Full wwPDB EM Validation Report

Jun 1, 2024 – 07:43 am BST

PDB ID	:	8C8R
EMDB ID	:	EMD-16492
Title	:	In situ structure of the Nitrosopumilus maritimus S-layer - Composite map between C2 and C6
Authors	:	von Kuegelgen, A.; Bharat, T.
Deposited on	:	2023-01-20
Resolution	:	3.50 Å(reported)

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

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

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

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

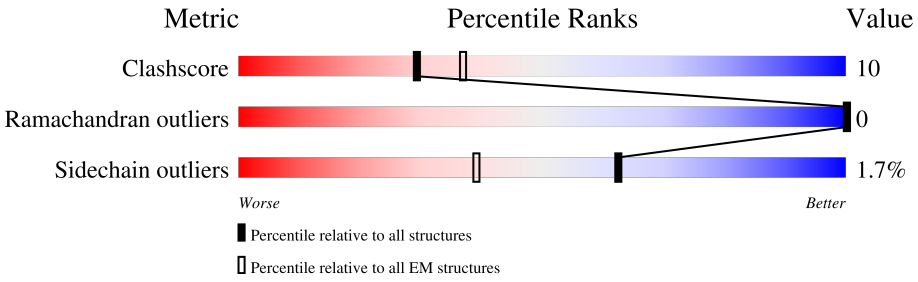
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1734	7% 66% 18% · 16%
1	B	1734	7% 67% 17% 16%
1	C	1734	7% 66% 18% 16%
1	D	1734	7% 67% 17% 16%
1	E	1734	7% 67% 17% · 16%
1	F	1734	7% 66% 18% · 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 65154 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.

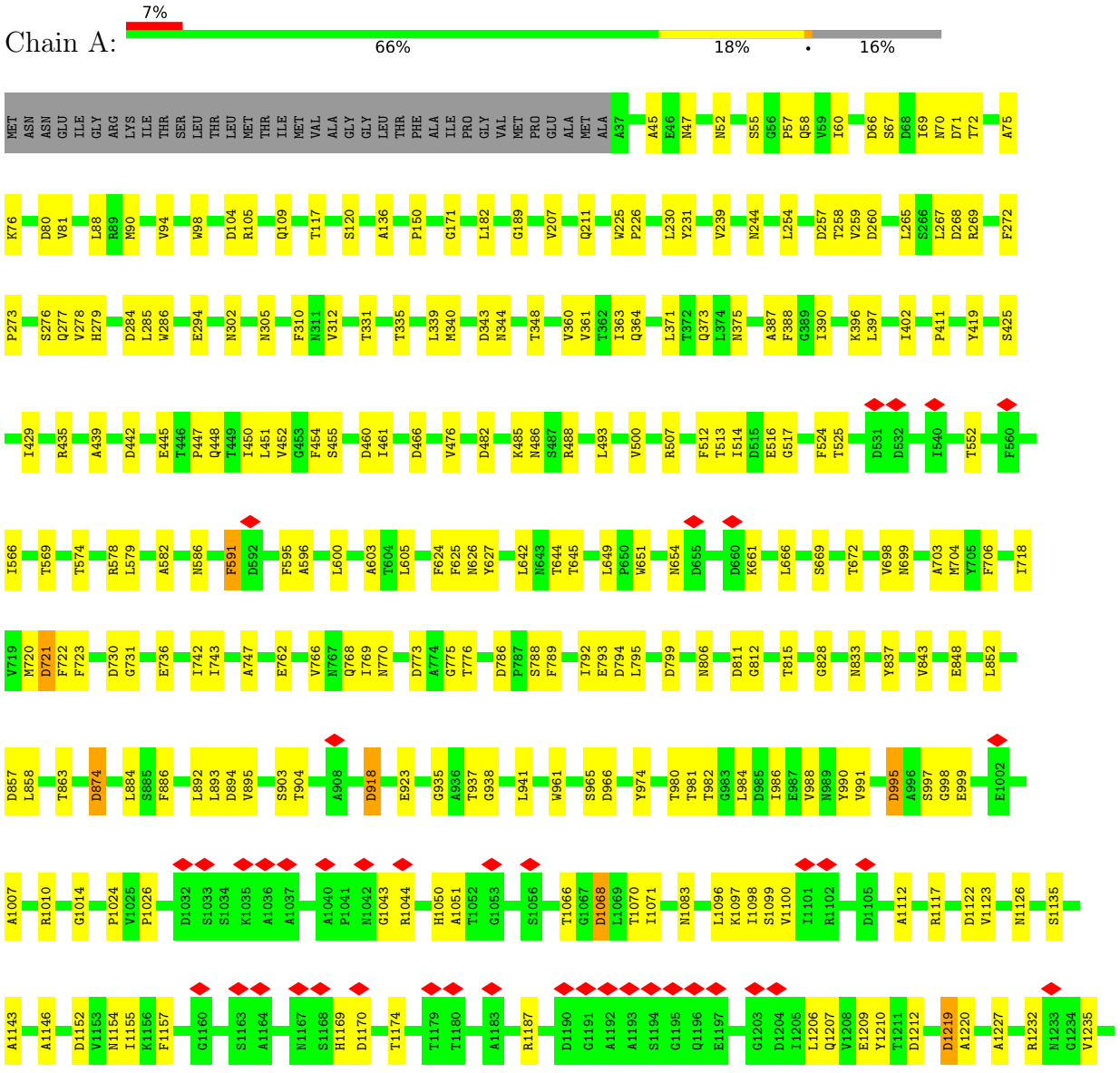
- Molecule 1 is a protein called Cell surface protein.

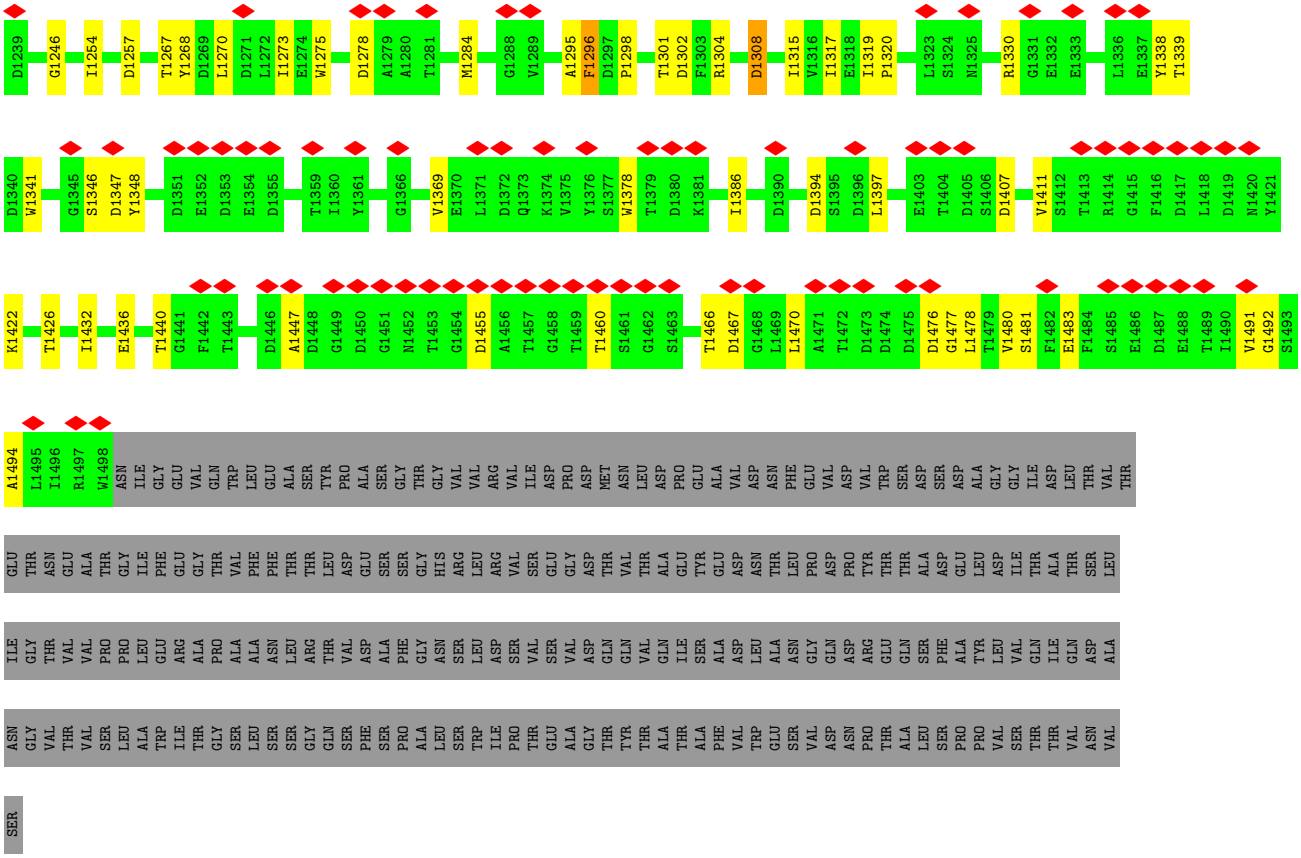
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	B	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	C	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	D	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	E	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	F	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		

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.

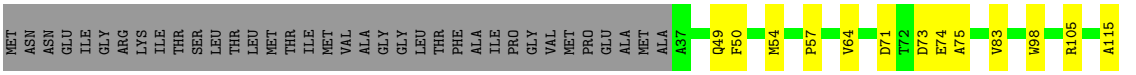
- Molecule 1: Cell surface protein

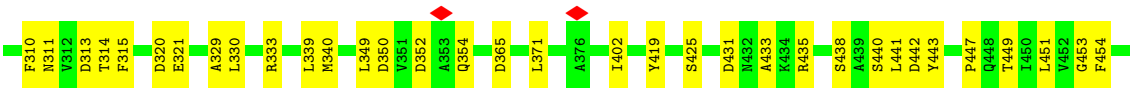


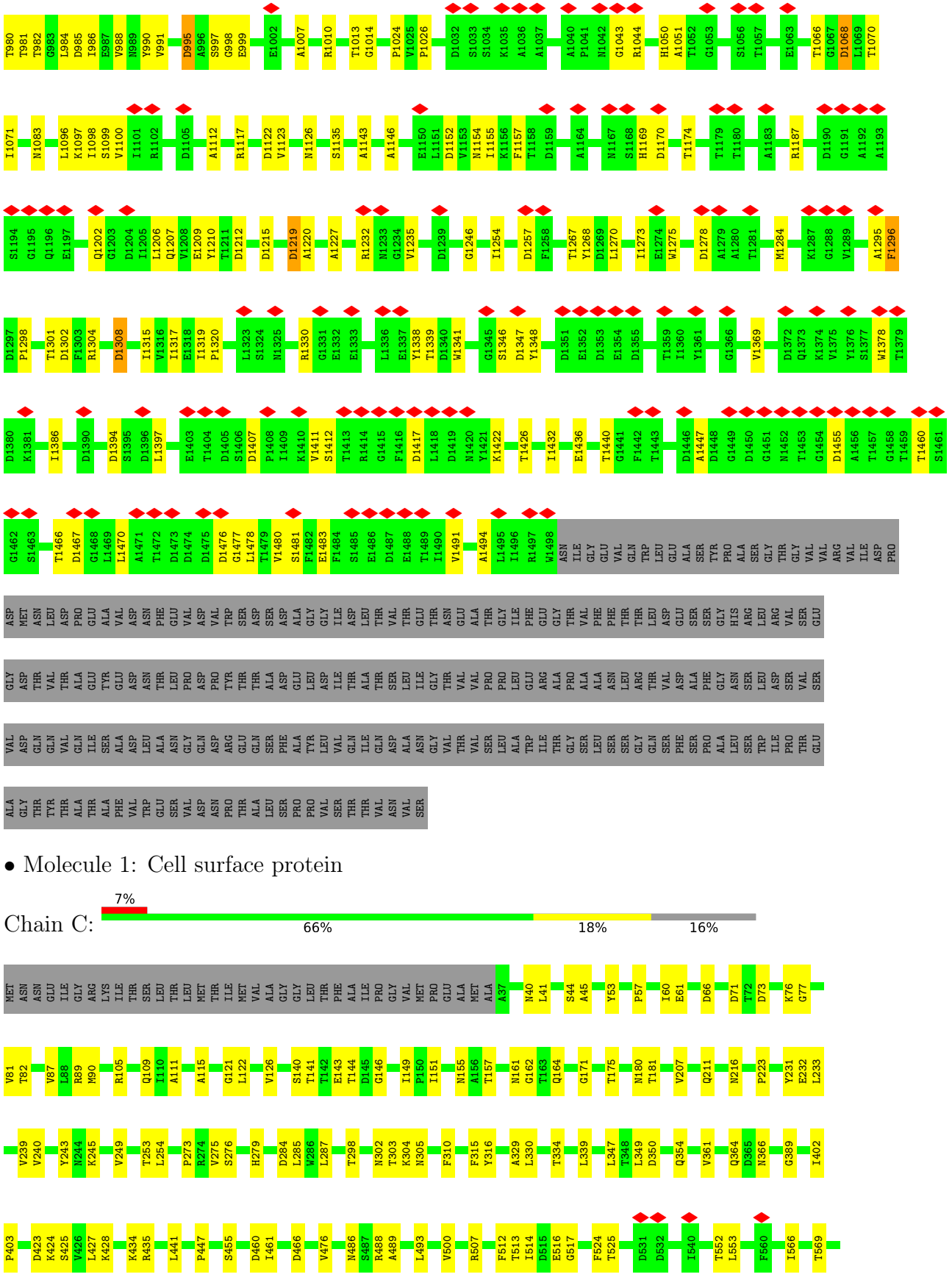


• Molecule 1: Cell surface protein

Chain B:

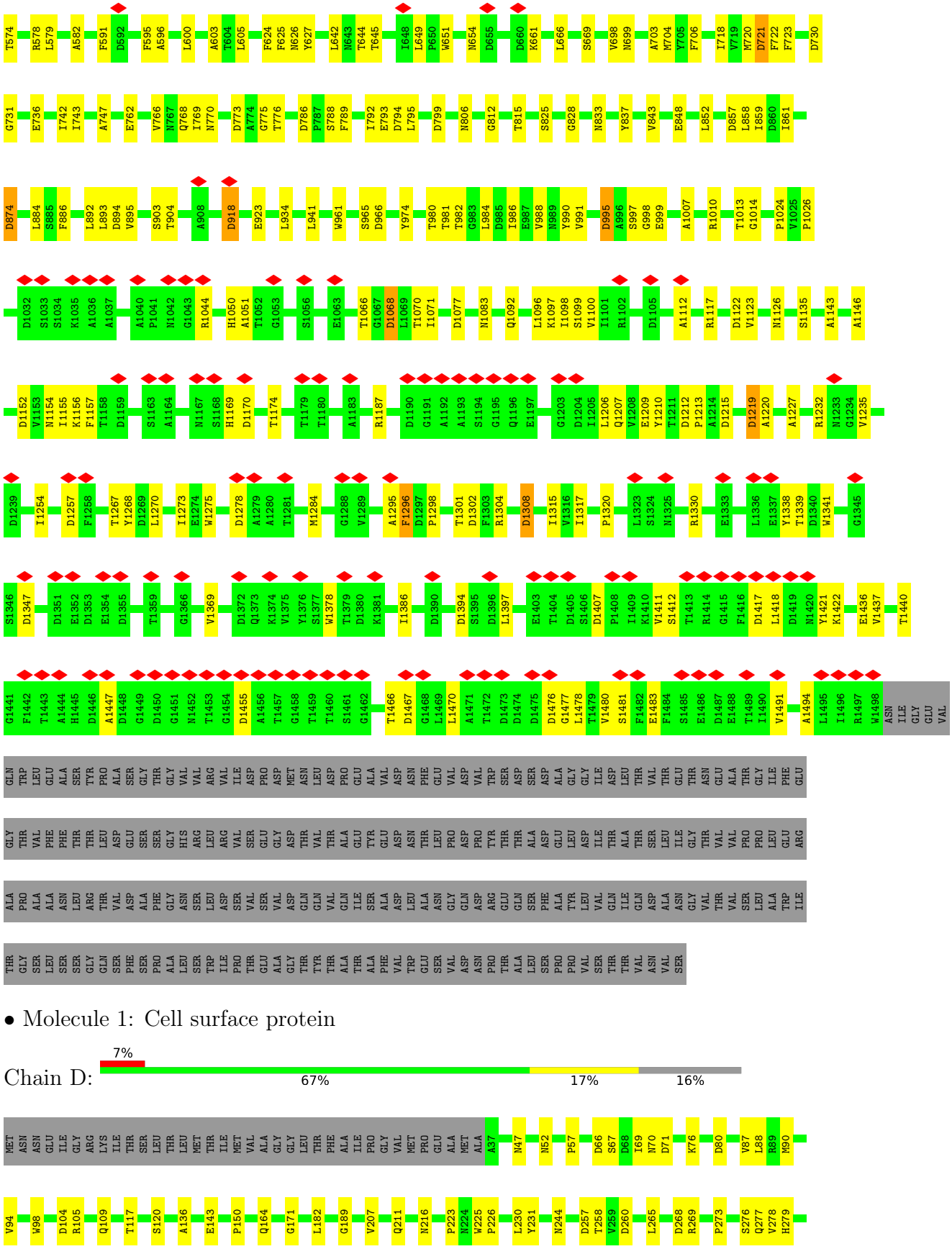






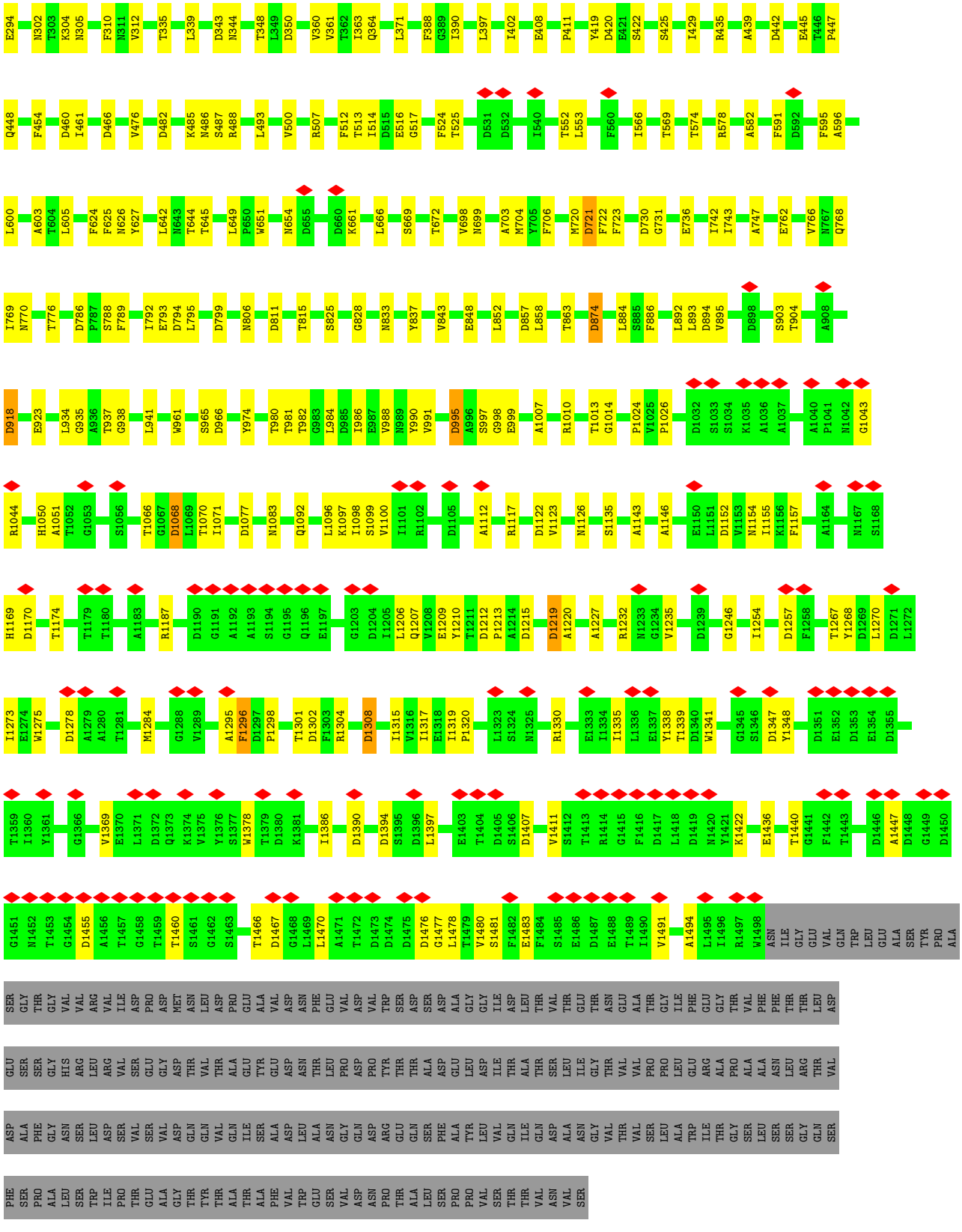
• Molecule 1: Cell surface protein

Chain C:



