Full wwPDB EM Validation Report ⓘ

Oct 18, 2023 – 07:03 PM JST

PDB ID	:	8GZN
EMDB ID	:	EMD-34399
Title	:	IgM-var2CSA complex
Authors	:	Akhouri, R.R.; Goel, S.; Skoglund, U.
Deposited on	:	2022-09-27
Resolution	:	3.60 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:

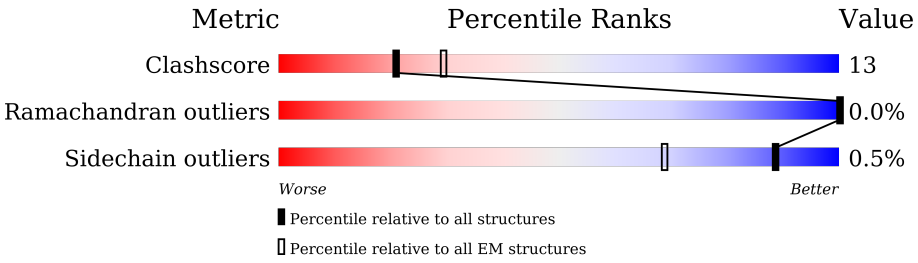
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 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	A	453	19% 10% 71%
1	B	453	33% 17% 50%
1	C	453	34% 16% 50%
1	D	453	35% 14% 51%
1	E	453	33% 17% 51%
1	F	453	35% 14% 51%
1	G	453	31% 18% 51%
1	H	453	38% 13% 49%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	453	
1	L	453	
2	I	2680	
2	M	2680	
3	J	136	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35322 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 Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total	C	N	O	S	0	0
			1026	648	174	198	6		
1	B	227	Total	C	N	O	S	0	0
			1764	1111	299	346	8		
1	C	225	Total	C	N	O	S	0	0
			1749	1103	297	341	8		
1	D	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	E	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	F	221	Total	C	N	O	S	0	0
			1723	1087	292	336	8		
1	G	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	H	230	Total	C	N	O	S	0	0
			1785	1124	301	351	9		
1	K	230	Total	C	N	O	S	0	0
			1786	1124	302	351	9		
1	L	127	Total	C	N	O	S	0	0
			993	626	168	193	6		

- Molecule 2 is a protein called Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1115	Total	C	N	O	S	0	0
			9208	5813	1571	1758	66		
2	M	1115	Total	C	N	O	S	0	0
			9208	5813	1571	1758	66		

- Molecule 3 is a protein called Immunoglobulin J chain.

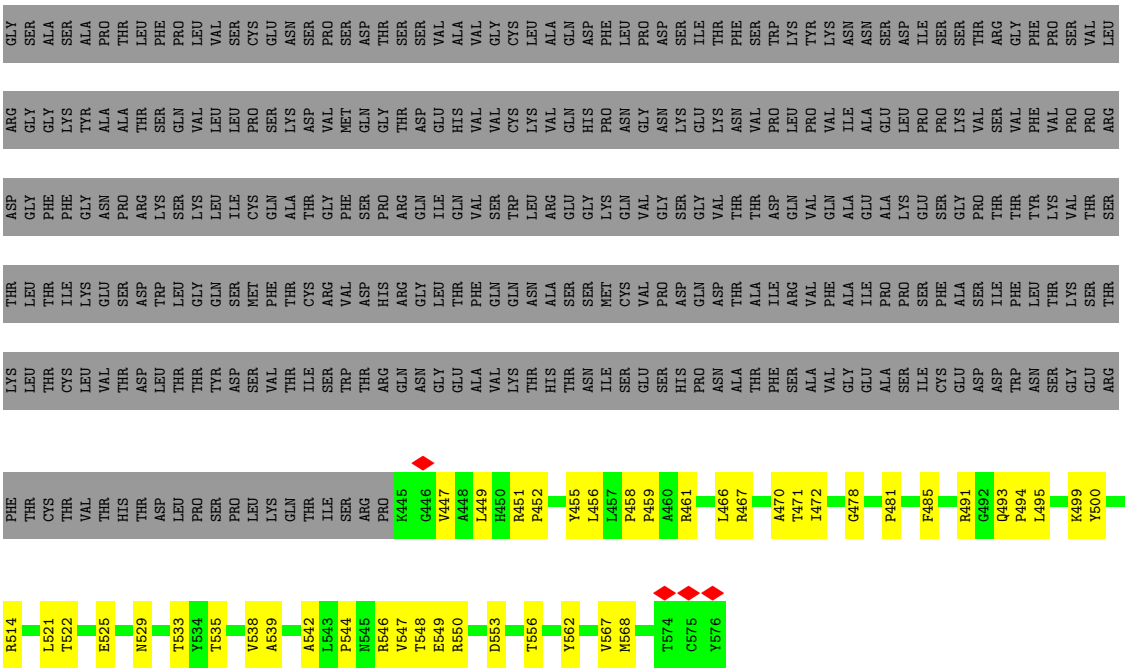
Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	106	Total	C	N	O	S	0	0
			851	528	150	166	7		

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.

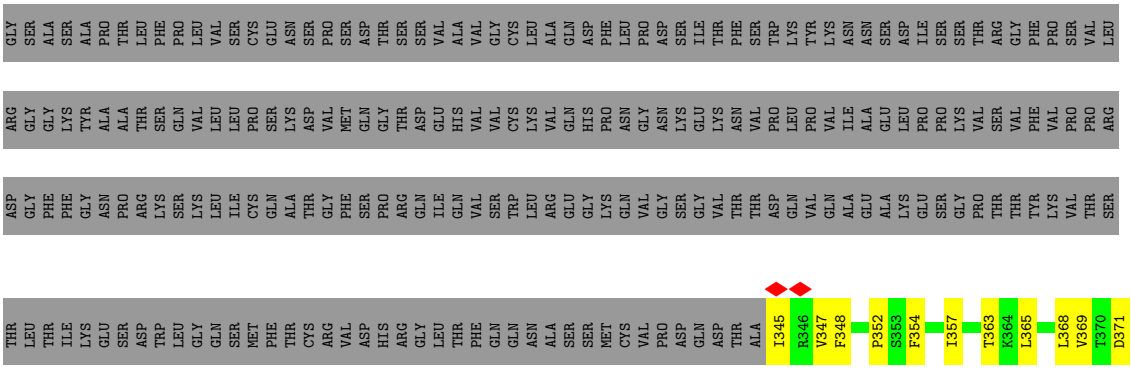
• Molecule 1: Immunoglobulin heavy constant mu

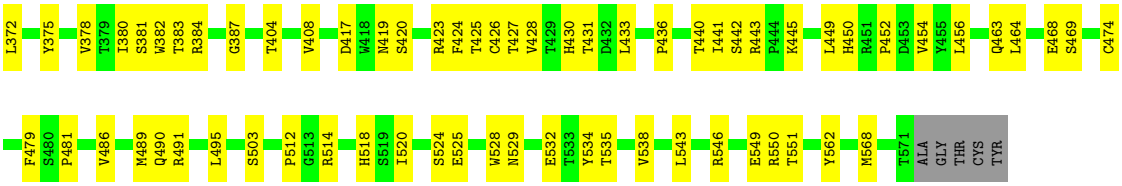
Chain A:



• Molecule 1: Immunoglobulin heavy constant mu

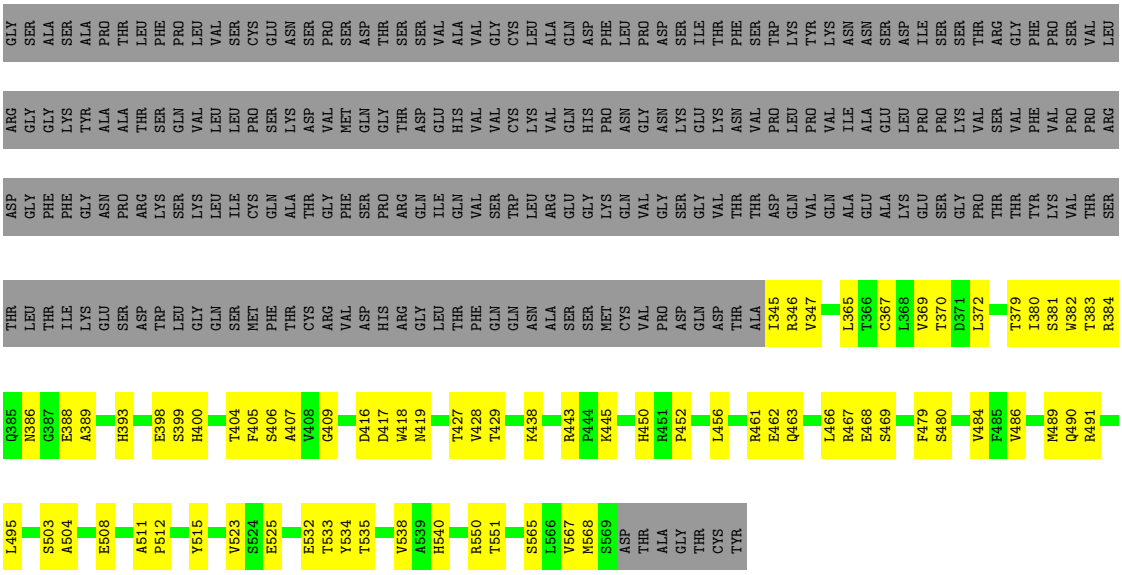
Chain B:





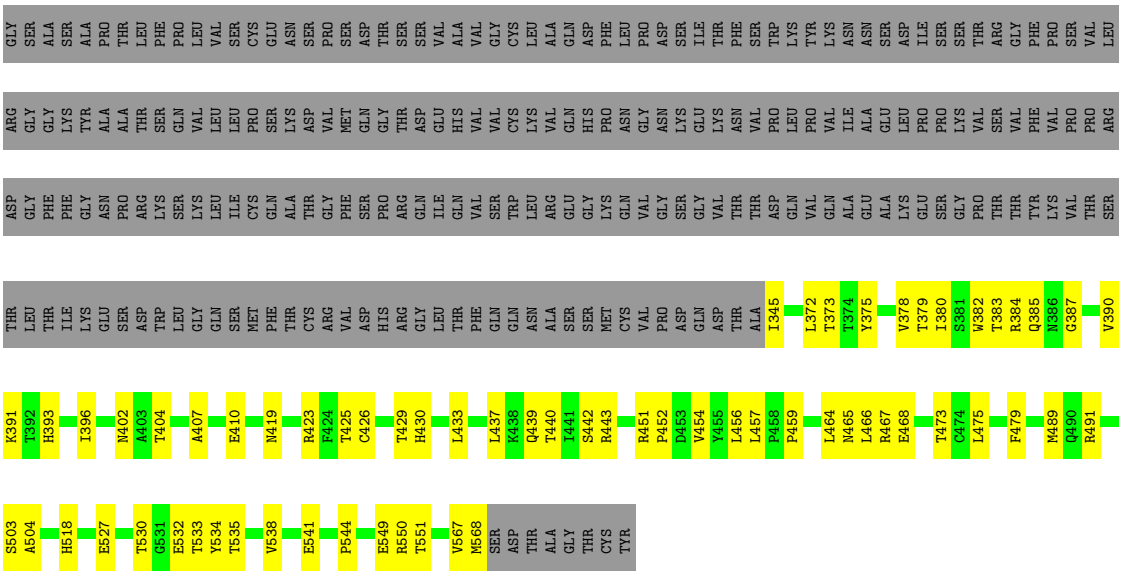
• Molecule 1: Immunoglobulin heavy constant mu

Chain C:



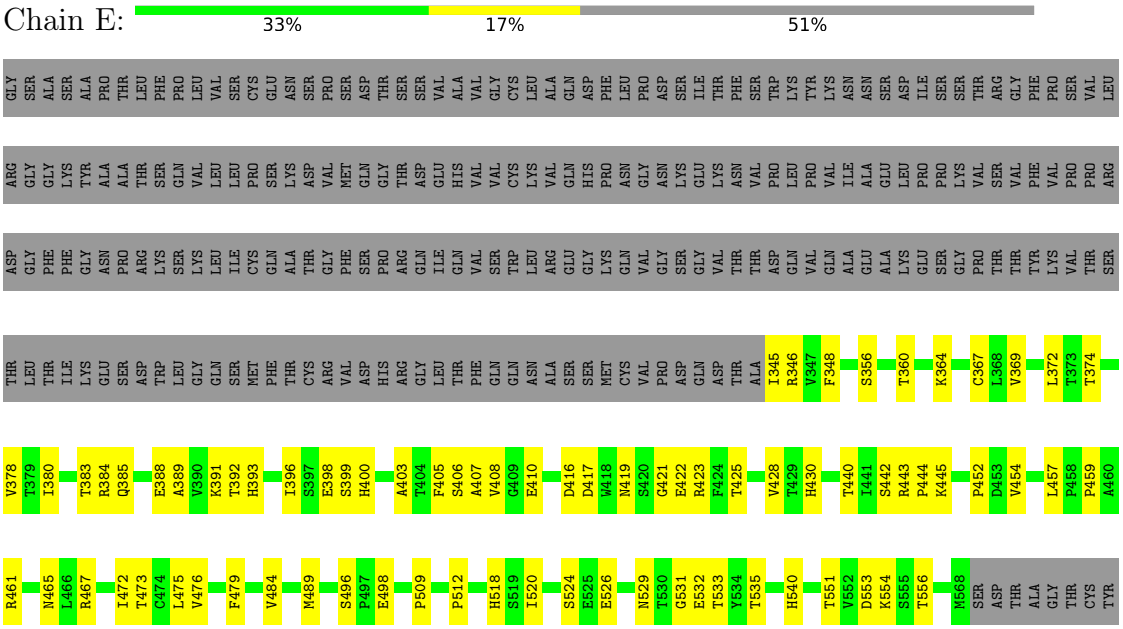
• Molecule 1: Immunoglobulin heavy constant mu

Chain D:



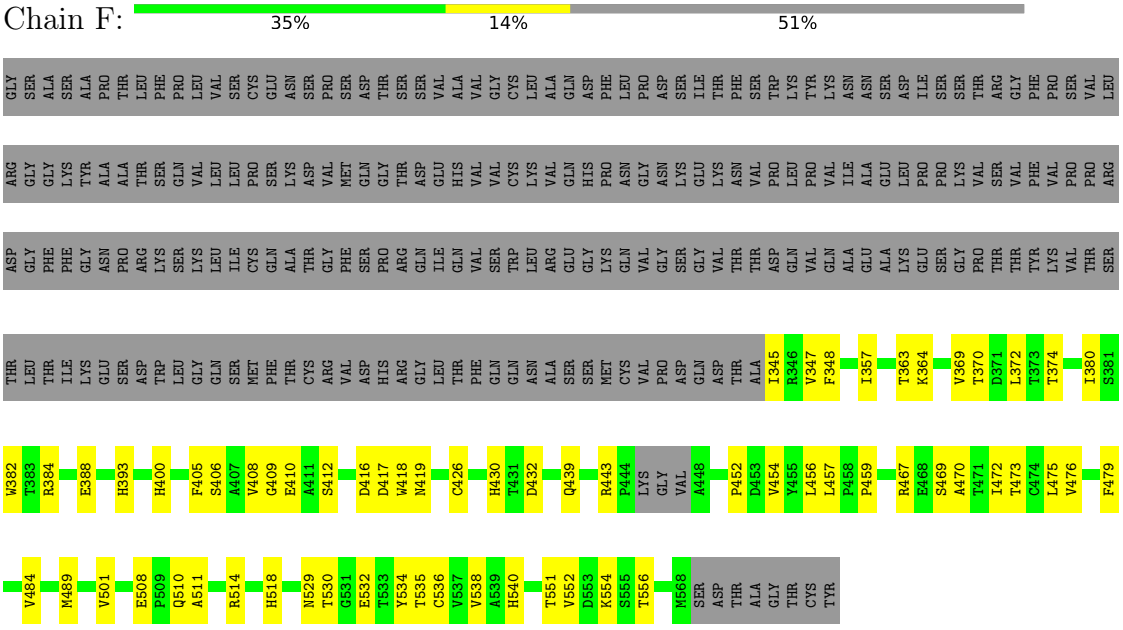
• Molecule 1: Immunoglobulin heavy constant mu

Chain E:



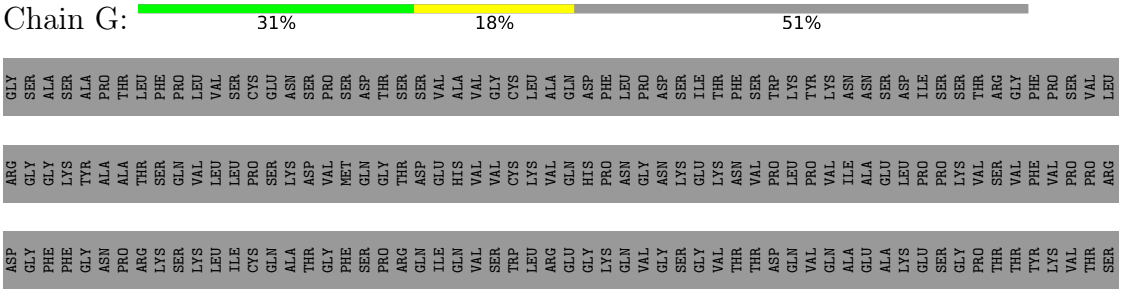
• Molecule 1: Immunoglobulin heavy constant mu

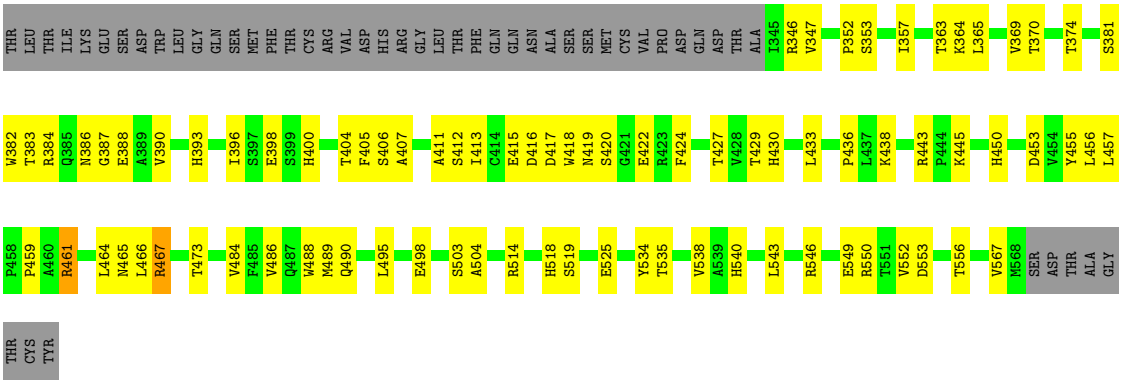
Chain F:



• Molecule 1: Immunoglobulin heavy constant mu

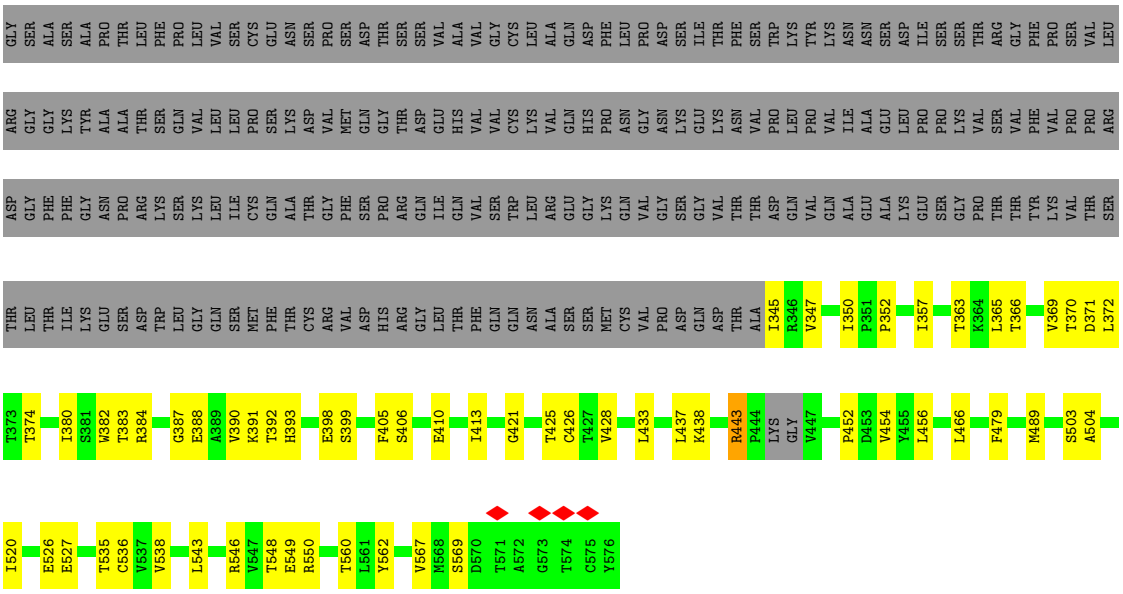
Chain G:





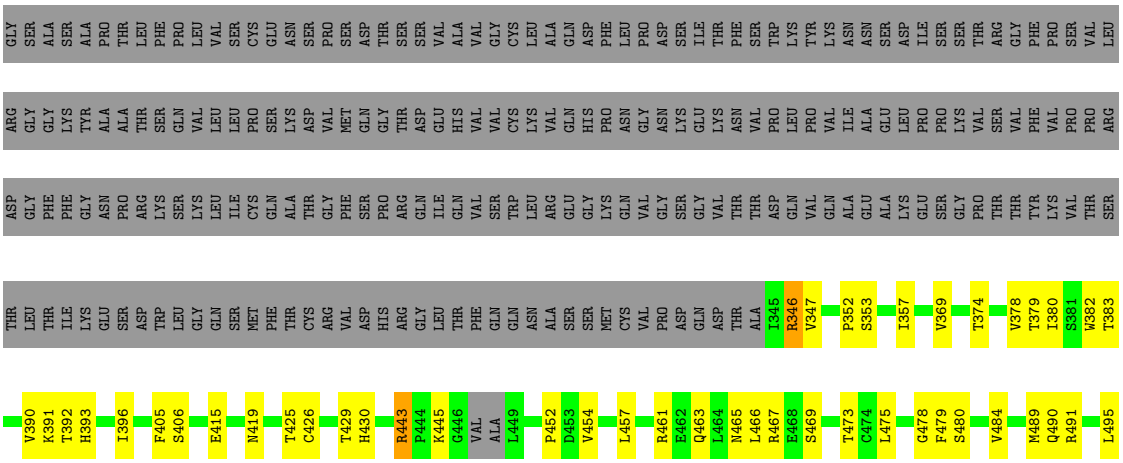
• Molecule 1: Immunoglobulin heavy constant mu

