45
12:L:1136:ASN:HB3	12:L:1139:VAL:HG12	1.96	0.45
12:L:2807:GLN:OE1	12:L:2807:GLN:HA	2.16	0.45
5:D:239:ASP:HA	5:D:242:ILE:HD12	1.97	0.45
8:K:462:ILE:HG23	8:K:463:PRO:HD3	1.98	0.45
1:M:166:VAL:HG22	1:M:210:GLY:O	2.17	0.45
8:K:562:GLN:CD	8:K:577:ALA:HB3	2.36	0.45
12:L:1916:ASP:OD1	12:L:1916:ASP:N	2.49	0.45
4:F:326:ARG:HD3	12:L:2751:LEU:HD21	1.97	0.45
10:H:17:TRP:HZ3	11:I:15:LEU:HD21	1.81	0.45
12:L:854:SER:C	12:L:856:LEU:N	2.69	0.45
12:L:1418:VAL:O	12:L:1422:VAL:HG13	2.17	0.45
9:G:460:ASP:O	9:G:468:LEU:HD12	2.17	0.45
9:G:546:HIS:NE2	9:G:591:GLY:HA2	2.32	0.45
9:G:594:LEU:CG	9:G:606:TRP:HB2	2.45	0.45
12:L:3461:GLY:N	12:L:3464:GLY:O	2.50	0.45
1:M:124:THR:CG2	1:M:125:GLY:N	2.80	0.45
1:M:189:LEU:HD13	5:D:84:LEU:HD22	1.98	0.45
8:K:465:ARG:HG3	12:L:2844:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:697:PHE:O	10:H:147:GLN:NE2	2.50	0.45
12:L:962:LEU:HG	12:L:2572:ALA:HB2	1.98	0.45
12:L:1543:PRO:O	12:L:1547:HIS:NE2	2.49	0.45
12:L:3494:GLU:HA	12:L:3497:ILE:HG12	1.99	0.45
1:M:135:ALA:O	1:M:139:TYR:CD2	2.70	0.45
5:D:27:THR:HG22	5:D:28:ASN:H	1.81	0.45
9:G:632:ARG:NH1	9:G:708:PHE:O	2.46	0.45
12:L:2708:LEU:HD21	12:L:3793:SER:HB2	1.98	0.45
12:L:2745:TRP:O	12:L:2749:THR:OG1	2.35	0.45
8:K:437:LEU:H	8:K:437:LEU:CD2	2.28	0.45
9:G:107:ILE:HD11	9:G:140:CYS:HB2	1.99	0.45
2:A:342:TYR:HD1	2:A:344:TYR:HH	1.64	0.44
4:F:305:SER:O	8:K:452:VAL:HG21	2.16	0.44
6:E:946:LYS:N	6:E:946:LYS:CD	2.79	0.44
9:G:450:VAL:HG22	9:G:451:GLY:N	2.29	0.44
8:K:465:ARG:HD3	8:K:465:ARG:H	1.83	0.44
12:L:271:ILE:O	12:L:275:VAL:N	2.48	0.44
12:L:854:SER:O	12:L:856:LEU:N	2.50	0.44
12:L:1425:PHE:C	12:L:1427:SER:N	2.70	0.44
12:L:1780:TYR:HA	12:L:1783:ILE:HG22	1.99	0.44
12:L:1876:ASP:OD1	12:L:1876:ASP:N	2.51	0.44
12:L:2539:THR:HG23	12:L:2541:GLY:H	1.83	0.44
9:G:371:LEU:HD12	9:G:372:SER:H	1.83	0.44
9:G:544:GLU:HG2	9:G:553:PHE:HB2	1.98	0.44
12:L:214:TYR:O	12:L:218:ALA:N	2.49	0.44
12:L:1340:CYS:HA	12:L:1343:LEU:HD13	1.98	0.44
12:L:2804:GLY:O	12:L:2809:LYS:N	2.50	0.44
12:L:3725:TYR:HA	12:L:3728:VAL:HG12	1.98	0.44
9:G:192:ILE:O	9:G:195:SER:OG	2.31	0.44
12:L:3172:GLN:O	12:L:3175:THR:OG1	2.34	0.44
8:K:465:ARG:O	12:L:2791:PRO:HG3	2.18	0.44
9:G:63:GLU:OE1	9:G:64:SER:OG	2.31	0.44
9:G:215:ASN:OD1	9:G:216:GLU:N	2.50	0.44
9:G:352:ALA:O	9:G:356:ARG:N	2.46	0.44
9:G:504:SER:OG	9:G:507:GLY:N	2.44	0.44
12:L:1610:LEU:O	12:L:1617:ARG:NH2	2.51	0.44
6:E:946:LYS:HD2	6:E:946:LYS:H	1.82	0.44
9:G:618:ARG:HD3	9:G:689:THR:HG21	2.00	0.44
12:L:1623:SER:OG	12:L:1626:ARG:NE	2.51	0.44
12:L:2393:SER:HA	12:L:2396:PHE:HB3	1.99	0.44
12:L:2446:GLU:O	12:L:2452:ARG:NE	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:CYS:SG	1:M:80:LEU:HD11	2.57	0.44
5:D:24:SER:HB3	5:D:210:CYS:CB	2.48	0.44
12:L:1356:ARG:N	12:L:1356:ARG:NE	2.65	0.44
12:L:1358:VAL:O	12:L:1359:GLN:C	2.56	0.44
12:L:1727:LYS:HD2	12:L:1734:PRO:HG3	1.99	0.44
9:G:138:VAL:O	9:G:142:LEU:HD23	2.18	0.44
9:G:596:SER:OG	9:G:604:CYS:HB2	2.18	0.44
12:L:404:ALA:HB3	12:L:407:VAL:HG22	1.99	0.44
12:L:1358:VAL:O	12:L:1360:GLU:N	2.51	0.44
12:L:3522:THR:O	12:L:3522:THR:OG1	2.33	0.44
8:K:461:LYS:HZ2	12:L:2792:ARG:NE	2.16	0.44
9:G:74:PRO:HB3	9:G:610:THR:CG2	2.47	0.44
12:L:722:LYS:HG2	12:L:768:LEU:HD21	2.00	0.44
12:L:2437:LEU:HA	12:L:2440:ILE:HD12	2.00	0.44
12:L:2897:ILE:HD12	12:L:2897:ILE:HA	1.86	0.44
1:M:76:LEU:O	1:M:78:CYS:N	2.51	0.43
6:E:880:LYS:C	6:E:881:LEU:HD12	2.38	0.43
8:K:461:LYS:HD2	12:L:2762:LEU:HD11	1.99	0.43
8:K:557:ASP:OD1	8:K:557:ASP:N	2.46	0.43
1:M:126:ALA:HB3	1:M:132:SER:OG	2.19	0.43
5:D:259:GLU:HA	5:D:262:ILE:HD12	2.00	0.43
12:L:408:GLN:OE1	12:L:445:ARG:NH1	2.39	0.43
12:L:850:VAL:N	12:L:851:PRO:CD	2.82	0.43
12:L:2860:VAL:HG13	12:L:2879:LEU:CD1	2.49	0.43
12:L:3151:ALA:HA	12:L:3154:VAL:HG12	2.01	0.43
1:M:79:ARG:O	1:M:80:LEU:HD12	2.17	0.43
5:D:215:PHE:HB3	5:D:223:PHE:HB2	2.01	0.43
8:K:452:VAL:O	12:L:2666:GLU:OE2	2.36	0.43
8:K:469:LEU:CD2	12:L:2790:THR:CG2	2.96	0.43
10:H:318:ALA:HB3	10:H:337:ARG:NH1	2.32	0.43
12:L:801:PHE:HD1	12:L:803:ASN:H	1.66	0.43
12:L:850:VAL:HG13	12:L:853:LEU:HD13	1.99	0.43
12:L:3765:GLN:HB3	12:L:3768:GLN:HB3	2.00	0.43
1:M:200:PRO:HD3	1:M:225:GLN:OE1	2.18	0.43
5:D:321:VAL:HG12	5:D:321:VAL:O	2.17	0.43
8:K:469:LEU:HD23	8:K:469:LEU:N	2.33	0.43
12:L:773:LEU:HD13	12:L:815:LEU:HD13	2.00	0.43
12:L:3541:ARG:HB2	12:L:3654:GLU:HB2	2.01	0.43
5:D:71:ILE:HD12	5:D:74:ILE:HD11	2.01	0.43
12:L:2741:LYS:NZ	12:L:2896:ASP:OD1	2.52	0.43
12:L:3099:THR:HG22	12:L:3103:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:3285:ASP:OD1	12:L:3285:ASP:N	2.48	0.43
12:L:2523:ASP:OD1	12:L:2523:ASP:N	2.42	0.43
4:F:204:GLN:OE1	4:F:204:GLN:HA	2.19	0.43
5:D:17:ILE:HG22	5:D:21:MET:SD	2.59	0.43
5:D:207:TRP:CD1	5:D:207:TRP:C	2.91	0.43
7:J:206:TYR:HB3	7:J:207:GLY:H	1.71	0.43
9:G:92:THR:OG1	9:G:93:ALA:N	2.51	0.43
12:L:560:ASP:N	12:L:560:ASP:OD1	2.51	0.43
12:L:1204:ASP:OD1	12:L:1204:ASP:N	2.52	0.43
12:L:1690:SER:O	12:L:1690:SER:OG	2.32	0.43
12:L:2447:LEU:HD23	12:L:2447:LEU:HA	1.89	0.43
1:M:177:PHE:CB	5:D:194:GLU:HA	2.49	0.43
2:A:243:MET:CB	2:A:268:ILE:HD12	2.49	0.43
6:E:883:SER:O	6:E:886:SER:OG	2.28	0.43
12:L:1884:ALA:HA	12:L:1887:VAL:HG12	2.00	0.43
12:L:1967:ILE:HD12	12:L:1967:ILE:HA	1.91	0.43
5:D:319:ARG:HD2	5:D:319:ARG:HA	1.65	0.42
6:E:885:VAL:HG13	10:H:128:PRO:HG2	2.01	0.42
6:E:929:LEU:CD1	6:E:955:ILE:HG22	2.49	0.42
6:E:950:VAL:O	6:E:950:VAL:HG23	2.19	0.42
12:L:1317:ILE:HD11	12:L:1333:ASN:HA	2.01	0.42
12:L:1357:LEU:N	12:L:1357:LEU:CD1	2.81	0.42
12:L:1736:VAL:HG13	12:L:1737:LEU:HD23	2.01	0.42
12:L:1060:LYS:HD2	12:L:1060:LYS:HA	1.72	0.42
12:L:1786:PRO:HA	12:L:1789:ILE:HG12	2.01	0.42
12:L:2805:PHE:HA	12:L:2810:ASP:O	2.19	0.42
5:D:240:ASP:OD1	5:D:241:VAL:N	2.52	0.42
9:G:581:ALA:O	9:G:582:ILE:HD13	2.19	0.42
10:H:122:LEU:HD12	10:H:123:ILE:HB	2.00	0.42
10:H:129:LYS:NZ	10:H:129:LYS:CB	2.82	0.42
10:H:129:LYS:HZ3	10:H:129:LYS:CB	2.31	0.42
12:L:1226:ARG:NH2	12:L:1275:ASP:OD2	2.52	0.42
12:L:1354:LEU:O	12:L:1357:LEU:HB2	2.19	0.42
12:L:2601:ARG:NE	12:L:2601:ARG:CA	2.81	0.42
2:A:183:GLU:O	2:A:184:SER:OG	2.26	0.42
8:K:581:ILE:HD12	11:I:52:ILE:HD11	2.01	0.42
10:H:317:LEU:HD12	10:H:318:ALA:N	2.34	0.42
12:L:848:VAL:O	12:L:851:PRO:HD2	2.19	0.42
12:L:1541:LEU:HD12	12:L:1541:LEU:HA	1.93	0.42