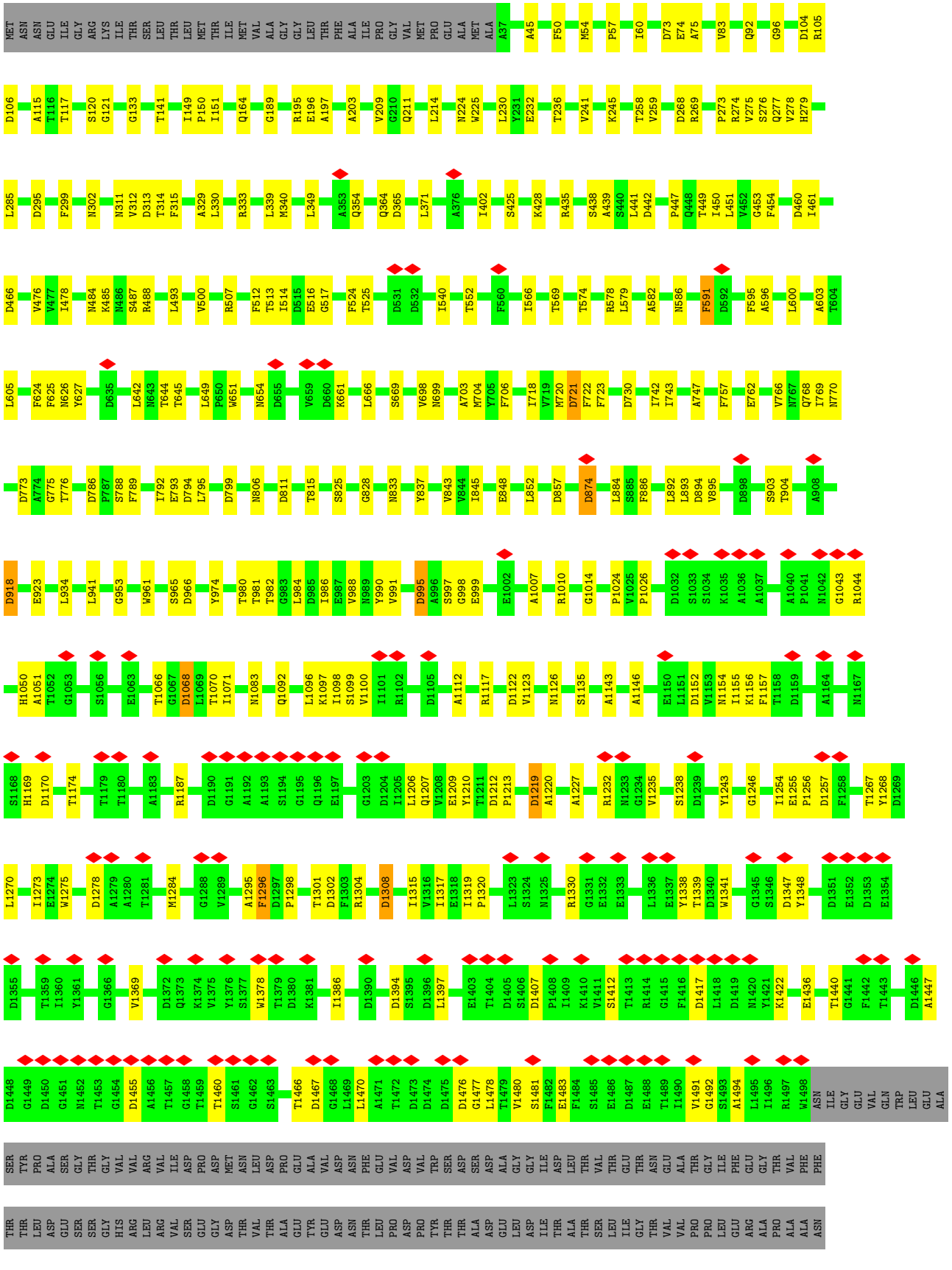
• Molecule 1: Cell surface protein

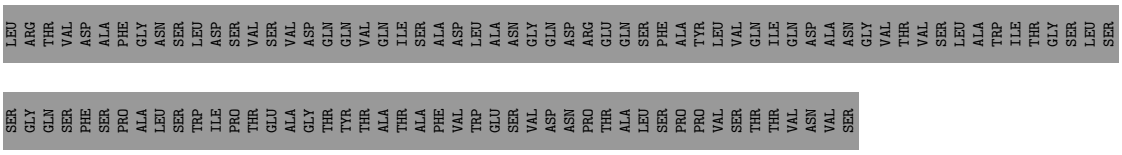
Chain D:



- Molecule 1: Cell surface protein

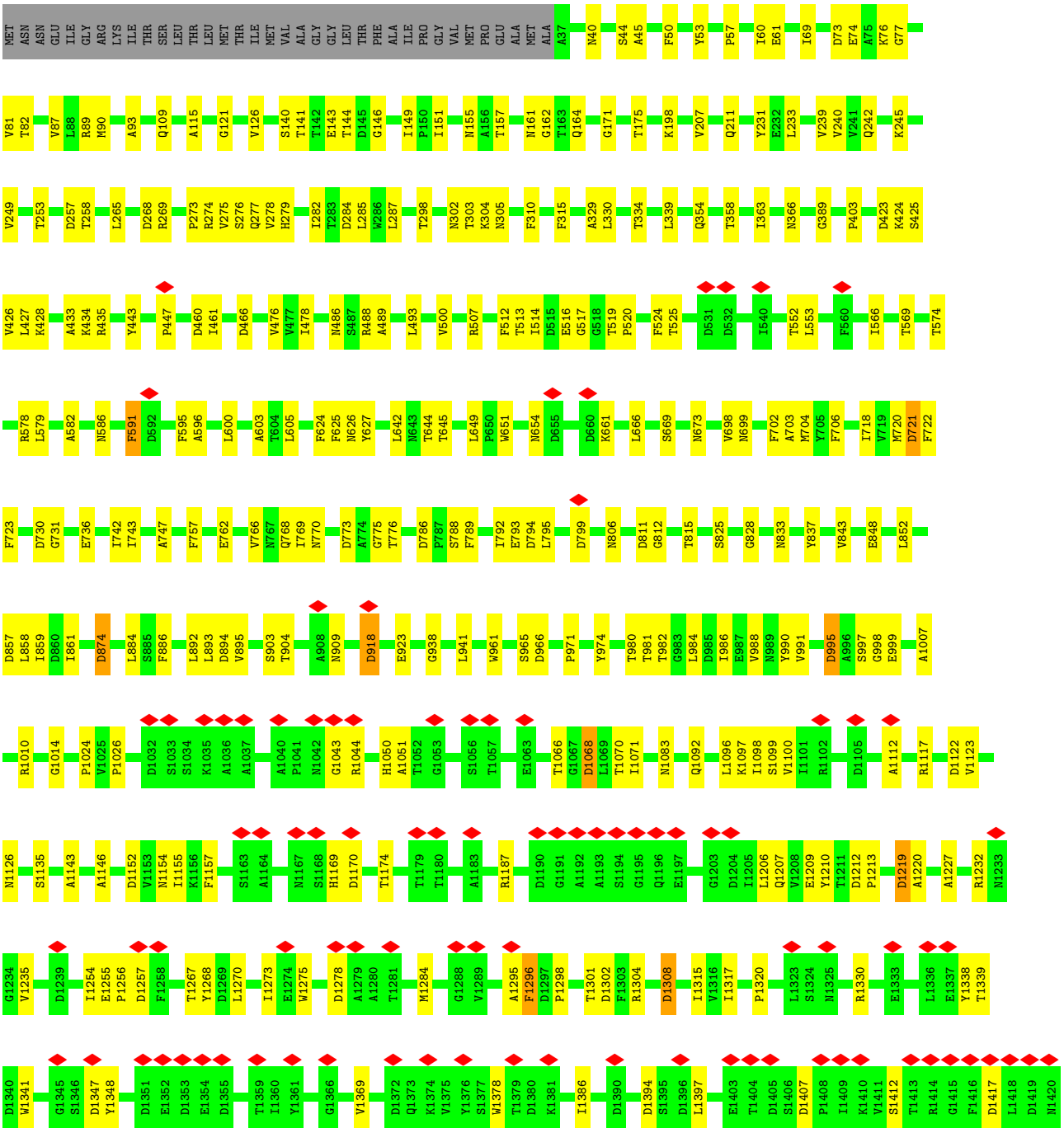
Chain E:

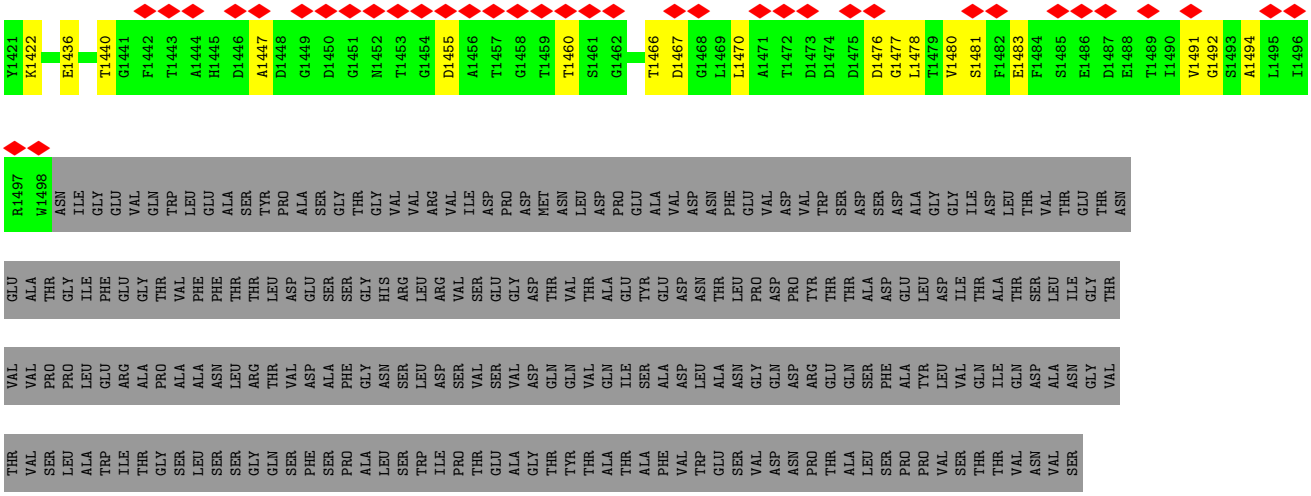

MET ASN ASN GLU ILE GLY ARG LYS ILE THR SER LEU THR LEU MET THR ILE MET VAL ALA GLY GLY LEU THR PHE ALA ILE PRO GLY VAL MET PRO GLU ALA MET ALA A37 A45 F50 M54 P57 I60 D73 E74 A75 V83 Q92 G96 D104 R105
D106 A115 T116 T117 S120 G121 G133 T141 I149 P150 I151 Q164 G189 R195 E196 A197 A203 V209 G210 Q211 L214 N224 W225 L230 Y231 E232 T236 V241 K245 T258 V259 D268 R269 P273 R274 V275 S276 Q277 V278 H279
L285 D295 F299 N302 N311 V312 D313 T314 F315 A329 L330 R333 L339 M340 L349 A353 Q354 Q364 D365 L371 A376 I402 S425 K428 R435 S438 A439 S440 L441 D442 P447 Q448 T449 I450 L451 V452 G453 F454 D460 I461
D466 V476 V477 I478 N484 K485 N486 S487 R488 L493 V500 R507 F512 T513 I514 D515 E516 G517 F524 T525 D531 D532 T540 T552 F560 I566 T569 T574 R578 L579 A582 N586 F591 D592 F595 A596 L600 A603 T604
L605 F624 F625 M626 Y627 D635 L642 N643 T644 T645 L649 P650 W651 N654 D655 V659 D660 K661 L666 S669 V698 N699 A703 M704 Y705 F706 I718 V719 M720 D721 F722 F723 D730 I742 I743 A747 F757 E762 V766 N767 Q768 I769 N770
D773 A774 G775 T776 D786 P787 S788 F789 I792 E793 D794 L795 D799 N806 D811 T815 S825 G828 N833 Y837 V843 V844 I845 E848 L852 D857 D874 L884 S885 F886 L892 L893 D894 V895 D898 S903 T904 A908
D918 E923 L934 L941 G953 W961 S965 D966 Y974 T980 T981 T982 G983 L984 D985 I986 E987 V988 N989 Y990 V991 D995 A996 S997 G998 E999 E1002 A1007 R1010 G1014 P1024 V1025 P1026 D1032 S1033 S1034 K1035 A1036 A1037 A1040 P1041 N1042 G1043 R1044
H1050 A1051 T1052 G1053 S1056 E1063 T1066 G1067 D1068 L1069 T1070 I1071 N1083 Q1092 L1096 K1097 I1098 S1099 V1100 I1101 R1102 D1105 A1112 R1117 D1122 V1123 N1126 S1135 A1143 A1146 E1150 L1151 D1152 V1153 N1154 I1155 K1156 F1157 T1158 D1159 A1164 N1167
S1168 H1169 D1170 T1174 T1179 T1180 A1183 R1187 D1190 G1191 A1192 A1193 S1194 G1195 Q1196 E1197 G1203 D1204 I1205 L1206 Q1207 V1208 E1209 Y1210 T1211 D1212 P1213 D1219 A1220 A1227 R1232 N1233 G1234 V1235 S1238 D1239 Y1243 G1246 I1254 E1255 P1256 D1257 F1258 T1267 Y1268 D1269
L1270 I1273 E1274 W1275 D1278 A1279 A1280 T1281 M1284 G1288 V1289 A1295 F1296 D1297 P1298 T1301 D1302 F1303 R1304 D1308 I1315 V1316 I1317 E1318 I1319 P1320 L1323 S1324 N1325 R1330 G1331 E1332 E1333 L1336 E1337 Y1338 T1339 D1340 W1341 G1345 S1346 D1347 Y1348 D1351 E1352 D1353 E1354
D1355 T1359 I1360 Y1361 G1366 V1369 D1372 Q1373 K1374 V1375 Y1376 S1377 W1378 T1379 D1380 K1381 I1386 D1390 D1394 S1395 D1396 L1397 E1403 T1404 D1405 S1406 D1407 P1408 I1409 K1410 V1411 S1412 T1413 R1414 G1415 F1416 D1417 L1418 D1419 N1420 Y1421 K1422 E1436 T1440 G1441 F1442 T1443 D1446 A1447
D1448 G1449 D1450 G1451 N1452 T1453 G1454 D1455 A1456 T1457 G1458 T1459 T1460 S1461 G1462 S1463 T1466 D1467 G1468 L1469 L1470 A1471 T1472 D1473 D1474 D1475 D1476 G1477 L1478 T1479 V1480 S1481 F1482 E1483 F1484 S1485 E1486 D1487 E1488 T1489 I1490 V1491 G1492 S1493 A1494 L1495 I1496 R1497 W1498 ASN ILE GLY GLU VAL GLN TRP LEU GLU ALA
SER TYR PRO ALA SER GLY THR GLY VAL VAL ARG VAL ILE ASP PRO ASP MET ASN LEU ASP PRO GLU ALA VAL ASP ASN PHE GLU VAL ASP VAL TRP SER ASP SER ASP ALA GLY GLY ILE ASP LEU THR VAL THR GLU THR ASN GLU ALA THR GLY ILE PHE GLU GLY THR VAL PHE PHE
THR THR LEU ASP GLU SER SER GLY HIS ARG LEU ARG VAL SER GLU GLY ASP THR VAL THR ALA GLU TYR GLU ASP ASN THR LEU PRO ASP PRO TYR THR THR ALA ASP GLU LEU ASP ILE THR ALA THR SER LEU ILE GLY THR VAL VAL PRO PRO LEU GLU ARG ALA PRO ALA ALA ASN



• Molecule 1: Cell surface protein

Chain F:




Y1421 K1422 E1436 T1440 G1441 F1442 T1443 A1444 H1445 D1446 A1447 D1448 G1449 D1450 G1451 N1452 T1453 G1454 D1455 A1456 T1457 G1458 T1459 T1460 S1461 G1462 T1466 D1467 G1468 L1469 L1470 A1471 T1472 D1473 D1474 D1475 D1476 G1477 L1478 T1479 V1480 S1481 F1482 E1483 F1484 S1485 E1486 D1487 E1488 T1489 I1490 V1491 G1492 S1493 A1494 L1495 I1496
R1497 W1498 ASN ILE GLY GLU VAL GLN TRP LEU GLU ALA SER TYR PRO ALA SER GLY THR GLY VAL VAL ARG VAL ILE ASP PRO ASP MET ASN LEU ASP PRO GLU ALA VAL ASP ASN PHE GLU VAL ASP VAL TRP SER ASP SER ASP ALA GLY GLY ILE ASP LEU THR VAL THR GLU THR ASN
GLU ALA THR GLY ILE PHE GLU GLY THR VAL PHE PHE THR THR LEU ASP GLU SER SER GLY HIS ARG LEU ARG VAL SER GLU GLY ASP THR VAL THR ALA GLU TYR GLU ASP ASN THR LEU PRO ASP PRO TYR THR THR ALA ASP GLU LEU ASP ILE THR ALA THR SER LEU ILE GLY THR
VAL VAL PRO PRO LEU GLU ARG ALA PRO ALA ALA ASN LEU ARG THR VAL ASP ALA PHE GLY ASN SER LEU ASP SER VAL SER VAL ASP GLN GLN VAL GLN ILE SER ALA ASP LEU ALA ASN GLY GLN ASP ARG GLU GLN SER PHE ALA TYR LEU VAL GLN ILE GLN ASP ALA ASN GLY VAL
THR VAL SER LEU ALA TRP ILE THR GLY SER LEU SER SER GLY GLN SER PHE SER PRO ALA LEU SER TRP ILE PRO THR GLU ALA GLY THR TYR THR ALA THR ALA PHE VAL TRP GLU SER VAL ASP ASN PRO THR ALA LEU SER PRO PRO VAL SER THR THR VAL ASN VAL SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	108621	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; PseudoSubtomograms as described in Zivanov 2022 (https://elifesciences.org/articles/83724)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	121	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.055	Depositor
Minimum map value	-6.789	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.582	Depositor
Recommended contour level	1.45621	Depositor
Map size (Å)	265.4, 265.4, 265.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.327, 1.327, 1.327	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	0.25	0/11032	0.49	0/15089
1	B	0.25	0/11032	0.49	0/15089
1	C	0.25	0/11032	0.49	0/15089
1	D	0.25	0/11032	0.49	0/15089
1	E	0.25	0/11032	0.49	0/15089
1	F	0.25	0/11032	0.49	0/15089
All	All	0.25	0/66192	0.49	0/90534

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	10859	0	10131	260	0
1	B	10859	0	10136	203	0
1	C	10859	0	10136	234	0
1	D	10859	0	10130	247	0
1	E	10859	0	10135	217	0
1	F	10859	0	10136	236	0
All	All	65154	0	60804	1279	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 10.