Chain H:



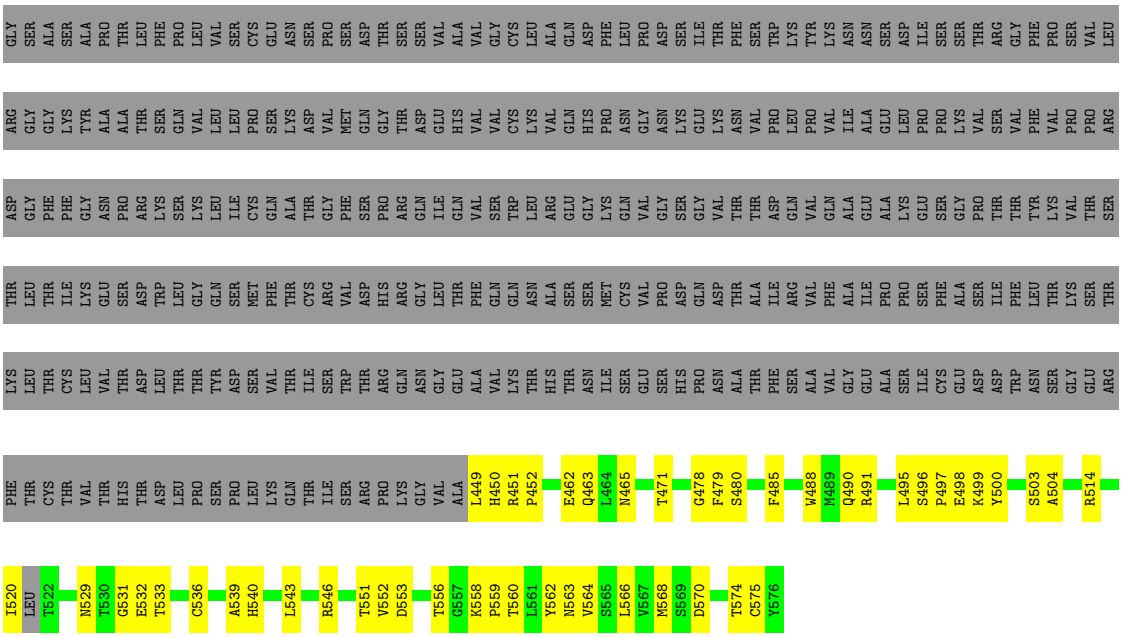
• Molecule 1: Immunoglobulin heavy constant mu

Chain K:



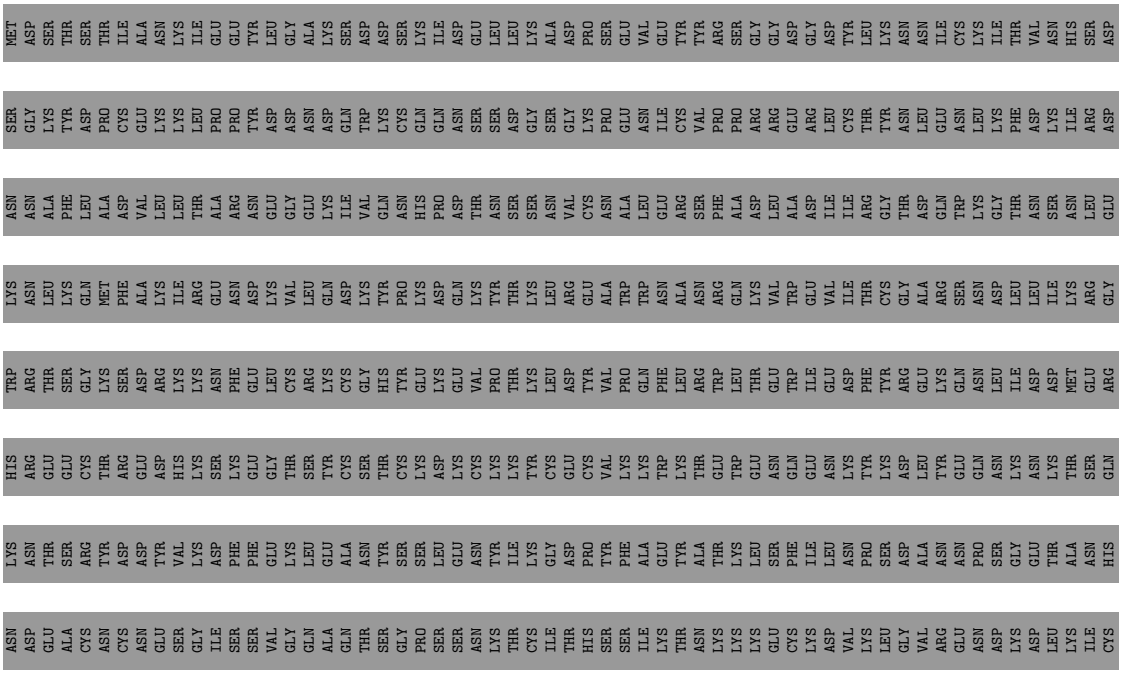
• Molecule 1: Immunoglobulin heavy constant mu

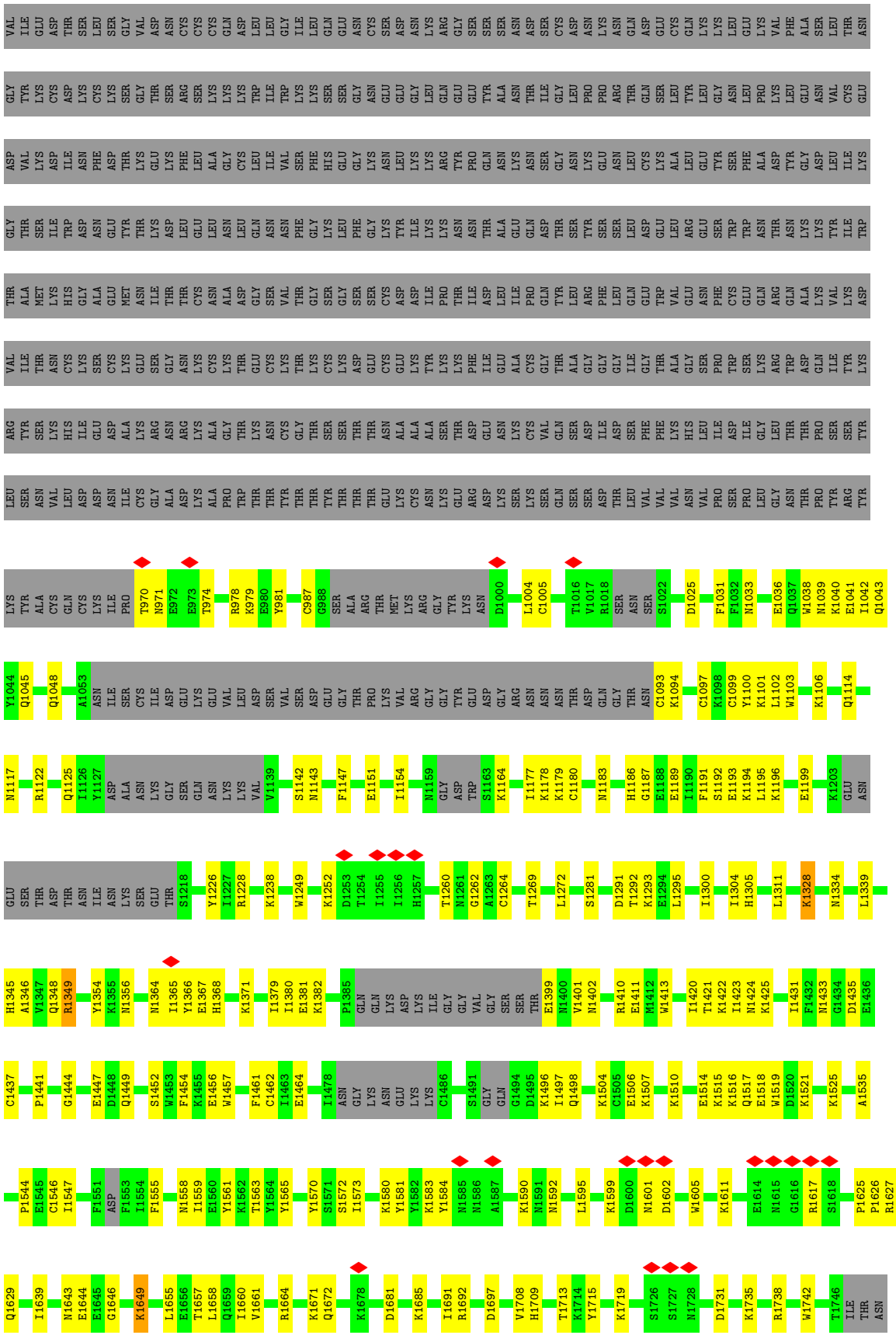
Chain L:

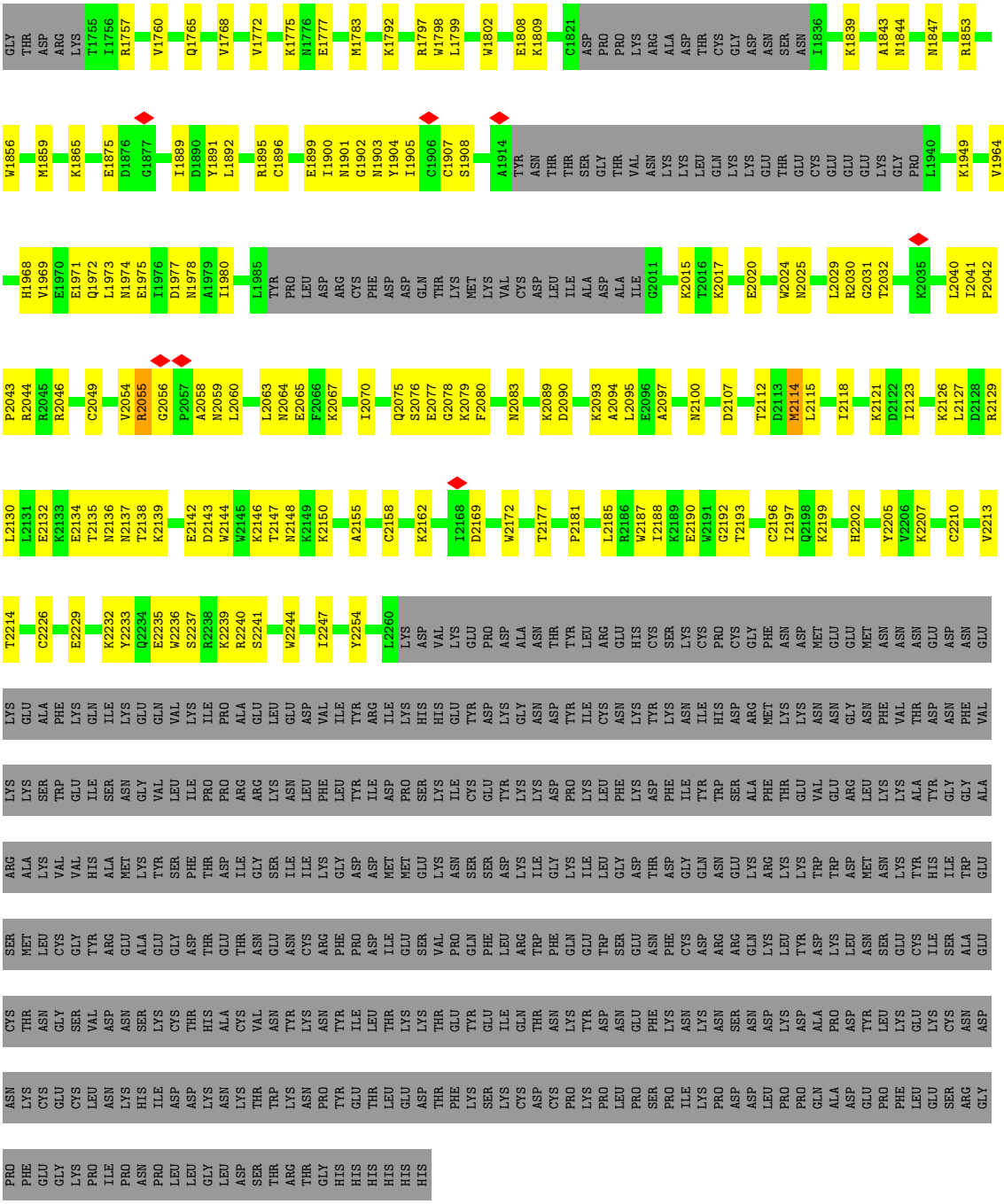


• Molecule 2: Erythrocyte membrane protein 1

Chain I:

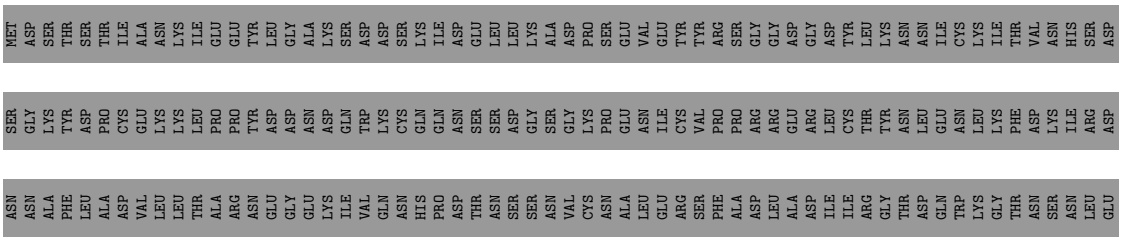


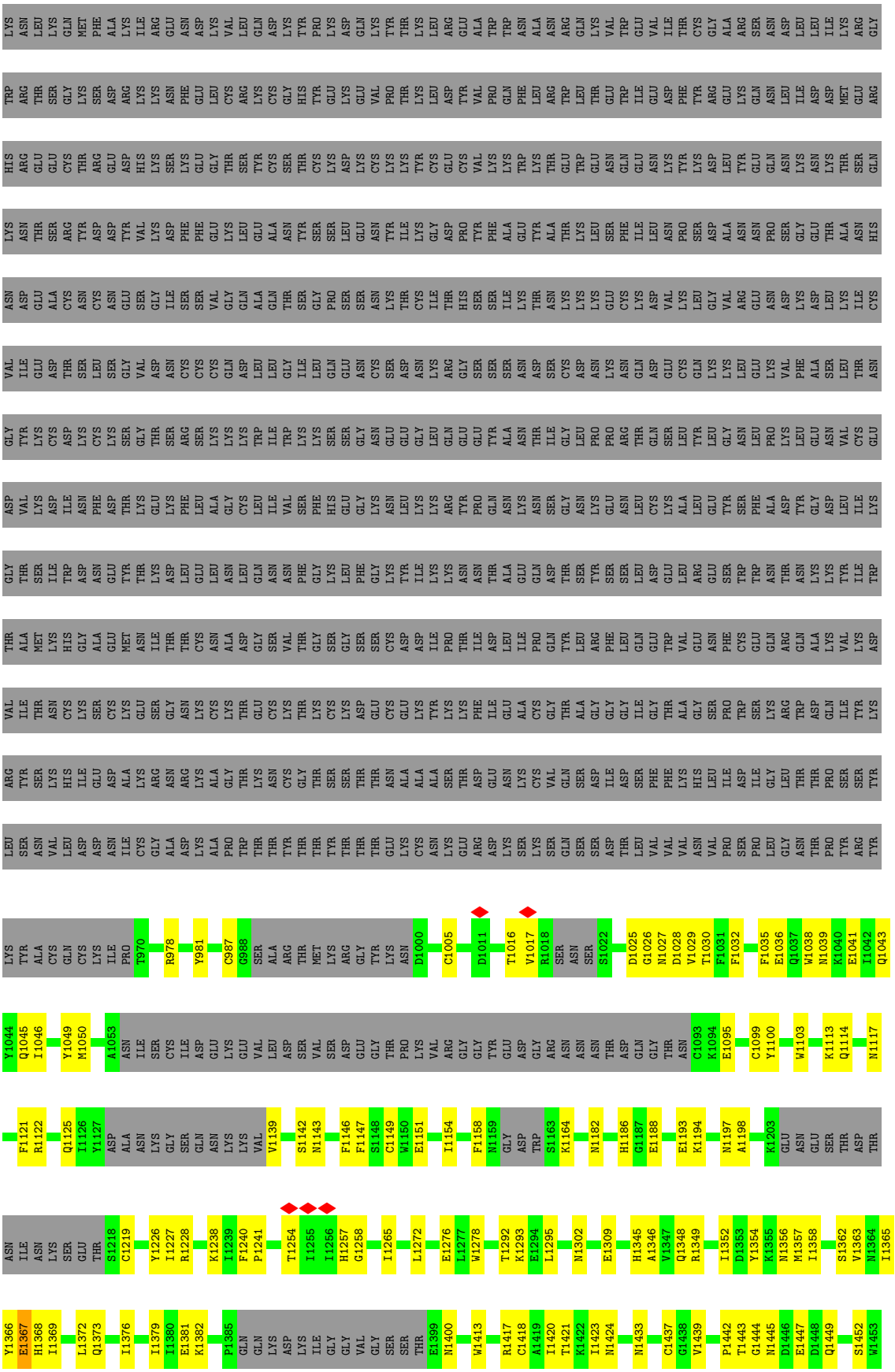

VAL ILE GLU ASP THR SER LEU SER GLY VAL ASP ASN CYS CYS CYS GLN ASP LEU LEU GLY ILE LEU GLN GLU ASN CYS SER ASP ASN LYS ARG GLY SER SER SER ASN ASP SER CYS ASP ASN LYS ASN GLN ASP GLU CYS GLN LYS LYS LEU GLU LYS VAL PHE ALA SER LEU THR ASN
GLY TYR LYS CYS ASP LYS CYS LYS SER GLY THR SER GLU GLU LYS LYS TRP ILE TRP LYS LYS SER SER GLY LYS HIS GLU GLY LEU GLN GLY GLU LYS PHE LEU ILE VAL SER PHE HIS GLU GLY ASP ASN GLU GLU GLY LEU GLN GLU GLU TYR ALA ASN THR ILE GLY LEU PRO PRO ARG THR GLN SER LEU TYR LEU GLY GLU GLU PRO LYS LEU GLU ASN VAL CYS GLU
ASP VAL LYS ASP ILE ASN PHE ASP THR LYS GLU LYS PHE LEU ALA GLY CYS LEU ILE ASN LEU LYS LYS ARG TYR PRO GLN ASN LYS ASN SER GLY ASN LYS GLU ASN LEU CYS LYS ALA LEU GLU TYR SER PHE ALA ASP TYR GLY ASP LEU ILE LYS
GLY THR SER ILE TRP ASP ASN GLU TYR THR LYS ASP LEU GLU LEU ASN LEU GLN GLN ASN THR ILE LYS ASN ASN THR ALA GLU GLN ASP THR SER TYR SER SER LEU ASP GLU LEU ARG GLU SER TRP TRP ASP THR ASN LYS LYS ALA LYS VAL LYS TYR ILE TRP
THR ALA MET LYS HIS GLY ALA GLU MET ASN ILE THR THR CYS ASN ALA ASP GLY SER VAL THR GLY SER LYS CYS SER GLY SER SER CYS ASP ILE PRO THR ILE ASP LEU ILE PRO GLY LEU GLN GLU ASP PHE CYS GLU GLN ARG GLN ALA LYS VAL LYS ASP
VAL ILE THR ASN CYS LYS SER CYS LYS GLU SER ASP GLU CYS LYS TYR LYS LYS PHE ILE GLU GLU ALA CYS GLY THR ALA GLY GLY GLY ILE GLY THR ALA GLY SER PRO TRP SER LYS ARG TRP ASP GLN ILE TYR TYR LYS
ARG TYR SER LYS HIS ILE GLU ASP ALA LYS ARG ASN ARG LYS ALA GLY THR LYS ASN CYS GLY THR SER SER SER THR THR ASN ALA ALA ALA SER THR THR ASN LYS CYS VAL GLN SER ASP ILE ASP SER PHE PHE LYS HIS LEU ILE SER PRO LEU GLY LEU THR THR PRO SER SER TYR
LEU SER ASN VAL LEU ASP ASP ASN ILE CYS GLY ALA ASP LYS ALA PRO TRP THR THR TYR THR THR THR GLU LYS CYS THR TYR THR GLN SER SER ASP THR LEU VAL VAL VAL ASN VAL PRO SER PRO LEU GLY ASN THR PRO TYR ARG TYR
LYS TYR ALA CYS GLN CYS LYS ILE PRO T970 N971 E972 E973 T974 R978 K979 E980 Y981 C987 G988 SER ALA ARG THR MET LYS ARG GLY TYR LYS ASN D1000 L1004 C1005 T1016 V1017 R1018 SER ASN SER S1022 D1025 F1031 F1032 N1033 E1036 Q1037 W1038 N1039 K1040 E1041 I1042 Q1043
Y1044 Q1045 Q1048 A1053 ASN ILE SER CYS ILE ASP GLU LYS GLU VAL LEU ASP SER VAL SER ASP GLU GLY THR PRO LYS VAL ARG GLY GLY TYR GLU ASP GLY ARG ASN ASN ASN THR ASP GLN GLY THR ASN C1093 K1094 C1097 K1098 C1099 Y1100 K1101 L1102 W1103 K1106 Q1114
N1117 R1122 Q1125 Y1126 Y1127 ASP ALA ASN LYS GLY SER GLN ASN LYS LYS VAL V1139 S1142 N1143 F1147 E1151 I1154 N1159 GLY ASP TRP S1163 K1164 I1177 K1178 K1179 C1180 N1183 H1186 G1187 E1188 E1189 I1190 F1191 S1192 E1193 K1194 L1196 K1196 E1199 K1203 GLU ASN
GLU SER THR ASP THR ASN ILE ASN LYS SER GLU THR S1218 Y1226 I1227 R1228 K1238 W1249 K1252 D1253 T1254 I1255 I1256 H1257 T1260 N1261 G1262 A1263 C1264 T1269 L1272 S1281 D1291 T1292 K1293 E1294 L1295 I1300 I1304 H1305 L1311 K1328 N1334 L1339
H1345 A1346 V1347 Q1348 R1349 Y1354 K1355 N1356 N1364 I1365 Y1366 E1367 H1368 K1371 I1379 I1380 E1381 K1382 P1385 GLN GLN LYS ASP LYS ILE GLY GLY VAL GLY SER SER THR E1399 N1400 V1401 N1402 R1410 E1411 M1412 W1413 I1420 T1421 K1422 I1423 N1424 K1425 I1431 F1432 N1433 G1434 D1435 E1436
C1437 P1441 G1444 E1447 D1448 Q1449 S1452 W1453 F1454 K1455 E1456 W1457 F1461 C1462 I1463 E1464 I1478 ASN GLY LYS ASN GLU LYS LYS C1486 S1491 GLY GLN G1494 D1495 K1496 I1497 Q1498 K1504 C1505 E1506 K1507 K1510 E1514 K1515 K1516 Q1517 E1518 W1519 D1520 K1521 K1525 A1535
P1544 E1545 C1546 I1547 F1551 ASP F1553 I1554 F1555 N1558 I1559 E1560 Y1561 K1562 T1563 Y1564 Y1565 Y1570 S1571 S1572 I1573 K1580 Y1581 Y1582 K1583 Y1584 N1585 N1586 A1587 K1590 N1591 N1592 L1595 K1599 D1600 N1601 D1602 W1605 K1611 E1614 N1615 G1616 R1617 S1618 P1625 P1626 R1627 R1628
Q1629 I1639 N1643 E1644 E1645 G1646 K1649 L1655 E1656 T1657 L1658 Q1659 I1660 V1661 R1664 K1671 Q1672 K1678 D1681 K1685 I1691 R1692 D1697 V1708 H1709 T1713 K1714 Y1715 K1719 S1726 S1727 N1728 D1731 K1735 R1738 W1742 T1746 ILE THR ASN