12:L:3173:LEU:HD21	12:L:3293:LEU:HD22	2.02	0.42
5:D:22:PHE:HE2	5:D:30:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:817:GLY:O	6:E:820:LYS:N	2.52	0.42
8:K:437:LEU:HD23	8:K:437:LEU:N	2.32	0.42
12:L:846:LEU:CA	12:L:850:VAL:HB	2.45	0.42
12:L:907:LYS:HE3	12:L:907:LYS:HB3	1.83	0.42
12:L:3111:SER:O	12:L:3111:SER:OG	2.33	0.42
9:G:416:LEU:N	9:G:447:ARG:O	2.52	0.42
10:H:242:GLU:OE1	10:H:242:GLU:N	2.52	0.42
12:L:1356:ARG:NE	12:L:1356:ARG:CA	2.82	0.42
12:L:1417:ARG:HH21	12:L:1417:ARG:HG3	1.85	0.42
12:L:2422:PHE:HE2	12:L:2441:LEU:HD22	1.85	0.42
12:L:2889:ARG:O	12:L:2889:ARG:HG2	2.20	0.42
3:C:288:LEU:CD2	3:C:292:THR:HG21	2.48	0.42
5:D:72:PHE:HD1	5:D:72:PHE:HA	1.70	0.42
12:L:1727:LYS:O	12:L:1776:ARG:NH2	2.53	0.42
1:M:186:GLU:HB3	1:M:189:LEU:HB2	2.01	0.42
5:D:244:ILE:O	5:D:248:LEU:HG	2.20	0.42
6:E:947:PHE:HE1	6:E:949:LYS:HA	1.85	0.42
7:J:116:TYR:OH	7:J:120:ARG:NH2	2.53	0.42
8:K:582:ARG:NH1	11:I:71:GLY:O	2.52	0.42
10:H:315:LEU:O	10:H:318:ALA:HB2	2.20	0.42
12:L:2476:GLN:HG2	12:L:2548:ILE:HD12	2.02	0.42
12:L:2592:ASP:OD1	12:L:2592:ASP:N	2.53	0.42
12:L:2740:GLU:HB2	12:L:2745:TRP:CH2	2.55	0.42
1:M:187:PRO:HB3	5:D:211:ARG:HB2	2.02	0.42
2:A:204:LYS:HA	3:C:293:ALA:HB3	2.02	0.42
2:A:250:MET:O	2:A:253:ILE:N	2.52	0.42
3:C:253:ARG:NH2	10:H:49:TYR:OH	2.51	0.42
10:H:67:ARG:NH2	10:H:74:ASP:OD1	2.53	0.42
12:L:1863:LYS:HA	12:L:1863:LYS:HD2	1.78	0.42
2:A:259:LEU:HD21	8:K:549:LYS:HB2	2.02	0.41
9:G:600:ASP:OD1	9:G:601:SER:N	2.53	0.41
11:I:24:ILE:O	11:I:26:SER:N	2.51	0.41
12:L:328:ARG:HH11	12:L:370:THR:HG22	1.84	0.41
12:L:3149:LYS:HD3	12:L:3149:LYS:HA	1.89	0.41
6:E:930:LYS:O	6:E:934:GLU:HG2	2.21	0.41
9:G:144:LEU:HD22	9:G:156:PHE:CE2	2.56	0.41
9:G:450:VAL:HG13	9:G:451:GLY:N	2.35	0.41
10:H:155:SER:OG	10:H:157:ASN:OD1	2.36	0.41
12:L:718:ILE:HD12	12:L:718:ILE:HA	1.95	0.41
12:L:3634:ILE:HD12	12:L:3703:PHE:HB2	2.02	0.41
1:M:74:VAL:HG23	1:M:155:PHE:CA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:442:PRO:HB3	12:L:2817:ARG:NH1	2.35	0.41
8:K:469:LEU:CD2	12:L:2790:THR:HG23	2.50	0.41
9:G:515:HIS:NE2	10:H:57:GLN:OE1	2.53	0.41
9:G:585:LEU:HA	9:G:595:ALA:O	2.21	0.41
10:H:69:THR:HG23	10:H:71:HIS:HE1	1.84	0.41
12:L:764:HIS:NE2	12:L:1525:ASN:OD1	2.37	0.41
12:L:3603:THR:HG22	12:L:3711:LYS:HG2	2.01	0.41
2:A:223:GLN:OE1	2:A:223:GLN:CA	2.68	0.41
12:L:1444:LYS:HE3	12:L:1444:LYS:HB2	1.80	0.41
12:L:2798:THR:HA	12:L:2818:LEU:HD23	2.02	0.41
12:L:3705:LEU:HD12	12:L:3705:LEU:HA	1.95	0.41
1:M:146:ILE:O	1:M:147:GLY:C	2.58	0.41
8:K:466:PRO:HA	12:L:2791:PRO:CG	2.23	0.41
9:G:709:THR:HG22	9:G:710:ARG:N	2.35	0.41
1:M:185:TYR:HD2	5:D:204:TYR:HH	1.64	0.41
1:M:189:LEU:CD1	5:D:84:LEU:HD13	2.49	0.41
6:E:934:GLU:O	6:E:936:LYS:N	2.45	0.41
8:K:454:PRO:CD	8:K:455:PRO:HD2	2.50	0.41
9:G:460:ASP:OD1	9:G:461:PHE:N	2.54	0.41
12:L:388:TRP:HA	12:L:391:VAL:HG12	2.03	0.41
12:L:1587:SER:OG	12:L:1588:PHE:N	2.53	0.41
12:L:3133:TRP:CZ3	12:L:3441:ASP:HB3	2.56	0.41
1:M:84:THR:O	1:M:87:LEU:HB2	2.20	0.41
2:A:268:ILE:O	2:A:272:LEU:HD23	2.20	0.41
9:G:365:SER:O	9:G:370:LYS:N	2.49	0.41
9:G:563:MET:HE3	9:G:608:ILE:HD13	2.03	0.41
10:H:129:LYS:NZ	10:H:129:LYS:CA	2.82	0.41
12:L:268:GLY:O	12:L:272:ILE:N	2.53	0.41
12:L:672:PRO:O	12:L:676:ASN:ND2	2.54	0.41
12:L:1629:GLY:HA2	12:L:1632:HIS:HD2	1.86	0.41
12:L:2794:GLN:HG2	12:L:2822:GLY:HA3	2.02	0.41
1:M:231:TYR:HB3	1:M:232:PRO:HD3	2.03	0.41
8:K:469:LEU:HD22	12:L:2790:THR:HG23	2.03	0.41
12:L:1295:SER:OG	12:L:1305:MET:SD	2.68	0.41
12:L:3136:ILE:HA	12:L:3139:VAL:HG23	2.03	0.41
2:A:242:GLU:O	2:A:243:MET:C	2.58	0.41
4:F:133:VAL:HG23	4:F:134:GLN:CD	2.41	0.41
9:G:648:VAL:HG13	9:G:694:SER:H	1.86	0.41
9:G:701:THR:O	9:G:701:THR:OG1	2.39	0.41
10:H:396:ILE:HG23	10:H:397:ARG:N	2.36	0.41
11:I:51:THR:HG22	11:I:76:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:314:SER:O	12:L:314:SER:OG	2.33	0.41
12:L:853:LEU:H	12:L:853:LEU:CD2	2.34	0.41
12:L:858:LYS:HB2	12:L:858:LYS:HE3	1.87	0.41
12:L:1540:HIS:O	12:L:1582:ARG:NH2	2.54	0.41
12:L:2465:LEU:H	12:L:2465:LEU:HG	1.71	0.41
12:L:2778:LEU:HD23	12:L:2778:LEU:HA	1.96	0.41
12:L:3142:LEU:HB3	12:L:3158:LEU:HD11	2.03	0.41
10:H:335:ALA:O	10:H:339:LEU:HD23	2.20	0.41
1:M:105:ARG:O	1:M:106:ILE:CG2	2.69	0.40
1:M:115:ILE:HD13	1:M:121:MET:CG	2.51	0.40
2:A:199:GLN:NE2	3:C:305:PHE:O	2.54	0.40
8:K:460:MET:HG3	12:L:2758:THR:CG2	2.51	0.40
12:L:325:HIS:HA	12:L:328:ARG:HB3	2.03	0.40
12:L:1358:VAL:HG22	12:L:1359:GLN:N	2.36	0.40
12:L:1506:LEU:HA	12:L:1509:TRP:HD1	1.86	0.40
12:L:2231:ILE:O	12:L:2235:VAL:N	2.53	0.40
12:L:2721:PHE:HA	12:L:2722:PRO:HD3	1.90	0.40
12:L:3604:LEU:HD12	12:L:3604:LEU:HA	1.93	0.40
12:L:2687:TYR:HB2	12:L:2690:THR:HG22	2.02	0.40
12:L:2817:ARG:HA	12:L:2817:ARG:HD2	1.91	0.40
12:L:2907:ARG:HH11	12:L:2907:ARG:CG	2.25	0.40
12:L:3798:THR:HB	12:L:3801:VAL:HG22	2.04	0.40
1:M:78:CYS:SG	1:M:80:LEU:CD1	3.10	0.40
4:F:85:PHE:N	4:F:143:ARG:O	2.46	0.40
6:E:944:ASP:OD1	6:E:944:ASP:N	2.54	0.40
9:G:588:SER:HB3	9:G:593:TRP:HB2	2.04	0.40
10:H:127:LEU:HD12	10:H:127:LEU:C	2.39	0.40
10:H:217:LEU:HB2	10:H:221:LEU:HD22	2.02	0.40
12:L:833:ASP:HA	12:L:836:VAL:HG12	2.03	0.40
12:L:1611:ASP:OD1	12:L:1611:ASP:N	2.53	0.40
5:D:84:LEU:HA	5:D:87:TYR:CD2	2.56	0.40
8:K:461:LYS:HE2	8:K:463:PRO:HD2	2.03	0.40
9:G:45:ASP:OD1	9:G:45:ASP:N	2.55	0.40
12:L:2783:LYS:HA	12:L:2783:LYS:HD3	1.74	0.40
12:L:3063:GLY:O	12:L:3067:ASP:N	2.47	0.40
1:M:85:VAL:HG11	1:M:143:ILE:HG22	2.04	0.40
9:G:182:GLU:OE1	9:G:182:GLU:N	2.49	0.40
12:L:3778:GLU:HA	12:L:3781:THR:HG22	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	M	178/243 (73%)	147 (83%)	24 (14%)	7 (4%)	3 28
2	A	169/448 (38%)	151 (89%)	18 (11%)	0	100 100
3	C	61/698 (9%)	56 (92%)	5 (8%)	0	100 100
4	F	202/517 (39%)	177 (88%)	24 (12%)	1 (0%)	29 66
5	D	203/341 (60%)	177 (87%)	19 (9%)	7 (3%)	3 31
6	E	150/1191 (13%)	135 (90%)	13 (9%)	2 (1%)	12 48
7	J	92/217 (42%)	82 (89%)	9 (10%)	1 (1%)	14 51
8	K	150/609 (25%)	125 (83%)	23 (15%)	2 (1%)	12 48
9	G	512/722 (71%)	448 (88%)	63 (12%)	1 (0%)	47 79
10	H	413/485 (85%)	365 (88%)	48 (12%)	0	100 100
11	I	119/153 (78%)	98 (82%)	21 (18%)	0	100 100
12	L	2874/3825 (75%)	2623 (91%)	233 (8%)	18 (1%)	25 62
All	All	5123/9449 (54%)	4584 (90%)	500 (10%)	39 (1%)	24 57