All (1279) 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:A:269:ARG:HH12	1:A:485:LYS:C	0.98	1.48
1:C:435:ARG:NH1	1:C:812:GLY:HA3	1.24	1.44
1:A:269:ARG:HH12	1:A:486:ASN:N	1.17	1.38
1:A:269:ARG:NH1	1:A:485:LYS:C	1.76	1.37
1:B:354:GLN:NE2	1:C:861:ILE:HD11	1.37	1.36
1:E:354:GLN:NE2	1:F:861:ILE:HD11	1.42	1.32
1:F:435:ARG:NH1	1:F:812:GLY:CA	1.88	1.32
1:F:435:ARG:NH1	1:F:812:GLY:HA3	0.97	1.28
1:A:276:SER:HB2	1:A:485:LYS:O	1.34	1.25
1:D:435:ARG:NH2	1:D:811:ASP:O	1.73	1.21
1:D:276:SER:HB2	1:D:485:LYS:O	1.45	1.15
1:A:435:ARG:NH2	1:A:811:ASP:O	1.79	1.14
1:C:435:ARG:NH1	1:C:812:GLY:CA	2.10	1.14
1:D:268:ASP:OD2	1:D:488:ARG:NH1	1.81	1.13
1:A:269:ARG:NH1	1:A:486:ASN:N	1.90	1.10
1:D:269:ARG:HG3	1:D:487:SER:HB3	1.31	1.10
1:F:435:ARG:HH12	1:F:812:GLY:CA	1.50	1.10
1:B:275:VAL:HG12	1:B:485:LYS:HD3	1.33	1.06
1:F:423:ASP:OD2	1:F:486:ASN:ND2	1.88	1.05
1:E:275:VAL:HG12	1:E:485:LYS:HD3	1.36	1.04
1:A:435:ARG:NH1	1:A:812:GLY:HA3	1.74	1.01
1:C:435:ARG:CZ	1:C:812:GLY:HA3	1.92	0.99
1:B:354:GLN:NE2	1:C:861:ILE:CD1	2.27	0.97
1:D:273:PRO:CG	1:D:485:LYS:HG2	1.95	0.97
1:F:435:ARG:HH11	1:F:812:GLY:HA3	1.23	0.96
1:E:268:ASP:OD2	1:E:488:ARG:NH1	1.99	0.96
1:F:279:HIS:CD2	1:F:488:ARG:HH22	1.83	0.95
1:B:449:THR:CG2	1:C:858:LEU:HG	1.96	0.95
1:C:435:ARG:HH12	1:C:812:GLY:HA3	1.23	0.94
1:A:273:PRO:CG	1:A:485:LYS:HG2	1.99	0.93
1:A:435:ARG:HH12	1:A:812:GLY:HA3	1.34	0.93
1:A:279:HIS:H	1:A:488:ARG:HH22	1.16	0.92
1:E:354:GLN:NE2	1:F:861:ILE:CD1	2.33	0.91
1:E:275:VAL:CG1	1:E:485:LYS:HD3	2.01	0.91
1:A:276:SER:CB	1:A:485:LYS:O	2.20	0.90
1:D:273:PRO:HG2	1:D:485:LYS:HG2	1.53	0.90
1:B:449:THR:HG22	1:C:858:LEU:HG	1.55	0.89
1:A:863:THR:HG21	1:F:354:GLN:CD	1.93	0.89
1:B:268:ASP:OD2	1:B:488:ARG:NH1	2.05	0.88
1:F:435:ARG:CZ	1:F:812:GLY:HA3	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ARG:HH12	1:C:812:GLY:CA	1.77	0.88
1:D:268:ASP:CG	1:D:488:ARG:NH1	2.28	0.87
1:E:449:THR:CG2	1:F:858:LEU:HG	2.05	0.87
1:A:858:LEU:HD11	1:F:447:PRO:O	1.75	0.86
1:B:354:GLN:HE22	1:C:861:ILE:HD11	1.38	0.86
1:D:279:HIS:H	1:D:488:ARG:HH22	1.19	0.85
1:C:279:HIS:CD2	1:C:488:ARG:HH22	1.94	0.85
1:E:354:GLN:HE22	1:F:861:ILE:HD11	1.36	0.85
1:B:275:VAL:CG1	1:B:485:LYS:HD3	2.05	0.85
1:C:435:ARG:HG3	1:D:938:GLY:HA3	1.59	0.85
1:A:935:GLY:O	1:F:434:LYS:NZ	2.10	0.85
1:C:423:ASP:OD2	1:C:486:ASN:ND2	2.09	0.85
1:A:273:PRO:HG2	1:A:485:LYS:HG2	1.55	0.84
1:E:435:ARG:NH2	1:E:811:ASP:O	2.12	0.83
1:E:275:VAL:HG12	1:E:485:LYS:CD	2.09	0.83
1:B:105:ARG:HA	1:B:230:LEU:HD12	1.60	0.83
1:B:275:VAL:HG12	1:B:485:LYS:CD	2.08	0.83
1:F:279:HIS:CD2	1:F:488:ARG:NH2	2.46	0.83
1:A:269:ARG:NH1	1:A:485:LYS:O	2.10	0.82
1:E:105:ARG:HA	1:E:230:LEU:HD12	1.60	0.81
1:A:435:ARG:CZ	1:A:811:ASP:O	2.27	0.81
1:A:938:GLY:HA3	1:F:435:ARG:HG3	1.62	0.81
1:A:435:ARG:NH1	1:A:812:GLY:CA	2.44	0.80
1:A:269:ARG:NH1	1:A:486:ASN:CA	2.44	0.80
1:D:999:GLU:OE1	1:E:1304:ARG:NH1	2.15	0.80
1:A:268:ASP:OD2	1:A:488:ARG:NH1	2.15	0.80
1:A:279:HIS:N	1:A:488:ARG:NH2	2.24	0.80
1:B:268:ASP:OD2	1:B:487:SER:OG	2.01	0.79
1:C:434:LYS:NZ	1:D:935:GLY:O	2.13	0.79
1:D:279:HIS:N	1:D:488:ARG:HH22	1.78	0.79
1:D:273:PRO:HB2	1:D:485:LYS:NZ	1.98	0.79
1:E:449:THR:HG22	1:F:858:LEU:HG	1.62	0.79
1:A:279:HIS:N	1:A:488:ARG:HH22	1.77	0.79
1:A:999:GLU:OE1	1:B:1304:ARG:NH1	2.16	0.78
1:B:999:GLU:OE1	1:C:1304:ARG:NH1	2.17	0.78
1:C:999:GLU:OE1	1:D:1304:ARG:NH1	2.17	0.78
1:A:1304:ARG:NH1	1:F:999:GLU:OE1	2.17	0.78
1:E:999:GLU:OE1	1:F:1304:ARG:NH1	2.17	0.78
1:C:447:PRO:O	1:D:858:LEU:HD11	1.84	0.77
1:E:268:ASP:OD2	1:E:487:SER:OG	2.02	0.77
1:A:276:SER:CB	1:A:485:LYS:HB3	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PRO:HG2	1:A:485:LYS:HA	1.68	0.76
1:A:273:PRO:HB2	1:A:485:LYS:NZ	2.01	0.76
1:F:435:ARG:HH12	1:F:812:GLY:HA3	0.97	0.75
1:F:435:ARG:HH12	1:F:812:GLY:N	1.85	0.75
1:A:276:SER:HB3	1:A:485:LYS:HB3	1.70	0.74
1:B:768:GLN:HE21	1:B:991:VAL:HG12	1.53	0.74
1:D:105:ARG:HA	1:D:230:LEU:HD12	1.70	0.74
1:C:279:HIS:CD2	1:C:488:ARG:NH2	2.56	0.74
1:C:354:GLN:CD	1:D:863:THR:HG21	2.08	0.74
1:A:302:ASN:HB2	1:A:402:ILE:H	1.53	0.73
1:A:768:GLN:HE21	1:A:991:VAL:HG12	1.53	0.73
1:E:768:GLN:HE21	1:E:991:VAL:HG12	1.53	0.73
1:A:672:THR:HG21	1:F:334:THR:HG22	1.69	0.73
1:C:768:GLN:HE21	1:C:991:VAL:HG12	1.53	0.73
1:D:768:GLN:HE21	1:D:991:VAL:HG12	1.53	0.73
1:D:273:PRO:HB2	1:D:485:LYS:HZ2	1.51	0.73
1:F:768:GLN:HE21	1:F:991:VAL:HG12	1.53	0.72
1:A:863:THR:HG21	1:F:354:GLN:CG	2.18	0.72
1:D:302:ASN:HB2	1:D:402:ILE:H	1.53	0.72
1:D:269:ARG:NH1	1:D:485:LYS:CA	2.43	0.72
1:A:276:SER:CA	1:A:485:LYS:HB3	2.18	0.72
1:C:354:GLN:HG2	1:D:863:THR:HG21	1.70	0.72
1:D:276:SER:CB	1:D:485:LYS:HB3	2.19	0.71
1:B:274:ARG:NH1	1:B:433:ALA:O	2.24	0.71
1:C:155:ASN:O	1:C:161:ASN:ND2	2.24	0.71
1:E:269:ARG:NH2	1:E:484:ASN:O	2.24	0.71
1:A:863:THR:HG21	1:F:354:GLN:HG2	1.72	0.71
1:D:276:SER:CB	1:D:485:LYS:O	2.34	0.70
1:D:279:HIS:N	1:D:488:ARG:NH2	2.28	0.70
1:E:275:VAL:CG1	1:E:485:LYS:CD	2.68	0.70
1:C:334:THR:HG22	1:D:672:THR:HG21	1.71	0.70
1:A:863:THR:OG1	1:F:354:GLN:HG2	1.91	0.70
1:D:276:SER:CA	1:D:485:LYS:HB3	2.22	0.70
1:A:105:ARG:HA	1:A:230:LEU:HD12	1.74	0.70
1:F:155:ASN:O	1:F:161:ASN:ND2	2.25	0.69
1:D:273:PRO:HG2	1:D:485:LYS:HA	1.75	0.69
1:B:236:THR:OG1	1:C:489:ALA:HB2	1.93	0.69
1:A:863:THR:HG23	1:F:354:GLN:NE2	2.07	0.69
1:D:265:LEU:O	1:D:448:GLN:NE2	2.26	0.69
1:B:259:VAL:HG11	1:B:285:LEU:HD22	1.75	0.68
1:C:273:PRO:HG2	1:C:276:SER:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ARG:NH2	1:E:232:GLU:OE2	2.27	0.68
1:B:435:ARG:NH1	1:B:811:ASP:O	2.27	0.68
1:A:279:HIS:NE2	1:A:486:ASN:ND2	2.42	0.67
1:A:411:PRO:HG2	1:F:249:VAL:HG11	1.76	0.67
1:D:269:ARG:CG	1:D:487:SER:HB3	2.18	0.67
1:D:273:PRO:HG2	1:D:276:SER:HB3	1.75	0.67
1:D:279:HIS:NE2	1:D:486:ASN:ND2	2.42	0.67
1:A:273:PRO:HG2	1:A:276:SER:HB3	1.76	0.67
1:A:276:SER:HB2	1:A:485:LYS:C	2.14	0.67
1:C:354:GLN:CG	1:D:863:THR:HG21	2.24	0.67
1:A:273:PRO:CG	1:A:485:LYS:HA	2.24	0.67
1:E:259:VAL:HG11	1:E:285:LEU:HD22	1.76	0.67
1:E:743:ILE:HG13	1:E:789:PHE:HB3	1.77	0.67
1:D:743:ILE:HG13	1:D:789:PHE:HB3	1.77	0.67
1:B:574:THR:OG1	1:B:806:ASN:ND2	2.29	0.66
1:C:574:THR:OG1	1:C:806:ASN:ND2	2.29	0.66
1:C:354:GLN:NE2	1:D:863:THR:HG23	2.09	0.66
1:D:574:THR:OG1	1:D:806:ASN:ND2	2.29	0.66
1:E:574:THR:OG1	1:E:806:ASN:ND2	2.29	0.66
1:F:574:THR:OG1	1:F:806:ASN:ND2	2.29	0.66
1:F:743:ILE:HG13	1:F:789:PHE:HB3	1.77	0.66
1:C:743:ILE:HG13	1:C:789:PHE:HB3	1.77	0.66
1:D:1220:ALA:O	1:E:1466:THR:OG1	2.13	0.66
1:A:863:THR:CG2	1:F:354:GLN:NE2	2.59	0.66
1:F:240:VAL:HG22	1:F:253:THR:HG22	1.78	0.66
1:A:273:PRO:HB2	1:A:485:LYS:HZ2	1.61	0.66
1:A:276:SER:HB3	1:A:485:LYS:CB	2.25	0.66
1:A:574:THR:OG1	1:A:806:ASN:ND2	2.29	0.66
1:D:294:GLU:HB2	1:D:408:GLU:HB3	1.77	0.66
1:A:1220:ALA:O	1:B:1466:THR:OG1	2.13	0.66
1:A:743:ILE:HG13	1:A:789:PHE:HB3	1.77	0.65
1:C:354:GLN:NE2	1:D:863:THR:CG2	2.59	0.65
1:B:743:ILE:HG13	1:B:789:PHE:HB3	1.77	0.65
1:B:766:VAL:HG11	1:B:792:ILE:HD12	1.78	0.65
1:A:1097:LYS:HB3	1:A:1209:GLU:HB3	1.79	0.65
1:B:1097:LYS:HB3	1:B:1209:GLU:HB3	1.79	0.65
1:C:364:GLN:OE1	1:C:364:GLN:N	2.29	0.65
1:C:766:VAL:HG11	1:C:792:ILE:HD12	1.78	0.65
1:A:373:GLN:HE22	1:A:387:ALA:HB1	1.61	0.65
1:D:276:SER:HA	1:D:485:LYS:HB3	1.78	0.65
1:E:236:THR:OG1	1:F:489:ALA:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1097:LYS:HB3	1:C:1209:GLU:HB3	1.79	0.65
1:D:454:PHE:HA	1:D:482:ASP:OD1	1.97	0.65
1:F:1097:LYS:HB3	1:F:1209:GLU:HB3	1.79	0.65
1:E:1394:ASP:HB3	1:E:1397:LEU:HB3	1.79	0.64
1:A:1394:ASP:HB3	1:A:1397:LEU:HB3	1.79	0.64
1:E:512:PHE:HB3	1:E:722:PHE:HB2	1.80	0.64
1:D:71:ASP:OD2	1:D:76:LYS:NZ	2.30	0.64
1:D:269:ARG:NH1	1:D:486:ASN:N	2.35	0.64
1:F:512:PHE:HB3	1:F:722:PHE:HB2	1.80	0.64
1:A:766:VAL:HG11	1:A:792:ILE:HD12	1.78	0.64
1:B:269:ARG:NH2	1:B:484:ASN:O	2.31	0.64
1:B:1394:ASP:HB3	1:B:1397:LEU:HB3	1.79	0.64
1:C:249:VAL:HG11	1:D:411:PRO:HG2	1.80	0.64
1:D:273:PRO:HG2	1:D:485:LYS:CG	2.26	0.64
1:D:1097:LYS:HB3	1:D:1209:GLU:HB3	1.79	0.64
1:E:1097:LYS:HB3	1:E:1209:GLU:HB3	1.79	0.64
1:F:1394:ASP:HB3	1:F:1397:LEU:HB3	1.79	0.64
1:F:766:VAL:HG11	1:F:792:ILE:HD12	1.78	0.64
1:D:1394:ASP:HB3	1:D:1397:LEU:HB3	1.80	0.64
1:A:276:SER:HA	1:A:485:LYS:HB3	1.80	0.64
1:D:512:PHE:HB3	1:D:722:PHE:HB2	1.80	0.64
1:A:55:SER:O	1:A:58:GLN:NE2	2.28	0.64
1:A:265:LEU:O	1:A:448:GLN:NE2	2.31	0.64
1:A:273:PRO:HG2	1:A:485:LYS:CG	2.28	0.64
1:D:268:ASP:CG	1:D:488:ARG:HH12	1.97	0.64
1:A:331:THR:HG22	1:A:396:LYS:HE2	1.80	0.64
1:D:766:VAL:HG11	1:D:792:ILE:HD12	1.78	0.64
1:A:512:PHE:HB3	1:A:722:PHE:HB2	1.80	0.63
1:C:1394:ASP:HB3	1:C:1397:LEU:HB3	1.79	0.63
1:D:273:PRO:CG	1:D:485:LYS:HA	2.29	0.63
1:E:766:VAL:HG11	1:E:792:ILE:HD12	1.78	0.63
1:E:1220:ALA:O	1:F:1466:THR:OG1	2.16	0.63
1:A:455:SER:N	1:A:482:ASP:OD1	2.30	0.63
1:C:435:ARG:CG	1:D:938:GLY:HA3	2.29	0.63
1:C:512:PHE:HB3	1:C:722:PHE:HB2	1.80	0.63
1:D:268:ASP:OD2	1:D:488:ARG:CZ	2.46	0.63
1:C:1220:ALA:O	1:D:1466:THR:OG1	2.17	0.63
1:D:276:SER:HB3	1:D:485:LYS:HB3	1.80	0.63
1:E:1050:HIS:HD2	1:E:1051:ALA:N	1.97	0.63
1:D:1050:HIS:HD2	1:D:1051:ALA:N	1.97	0.62
1:B:1295:ALA:HB1	1:B:1320:PRO:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1050:HIS:HD2	1:C:1051:ALA:N	1.97	0.62
1:F:1050:HIS:HD2	1:F:1051:ALA:N	1.97	0.62
1:A:1050:HIS:HD2	1:A:1051:ALA:N	1.97	0.62
1:B:269:ARG:NH1	1:B:276:SER:OG	2.32	0.62
1:B:273:PRO:HG2	1:B:276:SER:HB2	1.82	0.62
1:B:512:PHE:HB3	1:B:722:PHE:HB2	1.80	0.62
1:B:1050:HIS:HD2	1:B:1051:ALA:N	1.97	0.62
1:F:366:ASN:ND2	1:F:424:LYS:O	2.32	0.62
1:A:268:ASP:CG	1:A:488:ARG:NH1	2.53	0.62
1:C:354:GLN:HG2	1:D:863:THR:OG1	1.99	0.62
1:C:1295:ALA:HB1	1:C:1320:PRO:HB3	1.81	0.62