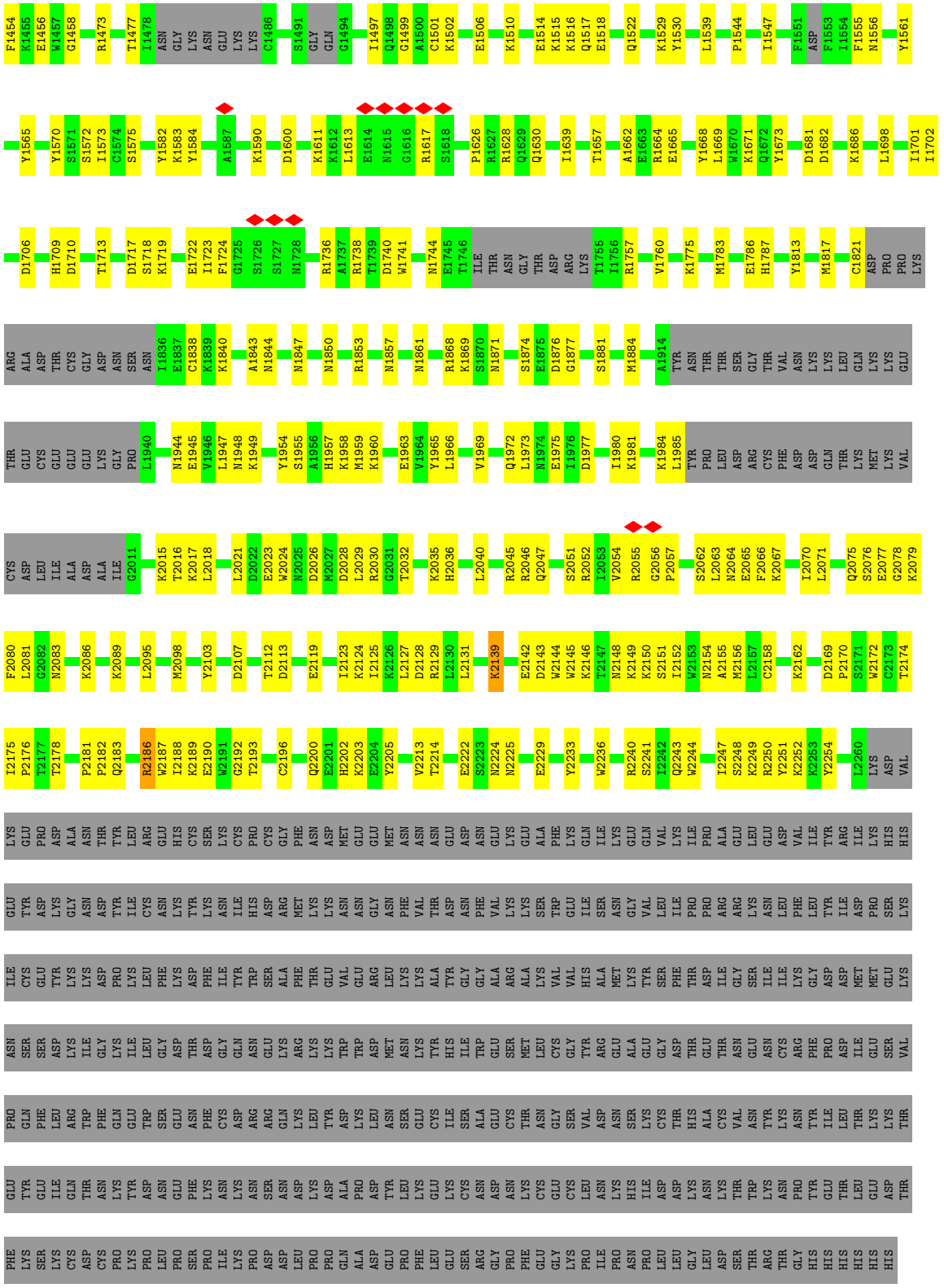


• Molecule 2: Erythrocyte membrane protein 1

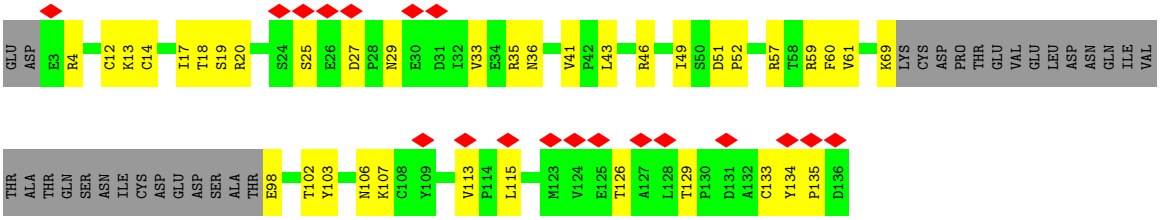
Chain M:




LYS ASN LEU LYS GLN MET PHE ALA LYS ILE ARG GLU ASN ASP LYS VAL LEU GLN ASP LYS TYR PRO LYS GLU LYS ASP GLN LYS TYR THR LYS LEU ARG GLU ALA TRP TRP ASN ALA ASN ARG GLN LYS VAL TRP GLU VAL ILE THR CYS GLY ALA ARG SER ASN ASP LEU LEU ILE LEU LYS GLY
TRP ARG THR SER GLY LYS SER ASP ARG LYS LYS ASN PHE GLU LEU CYS ARG CYS GLY HIS TYR GLU LYS GLU VAL PRO THR LYS LEU ASP TYR VAL PRO GLN PHE LEU ARG TRP ASN LEU LEU ILE ASP ASP MET GLU ARG
HIS ARG GLU GLU CYS THR ARG GLU ASP HIS LYS SER LYS GLU GLY THR SER TYR CYS SER THR CYS LYS ASP LYS CYS ASN GLN GLU ASN LYS TYR LYS TYR CYS GLU CYS VAL LYS LYS TRP LYS THR GLU TRP GLU ASN GLN GLU CYS LYS ASP LEU TYR ARG GLU LYS GLN ASN ASN LYS ASN THR SER GLN
LYS ASN THR SER ARG TYR ASP ASP TYR VAL LYS ASP PHE PHE GLU LYS LEU GLU GLU ALA ASN SER TYR SER SER LEU GLU ASN SER PHE ILE LEU ASN PRO SER ASP SER GLY ALA ASN ASN ASN PRO SER GLY GLU THR ALA THR LYS LEU SER PHE ILE LEU ASP TYR ALA GLU GLN TYR PHE ALA GLU TYR ALA THR LYS LEU GLU SER PHE ILE LEU ASP PHE ASP ASP ASP



• Molecule 3: Immunoglobulin J chain


GLU ASP E3 R4 C12 K13 C14 I17 T18 S19 R20 S24 S25 E26 D27 P28 N29 E30 D31 I32 V33 E34 R35 N36 V41 P42 L43 R46 I49 S50 D51 P52 R57 T58 R59 F60 V61 K69 LYS CYS ASP PRO THR GLU VAL GLU LEU ASP ASN GLN ILE VAL
THR ALA THR GLN SER ASN ILE CYS ASP GLU ASP SER ALA THR E98 T102 Y103 N106 K107 C108 Y109 V113 P114 L115 M123 V124 E125 T126 A127 L128 T129 P130 D131 A132 C133 Y134 P135 D136

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	371049	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00805	Depositor
Map size (Å)	594.0, 594.0, 594.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	A	0.24	0/1053	0.51	0/1442
1	B	0.25	0/1809	0.54	0/2478
1	C	0.24	0/1794	0.52	0/2457
1	D	0.25	0/1788	0.53	0/2449
1	E	0.25	0/1788	0.53	0/2449
1	F	0.25	0/1767	0.52	0/2420
1	G	0.25	0/1788	0.52	0/2449
1	H	0.25	0/1830	0.52	0/2507
1	K	0.25	0/1831	0.52	0/2506
1	L	0.25	0/1019	0.55	0/1395
2	I	0.24	0/9392	0.46	0/12593
2	M	0.25	0/9392	0.47	0/12593
3	J	0.23	0/864	0.55	0/1173
All	All	0.25	0/36115	0.49	0/48911

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1026	0	1001	33	0
1	B	1764	0	1724	61	0
1	C	1749	0	1713	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1743	0	1709	40	0
1	E	1743	0	1709	48	0
1	F	1723	0	1682	41	0
1	G	1743	0	1708	57	0
1	H	1785	0	1735	42	0
1	K	1786	0	1737	43	0
1	L	993	0	959	39	0
2	I	9208	0	8976	235	0
2	M	9208	0	8974	240	0
3	J	851	0	843	37	0
All	All	35322	0	34470	927	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 13.