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	77	GLY
1	M	99	PHE
1	M	110	LYS
5	D	200	THR
5	D	327	ARG
6	E	935	SER
8	K	459	ALA
12	L	66	VAL
12	L	204	PRO
12	L	828	ARG
12	L	854	SER
12	L	855	TYR

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Mol	Chain	Res	Type
12	L	1425	PHE
12	L	1426	LYS
12	L	2602	PRO
12	L	3428	GLU
12	L	3797	ALA
1	M	97	LYS
1	M	147	GLY
1	M	150	ALA
5	D	219	LYS
5	D	330	GLN
7	J	206	TYR
9	G	450	VAL
12	L	826	ALA
12	L	2597	GLN
1	M	201	LYS
5	D	77	ASP
6	E	941	VAL
12	L	1774	ASP
12	L	3460	ARG
8	K	442	PRO
12	L	2594	HIS
12	L	3439	HIS
4	F	80	PRO
5	D	218	ARG
12	L	3616	TYR
12	L	1359	GLN
5	D	321	VAL

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	M	152/208 (73%)	138 (91%)	14 (9%)	9 35
2	A	134/394 (34%)	132 (98%)	2 (2%)	65 81
3	C	55/627 (9%)	55 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	179/471 (38%)	179 (100%)	0	100	100
5	D	166/306 (54%)	154 (93%)	12 (7%)	14	45
6	E	142/1101 (13%)	136 (96%)	6 (4%)	30	58
7	J	85/183 (46%)	84 (99%)	1 (1%)	71	84
8	K	133/524 (25%)	130 (98%)	3 (2%)	50	72
9	G	439/635 (69%)	430 (98%)	9 (2%)	53	74
10	H	352/438 (80%)	348 (99%)	4 (1%)	73	85
11	I	104/130 (80%)	103 (99%)	1 (1%)	76	86
12	L	2156/3450 (62%)	2114 (98%)	42 (2%)	57	76
All	All	4097/8467 (48%)	4003 (98%)	94 (2%)	53	72