1:B:1436:GLU:N	1:B:1436:GLU:OE2	2.33	0.62
1:A:1295:ALA:HB1	1:A:1320:PRO:HB3	1.81	0.62
1:B:449:THR:HG21	1:C:859:ILE:H	1.64	0.62
1:F:1436:GLU:OE2	1:F:1436:GLU:N	2.33	0.62
1:A:1436:GLU:OE2	1:A:1436:GLU:N	2.33	0.62
1:E:1436:GLU:OE2	1:E:1436:GLU:N	2.33	0.62
1:C:1066:THR:OG1	1:C:1068:ASP:OD1	2.17	0.61
1:A:71:ASP:OD2	1:A:76:LYS:NZ	2.32	0.61
1:A:863:THR:CB	1:F:354:GLN:HG2	2.31	0.61
1:A:257:ASP:OD1	1:A:258:THR:N	2.33	0.61
1:A:863:THR:CG2	1:F:354:GLN:HG2	2.30	0.61
1:C:1436:GLU:OE2	1:C:1436:GLU:N	2.33	0.61
1:C:87:VAL:O	1:C:231:TYR:OH	2.19	0.61
1:A:886:PHE:HA	1:B:1301:THR:HG21	1.83	0.61
1:D:1295:ALA:HB1	1:D:1320:PRO:HB3	1.81	0.61
1:E:886:PHE:HA	1:F:1301:THR:HG21	1.82	0.61
1:E:1476:ASP:OD1	1:E:1477:GLY:N	2.31	0.61
1:B:1066:THR:OG1	1:B:1068:ASP:OD1	2.17	0.61
1:C:1476:ASP:OD1	1:C:1477:GLY:N	2.31	0.61
1:D:1122:ASP:OD1	1:D:1126:ASN:ND2	2.34	0.61
1:F:1295:ALA:HB1	1:F:1320:PRO:HB3	1.81	0.61
1:C:126:VAL:HG22	1:C:164:GLN:HA	1.83	0.60
1:D:1436:GLU:N	1:D:1436:GLU:OE2	2.33	0.60
1:D:1481:SER:HB3	1:D:1491:VAL:HG12	1.83	0.60
1:E:449:THR:HG21	1:F:859:ILE:H	1.64	0.60
1:E:115:ALA:HA	1:E:330:LEU:HD13	1.83	0.60
1:E:1066:THR:OG1	1:E:1068:ASP:OD1	2.17	0.60
1:D:87:VAL:O	1:D:231:TYR:OH	2.19	0.60
1:E:1122:ASP:OD1	1:E:1126:ASN:ND2	2.34	0.60
1:B:886:PHE:HA	1:C:1301:THR:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1122:ASP:OD1	1:C:1126:ASN:ND2	2.34	0.60
1:F:126:VAL:HG22	1:F:164:GLN:HA	1.82	0.60
1:E:1295:ALA:HB1	1:E:1320:PRO:HB3	1.81	0.60
1:A:90:MET:HB3	1:A:98:TRP:HB3	1.82	0.60
1:A:284:ASP:OD1	1:A:286:TRP:N	2.33	0.60
1:A:1466:THR:OG1	1:F:1220:ALA:O	2.18	0.60
1:B:354:GLN:CD	1:C:861:ILE:HD11	2.19	0.60
1:B:1481:SER:HB3	1:B:1491:VAL:HG12	1.83	0.60
1:E:1481:SER:HB3	1:E:1491:VAL:HG12	1.83	0.60
1:C:354:GLN:HG2	1:D:863:THR:CG2	2.32	0.60
1:C:240:VAL:HG22	1:C:253:THR:HG22	1.82	0.60
1:A:863:THR:CG2	1:F:354:GLN:CD	2.68	0.60
1:A:1122:ASP:OD1	1:A:1126:ASN:ND2	2.34	0.60
1:A:858:LEU:HD21	1:F:447:PRO:HB2	1.84	0.60
1:C:1481:SER:HB3	1:C:1491:VAL:HG12	1.82	0.60
1:F:144:THR:HG23	1:F:146:GLY:H	1.67	0.59
1:A:273:PRO:CB	1:A:485:LYS:HG2	2.31	0.59
1:C:303:THR:HG23	1:C:304:LYS:HG3	1.84	0.59
1:D:886:PHE:HA	1:E:1301:THR:HG21	1.83	0.59
1:F:435:ARG:HH12	1:F:811:ASP:C	1.97	0.59
1:F:1122:ASP:OD1	1:F:1126:ASN:ND2	2.34	0.59
1:D:273:PRO:CB	1:D:485:LYS:HG2	2.32	0.59
1:D:279:HIS:HD1	1:D:425:SER:HB2	1.67	0.59
1:B:1220:ALA:O	1:C:1466:THR:OG1	2.16	0.59
1:C:886:PHE:HA	1:D:1301:THR:HG21	1.84	0.59
1:F:1481:SER:HB3	1:F:1491:VAL:HG12	1.82	0.59
1:B:1122:ASP:OD1	1:B:1126:ASN:ND2	2.34	0.59
1:A:1481:SER:HB3	1:A:1491:VAL:HG12	1.83	0.59
1:E:273:PRO:HG2	1:E:276:SER:HB2	1.85	0.59
1:F:1476:ASP:OD1	1:F:1477:GLY:N	2.31	0.59
1:E:364:GLN:HE21	1:E:428:LYS:HB2	1.68	0.59
1:C:625:PHE:HE1	1:C:627:TYR:HB3	1.69	0.58
1:E:74:GLU:O	1:E:211:GLN:NE2	2.36	0.58
1:B:1476:ASP:OD1	1:B:1477:GLY:N	2.31	0.58
1:D:625:PHE:HE1	1:D:627:TYR:HB3	1.69	0.58
1:F:569:THR:HB	1:F:582:ALA:HB3	1.86	0.58
1:A:273:PRO:HG2	1:A:485:LYS:CA	2.34	0.58
1:D:57:PRO:HG3	1:D:339:LEU:HD22	1.85	0.58
1:A:569:THR:HB	1:A:582:ALA:HB3	1.85	0.58
1:A:937:THR:O	1:F:435:ARG:NE	2.37	0.58
1:A:1301:THR:HG21	1:F:886:PHE:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:PHE:HE1	1:B:627:TYR:HB3	1.69	0.58
1:F:257:ASP:OD1	1:F:258:THR:N	2.36	0.58
1:A:1066:THR:OG1	1:A:1068:ASP:OD1	2.17	0.58
1:D:257:ASP:OD1	1:D:258:THR:N	2.37	0.58
1:F:89:ARG:NH1	1:F:140:SER:O	2.36	0.58
1:E:569:THR:HB	1:E:582:ALA:HB3	1.85	0.58
1:F:109:GLN:NE2	1:F:171:GLY:O	2.31	0.58
1:A:1308:ASP:OD1	1:A:1308:ASP:N	2.37	0.58
1:A:1476:ASP:OD1	1:A:1477:GLY:N	2.31	0.57
1:D:569:THR:HB	1:D:582:ALA:HB3	1.85	0.57
1:E:625:PHE:HE1	1:E:627:TYR:HB3	1.69	0.57
1:F:87:VAL:O	1:F:231:TYR:OH	2.21	0.57
1:F:278:VAL:HB	1:F:427:LEU:HB2	1.86	0.57
1:E:1206:LEU:N	1:E:1227:ALA:O	2.32	0.57
1:D:279:HIS:ND1	1:D:425:SER:HB2	2.19	0.57
1:A:625:PHE:HE1	1:A:627:TYR:HB3	1.68	0.57
1:D:260:ASP:HA	1:D:344:ASN:HD22	1.70	0.57
1:A:80:ASP:OD2	1:A:244:ASN:ND2	2.35	0.57
1:E:624:PHE:HB2	1:E:723:PHE:HB2	1.87	0.57
1:B:214:LEU:HD22	1:B:224:ASN:HB3	1.85	0.57
1:C:1308:ASP:N	1:C:1308:ASP:OD1	2.37	0.57
1:B:569:THR:HB	1:B:582:ALA:HB3	1.85	0.57
1:D:624:PHE:HB2	1:D:723:PHE:HB2	1.87	0.57
1:D:995:ASP:OD2	1:D:997:SER:N	2.38	0.57
1:A:279:HIS:HD1	1:A:425:SER:HB2	1.69	0.57
1:C:995:ASP:OD2	1:C:997:SER:N	2.38	0.57
1:D:304:LYS:NZ	1:D:350:ASP:OD2	2.37	0.57
1:F:1308:ASP:OD1	1:F:1308:ASP:N	2.37	0.57
1:B:236:THR:HG21	1:C:489:ALA:HB1	1.86	0.56
1:C:569:THR:HB	1:C:582:ALA:HB3	1.85	0.56
1:A:276:SER:HB3	1:A:485:LYS:CA	2.35	0.56
1:A:524:PHE:HB2	1:A:566:ILE:HB	1.88	0.56
1:E:995:ASP:OD2	1:E:997:SER:N	2.38	0.56
1:A:442:ASP:HA	1:A:447:PRO:HA	1.86	0.56
1:C:524:PHE:HB2	1:C:566:ILE:HB	1.88	0.56
1:D:442:ASP:HA	1:D:447:PRO:HA	1.86	0.56
1:F:624:PHE:HB2	1:F:723:PHE:HB2	1.87	0.56
1:F:995:ASP:OD2	1:F:997:SER:N	2.38	0.56
1:F:273:PRO:HG2	1:F:276:SER:HB2	1.88	0.56
1:B:524:PHE:HB2	1:B:566:ILE:HB	1.88	0.56
1:B:624:PHE:HB2	1:B:723:PHE:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:THR:HG23	1:C:146:GLY:H	1.68	0.56
1:D:524:PHE:HB2	1:D:566:ILE:HB	1.88	0.56
1:F:524:PHE:HB2	1:F:566:ILE:HB	1.88	0.56
1:B:1206:LEU:N	1:B:1227:ALA:O	2.32	0.56
1:F:625:PHE:HE1	1:F:627:TYR:HB3	1.68	0.56
1:B:995:ASP:OD2	1:B:997:SER:N	2.38	0.56
1:C:105:ARG:NH2	1:C:232:GLU:OE2	2.38	0.56
1:D:1066:THR:OG1	1:D:1068:ASP:OD1	2.17	0.56
1:A:995:ASP:OD2	1:A:997:SER:N	2.38	0.56
1:A:1206:LEU:N	1:A:1227:ALA:O	2.32	0.56
1:D:1206:LEU:N	1:D:1227:ALA:O	2.32	0.56
1:E:195:ARG:NH2	1:E:295:ASP:OD1	2.36	0.56
1:F:837:TYR:O	1:F:1010:ARG:N	2.39	0.56
1:F:1206:LEU:N	1:F:1227:ALA:O	2.32	0.56
1:C:624:PHE:HB2	1:C:723:PHE:HB2	1.87	0.55
1:E:524:PHE:HB2	1:E:566:ILE:HB	1.88	0.55
1:F:45:ALA:HB2	1:F:60:ILE:HD12	1.87	0.55
1:B:837:TYR:O	1:B:1010:ARG:N	2.40	0.55
1:C:89:ARG:NH1	1:C:140:SER:O	2.39	0.55
1:F:1066:THR:OG1	1:F:1068:ASP:OD1	2.17	0.55
1:B:83:VAL:HG12	1:B:241:VAL:HG22	1.89	0.55
1:E:302:ASN:HB2	1:E:402:ILE:H	1.71	0.55
1:E:1308:ASP:N	1:E:1308:ASP:OD1	2.37	0.55
1:B:275:VAL:CG1	1:B:485:LYS:CD	2.76	0.55
1:B:313:ASP:OD1	1:B:314:THR:N	2.39	0.55
1:B:1308:ASP:OD1	1:B:1308:ASP:N	2.37	0.55
1:D:1308:ASP:OD1	1:D:1308:ASP:N	2.37	0.55
1:A:624:PHE:HB2	1:A:723:PHE:HB2	1.87	0.55
1:B:236:THR:OG1	1:C:489:ALA:CB	2.55	0.55
1:E:313:ASP:OD1	1:E:314:THR:N	2.40	0.55
1:A:279:HIS:ND1	1:A:425:SER:HB2	2.21	0.55
1:C:435:ARG:NE	1:D:937:THR:O	2.40	0.55
1:D:837:TYR:O	1:D:1010:ARG:N	2.39	0.55
1:A:150:PRO:HB2	1:A:189:GLY:HA2	1.89	0.54
1:A:837:TYR:O	1:A:1010:ARG:N	2.40	0.54
1:B:195:ARG:NH2	1:B:295:ASP:OD1	2.35	0.54
1:E:277:GLN:HE22	1:E:364:GLN:HE22	1.56	0.54
1:B:117:THR:HG22	1:B:330:LEU:HD21	1.89	0.54
1:B:449:THR:HG23	1:C:858:LEU:HG	1.86	0.54
1:D:360:VAL:HB	1:D:439:ALA:HB2	1.90	0.54
1:E:105:ARG:NH1	1:E:106:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1096:LEU:HB3	1:E:1112:ALA:HB3	1.89	0.54
1:A:938:GLY:HA3	1:F:435:ARG:CG	2.34	0.54
1:C:1096:LEU:HB3	1:C:1112:ALA:HB3	1.89	0.54
1:F:284:ASP:OD2	1:F:443:TYR:OH	2.16	0.54
1:C:837:TYR:O	1:C:1010:ARG:N	2.40	0.54
1:D:1476:ASP:OD1	1:D:1477:GLY:N	2.31	0.54
1:C:966:ASP:OD1	1:C:966:ASP:N	2.41	0.54
1:E:965:SER:OG	1:E:966:ASP:OD1	2.26	0.54
1:C:354:GLN:HG2	1:D:863:THR:CB	2.38	0.54
1:D:150:PRO:HB2	1:D:189:GLY:HA2	1.89	0.54
1:D:419:TYR:HA	1:D:425:SER:HA	1.90	0.54
1:A:1096:LEU:HB3	1:A:1112:ALA:HB3	1.89	0.53
1:B:1096:LEU:HB3	1:B:1112:ALA:HB3	1.89	0.53
1:A:966:ASP:OD1	1:A:966:ASP:N	2.41	0.53
1:C:45:ALA:HB2	1:C:60:ILE:HD12	1.89	0.53
1:F:966:ASP:OD1	1:F:966:ASP:N	2.41	0.53
1:E:214:LEU:HD22	1:E:224:ASN:HB3	1.89	0.53
1:E:1050:HIS:CD2	1:E:1051:ALA:N	2.77	0.53
1:F:1044:ARG:HA	1:F:1169:HIS:HB3	1.91	0.53
1:A:1044:ARG:HA	1:A:1169:HIS:HB3	1.91	0.53
1:B:320:ASP:OD1	1:B:321:GLU:N	2.42	0.53
1:B:500:VAL:O	1:B:578:ARG:NH2	2.40	0.53
1:C:144:THR:HA	1:C:231:TYR:HE1	1.73	0.53
1:C:1206:LEU:N	1:C:1227:ALA:O	2.32	0.53
1:D:642:LEU:HD11	1:D:703:ALA:HB2	1.91	0.53
1:F:1096:LEU:HB3	1:F:1112:ALA:HB3	1.89	0.53
1:C:447:PRO:HB2	1:D:858:LEU:HD21	1.90	0.53
1:C:642:LEU:HD11	1:C:703:ALA:HB2	1.91	0.53
1:D:966:ASP:OD1	1:D:966:ASP:N	2.41	0.53
1:E:83:VAL:HG12	1:E:241:VAL:HG22	1.90	0.53
1:E:837:TYR:O	1:E:1010:ARG:N	2.39	0.53
1:E:1296:PHE:HB3	1:E:1317:ILE:HG23	1.91	0.53
1:A:1098:ILE:HD11	1:A:1206:LEU:HD11	1.91	0.53
1:B:642:LEU:HD11	1:B:703:ALA:HB2	1.91	0.53
1:C:1098:ILE:HD11	1:C:1206:LEU:HD11	1.91	0.53
1:D:269:ARG:HH12	1:D:486:ASN:N	2.06	0.53
1:D:769:ILE:HD11	1:D:892:LEU:HB2	1.91	0.53
1:D:1050:HIS:CD2	1:D:1051:ALA:N	2.77	0.53
1:D:1096:LEU:HB3	1:D:1112:ALA:HB3	1.89	0.53
1:A:769:ILE:HD11	1:A:892:LEU:HB2	1.91	0.53
1:C:109:GLN:NE2	1:C:171:GLY:O	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1478:LEU:HB3	1:C:1494:ALA:HB3	1.91	0.53
1:A:642:LEU:HD11	1:A:703:ALA:HB2	1.91	0.53
1:B:596:ALA:HB3	1:B:704:MET:HB2	1.91	0.53
1:D:815:THR:OG1	1:E:1083:ASN:OD1	2.27	0.53
1:E:1044:ARG:HA	1:E:1169:HIS:HB3	1.91	0.53
1:A:269:ARG:NH1	1:A:485:LYS:CA	2.68	0.53
1:B:236:THR:CB	1:C:489:ALA:HA	2.39	0.53
1:E:236:THR:HG21	1:F:489:ALA:HB1	1.91	0.53
1:E:435:ARG:CZ	1:E:811:ASP:O	2.57	0.53
1:E:500:VAL:O	1:E:578:ARG:NH2	2.40	0.53
1:F:666:LEU:HD21	1:F:669:SER:HB2	1.91	0.53
1:F:1050:HIS:CD2	1:F:1051:ALA:N	2.77	0.53
1:A:419:TYR:HA	1:A:425:SER:HA	1.91	0.52
1:A:645:THR:HA	1:A:698:VAL:HA	1.91	0.52
1:A:768:GLN:NE2	1:A:991:VAL:HG12	2.23	0.52
1:A:1296:PHE:HB3	1:A:1317:ILE:HG23	1.91	0.52
1:B:1044:ARG:HA	1:B:1169:HIS:HB3	1.91	0.52
1:C:645:THR:HA	1:C:698:VAL:HA	1.92	0.52
1:D:109:GLN:NE2	1:D:171:GLY:O	2.38	0.52
1:D:273:PRO:HG2	1:D:485:LYS:CA	2.39	0.52
1:E:596:ALA:HB3	1:E:704:MET:HB2	1.91	0.52
1:F:596:ALA:HB3	1:F:704:MET:HB2	1.91	0.52
1:B:1478:LEU:HB3	1:B:1494:ALA:HB3	1.91	0.52