All (927) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:369:VAL:O	1:K:406:SER:HA	1.58	1.04
2:I:1191:PHE:O	2:I:1194:LYS:HB2	1.66	0.93
3:J:4:ARG:HH22	3:J:36:ASN:H	1.23	0.87
1:B:490:GLN:HG2	1:B:491:ARG:HG2	1.60	0.83
1:C:452:PRO:HB3	1:C:479:PHE:HB3	1.61	0.81
1:H:347:VAL:HG22	1:H:369:VAL:HG12	1.64	0.80
1:B:452:PRO:HB3	1:B:479:PHE:HB3	1.62	0.79
2:M:2075:GLN:NE2	2:M:2155:ALA:O	2.16	0.79
1:B:428:VAL:O	1:B:436:PRO:HA	1.84	0.78
1:D:426:CYS:HB3	1:D:439:GLN:HB2	1.67	0.77
1:D:527:GLU:OE1	1:D:534:TYR:OH	2.02	0.77
3:J:4:ARG:HH21	3:J:18:THR:HG23	1.49	0.77
2:M:1367:GLU:CD	2:M:1368:HIS:H	1.90	0.75
2:I:2067:LYS:HA	2:I:2070:ILE:HG12	1.69	0.73
1:K:452:PRO:HB3	1:K:479:PHE:HB3	1.70	0.73
2:I:2129:ARG:NH1	2:I:2132:GLU:O	2.21	0.73
2:M:2139:LYS:HD3	2:M:2142:GLU:HB3	1.71	0.73
2:I:1900:ILE:HB	2:I:1908:SER:HB2	1.71	0.72
2:M:2125:ILE:HG22	2:M:2129:ARG:HH11	1.54	0.72
3:J:4:ARG:HH11	3:J:20:ARG:HB2	1.53	0.71
1:B:454:VAL:HG21	1:B:538:VAL:HG11	1.70	0.71
1:D:425:THR:HG22	1:D:440:THR:HG22	1.73	0.70
2:I:1626:PRO:HA	2:I:1629:GLN:HE21	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2060:LEU:HD11	2:I:2064:ASN:HA	1.73	0.70
1:F:535:THR:HG22	1:F:551:THR:HB	1.74	0.70
1:K:378:VAL:HG12	1:K:430:HIS:HD2	1.56	0.69
2:I:1293:LYS:HE3	2:I:1380:ILE:HD13	1.74	0.69
1:D:489:MET:HB3	1:D:535:THR:HG23	1.75	0.69
2:I:2213:VAL:HG12	2:I:2214:THR:HG23	1.73	0.69
1:G:467:ARG:O	2:I:2059:ASN:ND2	2.26	0.69
2:M:1365:ILE:H	2:M:1369:ILE:HD11	1.57	0.69
1:L:478:GLY:O	1:L:514:ARG:NH2	2.27	0.68
2:M:1497:ILE:HG22	2:M:1499:GLY:H	1.57	0.68
1:C:463:GLN:NE2	1:C:469:SER:O	2.27	0.68
1:D:452:PRO:HB3	1:D:479:PHE:HB3	1.74	0.68
2:I:1122:ARG:NH1	2:I:1125:GLN:O	2.27	0.68
1:C:380:ILE:HG21	1:C:407:ALA:HB1	1.76	0.68
1:A:458:PRO:HA	1:A:472:ILE:HD12	1.76	0.68
1:B:489:MET:O	1:B:535:THR:OG1	2.08	0.68
2:I:1226:TYR:HE2	2:I:1228:ARG:HH12	1.42	0.68
1:D:393:HIS:HD2	1:D:396:ILE:HD11	1.58	0.68
2:I:2029:LEU:O	2:I:2032:THR:OG1	2.11	0.68
2:M:2054:VAL:HG12	2:M:2056:GLY:H	1.59	0.67
2:I:987:CYS:HA	2:I:1005:CYS:HA	1.76	0.67
2:M:1028:ASP:OD2	2:M:1125:GLN:NE2	2.27	0.67
1:G:383:THR:HB	1:G:387:GLY:HA2	1.74	0.67
1:G:567:VAL:HB	1:H:567:VAL:HG12	1.75	0.67
1:C:384:ARG:HB2	1:C:388:GLU:HB2	1.77	0.67
1:H:369:VAL:O	1:H:406:SER:HA	1.94	0.67
1:E:454:VAL:HG22	1:E:476:VAL:HG22	1.77	0.67
1:C:347:VAL:HG22	1:C:369:VAL:HG13	1.77	0.67
1:C:347:VAL:HG13	1:C:369:VAL:HG22	1.77	0.67
2:M:1869:LYS:HD3	2:M:1874:SER:HA	1.77	0.66
2:M:978:ARG:NH2	2:M:1099:CYS:SG	2.68	0.66
1:B:382:TRP:HB3	1:B:384:ARG:HH22	1.60	0.66
1:F:357:ILE:HD13	1:F:363:THR:HB	1.77	0.66
1:F:532:GLU:HB3	1:F:534:TYR:CZ	2.31	0.66
1:D:451:ARG:HH12	1:D:544:PRO:HD3	1.61	0.66
2:M:1572:SER:O	2:M:1575:SER:N	2.26	0.66
1:G:461:ARG:O	1:G:465:ASN:ND2	2.27	0.66
2:I:1757:ARG:HA	2:I:1760:VAL:HG22	1.78	0.66
1:G:427:THR:HG22	1:G:438:LYS:HG2	1.78	0.66
2:I:2079:LYS:HD2	2:I:2094:ALA:HB1	1.78	0.66
2:M:1348:GLN:NE2	2:M:1437:CYS:SG	2.69	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1736:ARG:HH22	2:M:1740:ASP:HB3	1.60	0.66
1:B:383:THR:HB	1:B:387:GLY:HA2	1.78	0.65
1:E:465:ASN:O	1:E:467:ARG:NH1	2.29	0.65
1:G:357:ILE:HD12	1:G:363:THR:HG22	1.76	0.65
1:B:456:LEU:HD13	1:B:474:CYS:HB3	1.77	0.65
1:H:384:ARG:HG3	1:H:388:GLU:HB2	1.78	0.65
1:K:465:ASN:HA	1:K:467:ARG:HH11	1.62	0.65
1:C:379:THR:HB	1:C:429:THR:HB	1.78	0.65
2:I:1420:ILE:O	2:I:1424:ASN:ND2	2.30	0.65
2:M:1346:ALA:HA	2:M:1349:ARG:HD2	1.78	0.65
1:G:384:ARG:NH1	1:G:388:GLU:OE1	2.29	0.65
1:A:548:THR:HB	1:A:550:ARG:HH12	1.61	0.65
1:G:489:MET:HB3	1:G:535:THR:OG1	1.97	0.65
2:I:2076:SER:HB3	2:I:2158:CYS:HB2	1.79	0.64
2:I:1515:LYS:NZ	2:I:1518:GLU:OE1	2.25	0.64
2:M:1226:TYR:O	2:M:1228:ARG:NH1	2.29	0.64
1:F:426:CYS:SG	1:F:439:GLN:NE2	2.70	0.64
2:I:1348:GLN:NE2	2:I:1437:CYS:SG	2.71	0.64
2:M:1032:PHE:O	2:M:1035:PHE:HB3	1.97	0.64
2:I:1004:LEU:HA	2:I:1031:PHE:HE1	1.62	0.64
2:I:1045:GLN:OE1	2:I:1048:GLN:NE2	2.31	0.64
2:I:1964:VAL:O	2:I:1968:HIS:ND1	2.30	0.64
2:M:1669:LEU:O	2:M:1673:TYR:HB2	1.97	0.64
1:G:369:VAL:HB	1:G:407:ALA:HB3	1.80	0.63
1:A:478:GLY:HA2	1:A:514:ARG:HB3	1.80	0.63
2:M:2247:ILE:HA	2:M:2250:ARG:HE	1.63	0.63
2:I:1100:TYR:HA	2:I:1103:TRP:CD1	2.32	0.63
1:L:450:HIS:HD1	1:L:480:SER:HG	1.44	0.63
2:I:2236:TRP:HA	2:I:2239:LYS:HD2	1.81	0.63
2:I:2148:ASN:HB3	2:I:2177:THR:HB	1.81	0.63
2:M:2150:LYS:O	2:M:2154:ASN:ND2	2.31	0.63
2:M:2236:TRP:HE3	2:M:2240:ARG:HH11	1.47	0.62
2:M:2248:SER:HA	2:M:2254:TYR:HB2	1.81	0.62
1:A:544:PRO:O	1:A:546:ARG:NH1	2.32	0.62
1:C:416:ASP:OD2	1:C:417:ASP:N	2.32	0.62
2:I:2144:TRP:O	2:I:2148:ASN:ND2	2.32	0.62
1:F:374:THR:HA	1:F:405:PHE:HB2	1.81	0.62
1:F:393:HIS:HB3	1:F:410:GLU:H	1.64	0.62
1:A:493:GLN:NE2	1:A:494:PRO:O	2.33	0.62
2:I:1293:LYS:NZ	2:I:1379:ILE:O	2.32	0.62
1:L:449:LEU:N	1:L:480:SER:O	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:VAL:HG11	1:E:428:VAL:HG11	1.81	0.62
1:F:345:ILE:HD12	1:F:372:LEU:HD11	1.82	0.62
1:K:380:ILE:O	1:K:393:HIS:ND1	2.31	0.62
1:B:491:ARG:HH21	2:M:2055:ARG:CZ	2.12	0.62
1:E:380:ILE:HG12	1:E:428:VAL:HG22	1.82	0.62
2:M:2083:ASN:HB3	2:M:2086:LYS:HB3	1.80	0.61
1:C:486:VAL:HG12	1:C:538:VAL:HG23	1.81	0.61
2:M:1357:MET:HA	2:M:1363:VAL:HG21	1.81	0.61
1:H:352:PRO:HB2	1:H:357:ILE:HD11	1.81	0.61
2:I:2044:ARG:NH2	2:I:2097:ALA:O	2.33	0.61
2:M:1257:HIS:ND1	2:M:1365:ILE:O	2.33	0.61
1:B:535:THR:HB	1:B:549:GLU:OE2	2.01	0.61
1:C:398:GLU:O	1:C:406:SER:OG	2.18	0.61
1:F:484:VAL:HG23	1:F:540:HIS:HB2	1.81	0.61
2:I:1262:GLY:HA2	2:I:1525:LYS:HE2	1.83	0.61
1:A:491:ARG:NH1	1:A:533:THR:O	2.30	0.61
1:G:352:PRO:HB2	1:G:357:ILE:HD11	1.83	0.61
1:L:452:PRO:HB3	1:L:479:PHE:HB3	1.83	0.61
2:M:1857:ASN:O	2:M:1861:ASN:ND2	2.33	0.61
1:L:451:ARG:HD3	1:L:452:PRO:HD2	1.83	0.60
2:M:1142:SER:OG	2:M:1188:GLU:OE1	2.19	0.60
2:M:2029:LEU:O	2:M:2032:THR:OG1	2.19	0.60
2:M:1017:VAL:HG21	2:M:1959:MET:HG3	1.83	0.60
2:M:1121:PHE:O	2:M:1125:GLN:NE2	2.33	0.60
2:M:2249:LYS:NZ	2:M:2250:ARG:O	2.33	0.60
1:K:346:ARG:NH1	1:K:347:VAL:O	2.35	0.60
2:M:1016:THR:HG22	2:M:1026:GLY:HA2	1.83	0.60
2:M:1420:ILE:O	2:M:1424:ASN:ND2	2.35	0.60
2:M:2052:ARG:HE	2:M:2057:PRO:HG3	1.66	0.60
1:G:413:ILE:HD13	1:G:424:PHE:HE2	1.65	0.60
1:C:427:THR:HG22	1:C:438:LYS:HD3	1.83	0.60
2:M:1673:TYR:HE2	2:M:1686:LYS:HG3	1.65	0.60
1:B:442:SER:OG	1:B:445:LYS:NZ	2.35	0.60
1:E:467:ARG:NH2	2:I:1281:SER:O	2.29	0.60
1:H:382:TRP:CD2	1:H:426:CYS:HB3	2.36	0.60
3:J:14:CYS:HB2	3:J:102:THR:HG21	1.84	0.60
2:I:1093:CYS:SG	2:I:1094:LYS:N	2.73	0.60
1:L:533:THR:O	1:L:551:THR:OG1	2.19	0.60
1:G:461:ARG:HD3	1:G:465:ASN:HD21	1.67	0.59
3:J:36:ASN:ND2	1:L:563:ASN:OD1	2.35	0.59
1:L:450:HIS:ND1	1:L:480:SER:OG	2.30	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1417:ARG:NH2	2:M:1439:VAL:O	2.34	0.59
2:M:2023:GLU:OE2	2:M:2046:ARG:NH2	2.34	0.59
1:G:346:ARG:NE	1:G:370:THR:OG1	2.35	0.59
1:C:533:THR:HG1	1:C:551:THR:HG1	1.33	0.59
1:H:345:ILE:HG21	1:H:433:LEU:HD12	1.84	0.59
1:H:489:MET:O	1:H:535:THR:OG1	2.17	0.59
2:I:1516:LYS:HD2	2:I:1555:PHE:HB3	1.83	0.59
2:I:2030:ARG:HE	2:I:2031:GLY:H	1.49	0.59
1:G:374:THR:HA	1:G:405:PHE:HB2	1.84	0.59
2:M:2241:SER:HA	2:M:2244:TRP:NE1	2.18	0.59
1:B:381:SER:OG	1:B:427:THR:OG1	2.19	0.59
1:K:443:ARG:HH12	1:K:445:LYS:HD3	1.68	0.59
1:L:496:SER:OG	1:L:498:GLU:OE1	2.20	0.59
1:F:452:PRO:HB3	1:F:479:PHE:HB3	1.84	0.59
2:I:1514:GLU:O	2:I:1517:GLN:NE2	2.36	0.59
2:I:2107:ASP:HB2	2:I:2112:THR:HB	1.83	0.59
2:M:1413:TRP:NE1	2:M:1439:VAL:O	2.33	0.59
1:G:553:ASP:OD1	1:G:556:THR:OG1	2.17	0.59
2:I:2147:THR:HG23	2:I:2150:LYS:HE2	1.85	0.59
1:D:383:THR:HB	1:D:387:GLY:HA2	1.85	0.59
2:M:2076:SER:HB3	2:M:2158:CYS:HB2	1.85	0.58
2:I:1334:ASN:ND2	2:I:1339:LEU:O	2.36	0.58
1:A:547:VAL:HG11	3:J:113:VAL:HG21	1.85	0.58
1:C:419:ASN:O	1:C:443:ARG:NH2	2.35	0.58
1:F:457:LEU:HB2	1:F:473:THR:HB	1.85	0.58
3:J:103:TYR:HB2	1:L:574:THR:HA	1.84	0.58
2:M:1100:TYR:HA	2:M:1103:TRP:HD1	1.68	0.58
2:M:1724:PHE:HD2	2:M:1738:ARG:HG2	1.69	0.58
2:I:2055:ARG:NH2	2:I:2059:ASN:OD1	2.36	0.58
1:H:370:THR:HG22	1:H:406:SER:HB2	1.85	0.58
1:H:391:LYS:NZ	1:H:392:THR:O	2.34	0.58
2:M:1702:ILE:O	2:M:1738:ARG:NH1	2.37	0.58
1:G:384:ARG:NE	1:G:386:ASN:OD1	2.36	0.58
1:L:562:TYR:HB3	1:L:564:VAL:HG23	1.86	0.58
1:G:459:PRO:HG2	1:G:464:LEU:HD11	1.86	0.58
2:I:2041:ILE:O	2:I:2046:ARG:NH2	2.37	0.58
2:M:981:TYR:HE2	2:M:1099:CYS:HB3	1.68	0.58
1:C:381:SER:HA	1:C:393:HIS:HE1	1.68	0.58
1:C:491:ARG:NH2	1:C:532:GLU:OE1	2.36	0.58
2:M:2075:GLN:HE22	2:M:2156:MET:HA	1.69	0.58
1:B:549:GLU:O	1:B:550:ARG:NH1	2.30	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:GLU:O	1:G:406:SER:OG	2.21	0.57
2:I:2029:LEU:HD22	2:I:2115:LEU:HD12	1.85	0.57
2:I:2015:LYS:HB3	2:I:2078:GLY:HA2	1.87	0.57
1:K:454:VAL:HG21	1:K:538:VAL:HG11	1.86	0.57
2:I:1305:HIS:HE1	2:I:1422:LYS:HD2	1.69	0.57
2:M:1038:TRP:O	2:M:1041:GLU:HG3	2.03	0.57
2:I:1033:ASN:HB3	2:I:1949:LYS:HD2	1.86	0.57
2:M:1036:GLU:O	2:M:1039:ASN:HB3	2.03	0.57
2:M:2143:ASP:OD1	2:M:2144:TRP:N	2.38	0.57
2:M:2145:TRP:HE1	2:M:2178:THR:HA	1.68	0.57
1:F:393:HIS:ND1	1:F:408:VAL:O	2.38	0.57
2:I:1799:LEU:HD13	2:I:1859:MET:HG3	1.87	0.57
2:M:1219:CYS:N	2:M:1418:CYS:SG	2.78	0.57
1:A:500:TYR:HB3	1:A:521:LEU:HD13	1.87	0.57
1:B:450:HIS:CE1	1:B:514:ARG:HH21	2.23	0.57
3:J:129:THR:OG1	3:J:133:CYS:SG	2.59	0.57
1:L:558:LYS:HZ3	1:L:560:THR:HA	1.69	0.57
1:A:451:ARG:NH2	1:A:542:ALA:O	2.38	0.57
1:F:454:VAL:HG22	1:F:476:VAL:HG22	1.86	0.57
2:M:1293:LYS:NZ	2:M:1379:ILE:O	2.36	0.57
2:M:1757:ARG:HA	2:M:1760:VAL:HG22	1.87	0.56
2:M:2026:ASP:OD2	2:M:2030:ARG:NH2	2.37	0.56
1:D:527:GLU:O	1:D:530:THR:OG1	2.18	0.56
1:E:399:SER:HA	1:E:405:PHE:HA	1.86	0.56
2:I:1356:ASN:HD22	2:I:1449:GLN:HG2	1.69	0.56
2:I:2024:TRP:CD1	2:I:2043:PRO:HD3	2.40	0.56
2:M:1113:LYS:O	2:M:1117:ASN:ND2	2.38	0.56
1:E:452:PRO:HB3	1:E:479:PHE:HB3	1.86	0.56
1:H:536:CYS:N	1:H:549:GLU:OE2	2.37	0.56
2:I:1452:SER:O	2:I:1456:GLU:HG2	2.05	0.56
3:J:33:VAL:HB	1:L:559:PRO:HA	1.85	0.56
1:G:430:HIS:HB3	1:G:433:LEU:HD13	1.87	0.56
1:H:452:PRO:HB3	1:H:479:PHE:HB3	1.88	0.56
2:M:2200:GLN:HA	2:M:2203:LYS:HZ3	1.71	0.56
2:I:2181:PRO:HB3	2:I:2185:LEU:HD22	1.86	0.56
2:I:2024:TRP:HD1	2:I:2042:PRO:HA	1.70	0.56
2:M:2077:GLU:HA	2:M:2080:PHE:HB3	1.86	0.56
2:M:2236:TRP:O	2:M:2240:ARG:NH1	2.39	0.56
1:C:565:SER:O	1:C:567:VAL:HG23	2.06	0.56
1:E:383:THR:HA	1:E:389:ALA:HA	1.87	0.56
1:E:416:ASP:OD1	1:E:417:ASP:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1599:LYS:O	2:I:1672:GLN:NE2	2.39	0.56
2:I:1856:TRP:HA	2:I:1859:MET:SD	2.46	0.56
2:M:1043:GLN:O	2:M:1046:ILE:HG22	2.06	0.56
2:I:1122:ARG:NH1	2:I:1125:GLN:OE1	2.39	0.56
1:D:423:ARG:HA	1:D:442:SER:HB3	1.88	0.55
1:G:382:TRP:HB2	1:G:390:VAL:HG21	1.87	0.55
1:G:486:VAL:HG12	1:G:538:VAL:HG23	1.88	0.55
1:K:391:LYS:NZ	1:K:392:THR:O	2.35	0.55
2:M:2213:VAL:HG12	2:M:2214:THR:HG23	1.88	0.55
2:M:1122:ARG:NH1	2:M:1139:VAL:O	2.39	0.55
2:M:1151:GLU:HA	2:M:1154:ILE:HG22	1.88	0.55
2:M:1100:TYR:HA	2:M:1103:TRP:CD1	2.41	0.55
1:E:459:PRO:HD3	1:E:472:ILE:HG13	1.87	0.55
3:J:4:ARG:NH2	3:J:18:THR:O	2.40	0.55
2:M:1421:THR:HA	2:M:1424:ASN:HD21	1.72	0.55
2:M:2075:GLN:HA	2:M:2079:LYS:H	1.72	0.55
2:M:2125:ILE:HG22	2:M:2129:ARG:NH1	2.22	0.55
2:M:2142:GLU:O	2:M:2146:LYS:N	2.34	0.55
2:I:1644:GLU:OE2	2:I:1719:LYS:NZ	2.39	0.55
2:M:1850:ASN:HD22	2:M:1853:ARG:HH12	1.55	0.55
2:I:978:ARG:NH2	2:I:1099:CYS:SG	2.72	0.55
2:M:1701:ILE:HG22	2:M:1706:ASP:HB2	1.88	0.55
2:I:1154:ILE:HG21	2:I:1164:LYS:HE2	1.89	0.55
1:K:465:ASN:HA	1:K:467:ARG:NH1	2.22	0.55
1:D:383:THR:OG1	1:D:425:THR:OG1	2.25	0.55
1:D:402:ASN:OD1	1:D:404:THR:OG1	2.21	0.55
1:H:503:SER:OG	1:H:504:ALA:N	2.40	0.55
2:M:2095:LEU:HD22	2:M:2172:TRP:HD1	1.72	0.55
1:C:369:VAL:HG11	1:C:428:VAL:HG21	1.88	0.54
2:M:1871:ASN:ND2	2:M:1877:GLY:O	2.38	0.54
2:I:1041:GLU:O	2:I:1045:GLN:N	2.38	0.54
1:K:374:THR:HA	1:K:405:PHE:HB2	1.89	0.54
2:M:1421:THR:HG22	2:M:1433:ASN:HA	1.89	0.54
1:C:400:HIS:CD2	1:C:406:SER:HB3	2.42	0.54
1:C:567:VAL:HG12	1:C:567:VAL:O	2.07	0.54
1:F:489:MET:HB3	1:F:535:THR:OG1	2.08	0.54
2:M:1821:CYS:O	2:M:1957:HIS:NE2	2.40	0.54
2:M:2036:HIS:CE1	2:M:2250:ARG:HH22	2.25	0.54
2:M:2107:ASP:HB3	2:M:2112:THR:HB	1.88	0.54
2:I:1151:GLU:HA	2:I:1154:ILE:HG22	1.89	0.54
1:K:353:SER:O	1:K:357:ILE:HG12	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2015:LYS:HB3	2:M:2078:GLY:HA2	1.88	0.54
1:A:459:PRO:HG3	1:A:470:ALA:HB1	1.89	0.54
3:J:57:ARG:NH2	3:J:59:ARG:O	2.40	0.54
2:M:1719:LYS:O	2:M:1723:ILE:HG12	2.06	0.54
2:I:1183:ASN:HB2	2:I:1186:HIS:HB3	1.90	0.54
2:M:1473:ARG:O	2:M:1477:THR:OG1	2.19	0.54
2:I:971:ASN:OD1	2:I:974:THR:OG1	2.26	0.54
2:I:1792:LYS:O	2:I:1797:ARG:NH1	2.41	0.54
2:M:1227:ILE:HD11	2:M:1302:ASN:HB3	1.90	0.54
2:M:2016:THR:HG21	2:M:2081:LEU:HD22	1.90	0.54
1:E:489:MET:HB3	1:E:535:THR:OG1	2.08	0.54
2:I:1605:TRP:CE2	2:I:1626:PRO:HD3	2.43	0.54
2:M:978:ARG:HH12	2:M:1095:GLU:HB2	1.73	0.54
1:E:393:HIS:HB3	1:E:410:GLU:H	1.73	0.54
1:H:393:HIS:HB2	1:H:410:GLU:HG3	1.88	0.54
2:I:1895:ARG:NH2	2:I:1904:TYR:O	2.40	0.53
2:M:1985:LEU:HB2	2:M:2149:LYS:HE3	1.90	0.53
2:I:1349:ARG:NH1	2:I:1456:GLU:OE1	2.41	0.53
2:M:1955:SER:HA	2:M:1958:LYS:HD3	1.89	0.53
1:B:535:THR:HG22	1:B:551:THR:HG23	1.89	0.53
1:H:345:ILE:N	1:H:371:ASP:O	2.42	0.53
2:I:2044:ARG:HH12	2:I:2100:ASN:HB2	1.72	0.53
2:I:2241:SER:HA	2:I:2244:TRP:CH2	2.44	0.53
1:L:503:SER:OG	1:L:504:ALA:N	2.41	0.53
2:M:1786:GLU:OE2	2:M:1787:HIS:ND1	2.41	0.53
1:B:383:THR:OG1	1:B:425:THR:OG1	2.26	0.53
2:I:1399:GLU:HG2	2:I:1401:VAL:HG22	1.89	0.53
2:I:2025:ASN:HA	2:I:2040:LEU:HD22	1.91	0.53
1:A:499:LYS:NZ	1:A:522:THR:O	2.41	0.53
1:D:380:ILE:HD13	1:D:407:ALA:HB1	1.89	0.53
1:D:433:LEU:HD21	1:D:437:LEU:HB2	1.90	0.53
2:I:1114:GLN:HA	2:I:1117:ASN:HD21	1.73	0.53
1:E:524:SER:OG	1:E:526:GLU:OE1	2.26	0.53
1:F:347:VAL:HG22	1:F:369:VAL:HG13	1.91	0.53
1:H:543:LEU:HD13	1:H:548:THR:HG23	1.91	0.53
2:I:2064:ASN:HB3	2:I:2067:LYS:HE3	1.90	0.53
3:J:46:ARG:NH1	3:J:51:ASP:O	2.30	0.53
1:K:480:SER:HB3	1:K:514:ARG:HE	1.74	0.53
1:B:380:ILE:HG23	1:B:428:VAL:HG12	1.91	0.53
2:M:1853:ARG:HE	2:M:1948:ASN:HA	1.72	0.53
1:C:450:HIS:HB2	1:C:480:SER:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:ILE:HG21	1:F:409:GLY:HA3	1.90	0.53
2:I:1345:HIS:C	2:I:1349:ARG:HE	2.13	0.53
2:I:1497:ILE:O	2:I:1498:GLN:NE2	2.34	0.53
2:I:2134:GLU:HG2	2:I:2136:ASN:H	1.74	0.53
3:J:4:ARG:HE	3:J:18:THR:HG23	1.74	0.53
1:B:532:GLU:HB3	1:B:534:TYR:CZ	2.44	0.53
1:H:393:HIS:HB3	1:H:410:GLU:H	1.73	0.53
2:I:1143:ASN:HB3	2:I:1973:LEU:HD21	1.91	0.53
2:I:1425:LYS:HA	2:I:1431:ILE:HG12	1.91	0.53