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	67	LEU
1	M	76	LEU
1	M	97	LYS
1	M	104	MET
1	M	141	ARG
1	M	148	PHE
1	M	153	THR
1	M	175	LEU
1	M	181	THR
1	M	185	TYR
1	M	202	ILE
1	M	215	THR
1	M	231	TYR
1	M	240	MET
2	A	229	PHE
2	A	291	LYS
5	D	18	GLN
5	D	74	ILE
5	D	78	LYS
5	D	83	ARG
5	D	85	ARG
5	D	87	TYR
5	D	211	ARG
5	D	212	GLN
5	D	218	ARG

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Mol	Chain	Res	Type
5	D	322	GLU
5	D	329	PHE
5	D	338	VAL
6	E	933	ILE
6	E	940	LYS
6	E	942	MET
6	E	946	LYS
6	E	948	GLN
6	E	949	LYS
7	J	205	GLU
8	K	437	LEU
8	K	449	ARG
8	K	465	ARG
9	G	115	LYS
9	G	194	ARG
9	G	230	ASN
9	G	452	HIS
9	G	537	LEU
9	G	542	CYS
9	G	560	THR
9	G	571	CYS
9	G	594	LEU
10	H	129	LYS
10	H	217	LEU
10	H	360	PRO
10	H	364	ARG
11	I	16	HIS
12	L	429	THR
12	L	800	ARG
12	L	849	LEU
12	L	852	HIS
12	L	971	THR
12	L	1122	ASN
12	L	1278	ASN
12	L	1314	LEU
12	L	1323	ARG
12	L	1356	ARG
12	L	1358	VAL
12	L	1413	ARG
12	L	1417	ARG
12	L	1419	LYS
12	L	1424	PHE

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Mol	Chain	Res	Type
12	L	1548	LYS
12	L	1665	LYS
12	L	1680	LEU
12	L	2427	ARG
12	L	2489	ARG
12	L	2595	ILE
12	L	2633	ASN
12	L	2807	GLN
12	L	2878	GLU
12	L	2880	LYS
12	L	2881	ARG
12	L	2883	LEU
12	L	2884	GLN
12	L	2887	ARG
12	L	2888	GLU
12	L	2907	ARG
12	L	2913	VAL
12	L	2914	ILE
12	L	2916	ARG
12	L	3314	ARG
12	L	3426	LYS
12	L	3440	LYS
12	L	3441	ASP
12	L	3489	ARG
12	L	3502	ARG
12	L	3542	TYR
12	L	3646	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	91	ASN
1	M	95	ASN
1	M	179	HIS
2	A	227	HIS
5	D	212	GLN
5	D	317	GLN
9	G	391	ASN
10	H	64	HIS
10	H	157	ASN
10	H	306	HIS
12	L	1632	HIS

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Continued from previous page...

Mol	Chain	Res	Type
12	L	2633	ASN
12	L	2698	GLN
12	L	2884	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	B	2
1	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	414:UNK	C	462:UNK	N	28.86
1	B	471:UNK	C	509:UNK	N	23.98
1	M	194:ILE	C	195:TYR	N	1.97

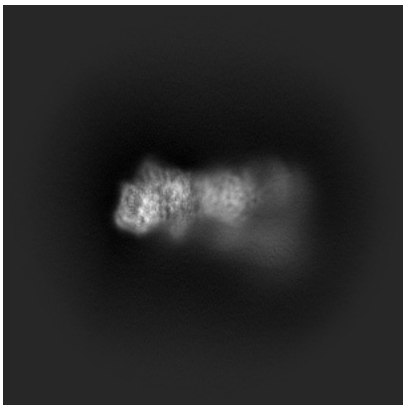
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10438. These allow visual inspection of the internal detail of the map and identification of artifacts.

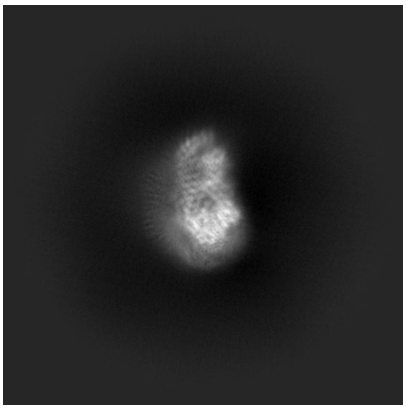
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

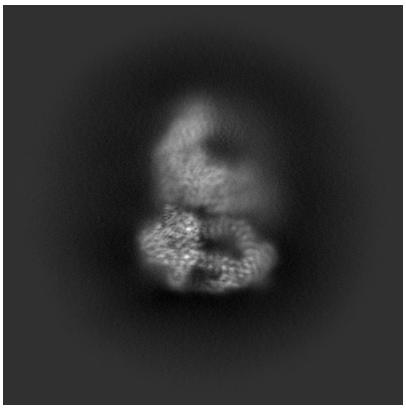
6.1.1 Primary map



X

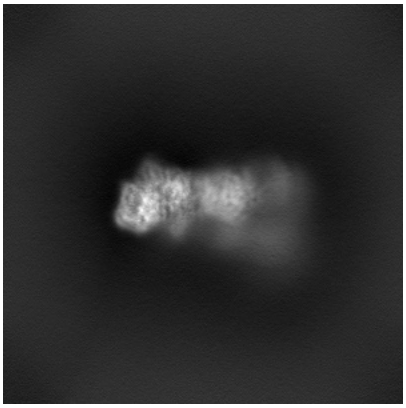


Y

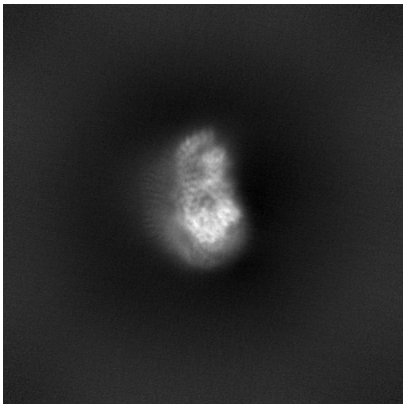


Z

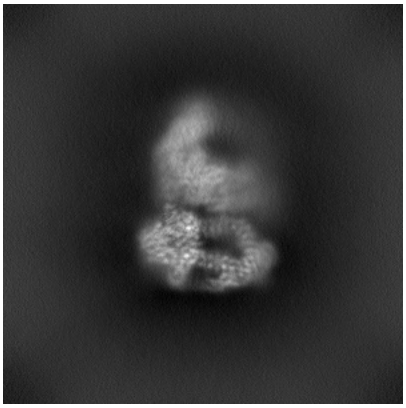
6.1.2 Raw map



X



Y

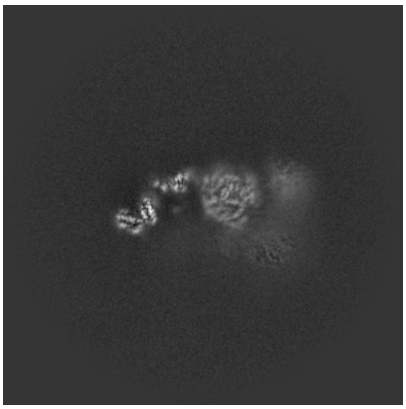


Z

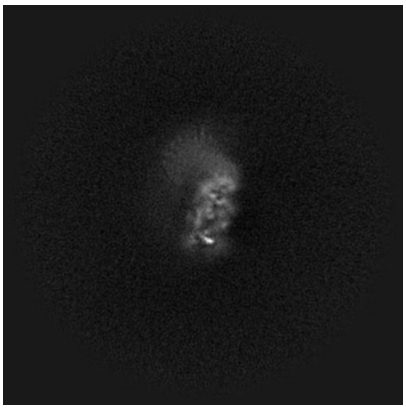
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