1:C:389:GLY:HA2	1:C:403:PRO:HG3	1.91	0.52
1:C:1050:HIS:CD2	1:C:1051:ALA:N	2.77	0.52
1:E:642:LEU:HD11	1:E:703:ALA:HB2	1.91	0.52
1:E:966:ASP:OD1	1:E:966:ASP:N	2.41	0.52
1:B:302:ASN:HB2	1:B:402:ILE:H	1.73	0.52
1:B:769:ILE:HD11	1:B:892:LEU:HB2	1.91	0.52
1:B:1296:PHE:HB3	1:B:1317:ILE:HG23	1.91	0.52
1:C:1296:PHE:HB3	1:C:1317:ILE:HG23	1.91	0.52
1:D:965:SER:OG	1:D:966:ASP:OD1	2.26	0.52
1:D:1478:LEU:HB3	1:D:1494:ALA:HB3	1.91	0.52
1:E:311:ASN:ND2	1:E:333:ARG:HD3	2.24	0.52
1:F:1296:PHE:HB3	1:F:1317:ILE:HG23	1.91	0.52
1:A:294:GLU:OE2	1:F:242:GLN:NE2	2.42	0.52
1:B:645:THR:HA	1:B:698:VAL:HA	1.92	0.52
1:E:769:ILE:HD11	1:E:892:LEU:HB2	1.91	0.52
1:A:1440:THR:N	1:A:1470:LEU:O	2.40	0.52
1:C:769:ILE:HD11	1:C:892:LEU:HB2	1.91	0.52
1:D:207:VAL:HG13	1:D:211:GLN:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:642:LEU:HD11	1:F:703:ALA:HB2	1.91	0.52
1:A:1050:HIS:CD2	1:A:1051:ALA:N	2.77	0.52
1:B:966:ASP:N	1:B:966:ASP:OD1	2.41	0.52
1:F:1478:LEU:HB3	1:F:1494:ALA:HB3	1.91	0.52
1:A:965:SER:OG	1:A:966:ASP:OD1	2.26	0.52
1:B:768:GLN:NE2	1:B:991:VAL:HG12	2.23	0.52
1:B:1050:HIS:CD2	1:B:1051:ALA:N	2.77	0.52
1:C:82:THR:HG22	1:C:87:VAL:HA	1.91	0.52
1:E:961:TRP:CD1	1:E:981:THR:HG22	2.45	0.52
1:E:1478:LEU:HB3	1:E:1494:ALA:HB3	1.91	0.52
1:F:1098:ILE:HD11	1:F:1206:LEU:HD11	1.91	0.52
1:A:596:ALA:HB3	1:A:704:MET:HB2	1.91	0.52
1:B:1098:ILE:HD11	1:B:1206:LEU:HD11	1.91	0.52
1:C:596:ALA:HB3	1:C:704:MET:HB2	1.91	0.52
1:C:961:TRP:CD1	1:C:981:THR:HG22	2.45	0.52
1:C:1044:ARG:HA	1:C:1169:HIS:HB3	1.91	0.52
1:D:645:THR:HA	1:D:698:VAL:HA	1.92	0.52
1:D:1044:ARG:HA	1:D:1169:HIS:HB3	1.91	0.52
1:F:768:GLN:NE2	1:F:991:VAL:HG12	2.23	0.52
1:A:72:THR:OG1	1:F:74:GLU:OE1	2.26	0.52
1:A:267:LEU:HD21	1:A:450:ILE:HG12	1.91	0.52
1:A:273:PRO:HB2	1:A:485:LYS:HZ3	1.73	0.52
1:A:454:PHE:HA	1:A:482:ASP:OD1	2.10	0.52
1:A:1467:ASP:OD1	1:A:1467:ASP:N	2.43	0.52
1:B:815:THR:OG1	1:C:1083:ASN:OD1	2.28	0.52
1:B:1050:HIS:HD2	1:B:1051:ALA:H	1.58	0.52
1:B:1235:VAL:HG13	1:B:1254:ILE:HG23	1.92	0.52
1:D:596:ALA:HB3	1:D:704:MET:HB2	1.91	0.52
1:D:1050:HIS:HD2	1:D:1051:ALA:H	1.58	0.52
1:D:1296:PHE:HB3	1:D:1317:ILE:HG23	1.91	0.52
1:E:1174:THR:OG1	1:E:1187:ARG:NH1	2.43	0.52
1:F:769:ILE:HD11	1:F:892:LEU:HB2	1.91	0.52
1:C:40:ASN:OD1	1:C:245:LYS:NZ	2.40	0.52
1:C:815:THR:OG1	1:D:1083:ASN:OD1	2.28	0.52
1:D:666:LEU:HD21	1:D:669:SER:HB2	1.91	0.52
1:F:645:THR:HA	1:F:698:VAL:HA	1.91	0.52
1:F:961:TRP:CD1	1:F:981:THR:HG22	2.45	0.52
1:A:273:PRO:HB2	1:A:485:LYS:HG2	1.91	0.51
1:A:666:LEU:HD21	1:A:669:SER:HB2	1.91	0.51
1:B:1174:THR:OG1	1:B:1187:ARG:NH1	2.43	0.51
1:F:466:ASP:OD2	1:F:466:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:TRP:CD1	1:A:981:THR:HG22	2.45	0.51
1:B:64:VAL:HB	1:B:98:TRP:HB2	1.92	0.51
1:B:517:GLY:HA3	1:B:603:ALA:HB2	1.93	0.51
1:D:961:TRP:CD1	1:D:981:THR:HG22	2.45	0.51
1:D:1098:ILE:HD11	1:D:1206:LEU:HD11	1.91	0.51
1:E:349:LEU:HD13	1:E:441:LEU:HD13	1.91	0.51
1:E:645:THR:HA	1:E:698:VAL:HA	1.91	0.51
1:E:666:LEU:HD21	1:E:669:SER:HB2	1.91	0.51
1:A:1174:THR:OG1	1:A:1187:ARG:NH1	2.43	0.51
1:C:1174:THR:OG1	1:C:1187:ARG:NH1	2.43	0.51
1:F:517:GLY:HA3	1:F:603:ALA:HB2	1.93	0.51
1:F:1467:ASP:OD1	1:F:1467:ASP:N	2.43	0.51
1:A:517:GLY:HA3	1:A:603:ALA:HB2	1.93	0.51
1:B:1467:ASP:OD1	1:B:1467:ASP:N	2.43	0.51
1:D:276:SER:HB2	1:D:485:LYS:C	2.25	0.51
1:D:276:SER:HB3	1:D:485:LYS:CB	2.39	0.51
1:F:1235:VAL:HG13	1:F:1254:ILE:HG23	1.92	0.51
1:B:961:TRP:CD1	1:B:981:THR:HG22	2.45	0.51
1:C:768:GLN:NE2	1:C:991:VAL:HG12	2.23	0.51
1:D:500:VAL:O	1:D:578:ARG:NH2	2.40	0.51
1:E:815:THR:OG1	1:F:1083:ASN:OD1	2.27	0.51
1:A:1478:LEU:HB3	1:A:1494:ALA:HB3	1.91	0.51
1:E:435:ARG:NH1	1:F:938:GLY:O	2.43	0.51
1:F:1174:THR:OG1	1:F:1187:ARG:NH1	2.43	0.51
1:C:284:ASP:HB3	1:C:287:LEU:HD12	1.93	0.51
1:C:666:LEU:HD21	1:C:669:SER:HB2	1.91	0.51
1:E:1071:ILE:HG12	1:E:1155:ILE:HD11	1.93	0.51
1:E:1098:ILE:HD11	1:E:1206:LEU:HD11	1.91	0.51
1:F:284:ASP:HB3	1:F:287:LEU:HD12	1.92	0.51
1:B:1071:ILE:HG12	1:B:1155:ILE:HD11	1.93	0.51
1:D:1219:ASP:OD2	1:E:1422:LYS:NZ	2.34	0.51
1:E:315:PHE:CD2	1:E:329:ALA:HB1	2.46	0.51
1:B:965:SER:OG	1:B:966:ASP:OD1	2.26	0.51
1:C:435:ARG:HD3	1:D:937:THR:O	2.11	0.51
1:D:903:SER:HG	1:D:974:TYR:HH	1.56	0.51
1:E:768:GLN:NE2	1:E:991:VAL:HG12	2.23	0.51
1:F:40:ASN:OD1	1:F:245:LYS:NZ	2.40	0.51
1:F:1050:HIS:HD2	1:F:1051:ALA:H	1.58	0.51
1:A:260:ASP:HA	1:A:344:ASN:HD22	1.77	0.50
1:A:269:ARG:NH1	1:A:486:ASN:HA	2.26	0.50
1:B:666:LEU:HD21	1:B:669:SER:HB2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:GLY:HA3	1:C:603:ALA:HB2	1.93	0.50
1:C:965:SER:OG	1:C:966:ASP:OD1	2.26	0.50
1:C:1467:ASP:N	1:C:1467:ASP:OD1	2.43	0.50
1:D:768:GLN:NE2	1:D:991:VAL:HG12	2.23	0.50
1:F:1071:ILE:HG12	1:F:1155:ILE:HD11	1.93	0.50
1:A:1235:VAL:HG13	1:A:1254:ILE:HG23	1.92	0.50
1:C:121:GLY:HA3	1:C:330:LEU:HD12	1.92	0.50
1:E:236:THR:CB	1:F:489:ALA:HA	2.42	0.50
1:E:517:GLY:HA3	1:E:603:ALA:HB2	1.93	0.50
1:E:1235:VAL:HG13	1:E:1254:ILE:HG23	1.92	0.50
1:E:1467:ASP:N	1:E:1467:ASP:OD1	2.43	0.50
1:B:105:ARG:NH1	1:B:232:GLU:OE2	2.42	0.50
1:C:57:PRO:HG3	1:C:339:LEU:HD22	1.93	0.50
1:C:115:ALA:HA	1:C:330:LEU:HD13	1.93	0.50
1:C:1235:VAL:HG13	1:C:1254:ILE:HG23	1.92	0.50
1:D:1235:VAL:HG13	1:D:1254:ILE:HG23	1.92	0.50
1:D:1467:ASP:OD1	1:D:1467:ASP:N	2.43	0.50
1:A:360:VAL:HB	1:A:439:ALA:HB2	1.94	0.50
1:C:354:GLN:NE2	1:D:863:THR:HG21	2.26	0.50
1:D:1174:THR:OG1	1:D:1187:ARG:NH1	2.43	0.50
1:E:197:ALA:HB1	1:E:225:TRP:NE1	2.27	0.50
1:E:236:THR:OG1	1:F:489:ALA:CB	2.58	0.50
1:F:82:THR:HG22	1:F:87:VAL:HA	1.94	0.50
1:A:276:SER:CB	1:A:485:LYS:CA	2.90	0.50
1:A:277:GLN:OE1	1:A:364:GLN:NE2	2.43	0.50
1:A:1050:HIS:HD2	1:A:1051:ALA:H	1.58	0.50
1:C:918:ASP:HB3	1:C:923:GLU:HG3	1.94	0.50
1:C:1050:HIS:HD2	1:C:1051:ALA:H	1.58	0.50
1:C:1071:ILE:HG12	1:C:1155:ILE:HD11	1.93	0.50
1:D:517:GLY:HA3	1:D:603:ALA:HB2	1.93	0.50
1:F:121:GLY:HA3	1:F:330:LEU:HD12	1.94	0.50
1:A:500:VAL:O	1:A:578:ARG:NH2	2.40	0.50
1:D:277:GLN:OE1	1:D:364:GLN:NE2	2.45	0.50
1:B:349:LEU:HD13	1:B:441:LEU:HD13	1.94	0.50
1:E:1050:HIS:HD2	1:E:1051:ALA:H	1.58	0.50
1:F:57:PRO:HG3	1:F:339:LEU:HD22	1.94	0.50
1:D:1071:ILE:HG12	1:D:1155:ILE:HD11	1.93	0.50
1:D:1440:THR:N	1:D:1470:LEU:O	2.40	0.50
1:E:1440:THR:N	1:E:1470:LEU:O	2.40	0.50
1:A:937:THR:O	1:F:435:ARG:HD3	2.11	0.49
1:C:1298:PRO:HB2	1:C:1301:THR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:THR:OG1	1:D:514:ILE:N	2.45	0.49
1:F:918:ASP:HB3	1:F:923:GLU:HG3	1.94	0.49
1:A:642:LEU:HD22	1:A:651:TRP:CZ2	2.47	0.49
1:A:1071:ILE:HG12	1:A:1155:ILE:HD11	1.93	0.49
1:B:642:LEU:HD22	1:B:651:TRP:CZ2	2.47	0.49
1:C:1440:THR:N	1:C:1470:LEU:O	2.40	0.49
1:D:642:LEU:HD22	1:D:651:TRP:CZ2	2.47	0.49
1:D:1339:THR:OG1	1:D:1341:TRP:NE1	2.46	0.49
1:E:513:THR:OG1	1:E:514:ILE:N	2.45	0.49
1:E:918:ASP:HB3	1:E:923:GLU:HG3	1.94	0.49
1:F:513:THR:OG1	1:F:514:ILE:N	2.45	0.49
1:A:373:GLN:NE2	1:A:375:ASN:O	2.42	0.49
1:A:1298:PRO:HB2	1:A:1301:THR:HA	1.94	0.49
1:A:1339:THR:OG1	1:A:1341:TRP:NE1	2.46	0.49
1:D:466:ASP:OD2	1:D:466:ASP:N	2.44	0.49
1:D:80:ASP:HB3	1:D:244:ASN:HB2	1.94	0.49
1:E:466:ASP:OD2	1:E:466:ASP:N	2.44	0.49
1:B:1298:PRO:HB2	1:B:1301:THR:HA	1.94	0.49
1:C:513:THR:OG1	1:C:514:ILE:N	2.45	0.49
1:D:1298:PRO:HB2	1:D:1301:THR:HA	1.94	0.49
1:F:157:THR:H	1:F:161:ASN:HD22	1.60	0.49
1:F:642:LEU:HD22	1:F:651:TRP:CZ2	2.47	0.49
1:F:1339:THR:OG1	1:F:1341:TRP:NE1	2.46	0.49
1:C:207:VAL:HG13	1:C:211:GLN:HG2	1.95	0.49
1:C:1270:LEU:HD12	1:C:1315:ILE:HD13	1.95	0.49
1:D:312:VAL:HG11	1:D:348:THR:HG22	1.94	0.49
1:D:918:ASP:HB3	1:D:923:GLU:HG3	1.94	0.49
1:F:1270:LEU:HD12	1:F:1315:ILE:HD13	1.95	0.49
1:A:980:THR:HG22	1:A:982:THR:H	1.78	0.49
1:A:995:ASP:N	1:A:999:GLU:O	2.45	0.49
1:B:315:PHE:CD2	1:B:329:ALA:HB1	2.48	0.49
1:C:435:ARG:NH1	1:C:812:GLY:C	2.64	0.49
1:C:893:LEU:HD23	1:C:941:LEU:HD21	1.95	0.49
1:A:513:THR:OG1	1:A:514:ILE:N	2.45	0.49
1:A:815:THR:OG1	1:B:1083:ASN:OD1	2.28	0.49
1:A:984:LEU:HA	1:B:1397:LEU:HD13	1.94	0.49
1:B:980:THR:HG22	1:B:982:THR:H	1.78	0.49
1:B:1339:THR:OG1	1:B:1341:TRP:NE1	2.46	0.49
1:C:1339:THR:OG1	1:C:1341:TRP:NE1	2.46	0.49
1:E:642:LEU:HD22	1:E:651:TRP:CZ2	2.47	0.49
1:E:893:LEU:HD23	1:E:941:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:980:THR:HG22	1:F:982:THR:H	1.78	0.49
1:A:837:TYR:CZ	1:A:843:VAL:HG23	2.48	0.49
1:A:1270:LEU:HD12	1:A:1315:ILE:HD13	1.95	0.49
1:B:918:ASP:HB3	1:B:923:GLU:HG3	1.94	0.49
1:F:965:SER:OG	1:F:966:ASP:OD1	2.26	0.49
1:A:1083:ASN:OD1	1:F:815:THR:OG1	2.28	0.48
1:D:893:LEU:HD23	1:D:941:LEU:HD21	1.95	0.48
1:D:1270:LEU:HD12	1:D:1315:ILE:HD13	1.95	0.48
1:E:1339:THR:OG1	1:E:1341:TRP:NE1	2.46	0.48
1:A:67:SER:HA	1:A:70:ASN:ND2	2.29	0.48
1:A:918:ASP:HB3	1:A:923:GLU:HG3	1.94	0.48
1:B:75:ALA:HA	1:B:211:GLN:HE22	1.78	0.48
1:C:642:LEU:HD22	1:C:651:TRP:CZ2	2.47	0.48
1:C:980:THR:HG22	1:C:982:THR:H	1.78	0.48
1:A:109:GLN:NE2	1:A:171:GLY:O	2.38	0.48
1:A:278:VAL:O	1:A:425:SER:OG	2.24	0.48
1:B:513:THR:OG1	1:B:514:ILE:N	2.45	0.48
1:B:837:TYR:CZ	1:B:843:VAL:HG23	2.48	0.48
1:B:893:LEU:HD23	1:B:941:LEU:HD21	1.95	0.48
1:B:1270:LEU:HD12	1:B:1315:ILE:HD13	1.95	0.48
1:C:1117:ARG:HG2	1:C:1135:SER:HB3	1.95	0.48
1:E:1117:ARG:HG2	1:E:1135:SER:HB3	1.95	0.48
1:E:1270:LEU:HD12	1:E:1315:ILE:HD13	1.95	0.48
1:E:1298:PRO:HB2	1:E:1301:THR:HA	1.94	0.48
1:F:903:SER:HG	1:F:974:TYR:HH	1.60	0.48
1:F:1298:PRO:HB2	1:F:1301:THR:HA	1.94	0.48
1:A:268:ASP:CG	1:A:488:ARG:HH12	2.17	0.48
1:A:273:PRO:HG2	1:A:485:LYS:CB	2.43	0.48
1:A:893:LEU:HD23	1:A:941:LEU:HD21	1.95	0.48
1:B:164:GLN:O	1:B:164:GLN:NE2	2.46	0.48
1:B:274:ARG:HD2	1:B:431:ASP:O	2.14	0.48