1:B:543:LEU:HB2	1:B:546:ARG:HA	1.91	0.52
2:I:2233:TYR:HA	2:I:2236:TRP:NE1	2.24	0.52
1:K:489:MET:HB3	1:K:535:THR:OG1	2.08	0.52
2:M:1143:ASN:HB3	2:M:1973:LEU:HD11	1.91	0.52
2:M:1681:ASP:OD1	2:M:1682:ASP:N	2.40	0.52
1:E:396:ILE:HG23	1:E:407:ALA:HA	1.91	0.52
1:G:503:SER:OG	1:G:504:ALA:N	2.42	0.52
2:I:1580:LYS:O	2:I:1590:LYS:NZ	2.42	0.52
2:M:1154:ILE:HG21	2:M:1164:LYS:HE2	1.91	0.52
2:M:1740:ASP:OD1	2:M:1741:TRP:N	2.42	0.52
2:M:2247:ILE:HA	2:M:2250:ARG:NE	2.24	0.52
1:E:398:GLU:O	1:E:406:SER:OG	2.23	0.52
2:I:2137:ASN:OD1	2:I:2139:LYS:NZ	2.42	0.52
3:J:4:ARG:NH2	3:J:36:ASN:HB2	2.24	0.52
1:B:503:SER:HG	1:B:518:HIS:H	1.58	0.52
2:M:2017:LYS:HE3	2:M:2047:GLN:HB3	1.92	0.52
1:G:365:LEU:HB2	1:G:411:ALA:HB3	1.92	0.52
1:K:463:GLN:NE2	1:K:469:SER:O	2.43	0.52
2:M:1147:PHE:CE1	2:M:1969:VAL:HG22	2.44	0.52
2:M:1193:GLU:O	2:M:1197:ASN:ND2	2.42	0.52
2:M:1572:SER:OG	2:M:1573:ILE:N	2.41	0.52
1:C:393:HIS:CD2	1:C:409:GLY:HA2	2.45	0.52
1:D:475:LEU:HD12	1:D:518:HIS:HE2	1.75	0.52
1:F:347:VAL:HG13	1:F:369:VAL:HG22	1.92	0.52
2:I:1681:ASP:O	2:I:1685:LYS:HG2	2.10	0.52
1:H:383:THR:HB	1:H:387:GLY:HA2	1.92	0.52
2:I:1639:ILE:O	2:I:1643:ASN:ND2	2.43	0.52
2:I:1655:LEU:HD12	2:I:1658:LEU:HD11	1.91	0.52
2:M:1354:TYR:O	2:M:1358:ILE:HG23	2.09	0.52
1:F:530:THR:OG1	2:M:1238:LYS:NZ	2.41	0.51
2:I:2015:LYS:HG3	2:I:2077:GLU:HB3	1.91	0.51
2:M:1356:ASN:HD22	2:M:1449:GLN:HG2	1.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2060:LEU:HB2	2:I:2127:LEU:HD12	1.92	0.51
2:I:2095:LEU:HD13	2:I:2172:TRP:CD1	2.44	0.51
2:M:1381:GLU:OE1	2:M:1400:ASN:ND2	2.44	0.51
2:I:1627:ARG:NH1	2:I:1697:ASP:OD2	2.43	0.51
1:H:569:SER:OG	1:H:569:SER:O	2.29	0.51
2:I:1399:GLU:N	2:I:1402:ASN:OD1	2.44	0.51
2:M:2080:PHE:HB2	2:M:2162:LYS:HG3	1.93	0.51
2:M:2175:ILE:HD12	2:M:2176:PRO:HD2	1.92	0.51
1:L:488:TRP:HB3	1:L:495:LEU:HD12	1.93	0.51
2:M:1710:ASP:OD1	2:M:1713:THR:OG1	2.27	0.51
1:C:367:CYS:HB2	1:C:382:TRP:CZ2	2.46	0.51
1:D:503:SER:OG	1:D:504:ALA:N	2.43	0.51
2:I:1421:THR:HA	2:I:1424:ASN:HD21	1.76	0.51
2:I:1457:TRP:NE1	2:I:1518:GLU:OE1	2.36	0.51
2:I:2118:ILE:HA	2:I:2121:LYS:HZ3	1.74	0.51
2:I:2129:ARG:NH2	2:I:2135:THR:HG22	2.25	0.51
2:M:2244:TRP:O	2:M:2247:ILE:HG22	2.11	0.51
1:G:416:ASP:OD1	1:G:417:ASP:N	2.44	0.51
1:G:466:LEU:HD11	2:I:2056:GLY:HA3	1.92	0.51
3:J:4:ARG:NH2	3:J:18:THR:HG23	2.21	0.51
3:J:29:ASN:HD22	1:L:529:ASN:HD22	1.57	0.51
1:C:346:ARG:NE	1:C:370:THR:OG1	2.42	0.51
1:C:489:MET:HB3	1:C:535:THR:HG23	1.92	0.51
2:I:1147:PHE:CE2	2:I:1969:VAL:HG22	2.46	0.51
2:I:1975:GLU:HA	2:I:1978:ASN:HD21	1.75	0.51
1:B:486:VAL:HG12	1:B:538:VAL:HG23	1.92	0.51
1:K:568:MET:HA	1:L:568:MET:SD	2.51	0.51
2:M:1443:THR:OG1	2:M:1445:ASN:OD1	2.20	0.51
1:A:467:ARG:HD2	1:A:525:GLU:HG3	1.92	0.51
1:E:384:ARG:HD2	1:E:388:GLU:HB2	1.93	0.51
1:H:380:ILE:HG13	1:H:428:VAL:HG22	1.92	0.51
1:K:563:ASN:HB3	1:L:563:ASN:HA	1.93	0.51
1:K:383:THR:HG22	1:K:390:VAL:HG11	1.93	0.50
2:M:1582:TYR:HB2	2:M:1590:LYS:HD3	1.92	0.50
1:G:467:ARG:HA	1:G:525:GLU:HG3	1.93	0.50
2:I:1305:HIS:CE1	2:I:1422:LYS:HD2	2.46	0.50
2:I:1249:TRP:HB3	2:I:1264:CYS:HB3	1.92	0.50
1:K:352:PRO:HB2	1:K:357:ILE:HD11	1.92	0.50
2:M:1723:ILE:HG13	2:M:1724:PHE:N	2.27	0.50
2:M:2169:ASP:OD1	2:M:2169:ASP:N	2.44	0.50
1:A:459:PRO:HB3	1:A:471:THR:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2015:LYS:HE2	2:I:2077:GLU:HB2	1.92	0.50
1:A:553:ASP:H	1:A:556:THR:HG22	1.77	0.50
1:F:467:ARG:HB2	1:F:467:ARG:NH1	2.25	0.50
1:G:484:VAL:HG12	1:G:540:HIS:CD2	2.47	0.50
2:I:1772:VAL:HG13	2:I:1777:GLU:HG3	1.94	0.50
1:K:496:SER:HB3	1:K:499:LYS:HD3	1.93	0.50
2:M:1723:ILE:HG13	2:M:1724:PHE:H	1.77	0.50
2:I:1671:LYS:HD3	2:I:1775:LYS:HE2	1.94	0.50
2:I:2169:ASP:N	2:I:2169:ASP:OD1	2.44	0.50
2:M:1452:SER:O	2:M:1456:GLU:HG2	2.11	0.50
2:M:2123:ILE:O	2:M:2127:LEU:HD23	2.12	0.50
1:E:443:ARG:O	1:E:445:LYS:NZ	2.45	0.50
2:I:1839:LYS:HB2	2:I:1964:VAL:HG21	1.93	0.50
1:D:384:ARG:HG2	1:D:385:GLN:H	1.75	0.50
2:I:1097:CYS:SG	2:I:1101:LYS:NZ	2.84	0.50
2:M:2183:GLN:HA	2:M:2186:ARG:HB3	1.92	0.50
1:D:382:TRP:HB2	1:D:390:VAL:HG21	1.94	0.50
1:K:465:ASN:OD1	1:K:466:LEU:HD12	2.11	0.50
2:M:1838:CYS:SG	2:M:1960:LYS:NZ	2.82	0.50
1:B:491:ARG:NH2	2:M:2055:ARG:HG2	2.27	0.49
1:D:466:LEU:HG	1:D:468:GLU:OE1	2.12	0.49
1:G:347:VAL:HG23	1:G:369:VAL:HG22	1.94	0.49
2:I:1768:VAL:O	2:I:1772:VAL:HG23	2.12	0.49
2:I:2188:ILE:O	2:I:2192:GLY:N	2.41	0.49
1:K:553:ASP:O	1:K:556:THR:OG1	2.26	0.49
2:M:2222:GLU:HG3	2:M:2224:ASN:H	1.77	0.49
1:F:454:VAL:HG21	1:F:538:VAL:HG11	1.92	0.49
2:I:1570:TYR:C	2:I:1572:SER:H	2.15	0.49
1:K:378:VAL:HG12	1:K:430:HIS:CD2	2.41	0.49
2:M:1349:ARG:NE	2:M:1456:GLU:OE2	2.45	0.49
1:G:457:LEU:HB2	1:G:473:THR:OG1	2.13	0.49
2:I:1896:CYS:O	2:I:1907:CYS:HB2	2.13	0.49
1:K:484:VAL:HG12	1:K:540:HIS:CD2	2.47	0.49
2:M:2186:ARG:NH1	2:M:2190:GLU:HB2	2.28	0.49
1:B:463:GLN:NE2	1:B:469:SER:O	2.46	0.49
2:I:1177:ILE:HD11	2:I:1980:ILE:HD11	1.93	0.49
2:I:1411:GLU:N	2:I:1411:GLU:OE1	2.41	0.49
1:K:461:ARG:NH1	1:K:465:ASN:HB3	2.28	0.49
1:E:345:ILE:HG13	1:E:372:LEU:HG	1.95	0.49
2:M:1345:HIS:HB3	2:M:1349:ARG:CZ	2.43	0.49
2:M:2152:ILE:HG12	2:M:2175:ILE:HG22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:454:VAL:HG21	1:H:538:VAL:HG11	1.95	0.49
2:I:1365:ILE:HG13	2:I:1366:TYR:N	2.28	0.49
2:I:1457:TRP:CH2	2:I:1519:TRP:HB2	2.48	0.49
2:M:1497:ILE:HB	2:M:1502:LYS:HB3	1.95	0.49
1:F:416:ASP:N	1:F:416:ASP:OD1	2.46	0.49
1:L:485:PHE:HB2	1:L:539:ALA:HB3	1.93	0.49
2:M:2188:ILE:O	2:M:2192:GLY:N	2.42	0.49
1:F:430:HIS:CD2	1:F:432:ASP:H	2.31	0.49
2:I:2076:SER:OG	2:I:2077:GLU:N	2.46	0.49
1:L:540:HIS:H	1:L:543:LEU:HD12	1.77	0.49
2:M:1045:GLN:HB3	2:M:1049:TYR:CE2	2.47	0.49
2:I:2075:GLN:NE2	2:I:2155:ALA:O	2.46	0.49
2:I:2126:LYS:NZ	2:I:2130:LEU:HD11	2.27	0.49
2:I:2196:CYS:O	2:I:2199:LYS:HG2	2.13	0.49
1:C:503:SER:OG	1:C:504:ALA:N	2.46	0.49
1:G:490:GLN:HE22	1:G:534:TYR:HE1	1.58	0.49
2:I:1601:ASN:OD1	2:I:1672:GLN:NE2	2.45	0.49
2:M:1444:GLY:HA2	2:M:1447:GLU:HG3	1.95	0.49
2:M:2193:THR:HA	2:M:2196:CYS:SG	2.53	0.49
1:A:452:PRO:HD3	1:A:542:ALA:HB3	1.95	0.48
2:I:1572:SER:OG	2:I:1573:ILE:N	2.32	0.48
1:L:488:TRP:CZ3	1:L:536:CYS:HB3	2.47	0.48
1:D:491:ARG:HH21	1:D:532:GLU:HG2	1.78	0.48
1:H:382:TRP:HB2	1:H:390:VAL:HG21	1.94	0.48
2:I:1681:ASP:N	2:I:1681:ASP:OD1	2.44	0.48
2:I:2049:CYS:O	2:I:2070:ILE:HD12	2.14	0.48
2:M:1981:LYS:HD3	2:M:1984:LYS:HZ3	1.77	0.48
2:M:2064:ASN:HB3	2:M:2067:LYS:HD3	1.95	0.48
2:I:1193:GLU:O	2:I:1196:LYS:HB2	2.13	0.48
1:L:491:ARG:NH1	1:L:532:GLU:O	2.46	0.48
2:M:2251:TYR:O	2:M:2252:LYS:HE2	2.13	0.48
1:H:357:ILE:HG12	1:H:363:THR:HB	1.96	0.48
2:M:1972:GLN:O	2:M:1975:GLU:HG3	2.13	0.48
1:E:475:LEU:HD13	1:E:518:HIS:CD2	2.49	0.48
1:H:560:THR:HG22	1:K:559:PRO:HA	1.95	0.48
2:I:1114:GLN:HA	2:I:1117:ASN:ND2	2.29	0.48
2:I:2210:CYS:HB3	2:I:2226:CYS:HB3	1.71	0.48
3:J:43:LEU:HD22	1:L:570:ASP:HB2	1.94	0.48
1:L:532:GLU:O	1:L:533:THR:HG22	2.14	0.48
2:M:1182:ASN:HB3	2:M:1186:HIS:HE1	1.77	0.48
2:M:1977:ASP:HA	2:M:1980:ILE:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HG21	1:A:481:PRO:HB3	1.96	0.48
1:E:425:THR:OG1	1:E:440:THR:HG22	2.13	0.48
1:G:381:SER:HA	1:G:393:HIS:HE1	1.77	0.48
2:I:1658:LEU:HA	2:I:1661:VAL:HG12	1.96	0.48
2:I:1735:LYS:HE2	2:I:1738:ARG:HD3	1.95	0.48
2:I:2132:GLU:HG2	2:I:2138:THR:HA	1.95	0.48
2:M:1029:VAL:O	2:M:1032:PHE:HB3	2.14	0.48
2:M:1154:ILE:HD12	2:M:1158:PHE:HD2	1.79	0.48
2:I:1356:ASN:ND2	2:I:1449:GLN:HG2	2.29	0.48
2:M:2103:TYR:HB3	2:M:2186:ARG:HE	1.77	0.48
1:B:525:GLU:O	1:B:529:ASN:ND2	2.46	0.48
1:G:429:THR:HG23	1:G:436:PRO:HG3	1.95	0.48
2:I:2213:VAL:O	2:I:2214:THR:OG1	2.31	0.48
3:J:43:LEU:HB3	1:L:570:ASP:HA	1.95	0.48
3:J:106:ASN:OD1	3:J:107:LYS:N	2.47	0.48
1:K:415:GLU:O	1:K:419:ASN:ND2	2.47	0.48
2:M:1254:THR:OG1	2:M:1258:GLY:O	2.25	0.48
2:M:1611:LYS:HB3	2:M:1709:HIS:CG	2.48	0.48
1:B:382:TRP:CZ2	1:B:426:CYS:HB2	2.49	0.47
1:D:379:THR:HB	1:D:429:THR:HB	1.96	0.47
1:E:461:ARG:O	1:E:461:ARG:NH1	2.46	0.47
2:I:1102:LEU:HD23	2:I:1106:LYS:HD3	1.95	0.47
2:I:1269:THR:O	2:I:1272:LEU:HB2	2.14	0.47
2:M:1844:ASN:HA	2:M:1847:ASN:HD21	1.79	0.47
2:M:1853:ARG:NE	2:M:1947:LEU:O	2.47	0.47
1:B:425:THR:HG22	1:B:440:THR:HG22	1.96	0.47
1:C:467:ARG:HA	1:C:525:GLU:OE2	2.14	0.47
1:E:348:PHE:O	1:E:367:CYS:HA	2.14	0.47
1:G:413:ILE:HD12	1:G:417:ASP:HB2	1.95	0.47
2:M:2124:LYS:NZ	2:M:2125:ILE:HG12	2.28	0.47
2:I:1506:GLU:HB3	2:I:1510:LYS:NZ	2.29	0.47
1:K:393:HIS:CD2	1:K:396:ILE:HD11	2.50	0.47
2:M:2079:LYS:NZ	2:M:2098:MET:SD	2.88	0.47
1:E:391:LYS:NZ	1:E:392:THR:O	2.36	0.47
1:G:400:HIS:HB2	1:G:404:THR:HB	1.96	0.47
2:M:1590:LYS:HB2	2:M:1664:ARG:HH22	1.79	0.47
1:B:423:ARG:HA	1:B:441:ILE:O	2.14	0.47
1:G:466:LEU:HD12	2:I:2058:ALA:H	1.79	0.47
2:I:1602:ASP:N	2:I:1602:ASP:OD1	2.48	0.47
1:G:552:VAL:HG23	1:G:556:THR:HG21	1.97	0.47
2:I:1381:GLU:O	2:I:1382:LYS:NZ	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1581:TYR:HB2	2:I:1660:ILE:HD11	1.97	0.47
2:I:2232:LYS:O	2:I:2235:GLU:HG2	2.15	0.47
2:M:1292:THR:H	2:M:1295:LEU:HD12	1.80	0.47
2:M:1843:ALA:O	2:M:1847:ASN:ND2	2.48	0.47
2:M:2063:LEU:HB2	2:M:2065:GLU:OE2	2.15	0.47
1:B:449:LEU:HD22	1:B:481:PRO:HD3	1.97	0.47
1:B:514:ARG:HD3	1:B:514:ARG:HA	1.71	0.47
1:B:518:HIS:HD2	1:B:520:ILE:HD11	1.80	0.47
1:F:384:ARG:NH1	1:F:388:GLU:OE1	2.47	0.47
1:G:413:ILE:HD13	1:G:424:PHE:CE2	2.49	0.47
2:I:1977:ASP:OD1	2:I:1978:ASN:N	2.48	0.47
2:M:1639:ILE:HD13	2:M:1657:THR:HG21	1.96	0.47
1:E:496:SER:OG	1:E:498:GLU:OE1	2.26	0.47
2:I:1504:LYS:HA	2:I:1507:LYS:HD2	1.97	0.47
3:J:113:VAL:HG13	3:J:126:THR:HG21	1.97	0.47
2:M:1497:ILE:HD13	2:M:1501:CYS:HB3	1.97	0.47
2:M:2240:ARG:HA	2:M:2243:GLN:HG3	1.96	0.47
1:B:417:ASP:O	1:B:420:SER:OG	2.33	0.47
1:C:466:LEU:HB2	1:C:468:GLU:OE1	2.14	0.47
1:F:456:LEU:HD11	1:F:536:CYS:SG	2.55	0.47
1:H:456:LEU:HD13	1:H:550:ARG:HB2	1.97	0.47
1:D:457:LEU:HB2	1:D:473:THR:OG1	2.15	0.47
1:F:417:ASP:OD1	1:F:418:TRP:N	2.47	0.47
2:M:1868:ARG:HA	2:M:1881:SER:HA	1.97	0.47
1:K:379:THR:HB	1:K:429:THR:OG1	2.15	0.46
1:H:345:ILE:HG12	1:H:372:LEU:HD23	1.97	0.46
2:I:1592:ASN:HB3	2:I:1595:LEU:HB2	1.97	0.46
2:M:2066:PHE:CE2	2:M:2070:ILE:HD11	2.50	0.46
1:E:356:SER:O	1:E:360:THR:OG1	2.25	0.46
2:I:2205:TYR:OH	2:I:2229:GLU:OE1	2.33	0.46
2:M:1960:LYS:O	2:M:1963:GLU:HG3	2.15	0.46
1:A:451:ARG:HH22	1:A:544:PRO:HD3	1.80	0.46
1:F:419:ASN:O	1:F:443:ARG:NH2	2.43	0.46
2:I:1260:THR:HG22	2:I:1262:GLY:H	1.81	0.46
2:I:2041:ILE:HD12	2:I:2042:PRO:HD2	1.98	0.46
1:K:383:THR:N	1:K:425:THR:O	2.42	0.46
2:M:987:CYS:HA	2:M:1005:CYS:HA	1.98	0.46
2:M:1556:ASN:ND2	2:M:1561:TYR:HB3	2.30	0.46
2:M:2045:ARG:NE	2:M:2113:ASP:OD2	2.48	0.46
1:B:512:PRO:O	1:B:514:ARG:N	2.39	0.46
1:D:541:GLU:OE1	1:D:541:GLU:N	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:ARG:HA	1:E:442:SER:HB3	1.97	0.46
1:F:456:LEU:HD23	1:F:552:VAL:HG12	1.96	0.46
2:M:1506:GLU:HB3	2:M:1510:LYS:NZ	2.31	0.46
1:E:457:LEU:HB2	1:E:473:THR:OG1	2.15	0.46
2:I:1291:ASP:OD1	2:I:1292:THR:N	2.48	0.46
1:L:462:GLU:HA	1:L:465:ASN:ND2	2.31	0.46
2:M:1278:TRP:HB2	2:M:1372:LEU:HD21	1.97	0.46
1:B:375:TYR:HE2	1:B:431:THR:HB	1.81	0.46
1:C:384:ARG:HH21	1:C:386:ASN:HB2	1.79	0.46
1:H:366:THR:HG23	1:H:410:GLU:HB3	1.97	0.46
2:I:1038:TRP:O	2:I:1041:GLU:HG3	2.15	0.46
2:I:1971:GLU:OE1	2:I:1972:GLN:NE2	2.46	0.46
1:L:552:VAL:HG13	1:L:556:THR:HB	1.97	0.46
2:I:970:THR:OG1	2:I:971:ASN:N	2.49	0.46
1:B:525:GLU:HA	1:B:528:TRP:HB3	1.97	0.46
1:D:465:ASN:O	1:D:467:ARG:HG3	2.16	0.46
2:M:1420:ILE:HA	2:M:1423:ILE:HG22	1.98	0.46
2:M:2189:LYS:O	2:M:2193:THR:N	2.32	0.46
1:G:418:TRP:O	1:G:443:ARG:HD3	2.16	0.45
2:I:1559:ILE:O	2:I:1563:THR:HG22	2.16	0.45
2:M:1664:ARG:HD2	2:M:1668:TYR:CZ	2.51	0.45
1:B:348:PHE:HD2	1:B:368:LEU:HD11	1.81	0.45
2:M:2202:HIS:HA	2:M:2205:TYR:CD2	2.50	0.45
1:B:378:VAL:HG22	1:B:430:HIS:ND1	2.31	0.45
1:C:490:GLN:HB2	1:C:495:LEU:HD11	1.97	0.45
1:G:450:HIS:CD2	1:G:514:ARG:HH21	2.34	0.45
2:I:1189:GLU:O	2:I:1192:SER:HB3	2.17	0.45
2:I:1346:ALA:N	2:I:1349:ARG:HH21	2.14	0.45
2:I:1420:ILE:HA	2:I:1423:ILE:HG22	1.98	0.45
2:I:2114:MET:SD	2:I:2114:MET:N	2.87	0.45
3:J:46:ARG:CZ	3:J:52:PRO:HA	2.47	0.45
1:A:538:VAL:HG12	1:A:548:THR:H	1.82	0.45
2:I:2193:THR:HA	2:I:2196:CYS:SG	2.56	0.45
1:A:449:LEU:HB3	1:A:542:ALA:HA	1.98	0.45
1:F:348:PHE:HE1	1:F:370:THR:HG22	1.82	0.45
1:H:421:GLY:HA2	1:H:443:ARG:HD2	1.97	0.45
2:I:1349:ARG:HH11	2:I:1456:GLU:HG3	1.82	0.45
2:I:1691:ILE:HD11	2:I:1783:MET:HG3	1.98	0.45
2:I:1715:TYR:O	2:I:1719:LYS:HG2	2.17	0.45
3:J:57:ARG:HB3	3:J:60:PHE:CE2	2.51	0.45
2:M:1376:ILE:HA	2:M:1379:ILE:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2181:PRO:HB2	2:M:2186:ARG:HB2	1.98	0.45
1:A:549:GLU:O	1:A:550:ARG:NH1	2.43	0.45
1:C:484:VAL:HG12	1:C:540:HIS:CD2	2.51	0.45
1:F:364:LYS:NZ	1:F:412:SER:OG	2.35	0.45
1:G:400:HIS:NE2	1:G:406:SER:HB3	2.32	0.45
2:I:2129:ARG:HH22	2:I:2135:THR:HG22	1.82	0.45
2:M:1027:ASN:O	2:M:1030:THR:OG1	2.28	0.45
2:M:1039:ASN:OD1	2:M:1043:GLN:NE2	2.46	0.45
2:M:1949:LYS:HB2	2:M:1954:TYR:CE2	2.51	0.45
1:C:399:SER:HA	1:C:405:PHE:HA	1.97	0.45
1:D:378:VAL:HG22	1:D:430:HIS:CE1	2.51	0.45
1:D:530:THR:OG1	1:D:532:GLU:OE2	2.34	0.45
1:G:384:ARG:HB2	1:G:422:GLU:HG2	1.99	0.45
1:H:466:LEU:HD23	1:H:466:LEU:H	1.82	0.45
2:M:2051:SER:OG	2:M:2052:ARG:NH1	2.50	0.45
1:A:535:THR:OG1	1:A:549:GLU:OE1	2.22	0.45
1:B:347:VAL:HG22	1:B:369:VAL:HG13	1.99	0.45
1:C:400:HIS:N	1:C:404:THR:O	2.50	0.45
1:D:456:LEU:HD23	1:D:550:ARG:HB2	1.99	0.45
1:D:535:THR:HB	1:D:551:THR:HG22	1.99	0.45
1:G:549:GLU:OE1	1:G:549:GLU:N	2.50	0.45
2:I:1039:ASN:O	2:I:1043:GLN:NE2	2.50	0.45
2:I:1583:LYS:HG3	2:I:1584:TYR:H	1.82	0.45
2:M:1514:GLU:HG2	2:M:1515:LYS:N	2.32	0.45
2:M:1965:TYR:O	2:M:1969:VAL:HG23	2.17	0.45
1:D:568:MET:SD	1:D:568:MET:N	2.86	0.45
1:E:535:THR:HG22	1:E:551:THR:HB	1.98	0.45
3:J:134:TYR:HD1	3:J:135:PRO:HD2	1.81	0.45
1:B:384:ARG:HA	1:B:424:PHE:HD1	1.83	0.45
1:E:423:ARG:HB3	1:E:440:THR:HB	1.98	0.45
1:E:509:PRO:HD3	1:F:501:VAL:HG21	1.99	0.45
2:I:1544:PRO:HA	2:I:1547:ILE:HD11	1.99	0.45
1:K:478:GLY:HA2	1:K:514:ARG:HB3	1.99	0.45
2:M:1100:TYR:OH	2:M:1198:ALA:O	2.29	0.45
2:M:1783:MET:O	2:M:1783:MET:HG2	2.17	0.45
1:B:382:TRP:HB3	1:B:384:ARG:NH2	2.28	0.44
1:C:523:VAL:HG11	1:C:534:TYR:CE2	2.52	0.44
2:I:979:LYS:HD3	2:I:1865:LYS:HD2	1.98	0.44
2:M:1352:ILE:HD11	2:M:1442:PRO:HB2	1.98	0.44
2:M:1515:LYS:HA	2:M:1518:GLU:HG3	1.99	0.44
2:M:1515:LYS:HD2	2:M:1518:GLU:OE2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2035:LYS:HG3	2:M:2036:HIS:H	1.82	0.44