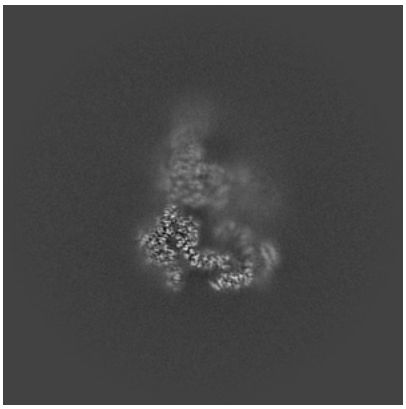
6.2.1 Primary map



X Index: 256

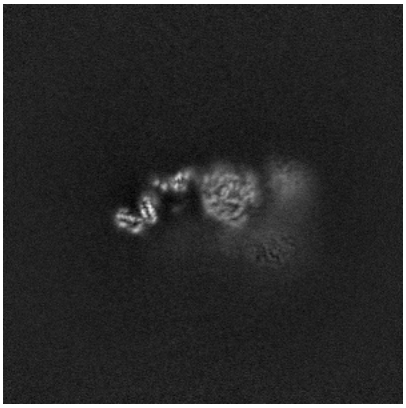


Y Index: 256

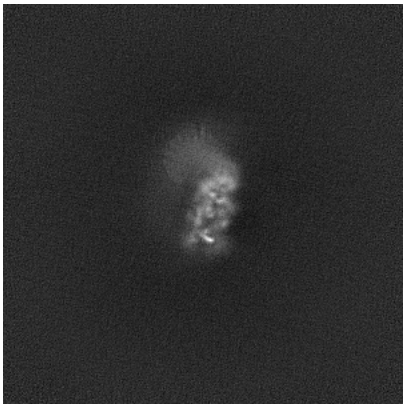


Z Index: 256

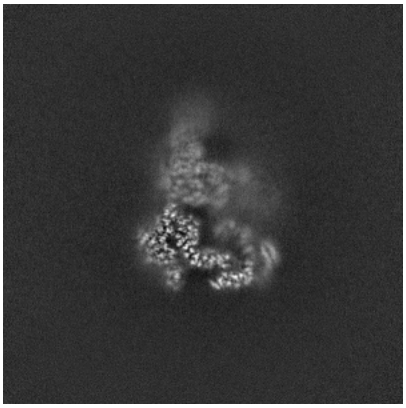
6.2.2 Raw map



X Index: 256



Y Index: 256

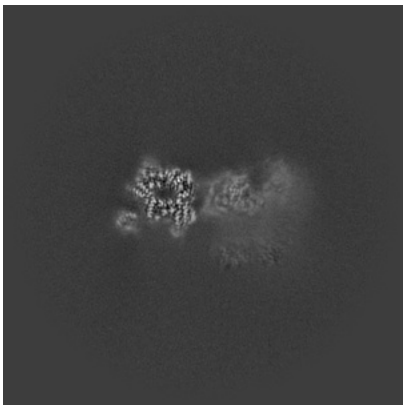


Z Index: 256

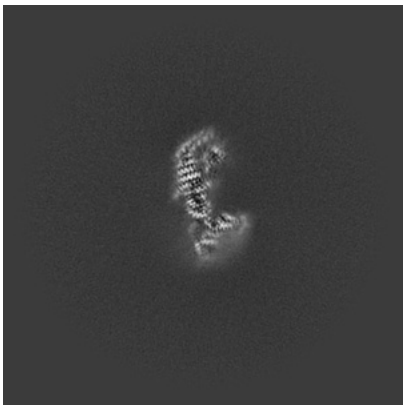
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

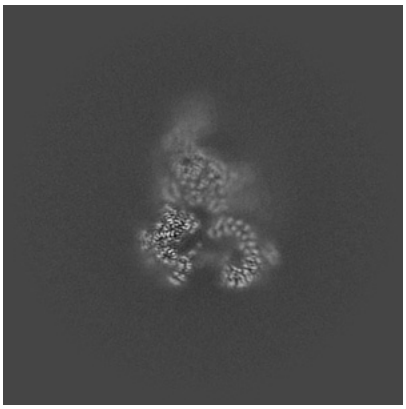
6.3.1 Primary map



X Index: 236

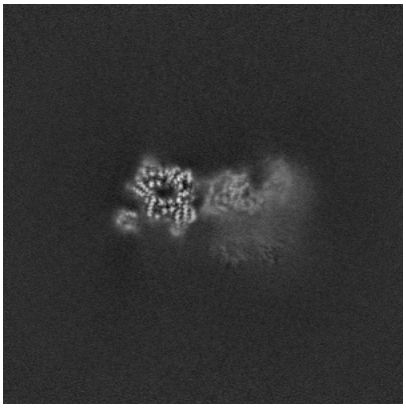


Y Index: 182

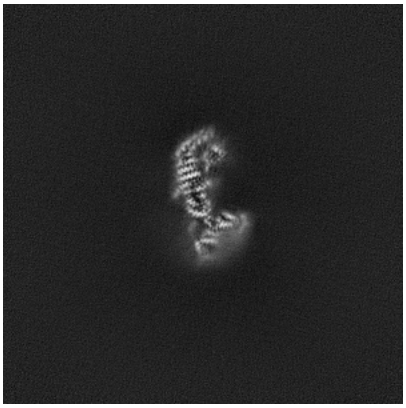


Z Index: 268

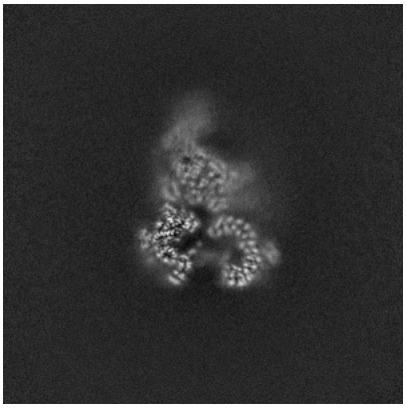
6.3.2 Raw map



X Index: 236



Y Index: 182

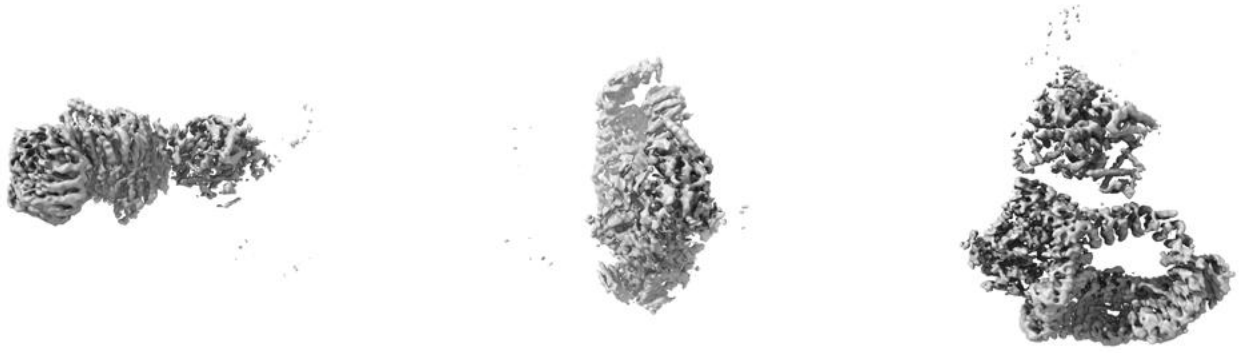


Z Index: 268

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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.

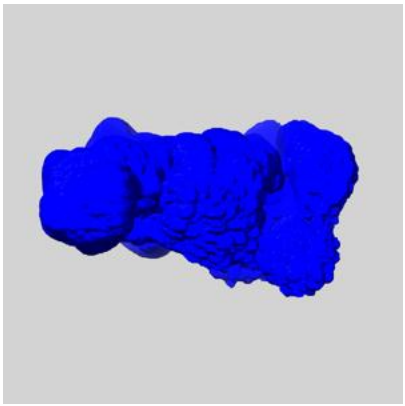
6.5 Mask visualisation (i)

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

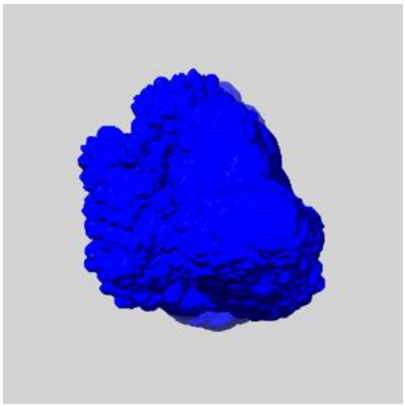
A mask typically either:

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

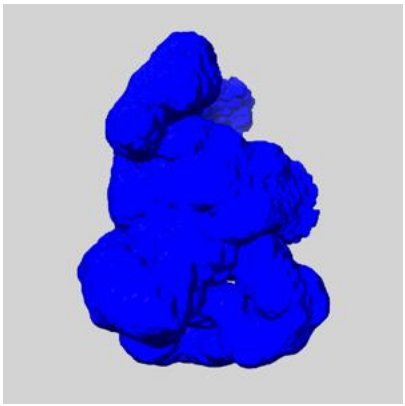
6.5.1 emd_10438_msk_1.map (i)



X



Y

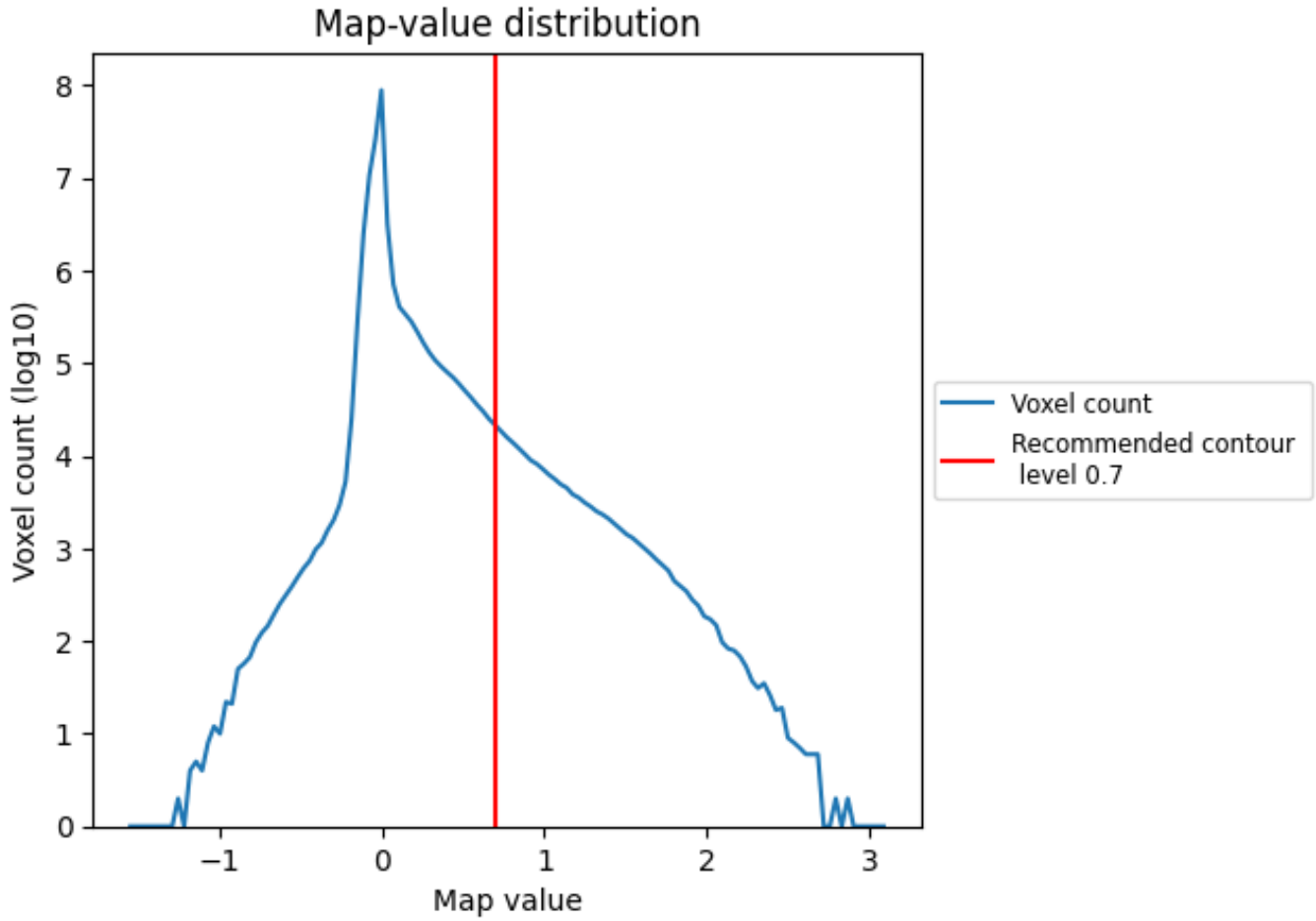


Z

7 Map analysis

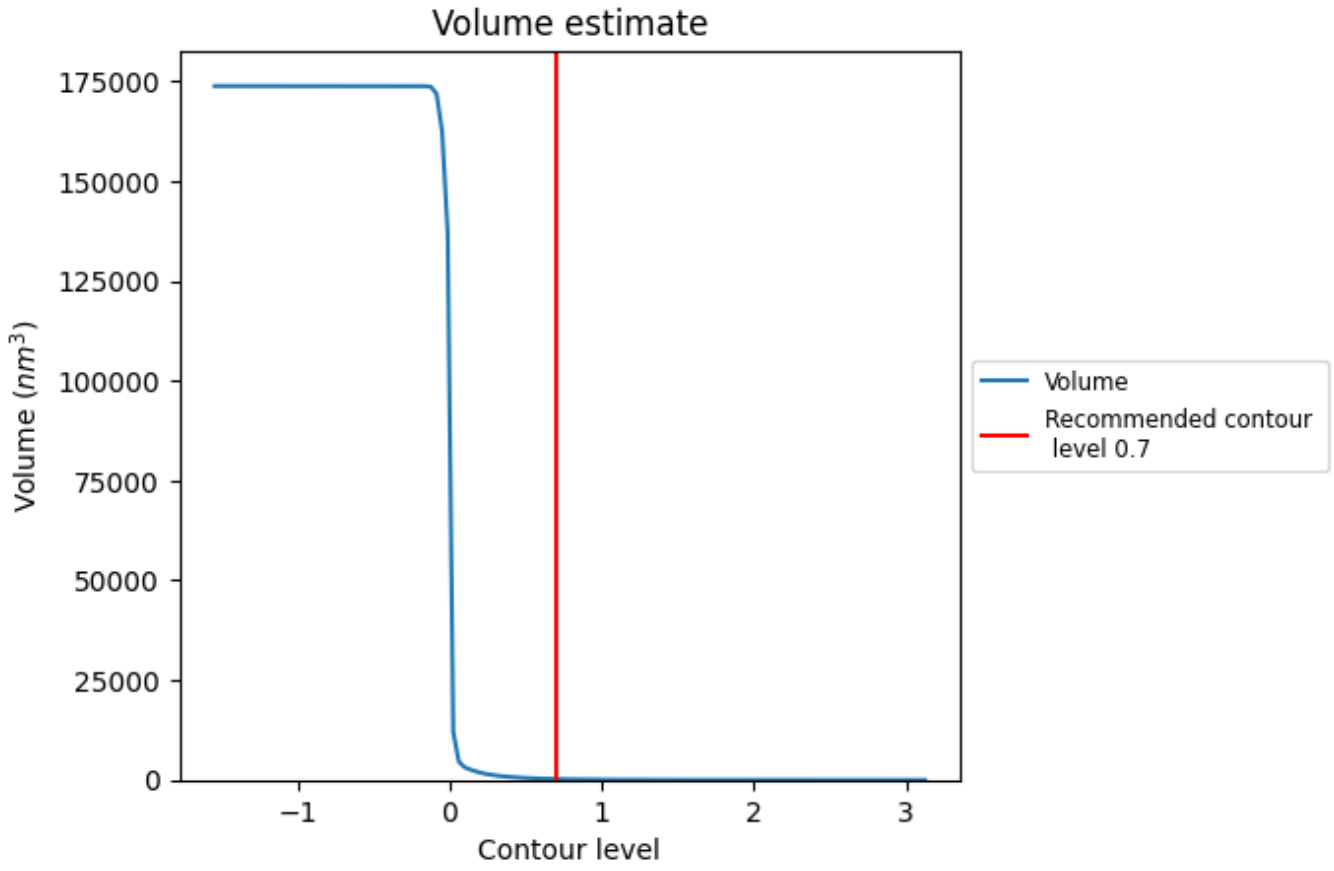
This section contains the results of statistical analysis of the map.

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.