1:E:837:TYR:CZ	1:E:843:VAL:HG23	2.48	0.48
1:E:274:ARG:HG2	1:E:454:PHE:HE1	1.78	0.48
1:B:833:ASN:OD1	1:B:833:ASN:N	2.46	0.48
1:B:1275:TRP:HB2	1:B:1284:MET:HG2	1.96	0.48
1:C:435:ARG:CZ	1:D:937:THR:O	2.62	0.48
1:C:837:TYR:CZ	1:C:843:VAL:HG23	2.48	0.48
1:D:273:PRO:HG2	1:D:485:LYS:CB	2.44	0.48
1:D:1407:ASP:HA	1:D:1483:GLU:OE2	2.14	0.48
1:E:279:HIS:CE1	1:E:488:ARG:NE	2.62	0.48
1:F:837:TYR:CZ	1:F:843:VAL:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:893:LEU:HD23	1:F:941:LEU:HD21	1.95	0.48
1:A:276:SER:HB3	1:A:485:LYS:HA	1.96	0.48
1:C:1275:TRP:HB2	1:C:1284:MET:HG2	1.96	0.48
1:D:273:PRO:HB2	1:D:485:LYS:HZ3	1.77	0.48
1:D:837:TYR:CZ	1:D:843:VAL:HG23	2.48	0.48
1:E:1407:ASP:HA	1:E:1483:GLU:OE2	2.14	0.48
1:F:1407:ASP:HA	1:F:1483:GLU:OE2	2.14	0.48
1:A:512:PHE:HA	1:A:516:GLU:HG3	1.96	0.48
1:C:1407:ASP:HA	1:C:1483:GLU:OE2	2.14	0.48
1:D:980:THR:HG22	1:D:982:THR:H	1.78	0.48
1:D:1117:ARG:HG2	1:D:1135:SER:HB3	1.95	0.48
1:E:980:THR:HG22	1:E:982:THR:H	1.78	0.48
1:F:207:VAL:HG13	1:F:211:GLN:HG2	1.96	0.48
1:F:1275:TRP:HB2	1:F:1284:MET:HG2	1.96	0.48
1:A:1407:ASP:HA	1:A:1483:GLU:OE2	2.14	0.48
1:B:1440:THR:N	1:B:1470:LEU:O	2.40	0.48
1:C:512:PHE:HA	1:C:516:GLU:HG3	1.96	0.48
1:D:66:ASP:HB3	1:D:69:ILE:HG12	1.96	0.48
1:A:863:THR:CG2	1:F:354:GLN:CG	2.89	0.47
1:A:1275:TRP:HB2	1:A:1284:MET:HG2	1.96	0.47
1:B:512:PHE:HA	1:B:516:GLU:HG3	1.96	0.47
1:B:1407:ASP:HA	1:B:1483:GLU:OE2	2.14	0.47
1:C:466:ASP:N	1:C:466:ASP:OD2	2.43	0.47
1:C:500:VAL:O	1:C:578:ARG:NH2	2.40	0.47
1:D:984:LEU:HA	1:E:1397:LEU:HD13	1.94	0.47
1:D:995:ASP:N	1:D:999:GLU:O	2.45	0.47
1:F:552:THR:HG22	1:F:654:ASN:H	1.79	0.47
1:A:644:THR:O	1:A:699:ASN:N	2.45	0.47
1:F:1440:THR:N	1:F:1470:LEU:O	2.40	0.47
1:A:207:VAL:HG13	1:A:211:GLN:HG2	1.96	0.47
1:A:552:THR:HG22	1:A:654:ASN:H	1.79	0.47
1:B:1117:ARG:HG2	1:B:1135:SER:HB3	1.95	0.47
1:C:833:ASN:OD1	1:C:833:ASN:N	2.46	0.47
1:E:203:ALA:HB2	1:E:209:VAL:HG23	1.96	0.47
1:E:365:ASP:HB2	1:E:371:LEU:HB3	1.96	0.47
1:E:984:LEU:HA	1:F:1397:LEU:HD13	1.96	0.47
1:F:512:PHE:HA	1:F:516:GLU:HG3	1.96	0.47
1:A:312:VAL:HG11	1:A:348:THR:HG22	1.95	0.47
1:B:644:THR:O	1:B:699:ASN:N	2.45	0.47
1:F:87:VAL:HG12	1:F:143:GLU:HB2	1.96	0.47
1:A:833:ASN:OD1	1:A:833:ASN:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ASP:OD2	1:D:244:ASN:ND2	2.41	0.47
1:D:512:PHE:HA	1:D:516:GLU:HG3	1.96	0.47
1:E:121:GLY:HA3	1:E:330:LEU:HD12	1.97	0.47
1:F:704:MET:HB3	1:F:706:PHE:CE2	2.50	0.47
1:A:75:ALA:HB3	1:B:73:ASP:HB3	1.97	0.47
1:A:863:THR:OG1	1:F:354:GLN:CG	2.59	0.47
1:A:1117:ARG:HG2	1:A:1135:SER:HB3	1.95	0.47
1:B:236:THR:HB	1:C:489:ALA:HA	1.97	0.47
1:B:1447:ALA:N	1:B:1455:ASP:OD2	2.48	0.47
1:C:40:ASN:HD22	1:C:66:ASP:HA	1.80	0.47
1:C:44:SER:OG	1:C:61:GLU:HB3	2.14	0.47
1:D:67:SER:HA	1:D:70:ASN:ND2	2.30	0.47
1:D:164:GLN:O	1:D:164:GLN:NE2	2.46	0.47
1:E:1099:SER:OG	1:E:1207:GLN:NE2	2.46	0.47
1:F:1044:ARG:HG2	1:F:1169:HIS:HB3	1.97	0.47
1:A:335:THR:HG22	1:A:339:LEU:HG	1.97	0.47
1:B:1043:GLY:O	1:B:1348:TYR:OH	2.31	0.47
1:D:1447:ALA:N	1:D:1455:ASP:OD2	2.48	0.47
1:E:1044:ARG:HG2	1:E:1169:HIS:HB3	1.97	0.47
1:E:1447:ALA:N	1:E:1455:ASP:OD2	2.48	0.47
1:F:1099:SER:OG	1:F:1207:GLN:NE2	2.46	0.47
1:A:45:ALA:HB2	1:A:60:ILE:HD12	1.97	0.47
1:A:704:MET:HB3	1:A:706:PHE:CE2	2.50	0.47
1:A:1447:ALA:N	1:A:1455:ASP:OD2	2.48	0.47
1:B:704:MET:HB3	1:B:706:PHE:CE2	2.50	0.47
1:C:1044:ARG:HG2	1:C:1169:HIS:HB3	1.97	0.47
1:D:360:VAL:HG12	1:D:361:VAL:HG13	1.96	0.47
1:F:1447:ALA:N	1:F:1455:ASP:OD2	2.48	0.47
1:A:269:ARG:CZ	1:A:486:ASN:N	2.70	0.47
1:C:1447:ALA:N	1:C:1455:ASP:OD2	2.48	0.47
1:D:279:HIS:HD1	1:D:419:TYR:HB3	1.80	0.47
1:E:258:THR:HG22	1:E:340:MET:HB3	1.97	0.47
1:E:552:THR:HG22	1:E:654:ASN:H	1.79	0.47
1:E:1275:TRP:HB2	1:E:1284:MET:HG2	1.96	0.47
1:F:303:THR:HG23	1:F:304:LYS:HG3	1.97	0.47
1:B:552:THR:HG22	1:B:654:ASN:H	1.79	0.46
1:E:442:ASP:HA	1:E:447:PRO:HA	1.96	0.46
1:F:1117:ARG:HG2	1:F:1135:SER:HB3	1.95	0.46
1:B:1044:ARG:HG2	1:B:1169:HIS:HB3	1.97	0.46
1:D:1099:SER:OG	1:D:1207:GLN:NE2	2.46	0.46
1:E:512:PHE:HA	1:E:516:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ARG:NH1	1:F:433:ALA:O	2.49	0.46
1:A:57:PRO:HG3	1:A:339:LEU:HD22	1.97	0.46
1:A:279:HIS:HD1	1:A:419:TYR:HB3	1.79	0.46
1:A:1099:SER:OG	1:A:1207:GLN:NE2	2.46	0.46
1:C:786:ASP:OD1	1:C:786:ASP:N	2.49	0.46
1:E:625:PHE:CE1	1:E:627:TYR:HB3	2.50	0.46
1:F:358:THR:HG21	1:F:434:LYS:H	1.79	0.46
1:B:995:ASP:N	1:B:999:GLU:O	2.45	0.46
1:D:704:MET:HB3	1:D:706:PHE:CE2	2.50	0.46
1:D:1044:ARG:HG2	1:D:1169:HIS:HB3	1.97	0.46
1:D:1275:TRP:HB2	1:D:1284:MET:HG2	1.96	0.46
1:E:786:ASP:N	1:E:786:ASP:OD1	2.49	0.46
1:E:794:ASP:OD1	1:E:998:GLY:HA3	2.16	0.46
1:F:1270:LEU:HD21	1:F:1284:MET:HB2	1.98	0.46
1:A:360:VAL:HG12	1:A:361:VAL:HG13	1.98	0.46
1:B:133:GLY:HA3	1:B:141:THR:HG22	1.98	0.46
1:B:626:ASN:O	1:B:720:MET:HA	2.16	0.46
1:C:773:ASP:OD2	1:C:775:GLY:N	2.43	0.46
1:E:995:ASP:N	1:E:999:GLU:O	2.45	0.46
1:E:1050:HIS:CD2	1:E:1051:ALA:H	2.33	0.46
1:E:1238:SER:HG	1:E:1243:TYR:HH	1.60	0.46
1:F:500:VAL:O	1:F:578:ARG:NH2	2.40	0.46
1:F:605:LEU:HD13	1:F:698:VAL:HG13	1.98	0.46
1:A:66:ASP:HB3	1:A:69:ILE:HG12	1.97	0.46
1:A:1397:LEU:HD13	1:F:984:LEU:HA	1.98	0.46
1:B:625:PHE:CE1	1:B:627:TYR:HB3	2.50	0.46
1:C:704:MET:HB3	1:C:706:PHE:CE2	2.50	0.46
1:D:1050:HIS:CD2	1:D:1051:ALA:H	2.34	0.46
1:E:1270:LEU:HD21	1:E:1284:MET:HB2	1.98	0.46
1:A:770:ASN:HB2	1:A:776:THR:HG21	1.98	0.46
1:C:71:ASP:OD1	1:C:76:LYS:HE2	2.16	0.46
1:C:552:THR:HG22	1:C:654:ASN:H	1.79	0.46
1:C:644:THR:O	1:C:699:ASN:N	2.45	0.46
1:D:552:THR:HG22	1:D:654:ASN:H	1.79	0.46
1:E:449:THR:HG23	1:F:858:LEU:HG	1.93	0.46
1:F:1050:HIS:CD2	1:F:1051:ALA:H	2.33	0.46
1:A:1050:HIS:CD2	1:A:1051:ALA:H	2.33	0.46
1:B:730:ASP:HA	1:B:884:LEU:HD23	1.98	0.46
1:C:77:GLY:H	1:D:94:VAL:HG21	1.81	0.46
1:C:626:ASN:O	1:C:720:MET:HA	2.16	0.46
1:D:90:MET:HB3	1:D:98:TRP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:704:MET:HB3	1:E:706:PHE:CE2	2.50	0.46
1:F:389:GLY:HA2	1:F:403:PRO:HG3	1.98	0.46
1:F:644:THR:O	1:F:699:ASN:N	2.45	0.46
1:A:269:ARG:CZ	1:A:485:LYS:C	2.72	0.46
1:A:1044:ARG:HG2	1:A:1169:HIS:HB3	1.97	0.46
1:B:984:LEU:HA	1:C:1397:LEU:HD13	1.97	0.46
1:C:180:ASN:OD1	1:C:181:THR:N	2.49	0.46
1:C:730:ASP:HA	1:C:884:LEU:HD23	1.98	0.46
1:C:1050:HIS:CD2	1:C:1051:ALA:H	2.33	0.46
1:D:136:ALA:O	1:D:182:LEU:HD11	2.16	0.46
1:D:143:GLU:HB2	1:E:196:GLU:OE2	2.16	0.46
1:E:605:LEU:HD13	1:E:698:VAL:HG13	1.98	0.46
1:A:626:ASN:O	1:A:720:MET:HA	2.16	0.45
1:B:786:ASP:OD1	1:B:786:ASP:N	2.49	0.45
1:C:81:VAL:HG11	1:C:90:MET:HE2	1.98	0.45
1:C:1369:VAL:HG22	1:C:1386:ILE:HG12	1.98	0.45
1:D:895:VAL:HG12	1:D:988:VAL:HG12	1.98	0.45
1:F:115:ALA:HA	1:F:330:LEU:HD13	1.98	0.45
1:F:794:ASP:OD1	1:F:998:GLY:HA3	2.16	0.45
1:A:1206:LEU:O	1:A:1227:ALA:N	2.40	0.45
1:B:299:PHE:CE1	1:B:314:THR:HG23	2.51	0.45
1:C:275:VAL:HG12	1:C:275:VAL:O	2.16	0.45
1:D:794:ASP:OD1	1:D:998:GLY:HA3	2.16	0.45
1:E:626:ASN:O	1:E:720:MET:HA	2.16	0.45
1:C:794:ASP:OD1	1:C:998:GLY:HA3	2.16	0.45
1:C:984:LEU:HA	1:D:1397:LEU:HD13	1.97	0.45
1:D:1043:GLY:O	1:D:1348:TYR:OH	2.31	0.45
1:E:92:GLN:OE1	1:E:211:GLN:HG3	2.17	0.45
1:A:794:ASP:OD1	1:A:998:GLY:HA3	2.16	0.45
1:B:794:ASP:OD1	1:B:998:GLY:HA3	2.16	0.45
1:B:795:LEU:HB3	1:B:799:ASP:O	2.17	0.45
1:B:1270:LEU:HD21	1:B:1284:MET:HB2	1.98	0.45
1:C:1270:LEU:HD21	1:C:1284:MET:HB2	1.98	0.45
1:E:439:ALA:HB3	1:E:450:ILE:HD12	1.98	0.45
1:F:315:PHE:CD2	1:F:329:ALA:HB1	2.52	0.45
1:F:833:ASN:OD1	1:F:833:ASN:N	2.46	0.45
1:A:605:LEU:HD13	1:A:698:VAL:HG13	1.98	0.45
1:B:723:PHE:HE1	1:B:742:ILE:HG22	1.82	0.45
1:B:770:ASN:HB2	1:B:776:THR:HG21	1.98	0.45
1:B:1050:HIS:CD2	1:B:1051:ALA:H	2.33	0.45
1:C:770:ASN:HB2	1:C:776:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ALA:HA	1:E:211:GLN:HE22	1.82	0.45
1:E:299:PHE:CE1	1:E:314:THR:HG23	2.51	0.45
1:E:723:PHE:HE1	1:E:742:ILE:HG22	1.82	0.45
1:E:773:ASP:OD2	1:E:775:GLY:N	2.43	0.45
1:F:69:ILE:HA	1:F:76:LYS:HE3	1.97	0.45
1:F:625:PHE:CE1	1:F:627:TYR:HB3	2.50	0.45
1:A:363:ILE:HD11	1:A:388:PHE:HB2	1.97	0.45
1:B:1014:GLY:N	1:B:1212:ASP:OD2	2.50	0.45
1:C:848:GLU:O	1:C:848:GLU:HG3	2.17	0.45
1:D:273:PRO:HB2	1:D:485:LYS:HG2	1.97	0.45
1:D:605:LEU:HD13	1:D:698:VAL:HG13	1.98	0.45
1:D:770:ASN:HB2	1:D:776:THR:HG21	1.98	0.45
1:D:848:GLU:HG3	1:D:848:GLU:O	2.17	0.45
1:E:278:VAL:O	1:E:425:SER:OG	2.22	0.45
1:F:461:ILE:HG12	1:F:476:VAL:HG22	1.98	0.45
1:A:1270:LEU:O	1:A:1273:ILE:HG22	2.17	0.45
1:C:53:TYR:O	1:C:285:LEU:HD11	2.17	0.45
1:D:1014:GLY:N	1:D:1212:ASP:OD2	2.50	0.45
1:D:1369:VAL:HG22	1:D:1386:ILE:HG12	1.98	0.45
1:E:1369:VAL:HG22	1:E:1386:ILE:HG12	1.98	0.45
1:F:302:ASN:ND2	1:F:305:ASN:HB2	2.32	0.45
1:F:1369:VAL:HG22	1:F:1386:ILE:HG12	1.98	0.45
1:A:272:PHE:HB3	1:A:429:ILE:HG13	1.99	0.45
1:B:311:ASN:ND2	1:B:333:ARG:HD3	2.31	0.45
1:C:354:GLN:HE21	1:D:863:THR:HG23	1.79	0.45
1:C:895:VAL:HG12	1:C:988:VAL:HG12	1.98	0.45
1:D:1270:LEU:HD21	1:D:1284:MET:HB2	1.98	0.45
1:E:895:VAL:HG12	1:E:988:VAL:HG12	1.98	0.45
1:E:1043:GLY:O	1:E:1348:TYR:OH	2.31	0.45
1:F:1270:LEU:O	1:F:1273:ILE:HG22	2.17	0.45
1:A:625:PHE:CE1	1:A:627:TYR:HB3	2.50	0.45
1:A:1369:VAL:HG22	1:A:1386:ILE:HG12	1.98	0.45
1:B:258:THR:HG22	1:B:340:MET:HB3	1.99	0.45
1:B:466:ASP:OD2	1:B:466:ASP:N	2.43	0.45
1:B:605:LEU:HD13	1:B:698:VAL:HG13	1.98	0.45
1:C:304:LYS:NZ	1:C:350:ASP:OD1	2.49	0.45
1:C:315:PHE:CD2	1:C:329:ALA:HB1	2.52	0.45
1:C:795:LEU:HB3	1:C:799:ASP:O	2.17	0.45
1:C:1068:ASP:OD2	1:C:1156:LYS:NZ	2.34	0.45
1:D:67:SER:HA	1:D:70:ASN:HD21	1.82	0.45
1:D:626:ASN:O	1:D:720:MET:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:GLN:HE21	1:E:96:GLY:HA2	1.82	0.45