1:A:467:ARG:HH12	1:A:529:ASN:HD21	1.64	0.44
1:D:393:HIS:HA	1:D:410:GLU:HG2	1.98	0.44
1:D:491:ARG:HA	1:D:533:THR:HG21	2.00	0.44
1:E:374:THR:OG1	1:E:403:ALA:O	2.35	0.44
2:I:1692:ARG:NH1	2:I:1902:GLY:O	2.51	0.44
2:I:1843:ALA:O	2:I:1847:ASN:ND2	2.50	0.44
1:L:566:LEU:HD23	1:L:566:LEU:H	1.82	0.44
2:I:1611:LYS:HD2	2:I:1709:HIS:HE1	1.82	0.44
2:I:2054:VAL:HG23	2:I:2123:ILE:HD12	1.98	0.44
2:M:1362:SER:O	2:M:1362:SER:OG	2.33	0.44
2:M:1516:LYS:NZ	2:M:1555:PHE:O	2.35	0.44
2:M:1570:TYR:C	2:M:1572:SER:H	2.20	0.44
2:M:2124:LYS:HG3	2:M:2125:ILE:N	2.32	0.44
1:B:345:ILE:HA	1:B:371:ASP:HB3	2.00	0.44
1:B:433:LEU:O	1:B:433:LEU:HD12	2.18	0.44
2:I:1367:GLU:OE1	2:I:1368:HIS:ND1	2.51	0.44
2:I:1742:TRP:CE2	2:I:1757:ARG:HB3	2.52	0.44
1:K:558:LYS:HE2	1:K:558:LYS:HA	1.99	0.44
2:M:1454:PHE:HD1	2:M:1522:GLN:HG2	1.82	0.44
2:M:1813:TYR:O	2:M:1817:MET:HG2	2.18	0.44
2:M:1853:ARG:HH22	2:M:1949:LYS:HZ1	1.65	0.44
2:M:2233:TYR:HA	2:M:2236:TRP:CD1	2.52	0.44
1:B:491:ARG:NH1	1:B:532:GLU:OE2	2.51	0.44
1:H:382:TRP:CE2	1:H:426:CYS:HB3	2.52	0.44
2:I:2030:ARG:NE	2:I:2031:GLY:H	2.14	0.44
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.88	0.44
1:C:383:THR:HG22	1:C:389:ALA:HA	2.00	0.44
1:E:385:GLN:HB3	1:E:422:GLU:HG3	1.99	0.44
1:E:512:PRO:HD2	2:M:1226:TYR:CZ	2.53	0.44
1:E:553:ASP:OD1	1:E:556:THR:OG1	2.29	0.44
1:G:415:GLU:HG3	1:G:419:ASN:HD22	1.83	0.44
2:I:1291:ASP:OD1	2:I:1295:LEU:HB2	2.17	0.44
2:I:1625:PRO:HG3	2:I:1798:TRP:CD1	2.52	0.44
2:I:2185:LEU:HA	2:I:2188:ILE:HG12	1.99	0.44
2:M:1583:LYS:HG2	2:M:1584:TYR:H	1.82	0.44
2:M:2124:LYS:HB2	2:M:2124:LYS:HE2	1.80	0.44
1:G:353:SER:O	1:G:357:ILE:HG12	2.17	0.44
1:H:365:LEU:HD22	1:H:413:ILE:HG12	2.00	0.44
1:L:531:GLY:C	1:L:533:THR:H	2.20	0.44
2:M:1194:LYS:HA	2:M:1197:ASN:HD21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1544:PRO:HA	2:M:1547:ILE:HD11	2.00	0.44
1:A:455:TYR:CE2	1:B:463:GLN:HB2	2.52	0.44
1:E:400:HIS:CD2	1:E:406:SER:HB3	2.53	0.44
1:E:531:GLY:C	1:E:533:THR:H	2.20	0.44
2:I:1708:VAL:HG23	2:I:1713:THR:HG21	1.99	0.44
2:M:1041:GLU:OE1	2:M:1045:GLN:NE2	2.51	0.44
2:M:1365:ILE:HG13	2:M:1366:TYR:N	2.32	0.44
2:M:1561:TYR:O	2:M:1565:TYR:HB2	2.18	0.44
2:M:2062:SER:O	2:M:2131:LEU:HD11	2.18	0.44
3:J:19:SER:HB2	3:J:35:ARG:HD2	2.00	0.44
1:L:490:GLN:HG2	1:L:491:ARG:HG2	1.99	0.44
1:B:468:GLU:OE1	1:B:468:GLU:N	2.51	0.43
1:F:469:SER:OG	1:F:470:ALA:N	2.51	0.43
2:I:1901:ASN:HD21	2:I:1903:ASN:HB2	1.83	0.43
2:I:2207:LYS:HD3	2:I:2207:LYS:HA	1.70	0.43
3:J:102:THR:HG21	1:L:575:CYS:HB2	1.99	0.43
2:M:2170:PRO:O	2:M:2174:THR:N	2.51	0.43
1:A:567:VAL:HG12	3:J:61:VAL:HA	2.00	0.43
1:C:461:ARG:HD2	1:C:462:GLU:N	2.34	0.43
1:E:484:VAL:HG23	1:E:540:HIS:HB2	1.99	0.43
1:G:456:LEU:HD23	1:G:550:ARG:HB2	1.99	0.43
2:I:1605:TRP:CH2	2:I:1802:TRP:HB2	2.54	0.43
2:I:1646:GLY:HA3	2:I:1649:LYS:HE3	1.99	0.43
2:M:1046:ILE:O	2:M:1050:MET:HG2	2.18	0.43
2:M:1740:ASP:O	2:M:1744:ASN:N	2.52	0.43
2:M:2236:TRP:O	2:M:2240:ARG:HG2	2.18	0.43
1:E:529:ASN:HA	1:E:554:LYS:HD2	1.99	0.43
1:F:552:VAL:HG23	1:F:556:THR:HG21	1.99	0.43
1:K:506:MET:SD	1:K:507:PRO:HD2	2.59	0.43
2:M:1365:ILE:HG13	2:M:1366:TYR:H	1.82	0.43
2:I:2237:SER:O	2:I:2241:SER:N	2.48	0.43
2:M:1853:ARG:HG2	2:M:1947:LEU:HB3	2.01	0.43
1:C:345:ILE:HG12	1:C:372:LEU:HD23	2.00	0.43
1:C:418:TRP:O	1:C:443:ARG:NH1	2.52	0.43
1:C:443:ARG:O	1:C:445:LYS:NZ	2.46	0.43
1:G:490:GLN:HB2	1:G:495:LEU:HD11	2.00	0.43
2:I:1382:LYS:HA	2:I:1382:LYS:HD3	1.79	0.43
2:I:2090:ASP:HB3	2:I:2093:LYS:HD3	2.00	0.43
1:B:568:MET:HB3	1:C:568:MET:HG2	2.00	0.43
1:E:421:GLY:HA3	1:E:445:LYS:HD3	2.01	0.43
1:G:453:ASP:OD2	1:G:455:TYR:OH	2.28	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2247:ILE:O	2:I:2254:TYR:HB2	2.18	0.43
1:K:490:GLN:HG3	1:K:491:ARG:HG2	1.99	0.43
2:M:1506:GLU:HB3	2:M:1510:LYS:HZ1	1.84	0.43
2:M:1514:GLU:HA	2:M:1517:GLN:NE2	2.34	0.43
2:M:1671:LYS:HD3	2:M:1775:LYS:HZ1	1.83	0.43
2:M:2028:ASP:N	2:M:2028:ASP:OD1	2.51	0.43
2:M:2139:LYS:HD2	2:M:2139:LYS:O	2.19	0.43
2:M:2144:TRP:O	2:M:2148:ASN:ND2	2.52	0.43
1:B:354:PHE:HA	1:B:357:ILE:HD12	2.00	0.43
1:C:365:LEU:HD23	1:C:365:LEU:H	1.84	0.43
1:C:567:VAL:HG13	1:D:567:VAL:HG13	2.00	0.43
1:H:425:THR:HG21	1:H:438:LYS:HD3	2.01	0.43
2:I:1413:TRP:CG	2:I:1441:PRO:HD3	2.54	0.43
1:L:497:PRO:HA	1:L:500:TYR:CZ	2.54	0.43
1:A:485:PHE:HB3	1:A:539:ALA:HB3	2.00	0.43
1:E:419:ASN:HA	1:E:443:ARG:NE	2.33	0.43
1:H:543:LEU:HB2	1:H:546:ARG:HA	2.01	0.43
2:I:1272:LEU:HD11	2:I:1354:TYR:CE1	2.54	0.43
2:I:1808:GLU:HG3	2:I:1809:LYS:HE2	2.00	0.43
2:I:2064:ASN:CB	2:I:2067:LYS:HE3	2.49	0.43
2:M:1227:ILE:HG23	2:M:1276:GLU:OE2	2.19	0.43
2:M:2125:ILE:HA	2:M:2128:ASP:OD2	2.18	0.43
1:A:568:MET:HB3	1:B:568:MET:SD	2.58	0.43
1:B:469:SER:HA	1:B:524:SER:HA	1.99	0.43
2:I:1899:GLU:HG3	2:I:1901:ASN:H	1.84	0.43
2:I:1639:ILE:HG21	2:I:1657:THR:HG21	2.01	0.43
2:I:1660:ILE:O	2:I:1664:ARG:HG2	2.19	0.43
2:I:1844:ASN:HA	2:I:1847:ASN:HD21	1.84	0.43
3:J:4:ARG:HD2	3:J:20:ARG:HB2	2.01	0.43
2:M:1265:ILE:HG12	2:M:1365:ILE:HG21	2.01	0.43
1:A:495:LEU:HD23	1:A:495:LEU:HA	1.84	0.42
1:C:508:GLU:OE2	1:C:511:ALA:HB3	2.19	0.42
1:D:372:LEU:HD23	1:D:430:HIS:CD2	2.54	0.42
2:I:1454:PHE:HE2	2:I:1535:ALA:HB1	1.83	0.42
2:I:2236:TRP:O	2:I:2240:ARG:N	2.46	0.42
2:M:1309:GLU:HG2	2:M:1423:ILE:HD12	2.01	0.42
2:M:1458:GLY:HA3	2:M:1539:LEU:HD11	2.01	0.42
2:M:1719:LYS:O	2:M:1722:GLU:HG3	2.19	0.42
2:M:2075:GLN:NE2	2:M:2156:MET:HA	2.33	0.42
2:M:2182:PRO:O	2:M:2186:ARG:N	2.31	0.42
1:B:419:ASN:O	1:B:443:ARG:NH2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLN:HG3	1:B:464:LEU:HD12	2.01	0.42
1:E:346:ARG:HD2	1:E:348:PHE:CZ	2.54	0.42
1:F:459:PRO:HD3	1:F:472:ILE:HG12	2.01	0.42
1:H:382:TRP:HA	1:H:426:CYS:HA	2.01	0.42
2:I:1142:SER:HB3	2:I:1187:GLY:HA2	2.01	0.42
1:L:533:THR:HA	1:L:553:ASP:HA	2.01	0.42
2:M:1240:PHE:CD1	2:M:1241:PRO:HA	2.54	0.42
2:M:1600:ASP:N	2:M:1630:GLN:OE1	2.52	0.42
2:M:1698:LEU:HA	2:M:1701:ILE:HG12	2.00	0.42
2:M:2148:ASN:HA	2:M:2151:SER:HB3	2.02	0.42
1:C:418:TRP:CZ2	1:C:443:ARG:HB3	2.54	0.42
1:F:400:HIS:NE2	1:F:406:SER:OG	2.46	0.42
2:I:1462:CYS:HB3	2:I:1546:CYS:HB3	1.85	0.42
2:M:2107:ASP:OD2	2:M:2187:TRP:NE1	2.52	0.42
1:G:417:ASP:O	1:G:420:SER:OG	2.36	0.42
2:I:1903:ASN:O	2:I:1905:ILE:N	2.49	0.42
2:I:2063:LEU:HB3	2:I:2065:GLU:HG3	1.99	0.42
3:J:25:SER:O	3:J:27:ASP:N	2.52	0.42
1:K:490:GLN:HB2	1:K:495:LEU:HD11	2.02	0.42
2:M:1357:MET:O	2:M:1373:GLN:NE2	2.49	0.42
2:M:2024:TRP:HB2	2:M:2040:LEU:HD13	2.01	0.42
1:A:539:ALA:HB2	3:J:115:LEU:HD11	2.01	0.42
1:C:511:ALA:HB1	1:C:512:PRO:HD2	2.01	0.42
2:I:2202:HIS:CE1	2:I:2233:TYR:HB3	2.54	0.42
2:M:2225:ASN:ND2	2:M:2229:GLU:OE2	2.52	0.42
2:I:1617:ARG:NH1	2:I:1875:GLU:OE1	2.53	0.42
2:I:1731:ASP:O	2:I:1735:LYS:HG2	2.19	0.42
2:I:2080:PHE:O	2:I:2083:ASN:N	2.52	0.42
1:L:543:LEU:HB2	1:L:546:ARG:HA	2.02	0.42
2:M:2035:LYS:HG3	2:M:2036:HIS:CD2	2.55	0.42
1:A:466:LEU:H	1:A:466:LEU:HD23	1.83	0.42
1:D:549:GLU:N	1:D:549:GLU:OE1	2.53	0.42
1:E:419:ASN:HA	1:E:443:ARG:HE	1.85	0.42
2:I:1311:LEU:HD23	2:I:1311:LEU:HA	1.85	0.42
2:M:1025:ASP:OD1	2:M:1025:ASP:N	2.50	0.42
2:M:1029:VAL:HA	2:M:1032:PHE:HB3	2.00	0.42
2:M:1114:GLN:HA	2:M:1117:ASN:HD21	1.84	0.42
1:G:498:GLU:OE1	1:G:498:GLU:N	2.53	0.42
2:I:1042:ILE:HD13	2:I:1042:ILE:HA	1.90	0.42
2:I:1252:LYS:HD3	2:I:1521:LYS:HG2	2.01	0.42
2:I:1974:ASN:HA	2:I:1977:ASP:OD2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2162:LYS:HD3	2:I:2162:LYS:HA	1.86	0.42
2:M:1626:PRO:O	2:M:1630:GLN:HG2	2.19	0.42
1:B:419:ASN:HA	1:B:443:ARG:NH1	2.35	0.42
1:E:396:ILE:HA	1:E:408:VAL:HG22	2.02	0.42
1:E:473:THR:HG22	1:E:520:ILE:HG22	2.02	0.42
1:F:384:ARG:HB2	1:F:388:GLU:HB2	2.01	0.42
1:G:419:ASN:O	1:G:445:LYS:NZ	2.44	0.42
2:I:1410:ARG:HD2	2:I:1410:ARG:HA	1.86	0.42
2:I:1765:GLN:HA	2:I:1768:VAL:HG12	2.01	0.42
1:K:475:LEU:HD13	1:K:518:HIS:CE1	2.55	0.42
2:M:2119:GLU:OE1	2:M:2124:LYS:HB3	2.20	0.42
1:A:455:TYR:CZ	1:B:463:GLN:HB2	2.55	0.42
1:D:373:THR:HG23	1:D:375:TYR:HB3	2.01	0.42
1:E:378:VAL:HG22	1:E:430:HIS:CD2	2.55	0.42
1:G:384:ARG:HE	1:G:386:ASN:CG	2.20	0.42
1:H:569:SER:N	1:K:569:SER:HB2	2.35	0.42
2:I:1036:GLU:O	2:I:1040:LYS:HG2	2.19	0.42
2:I:2143:ASP:OD1	2:I:2144:TRP:N	2.52	0.42
3:J:17:ILE:HD11	3:J:35:ARG:HH21	1.83	0.42
2:M:1146:PHE:HA	2:M:1149:CYS:SG	2.60	0.42
2:M:1944:ASN:OD1	2:M:1945:GLU:N	2.52	0.42
1:D:419:ASN:O	1:D:443:ARG:NE	2.53	0.41
1:H:428:VAL:HB	1:H:437:LEU:HB2	2.01	0.41
2:I:1457:TRP:HZ2	2:I:1515:LYS:HD2	1.85	0.41
2:I:2197:ILE:HD12	2:I:2197:ILE:HA	1.94	0.41
3:J:49:ILE:HG13	3:J:103:TYR:CE1	2.55	0.41
1:L:463:GLN:HE22	1:L:471:THR:HG23	1.85	0.41
1:L:558:LYS:HZ3	1:L:560:THR:HG22	1.84	0.41
1:B:490:GLN:OE1	1:B:495:LEU:HD21	2.20	0.41
1:B:491:ARG:HH12	2:M:2054:VAL:HG13	1.85	0.41
1:D:475:LEU:HD12	1:D:518:HIS:NE2	2.34	0.41
1:E:364:LYS:HE3	1:E:364:LYS:HB3	1.92	0.41
1:F:475:LEU:HD13	1:F:518:HIS:CD2	2.55	0.41
1:G:364:LYS:HD3	1:G:412:SER:HA	2.02	0.41
3:J:69:LYS:NZ	3:J:98:GLU:OE2	2.39	0.41
1:A:562:TYR:HB2	1:B:562:TYR:HD1	1.85	0.41
1:H:350:ILE:O	1:H:350:ILE:HG13	2.20	0.41
2:I:1328:LYS:HD2	2:I:1328:LYS:O	2.20	0.41
1:K:543:LEU:HD13	1:K:548:THR:HG23	2.01	0.41
2:M:1381:GLU:O	2:M:1382:LYS:HE2	2.19	0.41
2:M:1963:GLU:O	2:M:1966:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:THR:OG1	1:C:551:THR:OG1	2.14	0.41
2:I:1444:GLY:HA2	2:I:1447:GLU:HG3	2.01	0.41
2:I:1561:TYR:O	2:I:1565:TYR:HB2	2.20	0.41
2:I:2020:GLU:HG3	2:I:2024:TRP:HZ2	1.84	0.41
2:I:2041:ILE:HG23	2:I:2046:ARG:HH21	1.85	0.41
1:K:527:GLU:OE1	1:K:534:TYR:OH	2.34	0.41
2:M:1356:ASN:ND2	2:M:1449:GLN:HG2	2.35	0.41
2:M:1669:LEU:O	2:M:1673:TYR:CB	2.68	0.41
2:M:2247:ILE:O	2:M:2250:ARG:HG2	2.20	0.41
1:C:479:PHE:CE1	1:C:515:TYR:HB2	2.55	0.41
1:F:382:TRP:CD2	1:F:426:CYS:HB3	2.55	0.41
2:I:2187:TRP:O	2:I:2190:GLU:HG3	2.20	0.41
2:M:1272:LEU:HD12	2:M:1272:LEU:O	2.20	0.41
2:M:1497:ILE:HG21	2:M:1501:CYS:HB3	2.03	0.41
2:M:1529:LYS:HG3	2:M:1530:TYR:HD1	1.85	0.41
2:M:2089:LYS:HD3	2:M:2089:LYS:HA	1.77	0.41
1:B:368:LEU:HB3	1:B:408:VAL:HA	2.02	0.41
1:G:518:HIS:CE1	1:H:520:ILE:HD11	2.56	0.41
1:G:488:TRP:HE1	1:G:519:SER:HG	1.68	0.41
2:I:1272:LEU:O	2:I:1272:LEU:HD12	2.21	0.41
2:I:1300:ILE:O	2:I:1304:ILE:HG12	2.20	0.41
2:I:1368:HIS:CD2	2:I:1371:LYS:HB2	2.56	0.41
2:I:1558:ASN:HB3	2:I:1561:TYR:HD2	1.86	0.41
3:J:41:VAL:HG12	1:L:568:MET:HB2	2.02	0.41
1:G:543:LEU:HB2	1:G:546:ARG:HA	2.02	0.41
1:H:526:GLU:HG2	1:H:527:GLU:N	2.36	0.41
2:I:981:TYR:CE2	2:I:1099:CYS:HB3	2.55	0.41
2:I:1179:LYS:HG2	2:I:1180:CYS:SG	2.61	0.41
2:I:1611:LYS:HD2	2:I:1709:HIS:CE1	2.56	0.41
2:I:2142:GLU:O	2:I:2146:LYS:N	2.37	0.41
1:A:451:ARG:HH12	1:A:544:PRO:HD2	1.86	0.41
1:A:456:LEU:HD23	1:A:550:ARG:HG3	2.01	0.41
1:B:352:PRO:HD3	1:B:365:LEU:HB3	2.03	0.41
1:B:372:LEU:O	1:B:404:THR:HA	2.21	0.41
1:E:443:ARG:HA	1:E:444:PRO:HD3	1.93	0.41
1:F:364:LYS:HE3	1:F:364:LYS:HB3	1.77	0.41
1:F:529:ASN:HA	1:F:554:LYS:HD3	2.02	0.41
1:H:374:THR:HA	1:H:405:PHE:HB2	2.03	0.41
2:I:1025:ASP:OD1	2:I:1025:ASP:N	2.53	0.41
2:I:1195:LEU:O	2:I:1199:GLU:N	2.54	0.41
2:I:1742:TRP:CZ2	2:I:1757:ARG:HB3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1891:TYR:O	2:I:1895:ARG:HB2	2.21	0.41
2:I:1975:GLU:HA	2:I:1978:ASN:ND2	2.34	0.41
2:I:2089:LYS:HD3	2:I:2089:LYS:HA	1.77	0.41
3:J:4:ARG:HH11	3:J:20:ARG:CB	2.29	0.41
2:M:1662:ALA:O	2:M:1665:GLU:HG3	2.20	0.41
2:M:1717:ASP:OD1	2:M:1718:SER:N	2.54	0.41
2:M:1874:SER:OG	2:M:1876:ASP:O	2.36	0.41
2:M:2018:LEU:HD21	2:M:2021:LEU:HD13	2.02	0.41
2:M:2071:LEU:HD11	2:M:2154:ASN:OD1	2.21	0.41
1:C:456:LEU:HD13	1:C:550:ARG:HB2	2.03	0.41
1:E:532:GLU:OE2	2:I:1238:LYS:NZ	2.51	0.41
1:H:562:TYR:HB2	1:K:562:TYR:HB2	2.03	0.41
2:I:1042:ILE:O	2:I:1045:GLN:HB3	2.21	0.41
2:I:1515:LYS:HD3	2:I:1515:LYS:HA	1.83	0.41
3:J:59:ARG:HD2	3:J:60:PHE:N	2.36	0.41
1:K:509:PRO:HG2	1:K:510:GLN:OE1	2.21	0.41
2:M:1613:LEU:HD11	2:M:1617:ARG:HG3	2.03	0.41
2:M:1724:PHE:CD2	2:M:1738:ARG:HG2	2.53	0.41
1:G:396:ILE:HD11	1:G:407:ALA:HA	2.03	0.40
2:I:1899:GLU:O	2:I:1905:ILE:HG12	2.20	0.40
1:D:345:ILE:HD12	1:D:372:LEU:HG	2.02	0.40
1:D:454:VAL:HG21	1:D:538:VAL:HG11	2.03	0.40
1:F:511:ALA:HB3	1:F:514:ARG:HB2	2.03	0.40
1:H:398:GLU:HG2	1:H:399:SER:H	1.87	0.40
3:J:106:ASN:OD1	3:J:107:LYS:HG3	2.21	0.40
1:K:382:TRP:CE2	1:K:426:CYS:HB2	2.57	0.40
2:M:1868:ARG:NH2	2:M:1884:MET:SD	2.94	0.40
1:F:508:GLU:OE1	1:F:510:GLN:N	2.54	0.40
1:G:364:LYS:HE2	1:G:364:LYS:HB2	1.90	0.40
2:I:1433:ASN:C	2:I:1435:ASP:H	2.25	0.40
2:I:2043:PRO:HA	2:I:2046:ARG:NE	2.36	0.40
1:K:457:LEU:HB2	1:K:473:THR:CG2	2.52	0.40
1:L:471:THR:HB	1:L:520:ILE:HD11	2.03	0.40
1:L:496:SER:H	1:L:499:LYS:HZ2	1.70	0.40
1:B:357:ILE:HG12	1:B:363:THR:HG22	2.03	0.40
1:B:568:MET:HB3	1:C:568:MET:CG	2.52	0.40
1:F:514:ARG:NH1	2:I:1226:TYR:OH	2.55	0.40
2:I:1461:PHE:O	2:I:1464:GLU:HG3	2.21	0.40
2:I:1889:ILE:HD12	2:I:1892:LEU:HD11	2.02	0.40
3:J:12:CYS:SG	3:J:13:LYS:N	2.94	0.40
1:D:459:PRO:HG2	1:D:464:LEU:HD11	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1178:LYS:HB3	2:I:1178:LYS:HE2	1.86	0.40
2:I:1364:ASN:N	2:I:1364:ASN:OD1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/453 (29%)	123 (95%)	7 (5%)	0	100	100
1	B	225/453 (50%)	206 (92%)	19 (8%)	0	100	100
1	C	223/453 (49%)	195 (87%)	28 (13%)	0	100	100
1	D	222/453 (49%)	204 (92%)	18 (8%)	0	100	100
1	E	222/453 (49%)	206 (93%)	16 (7%)	0	100	100
1	F	217/453 (48%)	198 (91%)	19 (9%)	0	100	100
1	G	222/453 (49%)	203 (91%)	19 (9%)	0	100	100
1	H	226/453 (50%)	206 (91%)	20 (9%)	0	100	100
1	K	226/453 (50%)	206 (91%)	20 (9%)	0	100	100
1	L	123/453 (27%)	112 (91%)	11 (9%)	0	100	100
2	I	1085/2680 (40%)	991 (91%)	94 (9%)	0	100	100
2	M	1085/2680 (40%)	976 (90%)	108 (10%)	1 (0%)	51	83
3	J	102/136 (75%)	89 (87%)	13 (13%)	0	100	100
All	All	4308/10026 (43%)	3915 (91%)	392 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	1367	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	115/399 (29%)	114 (99%)	1 (1%)	78 90
1	B	203/399 (51%)	203 (100%)	0	100 100
1	C	201/399 (50%)	201 (100%)	0	100 100
1	D	200/399 (50%)	199 (100%)	1 (0%)	88 95
1	E	200/399 (50%)	200 (100%)	0	100 100
1	F	198/399 (50%)	198 (100%)	0	100 100
1	G	200/399 (50%)	198 (99%)	2 (1%)	76 88
1	H	205/399 (51%)	204 (100%)	1 (0%)	88 95
1	K	205/399 (51%)	203 (99%)	2 (1%)	76 88
1	L	112/399 (28%)	112 (100%)	0	100 100
2	I	1013/2431 (42%)	1004 (99%)	9 (1%)	78 90
2	M	1013/2431 (42%)	1009 (100%)	4 (0%)	91 97
3	J	100/128 (78%)	100 (100%)	0	100 100
All	All	3965/8980 (44%)	3945 (100%)	20 (0%)	89 95