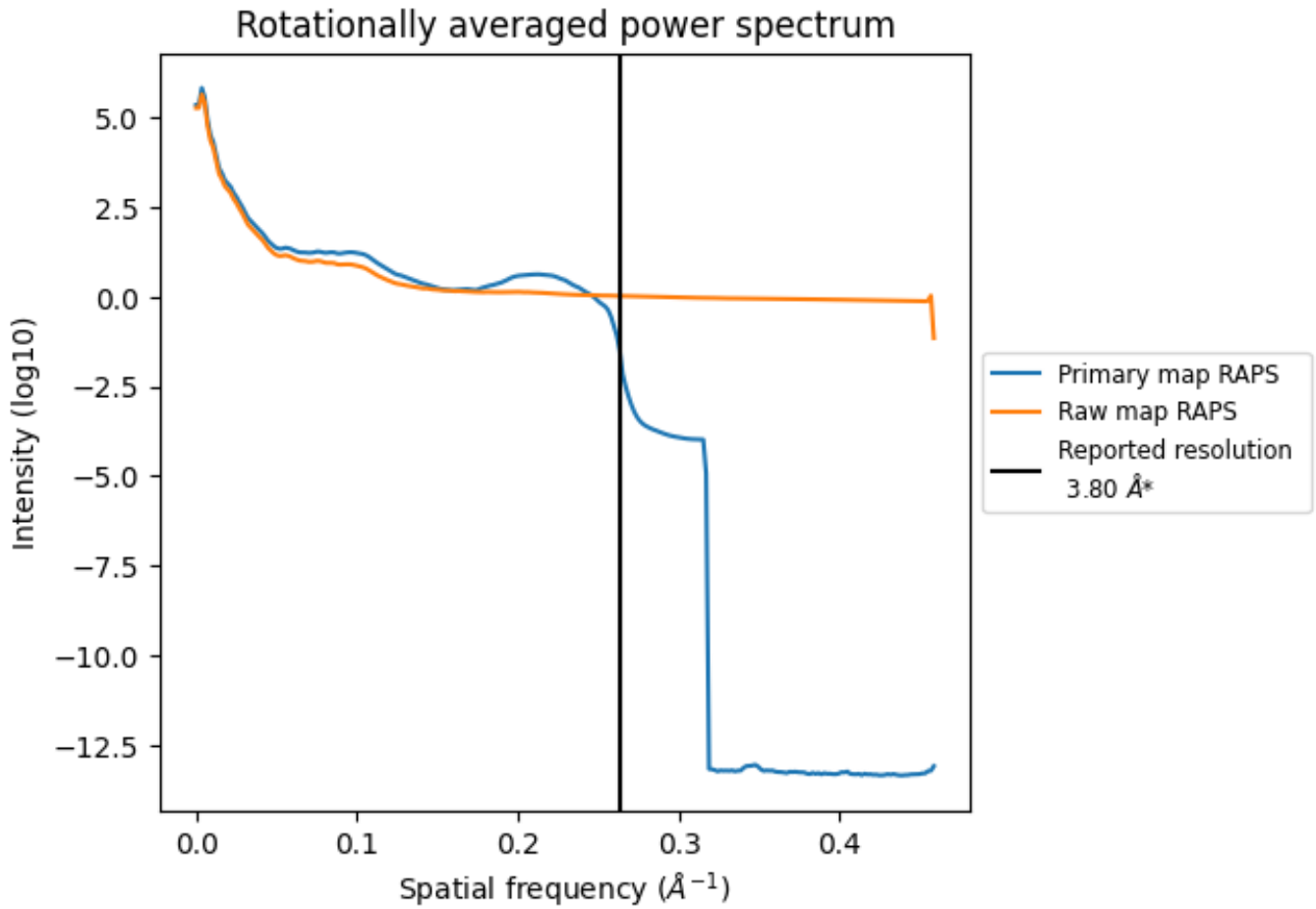
7.2 Volume estimate



The volume at the recommended contour level is 221 nm^3; this corresponds to an approximate mass of 199 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)

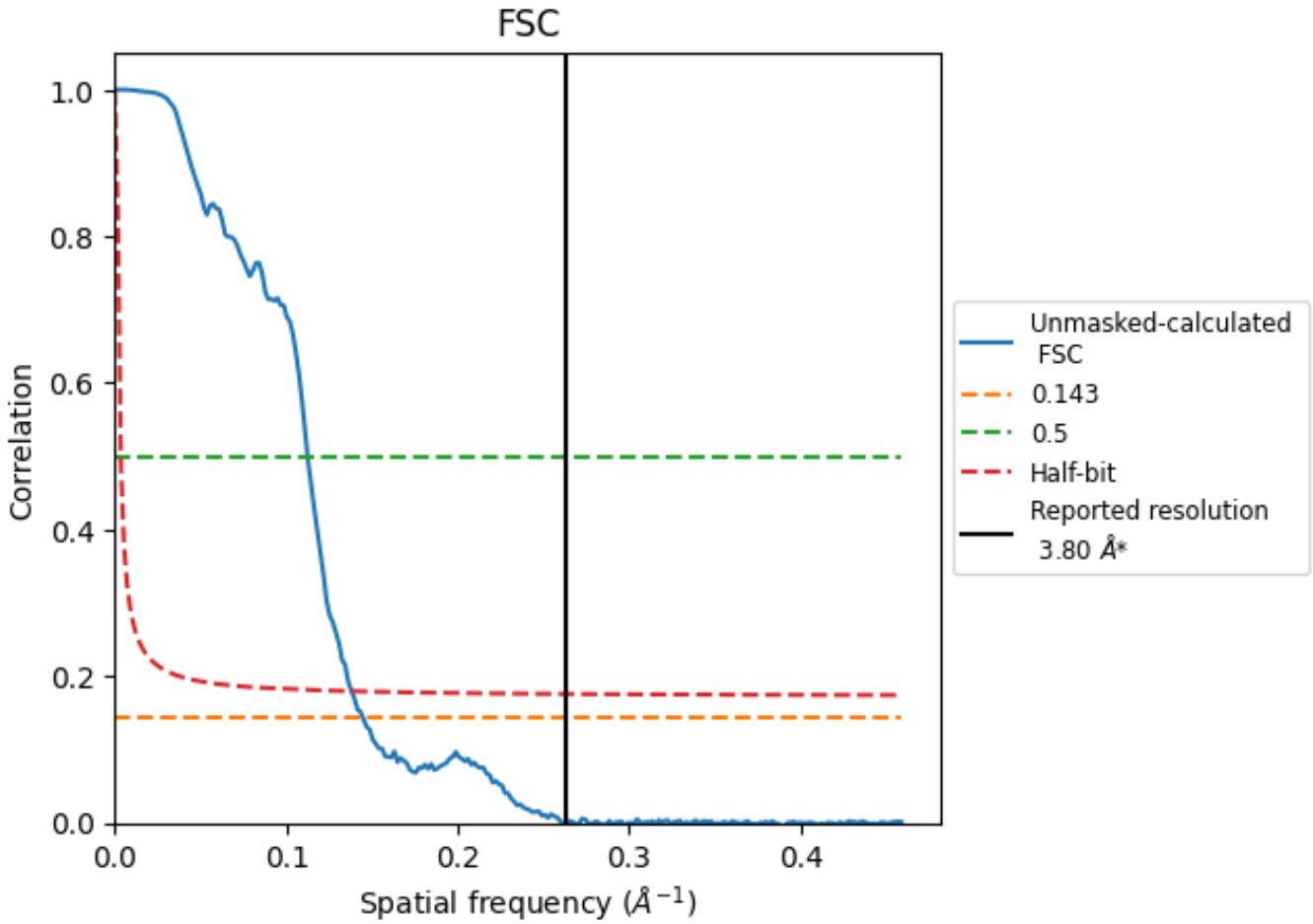


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

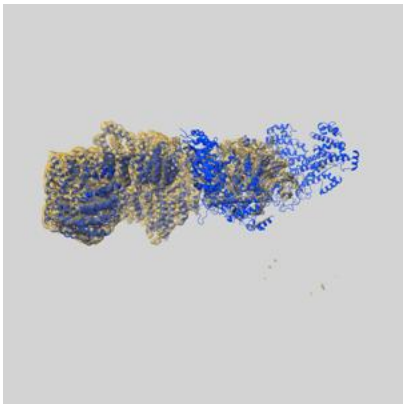
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.91	8.89	7.24

*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 6.91 differs from the reported value 3.8 by more than 10 %

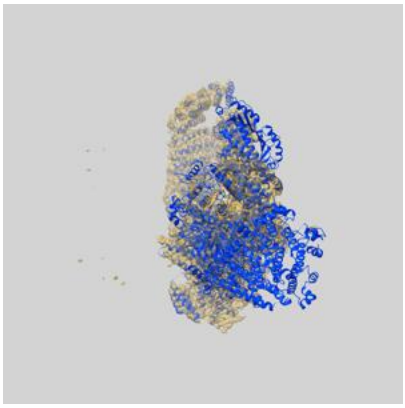
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10438 and PDB model 6TB4. Per-residue inclusion information can be found in section 3 on page 7.