1:F:786:ASP:OD1	1:F:786:ASP:N	2.49	0.45
1:A:723:PHE:HE1	1:A:742:ILE:HG22	1.82	0.45
1:A:795:LEU:HB3	1:A:799:ASP:O	2.17	0.45
1:B:115:ALA:HA	1:B:330:LEU:HD22	1.99	0.45
1:C:366:ASN:ND2	1:C:424:LYS:O	2.50	0.45
1:E:104:ASP:OD1	1:E:105:ARG:N	2.50	0.45
1:F:626:ASN:O	1:F:720:MET:HA	2.16	0.45
1:A:730:ASP:HA	1:A:884:LEU:HD23	1.98	0.44
1:A:903:SER:OG	1:A:974:TYR:OH	2.29	0.44
1:B:1369:VAL:HG22	1:B:1386:ILE:HG12	1.98	0.44
1:C:723:PHE:HE1	1:C:742:ILE:HG22	1.82	0.44
1:D:1270:LEU:O	1:D:1273:ILE:HG22	2.17	0.44
1:E:133:GLY:HA3	1:E:141:THR:HG22	1.99	0.44
1:C:302:ASN:ND2	1:C:305:ASN:HB2	2.32	0.44
1:C:460:ASP:OD2	1:C:461:ILE:N	2.50	0.44
1:C:1099:SER:OG	1:C:1207:GLN:NE2	2.46	0.44
1:C:1270:LEU:O	1:C:1273:ILE:HG22	2.17	0.44
1:D:723:PHE:HE1	1:D:742:ILE:HG22	1.82	0.44
1:E:461:ILE:HG12	1:E:476:VAL:HG22	1.99	0.44
1:F:44:SER:OG	1:F:61:GLU:HB3	2.16	0.44
1:C:605:LEU:HD13	1:C:698:VAL:HG13	1.98	0.44
1:C:903:SER:OG	1:C:974:TYR:OH	2.29	0.44
1:D:730:ASP:HA	1:D:884:LEU:HD23	1.98	0.44
1:E:57:PRO:HG3	1:E:339:LEU:HD22	1.99	0.44
1:E:848:GLU:O	1:E:848:GLU:HG3	2.17	0.44
1:F:848:GLU:O	1:F:848:GLU:HG3	2.17	0.44
1:A:461:ILE:HG12	1:A:476:VAL:HG22	1.98	0.44
1:A:786:ASP:OD1	1:A:786:ASP:N	2.49	0.44
1:A:1270:LEU:HD21	1:A:1284:MET:HB2	1.98	0.44
1:B:1270:LEU:O	1:B:1273:ILE:HG22	2.17	0.44
1:C:1014:GLY:N	1:C:1212:ASP:OD2	2.50	0.44
1:D:47:ASN:N	1:D:52:ASN:OD1	2.49	0.44
1:A:258:THR:HG22	1:A:340:MET:HG2	1.99	0.44
1:B:57:PRO:HG3	1:B:339:LEU:HD22	1.99	0.44
1:B:1273:ILE:HD12	1:B:1273:ILE:HA	1.85	0.44
1:C:162:GLY:HA2	1:C:175:THR:HB	2.00	0.44
1:D:269:ARG:NH1	1:D:485:LYS:HA	2.32	0.44
1:D:460:ASP:OD2	1:D:461:ILE:N	2.51	0.44
1:E:770:ASN:HB2	1:E:776:THR:HG21	1.98	0.44
1:E:1270:LEU:O	1:E:1273:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:730:ASP:HA	1:F:884:LEU:HD23	1.98	0.44
1:A:848:GLU:O	1:A:848:GLU:HG3	2.17	0.44
1:A:937:THR:O	1:F:435:ARG:CD	2.65	0.44
1:C:233:LEU:HD13	1:C:239:VAL:HG21	2.00	0.44
1:D:795:LEU:HB3	1:D:799:ASP:O	2.17	0.44
1:E:730:ASP:HA	1:E:884:LEU:HD23	1.98	0.44
1:A:55:SER:H	1:A:58:GLN:NE2	2.16	0.44
1:A:136:ALA:O	1:A:182:LEU:HD11	2.17	0.44
1:A:1026:PRO:HG2	1:A:1157:PHE:HA	2.00	0.44
1:B:848:GLU:HG3	1:B:848:GLU:O	2.17	0.44
1:C:157:THR:H	1:C:161:ASN:HD22	1.64	0.44
1:C:1143:ALA:HB3	1:C:1146:ALA:HB2	2.00	0.44
1:D:390:ILE:HD12	1:D:397:LEU:HD13	2.00	0.44
1:E:795:LEU:HB3	1:E:799:ASP:O	2.17	0.44
1:E:1096:LEU:HD12	1:E:1210:TYR:HB2	2.00	0.44
1:F:770:ASN:HB2	1:F:776:THR:HG21	1.98	0.44
1:A:1267:THR:HB	1:A:1304:ARG:HH12	1.83	0.44
1:B:1026:PRO:HG2	1:B:1157:PHE:HA	2.00	0.44
1:D:343:ASP:HB2	1:D:445:GLU:CD	2.39	0.44
1:E:644:THR:O	1:E:699:ASN:N	2.45	0.44
1:E:1014:GLY:N	1:E:1212:ASP:OD2	2.50	0.44
1:A:390:ILE:HD12	1:A:397:LEU:HD13	2.00	0.44
1:B:460:ASP:OD2	1:B:461:ILE:N	2.50	0.44
1:C:239:VAL:N	1:C:254:LEU:O	2.28	0.44
1:D:88:LEU:HD13	1:D:231:TYR:HE2	1.83	0.44
1:D:644:THR:O	1:D:699:ASN:N	2.45	0.44
1:E:460:ASP:OD2	1:E:461:ILE:N	2.50	0.44
1:F:460:ASP:OD2	1:F:461:ILE:N	2.50	0.44
1:F:1267:THR:HB	1:F:1304:ARG:HH12	1.83	0.44
1:C:41:LEU:HD13	1:C:243:TYR:HB2	2.00	0.43
1:C:461:ILE:HG12	1:C:476:VAL:HG22	1.99	0.43
1:D:1143:ALA:HB3	1:D:1146:ALA:HB2	2.00	0.43
1:E:493:LEU:HD22	1:E:747:ALA:HB3	2.00	0.43
1:F:723:PHE:HE1	1:F:742:ILE:HG22	1.82	0.43
1:F:1026:PRO:HG2	1:F:1157:PHE:HA	2.00	0.43
1:B:442:ASP:HA	1:B:447:PRO:HA	1.99	0.43
1:B:447:PRO:HB2	1:C:858:LEU:HD11	2.00	0.43
1:B:895:VAL:HG12	1:B:988:VAL:HG12	1.98	0.43
1:B:1143:ALA:HB3	1:B:1146:ALA:HB2	2.00	0.43
1:D:461:ILE:HG12	1:D:476:VAL:HG22	1.99	0.43
1:D:786:ASP:OD1	1:D:786:ASP:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:493:LEU:HD22	1:F:747:ALA:HB3	2.00	0.43
1:F:795:LEU:HB3	1:F:799:ASP:O	2.17	0.43
1:F:895:VAL:HG12	1:F:988:VAL:HG12	1.98	0.43
1:A:451:LEU:HD23	1:A:452:VAL:O	2.18	0.43
1:A:1096:LEU:HD12	1:A:1210:TYR:HB2	2.00	0.43
1:A:1422:LYS:NZ	1:F:1219:ASP:OD2	2.33	0.43
1:E:75:ALA:HB3	1:F:73:ASP:HB3	1.99	0.43
1:E:164:GLN:O	1:E:164:GLN:NE2	2.48	0.43
1:E:447:PRO:HB2	1:F:858:LEU:HD11	2.01	0.43
1:E:1267:THR:HB	1:E:1304:ARG:HH12	1.83	0.43
1:F:1143:ALA:HB3	1:F:1146:ALA:HB2	2.00	0.43
1:A:1122:ASP:OD1	1:A:1123:VAL:N	2.52	0.43
1:B:461:ILE:HG12	1:B:476:VAL:HG22	1.99	0.43
1:C:349:LEU:HD23	1:C:402:ILE:HG21	2.00	0.43
1:C:1206:LEU:O	1:C:1227:ALA:N	2.40	0.43
1:D:269:ARG:NH2	1:D:276:SER:HB2	2.31	0.43
1:E:149:ILE:HG13	1:E:151:ILE:HG12	2.01	0.43
1:F:233:LEU:HD13	1:F:239:VAL:HG21	2.00	0.43
1:F:1014:GLY:N	1:F:1212:ASP:OD2	2.50	0.43
1:A:460:ASP:OD2	1:A:461:ILE:N	2.50	0.43
1:B:493:LEU:HD22	1:B:747:ALA:HB3	2.00	0.43
1:B:1267:THR:HB	1:B:1304:ARG:HH12	1.83	0.43
1:C:435:ARG:CD	1:D:937:THR:O	2.67	0.43
1:E:268:ASP:CG	1:E:487:SER:OG	2.57	0.43
1:F:1273:ILE:HD12	1:F:1273:ILE:HA	1.85	0.43
1:A:47:ASN:N	1:A:52:ASN:OD1	2.51	0.43
1:A:117:THR:HG23	1:A:120:SER:HB2	1.99	0.43
1:A:1014:GLY:N	1:A:1212:ASP:OD2	2.50	0.43
1:C:435:ARG:CD	1:D:938:GLY:HA3	2.48	0.43
1:C:1026:PRO:HG2	1:C:1157:PHE:HA	2.00	0.43
1:E:269:ARG:NH1	1:E:276:SER:OG	2.52	0.43
1:E:279:HIS:ND1	1:E:425:SER:HB2	2.33	0.43
1:E:1026:PRO:HG2	1:E:1157:PHE:HA	2.00	0.43
1:F:162:GLY:HA2	1:F:175:THR:HB	2.00	0.43
1:F:1122:ASP:OD1	1:F:1123:VAL:N	2.52	0.43
1:B:75:ALA:HB3	1:C:73:ASP:HB3	2.00	0.43
1:C:493:LEU:HD22	1:C:747:ALA:HB3	2.00	0.43
1:C:1219:ASP:OD2	1:D:1422:LYS:NZ	2.33	0.43
1:D:1096:LEU:HD12	1:D:1210:TYR:HB2	2.00	0.43
1:E:333:ARG:NH2	1:F:673:ASN:OD1	2.51	0.43
1:A:895:VAL:HG12	1:A:988:VAL:HG12	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:ILE:N	1:B:1007:ALA:O	2.52	0.43
1:B:1096:LEU:HD12	1:B:1210:TYR:HB2	2.00	0.43
1:C:141:THR:O	1:C:144:THR:HG22	2.19	0.43
1:D:104:ASP:OD1	1:D:105:ARG:N	2.52	0.43
1:F:995:ASP:N	1:F:999:GLU:O	2.45	0.43
1:D:442:ASP:HB2	1:D:447:PRO:HB3	2.01	0.43
1:D:986:ILE:N	1:D:1007:ALA:O	2.52	0.43
1:E:833:ASN:OD1	1:E:833:ASN:N	2.46	0.43
1:F:93:ALA:HB1	1:F:198:LYS:HB3	2.01	0.43
1:F:265:LEU:HD12	1:F:282:ILE:HG12	2.00	0.43
1:A:1143:ALA:HB3	1:A:1146:ALA:HB2	2.00	0.43
1:B:985:ASP:OD1	1:B:985:ASP:N	2.49	0.43
1:B:1122:ASP:OD1	1:B:1123:VAL:N	2.52	0.43
1:E:209:VAL:HG12	1:E:214:LEU:HB2	2.00	0.43
1:E:986:ILE:N	1:E:1007:ALA:O	2.52	0.43
1:F:275:VAL:HG12	1:F:275:VAL:O	2.19	0.43
1:F:986:ILE:N	1:F:1007:ALA:O	2.52	0.43
1:F:1480:VAL:O	1:F:1492:GLY:N	2.42	0.43
1:C:361:VAL:HG11	1:C:427:LEU:HD23	2.00	0.42
1:C:1024:PRO:HB3	1:C:1257:ASP:HA	2.01	0.42
1:C:1096:LEU:HD12	1:C:1210:TYR:HB2	2.00	0.42
1:D:1122:ASP:OD1	1:D:1123:VAL:N	2.52	0.42
1:E:236:THR:HB	1:F:489:ALA:HA	2.00	0.42
1:E:874:ASP:OD2	1:E:904:THR:HG22	2.20	0.42
1:F:363:ILE:HA	1:F:426:VAL:O	2.19	0.42
1:A:466:ASP:OD2	1:A:466:ASP:N	2.44	0.42
1:A:986:ILE:N	1:A:1007:ALA:O	2.52	0.42
1:B:71:ASP:OD1	1:B:74:GLU:HB2	2.19	0.42
1:C:122:LEU:HD23	1:C:316:TYR:CD2	2.54	0.42
1:C:874:ASP:OD2	1:C:904:THR:HG22	2.19	0.42
1:C:1436:GLU:OE1	1:C:1466:THR:HG22	2.19	0.42
1:F:1096:LEU:HD12	1:F:1210:TYR:HB2	2.00	0.42
1:A:279:HIS:H	1:A:488:ARG:NH2	1.83	0.42
1:C:111:ALA:HB1	1:C:122:LEU:HB3	2.00	0.42
1:C:1122:ASP:OD1	1:C:1123:VAL:N	2.52	0.42
1:D:1024:PRO:HB3	1:D:1257:ASP:HA	2.01	0.42
1:D:1267:THR:HB	1:D:1304:ARG:HH12	1.83	0.42
1:E:1143:ALA:HB3	1:E:1146:ALA:HB2	2.00	0.42
1:F:773:ASP:OD2	1:F:775:GLY:N	2.43	0.42
1:A:259:VAL:HG21	1:A:285:LEU:HB2	2.01	0.42
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:PRO:HB3	1:A:1257:ASP:HA	2.01	0.42
1:A:1268:TYR:O	1:A:1302:ASP:HB3	2.20	0.42
1:B:1024:PRO:HB3	1:B:1257:ASP:HA	2.01	0.42
1:B:1436:GLU:OE1	1:B:1466:THR:HG22	2.19	0.42
1:C:347:LEU:HD11	1:C:441:LEU:HD21	2.02	0.42
1:D:420:ASP:OD2	1:D:422:SER:OG	2.38	0.42
1:F:1024:PRO:HB3	1:F:1257:ASP:HA	2.01	0.42
1:A:94:VAL:HG21	1:F:77:GLY:H	1.85	0.42
1:A:269:ARG:NH2	1:A:485:LYS:CA	2.82	0.42
1:A:493:LEU:HD22	1:A:747:ALA:HB3	2.00	0.42
1:B:305:ASN:HB3	1:B:310:PHE:CE2	2.54	0.42
1:B:419:TYR:HA	1:B:425:SER:HA	2.00	0.42
1:B:874:ASP:OD2	1:B:904:THR:HG22	2.19	0.42
1:C:249:VAL:HG21	1:D:411:PRO:HD2	2.02	0.42
1:D:1268:TYR:O	1:D:1302:ASP:HB3	2.20	0.42
1:E:45:ALA:HB2	1:E:60:ILE:HD12	2.01	0.42
1:E:1122:ASP:OD1	1:E:1123:VAL:N	2.52	0.42
1:F:81:VAL:HG21	1:F:90:MET:HE2	2.00	0.42
1:F:1268:TYR:O	1:F:1302:ASP:HB3	2.20	0.42
1:A:239:VAL:O	1:A:254:LEU:N	2.48	0.42
1:B:721:ASP:N	1:B:721:ASP:OD1	2.53	0.42
1:B:1099:SER:OG	1:B:1207:GLN:NE2	2.46	0.42
1:C:298:THR:HB	1:C:315:PHE:HB2	2.01	0.42
1:C:364:GLN:NE2	1:C:428:LYS:HD2	2.34	0.42
1:C:995:ASP:N	1:C:999:GLU:O	2.45	0.42
1:D:493:LEU:HD22	1:D:747:ALA:HB3	2.00	0.42
1:D:514:ILE:O	1:D:600:LEU:HD12	2.20	0.42
1:D:1026:PRO:HG2	1:D:1157:PHE:HA	2.00	0.42
1:E:435:ARG:HB3	1:E:454:PHE:HE2	1.84	0.42
1:E:1268:TYR:O	1:E:1302:ASP:HB3	2.20	0.42
1:F:435:ARG:NH1	1:F:812:GLY:C	2.67	0.42
1:F:909:ASN:ND2	1:F:971:PRO:O	2.46	0.42
1:A:514:ILE:O	1:A:600:LEU:HD12	2.20	0.42
1:B:278:VAL:O	1:B:425:SER:OG	2.23	0.42
1:B:579:LEU:HD22	1:B:718:ILE:HB	2.02	0.42
1:B:773:ASP:OD2	1:B:775:GLY:N	2.43	0.42
1:C:305:ASN:HB3	1:C:310:PHE:CE2	2.54	0.42
1:C:579:LEU:HD22	1:C:718:ILE:HB	2.02	0.42
1:D:104:ASP:HA	1:D:231:TYR:O	2.20	0.42
1:D:833:ASN:OD1	1:D:833:ASN:N	2.46	0.42
1:E:50:PHE:CD2	1:E:285:LEU:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:514:ILE:O	1:F:600:LEU:HD12	2.20	0.42
1:F:721:ASP:OD1	1:F:721:ASP:N	2.53	0.42
1:A:874:ASP:OD2	1:A:904:THR:HG22	2.20	0.42
1:C:514:ILE:O	1:C:600:LEU:HD12	2.20	0.42
1:C:595:PHE:N	1:C:595:PHE:CD2	2.88	0.42
1:C:1267:THR:HB	1:C:1304:ARG:HH12	1.83	0.42
1:E:453:GLY:C	1:E:454:PHE:CG	2.93	0.42
1:F:305:ASN:HB3	1:F:310:PHE:CE2	2.55	0.42
1:F:762:GLU:O	1:F:788:SER:HA	2.20	0.42
1:F:1255:GLU:HA	1:F:1256:PRO:HD3	1.89	0.42
1:A:852:LEU:HD11	1:A:990:TYR:OH	2.20	0.42
1:A:1273:ILE:HD12	1:A:1273:ILE:HA	1.85	0.42
1:B:54:MET:HA	1:B:285:LEU:HD21	2.01	0.42