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	ARG
1	D	391	LYS
1	G	461	ARG
1	G	467	ARG
1	H	443	ARG
2	I	1328	LYS
2	I	1349	ARG
2	I	1496	LYS
2	I	1628	ARG
2	I	1649	LYS
2	I	1853	ARG
2	I	2017	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	2055	ARG
2	I	2114	MET
1	K	346	ARG
1	K	443	ARG
2	M	1628	ARG
2	M	1840	LYS
2	M	2139	LYS
2	M	2186	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	529	ASN
1	B	529	ASN
1	D	393	HIS
1	D	430	HIS
1	G	465	ASN
1	H	490	GLN
2	I	1117	ASN
2	I	1305	HIS
2	I	1629	GLN
2	I	2148	ASN
2	M	1197	ASN
2	M	1400	ASN
2	M	1850	ASN
2	M	2036	HIS
2	M	2075	GLN
2	M	2148	ASN

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 (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.

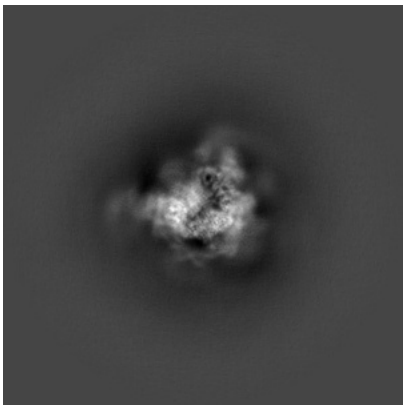
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34399. These allow visual inspection of the internal detail of the map and identification of artifacts.

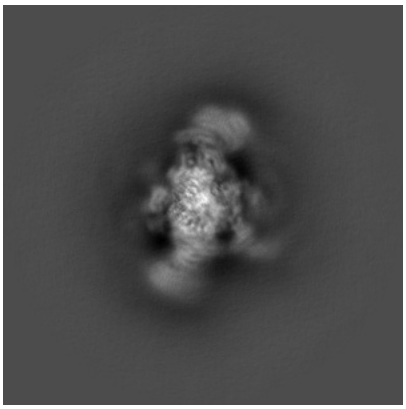
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

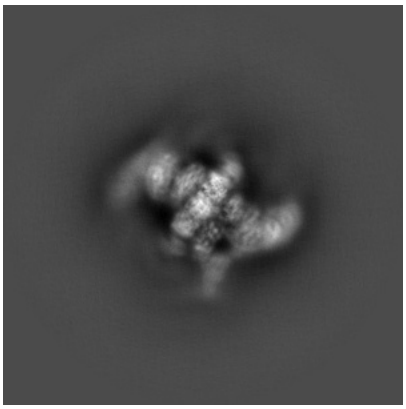
6.1.1 Primary map



X

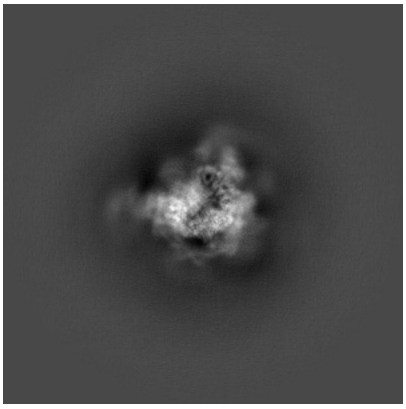


Y

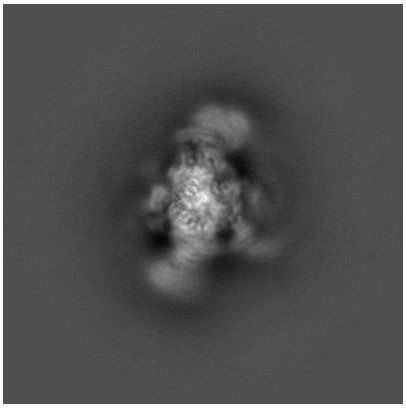


Z

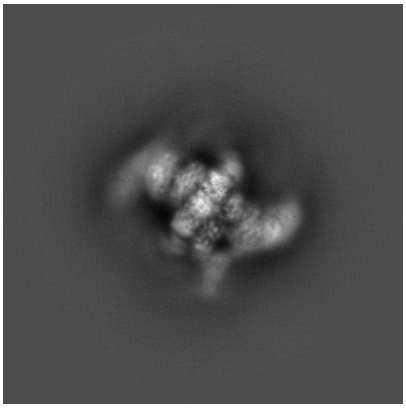
6.1.2 Raw map



X



Y

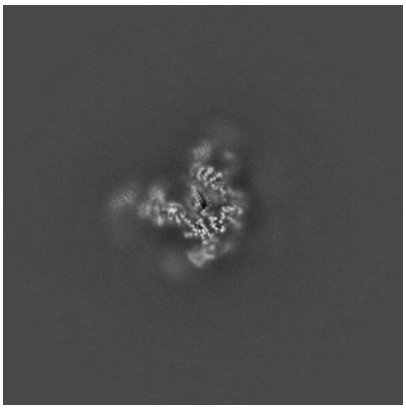


Z

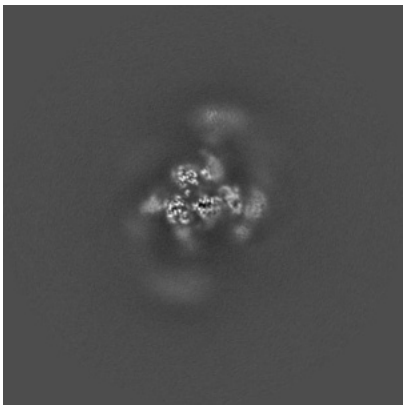
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

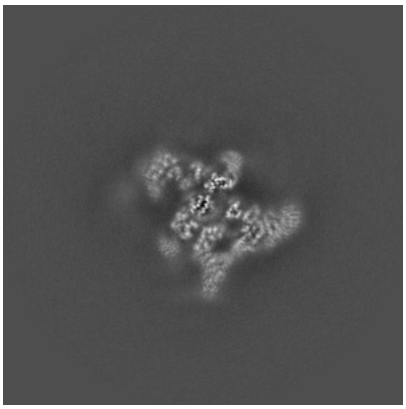
6.2.1 Primary map



X Index: 270

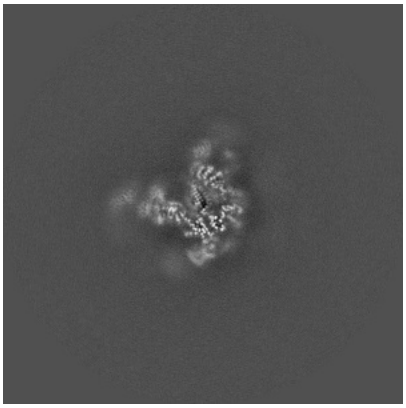


Y Index: 270

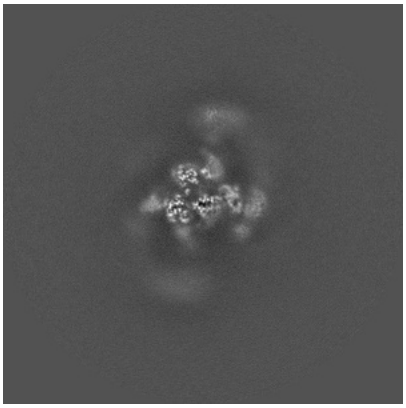


Z Index: 270

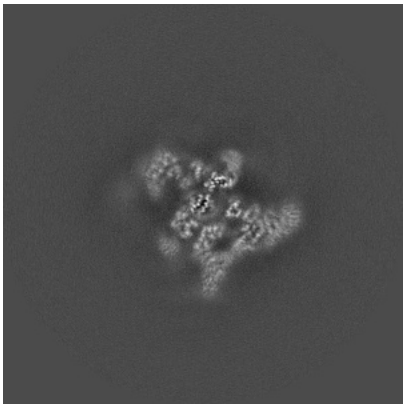
6.2.2 Raw map



X Index: 270



Y Index: 270

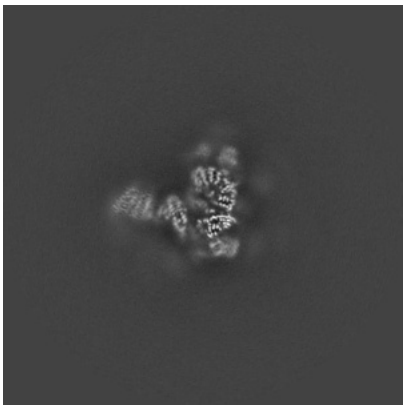


Z Index: 270

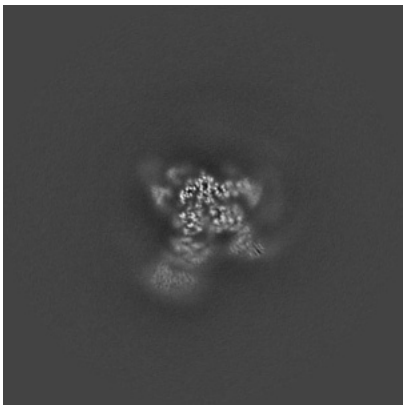
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

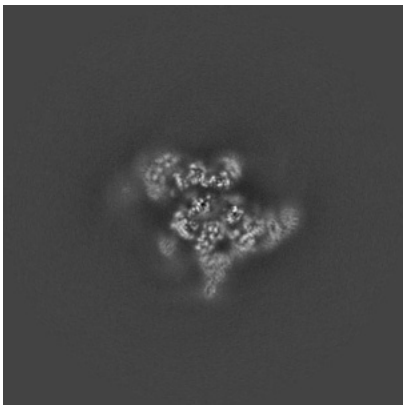
6.3.1 Primary map



X Index: 283

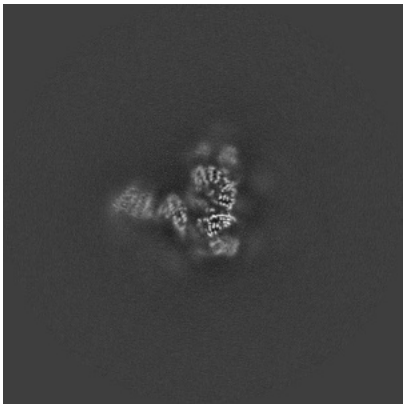


Y Index: 301

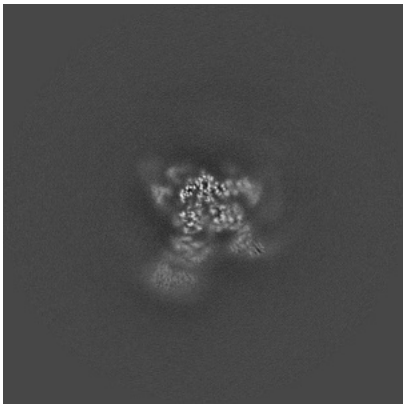


Z Index: 265

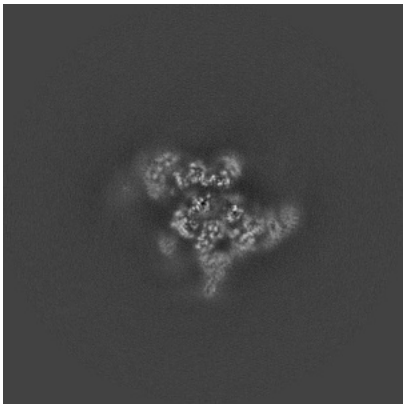
6.3.2 Raw map



X Index: 283



Y Index: 301

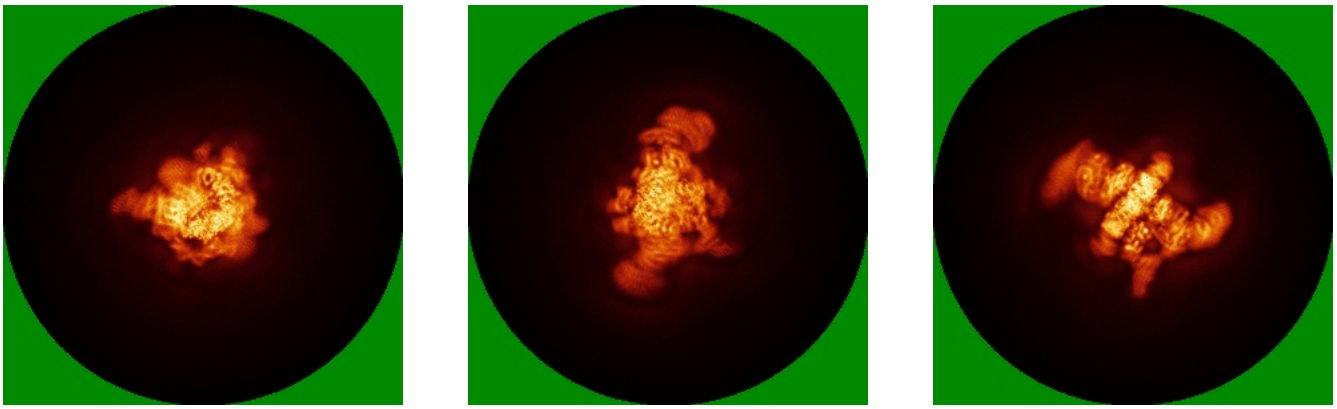


Z Index: 265

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

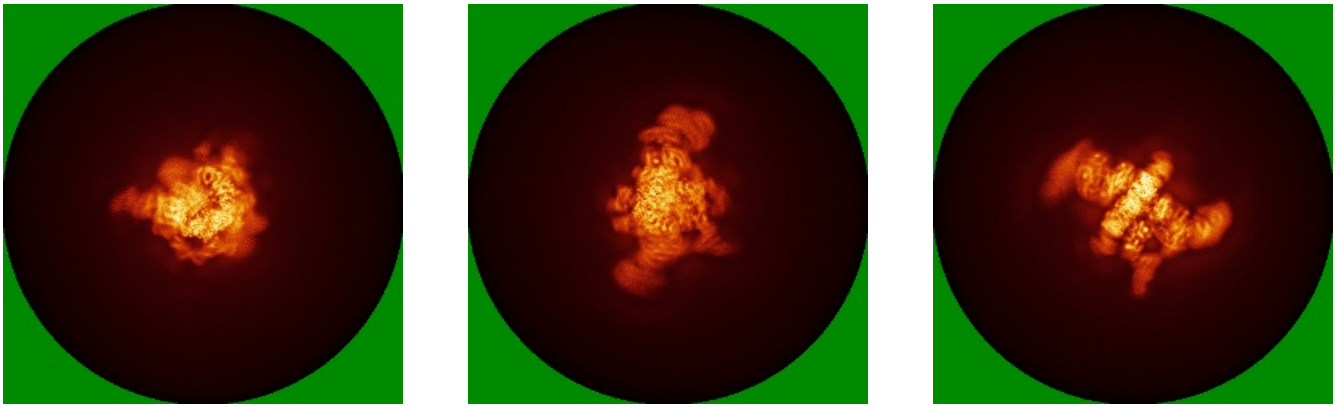
6.4 Orthogonal standard-deviation projections (False-color) (i)

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00805. 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

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.