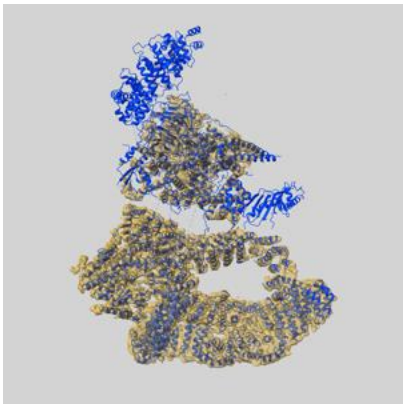
9.1 Map-model overlay



X



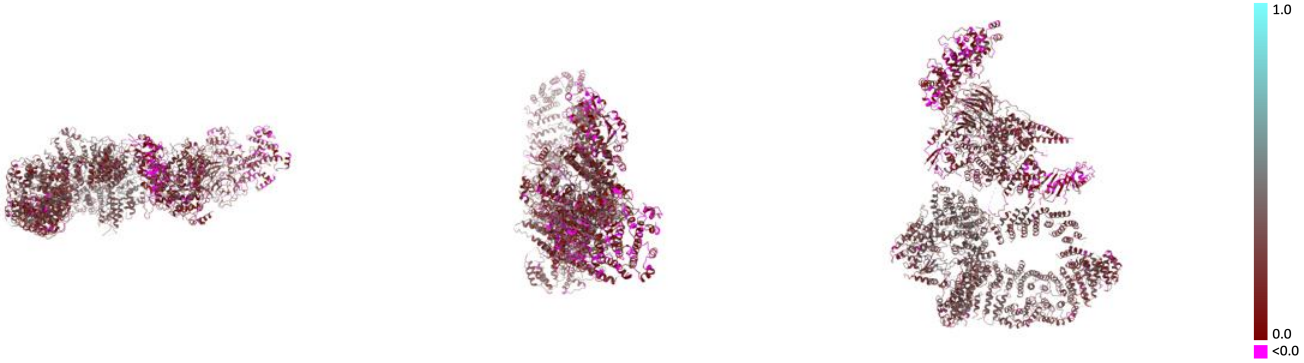
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

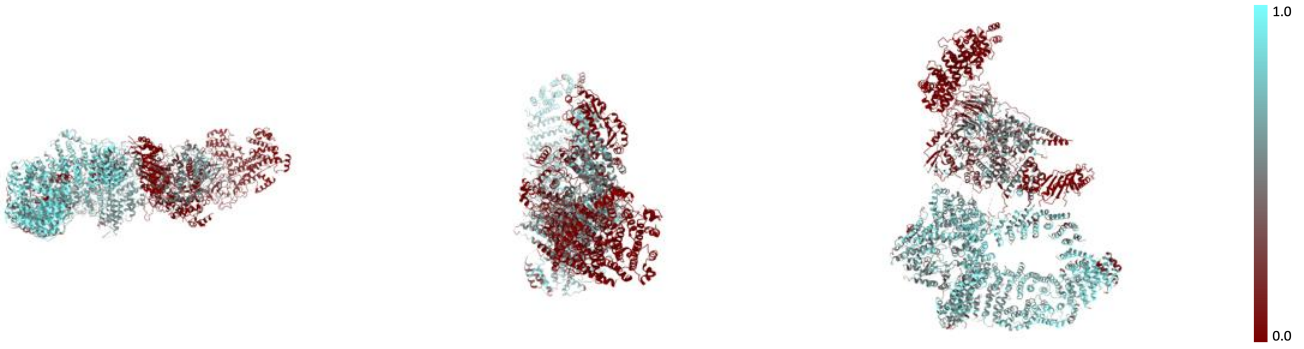
9.2 Q-score mapped to coordinate model (i)



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.

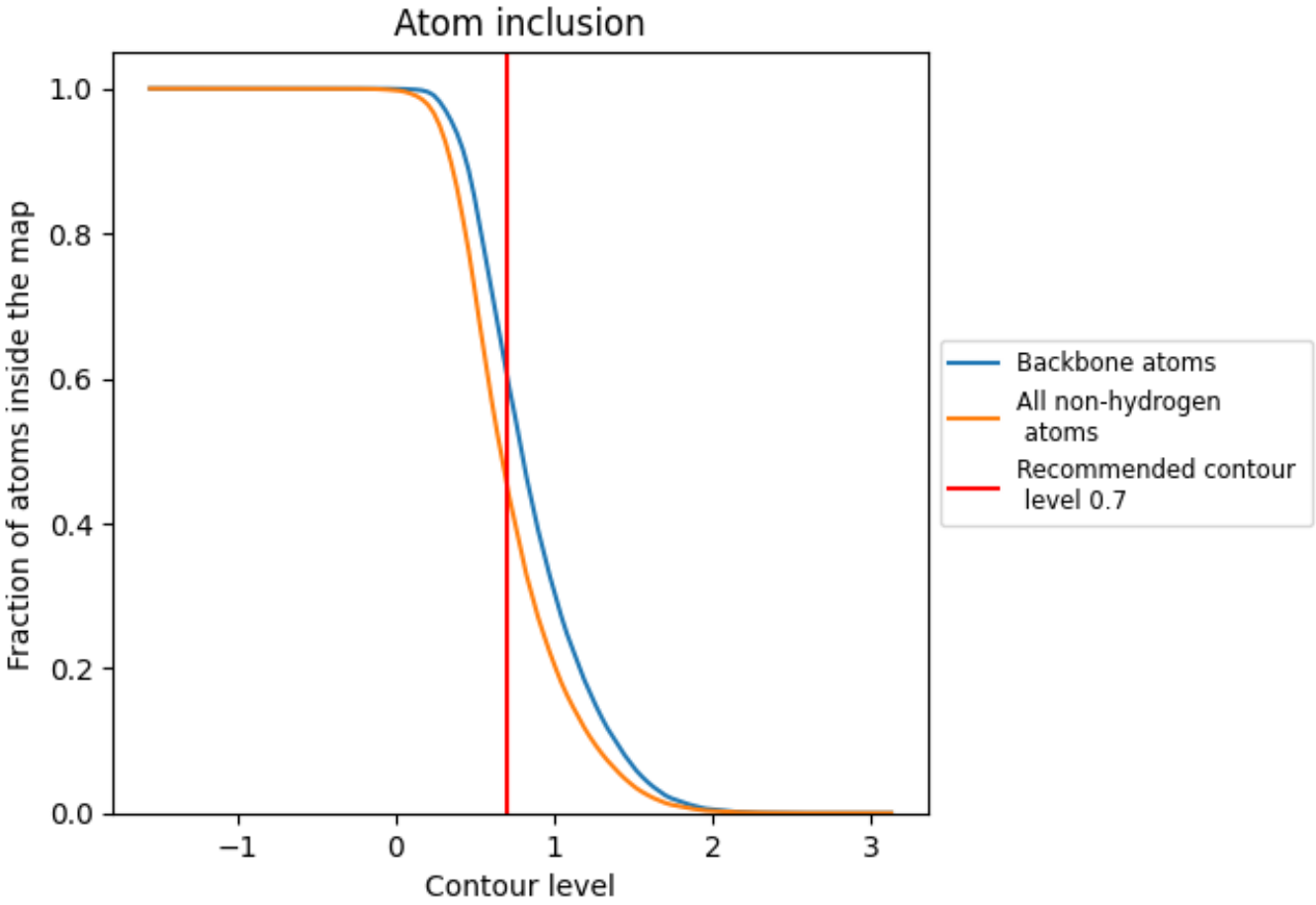
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 46% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4562	0.2310
A	0.2351	0.1830
B	0.0026	0.1280
C	0.0904	0.1570
D	0.2949	0.1690
E	0.4002	0.1980
F	0.1989	0.1540
G	0.1955	0.1800
H	0.0853	0.1350
I	0.2927	0.1750
J	0.4019	0.2060
K	0.3293	0.2160
L	0.6655	0.2880
M	0.0022	0.0490