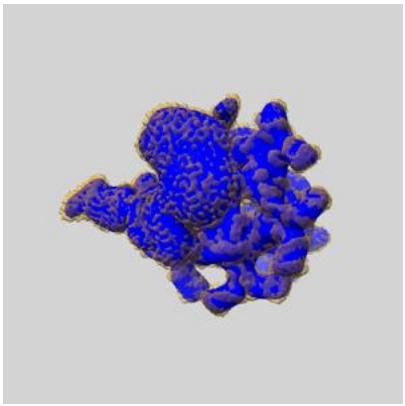
6.6 Mask visualisation (i)

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

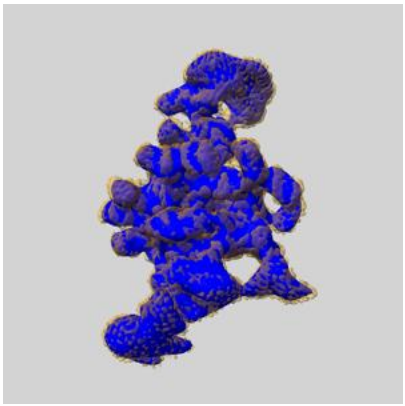
A mask typically either:

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

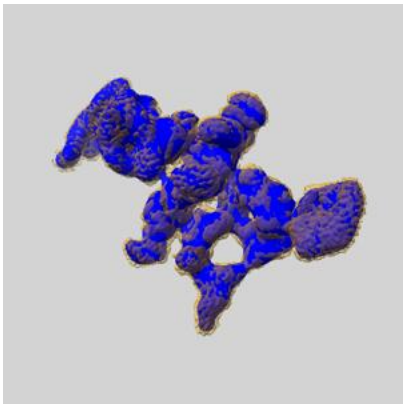
6.6.1 emd_34399_msk_1.map (i)



X



Y

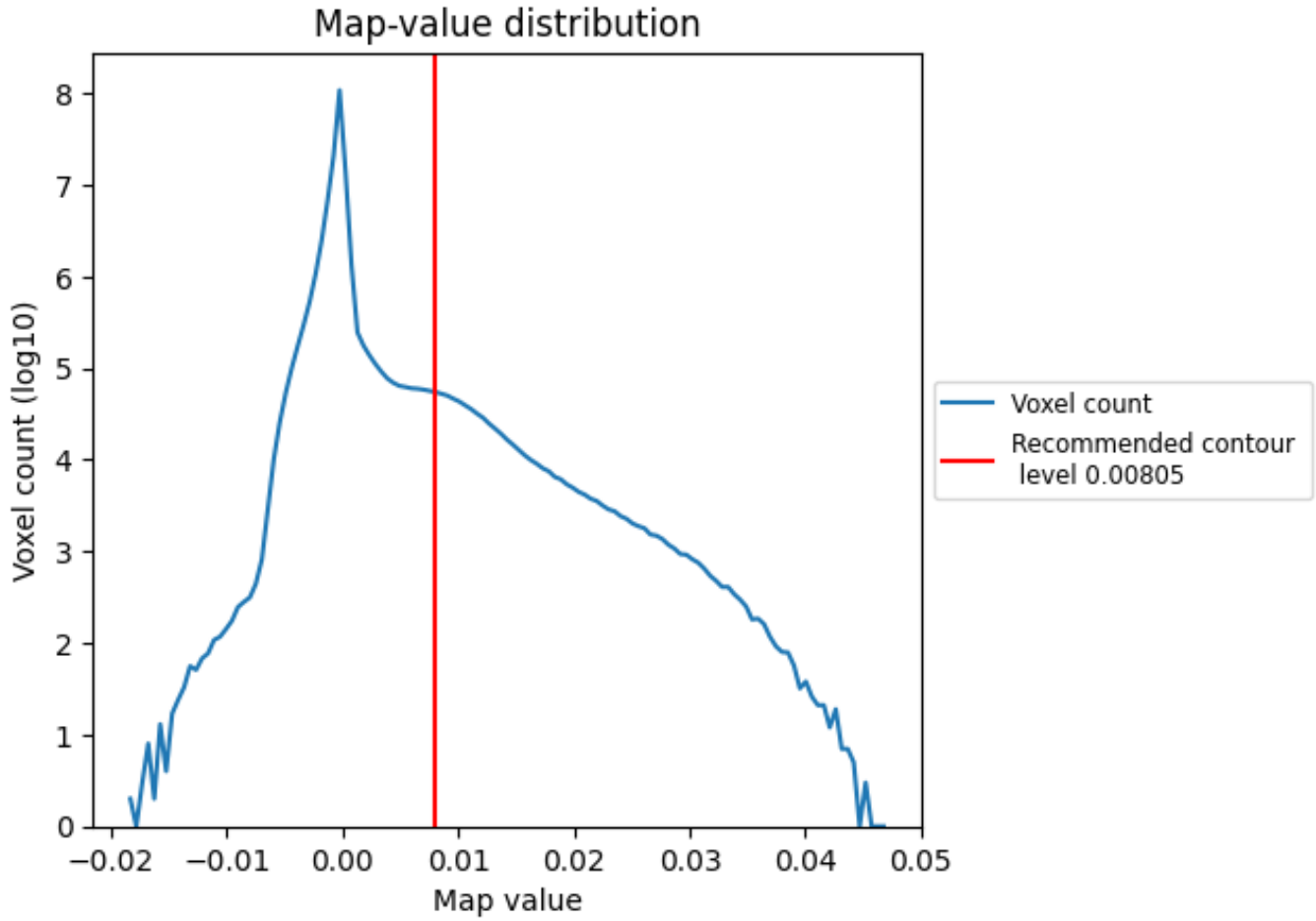


Z

7 Map analysis

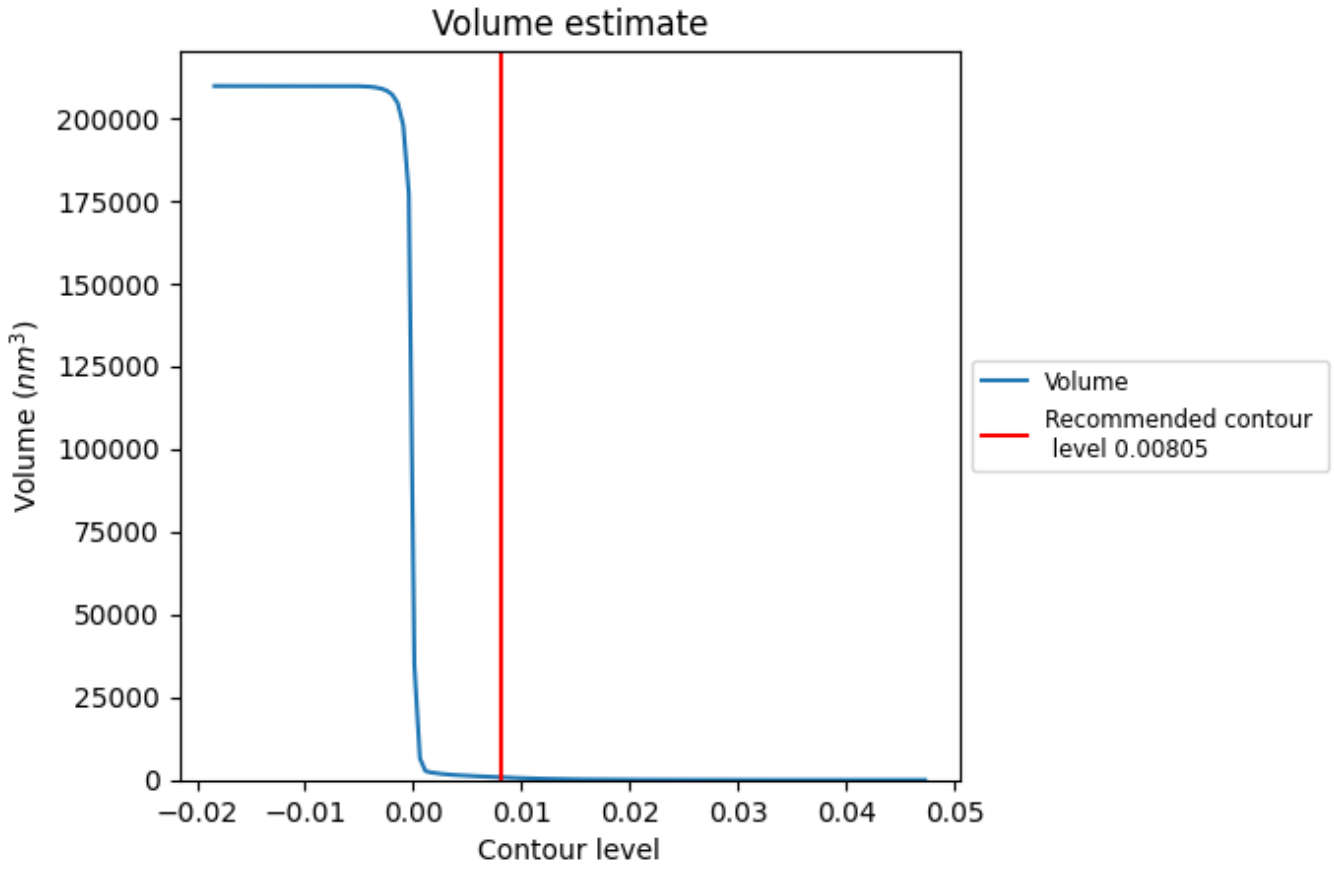
This section contains the results of statistical analysis of the map.

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.

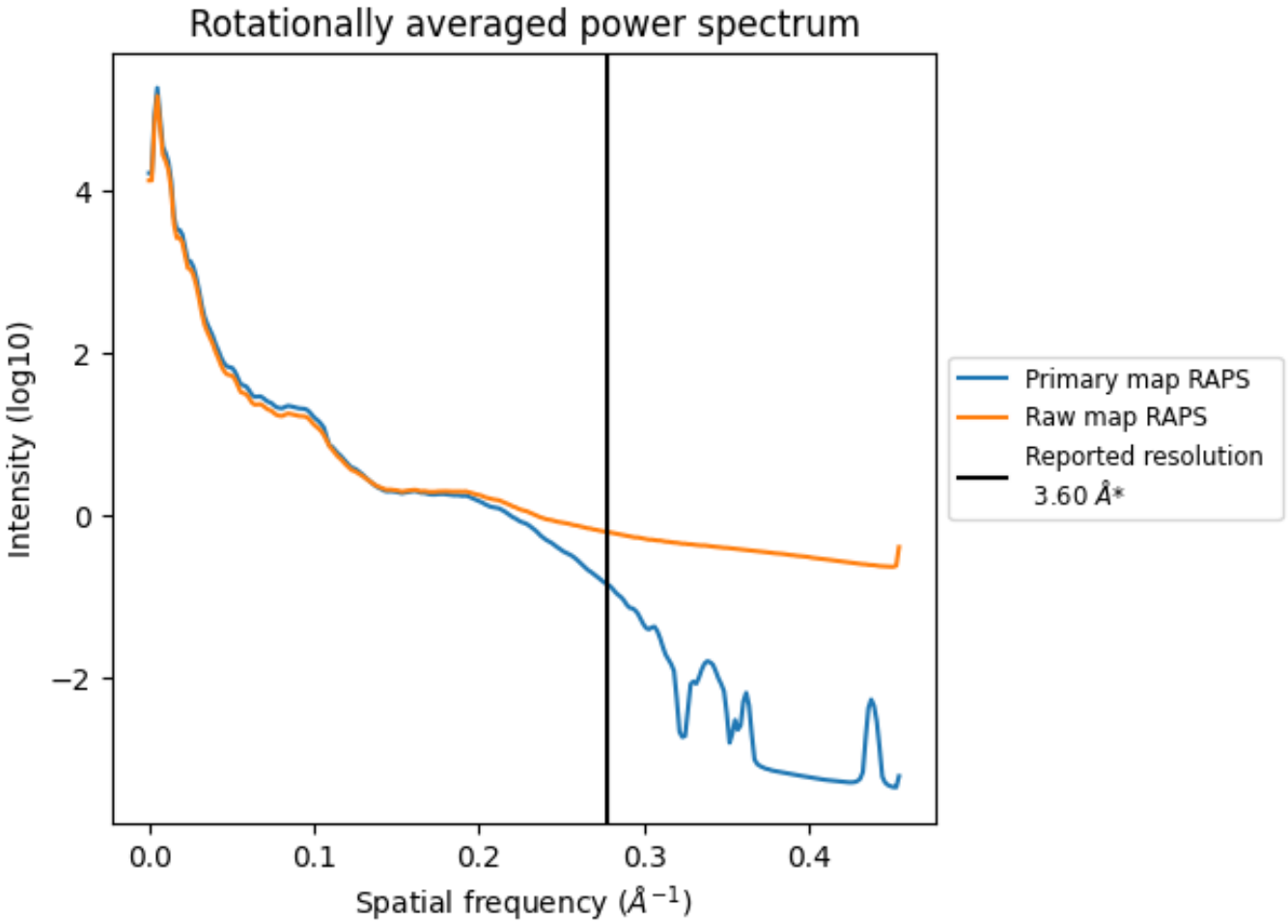
7.2 Volume estimate



The volume at the recommended contour level is 809 nm^3; this corresponds to an approximate mass of 731 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)

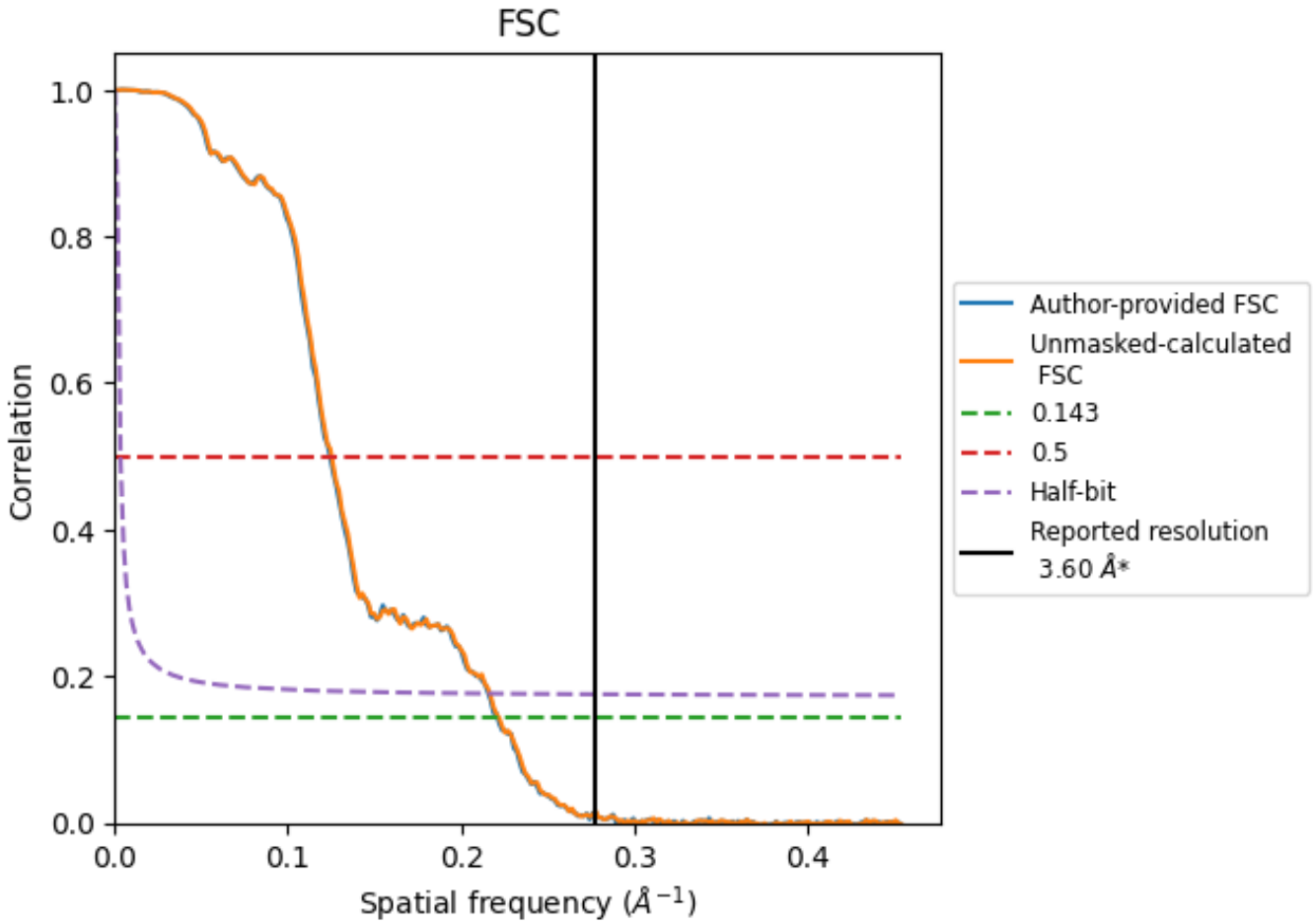


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

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 0.278 $Å^{-1}$

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	4.52	8.05	4.63
Unmasked-calculated*	4.50	7.98	4.61

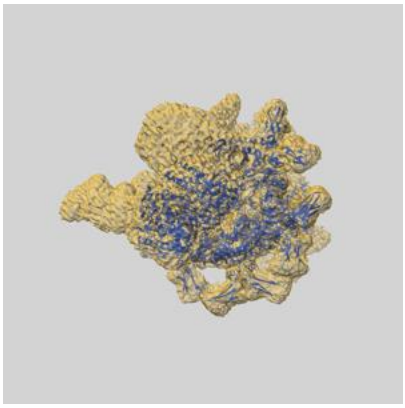
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.6 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.6 by more than 10 %

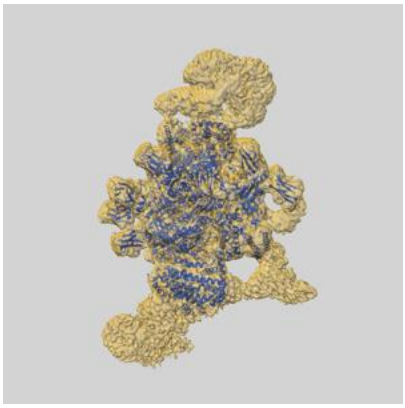
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34399 and PDB model 8GZN. Per-residue inclusion information can be found in section 3 on page 5.

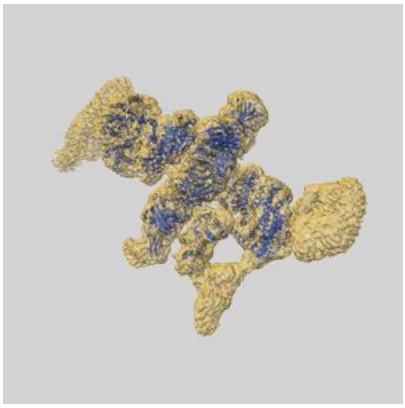
9.1 Map-model overlay



X



Y



Z

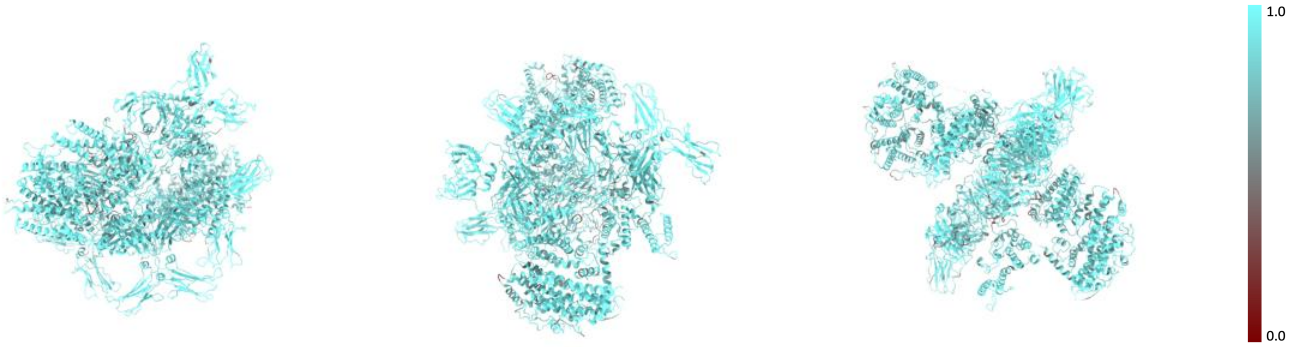
The images above show the 3D surface view of the map at the recommended contour level 0.00805 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

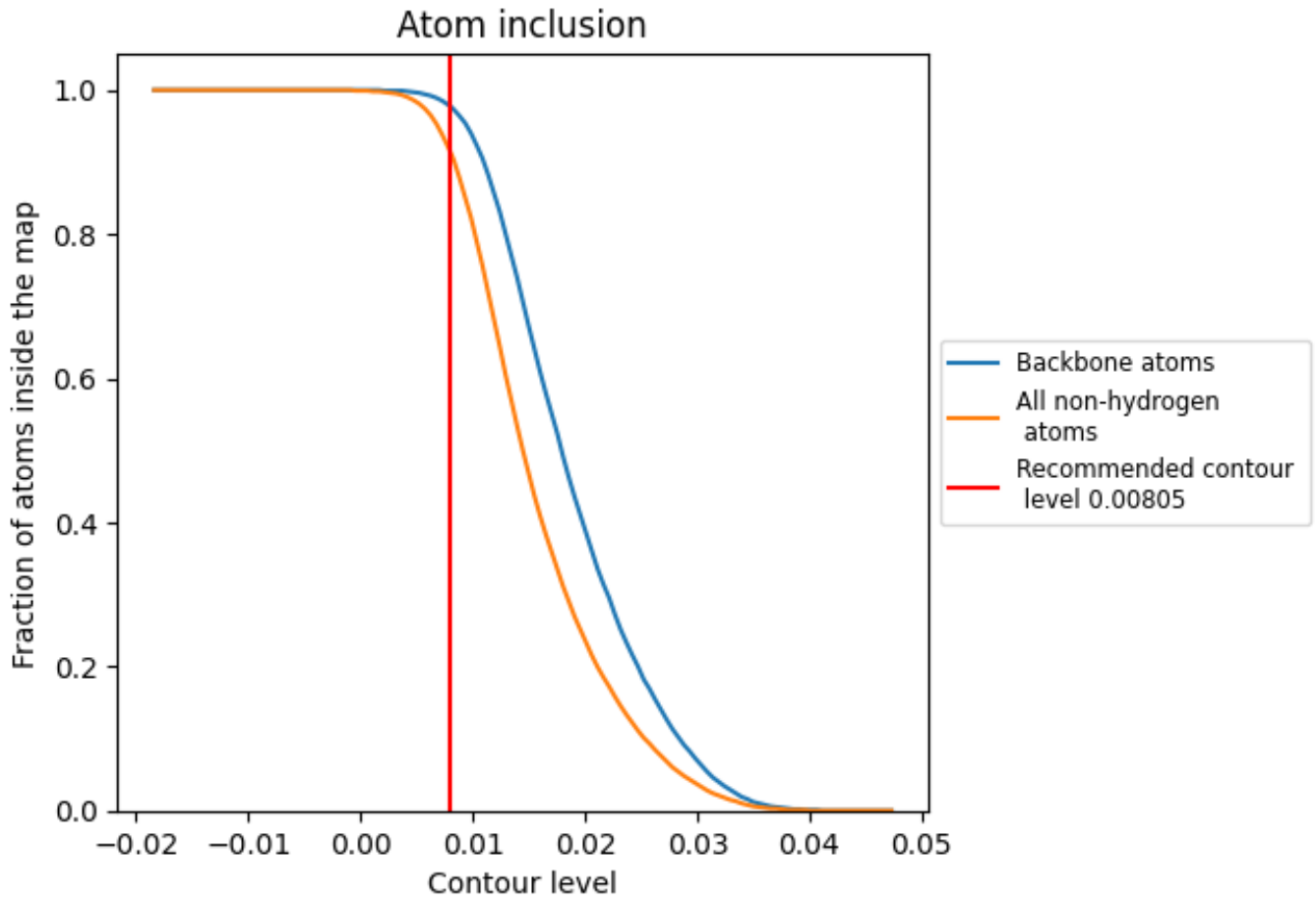
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00805).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00805) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.3040
A	0.9120	0.3280
B	0.9120	0.3300
C	0.9560	0.3410
D	0.9550	0.3630
E	0.9590	0.3830
F	0.9510	0.3730
G	0.9400	0.3620
H	0.9450	0.3300
I	0.8870	0.2540
J	0.7250	0.2720
K	0.9210	0.3080
L	0.9550	0.3170
M	0.9070	0.2840