1:B:279:HIS:ND1	1:B:425:SER:HB2	2.34	0.42
1:C:364:GLN:NE2	1:C:425:SER:O	2.53	0.42
1:C:986:ILE:N	1:C:1007:ALA:O	2.52	0.42
1:C:1268:TYR:O	1:C:1302:ASP:HB3	2.20	0.42
1:D:278:VAL:O	1:D:425:SER:OG	2.26	0.42
1:D:721:ASP:OD1	1:D:721:ASP:N	2.53	0.42
1:D:893:LEU:HD12	1:D:894:ASP:N	2.35	0.42
1:E:54:MET:HA	1:E:285:LEU:HD21	2.02	0.42
1:F:874:ASP:OD2	1:F:904:THR:HG22	2.19	0.42
1:A:273:PRO:HB3	1:A:482:ASP:O	2.20	0.42
1:A:595:PHE:N	1:A:595:PHE:CD2	2.88	0.42
1:A:762:GLU:O	1:A:788:SER:HA	2.20	0.42
1:A:828:GLY:HA3	1:A:990:TYR:HE2	1.85	0.42
1:A:1100:VAL:HG22	1:A:1206:LEU:HD13	2.02	0.42
1:B:595:PHE:N	1:B:595:PHE:CD2	2.88	0.42
1:B:893:LEU:HD12	1:B:894:ASP:N	2.35	0.42
1:C:893:LEU:HD12	1:C:894:ASP:N	2.35	0.42
1:D:276:SER:CB	1:D:485:LYS:CB	2.94	0.42
1:E:595:PHE:N	1:E:595:PHE:CD2	2.88	0.42
1:D:371:LEU:HD12	1:D:371:LEU:HA	1.92	0.41
1:D:1436:GLU:OE1	1:D:1466:THR:HG22	2.19	0.41
1:A:1043:GLY:O	1:A:1348:TYR:OH	2.31	0.41
1:B:197:ALA:HB1	1:B:225:TRP:NE1	2.35	0.41
1:B:304:LYS:NZ	1:B:352:ASP:O	2.53	0.41
1:B:453:GLY:C	1:B:454:PHE:CG	2.93	0.41
1:B:1268:TYR:O	1:B:1302:ASP:HB3	2.20	0.41
1:C:1070:THR:HG22	1:C:1154:ASN:HB3	2.02	0.41
1:D:625:PHE:CE1	1:D:627:TYR:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:874:ASP:OD2	1:D:904:THR:HG22	2.19	0.41
1:D:1100:VAL:HG22	1:D:1206:LEU:HD13	2.02	0.41
1:E:721:ASP:OD1	1:E:721:ASP:N	2.53	0.41
1:D:595:PHE:CD2	1:D:595:PHE:N	2.88	0.41
1:D:1070:THR:HG22	1:D:1154:ASN:HB3	2.02	0.41
1:E:762:GLU:O	1:E:788:SER:HA	2.20	0.41
1:E:852:LEU:HD11	1:E:990:TYR:OH	2.20	0.41
1:E:893:LEU:HD12	1:E:894:ASP:N	2.35	0.41
1:E:1100:VAL:HG22	1:E:1206:LEU:HD13	2.02	0.41
1:F:277:GLN:OE1	1:F:428:LYS:HG2	2.20	0.41
1:F:852:LEU:HD11	1:F:990:TYR:OH	2.20	0.41
1:A:104:ASP:HA	1:A:231:TYR:O	2.20	0.41
1:B:50:PHE:CD2	1:B:285:LEU:HD12	2.55	0.41
1:B:365:ASP:HB2	1:B:371:LEU:HB3	2.01	0.41
1:B:762:GLU:O	1:B:788:SER:HA	2.20	0.41
1:C:149:ILE:HG13	1:C:151:ILE:HG12	2.02	0.41
1:C:852:LEU:HD11	1:C:990:TYR:OH	2.20	0.41
1:D:117:THR:HG23	1:D:120:SER:HB2	2.03	0.41
1:E:1436:GLU:OE1	1:E:1466:THR:HG22	2.20	0.41
1:F:50:PHE:O	1:F:53:TYR:HD1	2.03	0.41
1:F:519:THR:HA	1:F:520:PRO:HD3	1.94	0.41
1:A:893:LEU:HD12	1:A:894:ASP:N	2.35	0.41
1:B:144:THR:HA	1:B:231:TYR:HE2	1.86	0.41
1:B:514:ILE:O	1:B:600:LEU:HD12	2.20	0.41
1:B:828:GLY:HA3	1:B:990:TYR:HE2	1.85	0.41
1:C:895:VAL:HG22	1:C:934:LEU:HD22	2.03	0.41
1:C:1100:VAL:HG22	1:C:1206:LEU:HD13	2.02	0.41
1:D:361:VAL:HG12	1:D:429:ILE:HD13	2.03	0.41
1:D:852:LEU:HD11	1:D:990:TYR:OH	2.20	0.41
1:D:895:VAL:HG22	1:D:934:LEU:HD22	2.03	0.41
1:E:73:ASP:OD1	1:E:73:ASP:N	2.45	0.41
1:F:268:ASP:OD1	1:F:269:ARG:N	2.54	0.41
1:F:277:GLN:HB3	1:F:425:SER:HB3	2.02	0.41
1:F:595:PHE:N	1:F:595:PHE:CD2	2.88	0.41
1:A:225:TRP:CE3	1:A:226:PRO:HA	2.56	0.41
1:A:373:GLN:HE21	1:A:375:ASN:C	2.23	0.41
1:A:525:THR:HB	1:A:595:PHE:HB2	2.03	0.41
1:A:1219:ASP:OD2	1:B:1422:LYS:NZ	2.35	0.41
1:A:1436:GLU:OE1	1:A:1466:THR:HG22	2.20	0.41
1:C:553:LEU:HB2	1:C:595:PHE:HE1	1.85	0.41
1:C:721:ASP:OD1	1:C:721:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1077:ASP:OD2	1:D:1210:TYR:OH	2.38	0.41
1:E:514:ILE:O	1:E:600:LEU:HD12	2.20	0.41
1:E:828:GLY:HA3	1:E:990:TYR:HE2	1.85	0.41
1:F:1043:GLY:O	1:F:1348:TYR:OH	2.31	0.41
1:B:49:GLN:HG2	1:B:50:PHE:CE1	2.56	0.41
1:B:354:GLN:HE21	1:C:861:ILE:CD1	2.26	0.41
1:C:525:THR:HB	1:C:595:PHE:HB2	2.03	0.41
1:C:1412:SER:HA	1:C:1417:ASP:HA	2.03	0.41
1:D:825:SER:HB3	1:D:995:ASP:O	2.21	0.41
1:D:828:GLY:HA3	1:D:990:TYR:HE2	1.85	0.41
1:E:845:ILE:N	1:E:953:GLY:O	2.35	0.41
1:E:1068:ASP:OD2	1:E:1156:LYS:NZ	2.34	0.41
1:E:1480:VAL:O	1:E:1492:GLY:N	2.42	0.41
1:F:149:ILE:HG13	1:F:151:ILE:HG12	2.01	0.41
1:F:1460:THR:HG23	1:F:1470:LEU:HD12	2.02	0.41
1:B:1070:THR:HG22	1:B:1154:ASN:HB3	2.02	0.41
1:C:1077:ASP:OD2	1:C:1210:TYR:OH	2.38	0.41
1:D:335:THR:HG22	1:D:339:LEU:HG	2.03	0.41
1:D:363:ILE:HD11	1:D:388:PHE:HB2	2.02	0.41
1:D:363:ILE:HD13	1:D:402:ILE:HG23	2.02	0.41
1:D:553:LEU:HB2	1:D:595:PHE:HE1	1.86	0.41
1:D:1092:GLN:NE2	1:D:1213:PRO:HB3	2.36	0.41
1:F:478:ILE:O	1:F:757:PHE:N	2.44	0.41
1:F:828:GLY:HA3	1:F:990:TYR:HE2	1.85	0.41
1:F:1100:VAL:HG22	1:F:1206:LEU:HD13	2.02	0.41
1:F:1436:GLU:OE1	1:F:1466:THR:HG22	2.20	0.41
1:A:305:ASN:HB3	1:A:310:PHE:CD2	2.56	0.41
1:A:586:ASN:HB3	1:A:591:PHE:CE1	2.56	0.41
1:A:721:ASP:OD1	1:A:721:ASP:N	2.53	0.41
1:A:773:ASP:OD2	1:A:775:GLY:N	2.43	0.41
1:A:793:GLU:O	1:A:795:LEU:N	2.54	0.41
1:A:1480:VAL:O	1:A:1492:GLY:N	2.43	0.41
1:B:279:HIS:CE1	1:B:425:SER:HB2	2.56	0.41
1:B:525:THR:HB	1:B:595:PHE:HB2	2.03	0.41
1:B:793:GLU:O	1:B:795:LEU:N	2.54	0.41
1:B:852:LEU:HD11	1:B:990:TYR:OH	2.20	0.41
1:B:1412:SER:HA	1:B:1417:ASP:HA	2.03	0.41
1:B:1460:THR:HG23	1:B:1470:LEU:HD12	2.02	0.41
1:C:1013:THR:HG22	1:C:1215:ASP:HB2	2.03	0.41
1:D:525:THR:HB	1:D:595:PHE:HB2	2.03	0.41
1:D:762:GLU:O	1:D:788:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1013:THR:HG22	1:D:1215:ASP:HB2	2.03	0.41
1:D:1460:THR:HG23	1:D:1470:LEU:HD12	2.02	0.41
1:E:150:PRO:HB2	1:E:189:GLY:HA2	2.02	0.41
1:E:279:HIS:CE1	1:E:425:SER:HB2	2.56	0.41
1:E:586:ASN:HB3	1:E:591:PHE:CE1	2.56	0.41
1:E:825:SER:HB3	1:E:995:ASP:O	2.21	0.41
1:E:903:SER:OG	1:E:974:TYR:OH	2.29	0.41
1:E:1024:PRO:HB3	1:E:1257:ASP:HA	2.01	0.41
1:E:1092:GLN:NE2	1:E:1213:PRO:HB3	2.36	0.41
1:E:1255:GLU:HA	1:E:1256:PRO:HD3	1.89	0.41
1:F:141:THR:O	1:F:144:THR:HG22	2.21	0.41
1:F:579:LEU:HD22	1:F:718:ILE:HB	2.02	0.41
1:F:586:ASN:HB3	1:F:591:PHE:CE1	2.56	0.41
1:F:793:GLU:O	1:F:795:LEU:N	2.54	0.41
1:F:893:LEU:HD12	1:F:894:ASP:N	2.35	0.41
1:F:1070:THR:HG22	1:F:1154:ASN:HB3	2.02	0.41
1:B:263:ALA:HB1	1:B:443:TYR:HE2	1.86	0.41
1:B:1100:VAL:HG22	1:B:1206:LEU:HD13	2.02	0.41
1:B:1219:ASP:OD2	1:C:1422:LYS:NZ	2.35	0.41
1:B:1411:VAL:HG23	1:B:1480:VAL:HG22	2.03	0.41
1:C:87:VAL:HG12	1:C:143:GLU:HB2	2.03	0.41
1:C:762:GLU:O	1:C:788:SER:HA	2.20	0.41
1:C:828:GLY:HA3	1:C:990:TYR:HE2	1.85	0.41
1:D:225:TRP:CE3	1:D:226:PRO:HA	2.56	0.41
1:D:305:ASN:HB3	1:D:310:PHE:CD2	2.56	0.41
1:D:793:GLU:O	1:D:795:LEU:N	2.54	0.41
1:D:1335:ILE:HD13	1:D:1335:ILE:HA	1.93	0.41
1:D:1411:VAL:HG23	1:D:1480:VAL:HG22	2.03	0.41
1:E:438:SER:HB3	1:E:451:LEU:HD12	2.03	0.41
1:F:525:THR:HB	1:F:595:PHE:HB2	2.03	0.41
1:F:553:LEU:HB2	1:F:595:PHE:HE1	1.85	0.41
1:A:1426:THR:HG22	1:A:1432:ILE:O	2.22	0.40
1:C:216:ASN:HB3	1:C:223:PRO:HD2	2.02	0.40
1:C:793:GLU:O	1:C:795:LEU:N	2.54	0.40
1:D:1246:GLY:H	1:D:1319:ILE:HB	1.86	0.40
1:E:312:VAL:O	1:E:333:ARG:HD2	2.21	0.40
1:E:540:ILE:HD13	1:E:540:ILE:HA	1.84	0.40
1:E:1070:THR:HG22	1:E:1154:ASN:HB3	2.02	0.40
1:E:1246:GLY:H	1:E:1319:ILE:HB	1.86	0.40
1:E:1412:SER:HA	1:E:1417:ASP:HA	2.03	0.40
1:E:1460:THR:HG23	1:E:1470:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:731:GLY:HA2	1:F:736:GLU:HG3	2.03	0.40
1:A:579:LEU:HD22	1:A:718:ILE:HB	2.02	0.40
1:A:1246:GLY:H	1:A:1319:ILE:HB	1.86	0.40
1:A:1460:THR:HG23	1:A:1470:LEU:HD12	2.02	0.40
1:B:150:PRO:HB2	1:B:189:GLY:HA2	2.02	0.40
1:B:438:SER:HB3	1:B:451:LEU:HD12	2.03	0.40
1:B:553:LEU:HB2	1:B:595:PHE:HE1	1.86	0.40
1:B:1013:THR:HG22	1:B:1215:ASP:HB2	2.03	0.40
1:B:1202:GLN:NE2	1:B:1346:SER:O	2.54	0.40
1:C:731:GLY:HA2	1:C:736:GLU:HG3	2.03	0.40
1:D:731:GLY:HA2	1:D:736:GLU:HG3	2.03	0.40
1:D:1390:ASP:N	1:D:1390:ASP:OD1	2.54	0.40
1:E:579:LEU:HD22	1:E:718:ILE:HB	2.02	0.40
1:E:895:VAL:HG22	1:E:934:LEU:HD22	2.03	0.40
1:E:1219:ASP:OD2	1:F:1422:LYS:NZ	2.34	0.40
1:F:53:TYR:O	1:F:285:LEU:HD11	2.20	0.40
1:F:298:THR:HB	1:F:315:PHE:HB2	2.02	0.40
1:F:1092:GLN:NE2	1:F:1213:PRO:HB3	2.36	0.40
1:B:895:VAL:HG22	1:B:934:LEU:HD22	2.03	0.40
1:B:1246:GLY:H	1:B:1319:ILE:HB	1.86	0.40
1:B:1346:SER:OG	1:B:1348:TYR:O	2.38	0.40
1:C:825:SER:HB3	1:C:995:ASP:O	2.21	0.40
1:C:1411:VAL:HG23	1:C:1480:VAL:HG22	2.03	0.40
1:E:117:THR:HG23	1:E:120:SER:HB2	2.03	0.40
1:F:1412:SER:HA	1:F:1417:ASP:HA	2.03	0.40
1:A:81:VAL:HG13	1:A:88:LEU:HB3	2.04	0.40
1:A:343:ASP:HB2	1:A:445:GLU:CD	2.41	0.40
1:A:731:GLY:HA2	1:A:736:GLU:HG3	2.03	0.40
1:A:1070:THR:HG22	1:A:1154:ASN:HB3	2.02	0.40
1:B:350:ASP:HB3	1:B:440:SER:OG	2.21	0.40
1:B:1426:THR:HG22	1:B:1432:ILE:O	2.22	0.40
1:C:1092:GLN:NE2	1:C:1213:PRO:HB3	2.36	0.40
1:D:736:GLU:H	1:D:736:GLU:HG2	1.65	0.40
1:E:245:LYS:HE3	1:E:245:LYS:HB2	1.93	0.40
1:E:478:ILE:O	1:E:757:PHE:N	2.44	0.40
1:E:1273:ILE:HD12	1:E:1273:ILE:HA	1.85	0.40
1:F:702:PHE:CZ	1:F:722:PHE:HE2	2.40	0.40
1:A:442:ASP:HB2	1:A:447:PRO:HB3	2.03	0.40
1:A:1346:SER:OG	1:A:1348:TYR:O	2.38	0.40
1:A:1411:VAL:HG23	1:A:1480:VAL:HG22	2.03	0.40
1:C:625:PHE:CE1	1:C:627:TYR:HB3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1411:VAL:CG1	1:C:1418:LEU:HB2	2.52	0.40
1:C:1421:TYR:CZ	1:C:1437:VAL:HG22	2.57	0.40
1:D:216:ASN:HB3	1:D:223:PRO:HD2	2.02	0.40
1:D:934:LEU:HD12	1:D:934:LEU:HA	1.92	0.40
1:E:525:THR:HB	1:E:595:PHE:HB2	2.03	0.40
1:E:793:GLU:O	1:E:795:LEU:N	2.54	0.40
1:E:995:ASP:OD2	1:E:995:ASP:C	2.60	0.40
1:F:825:SER:HB3	1:F:995:ASP:O	2.21	0.40
1:F:995:ASP:OD2	1:F:995:ASP:C	2.60	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	1460/1734 (84%)	1418 (97%)	42 (3%)	0	100	100
1	B	1460/1734 (84%)	1415 (97%)	45 (3%)	0	100	100
1	C	1460/1734 (84%)	1414 (97%)	46 (3%)	0	100	100
1	D	1460/1734 (84%)	1421 (97%)	39 (3%)	0	100	100
1	E	1460/1734 (84%)	1414 (97%)	46 (3%)	0	100	100
1	F	1460/1734 (84%)	1412 (97%)	48 (3%)	0	100	100
All	All	8760/10404 (84%)	8494 (97%)	266 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1212/1438 (84%)	1191 (98%)	21 (2%)	60	82
1	B	1212/1438 (84%)	1191 (98%)	21 (2%)	60	82
1	C	1212/1438 (84%)	1190 (98%)	22 (2%)	59	81
1	D	1212/1438 (84%)	1191 (98%)	21 (2%)	60	82
1	E	1212/1438 (84%)	1191 (98%)	21 (2%)	60	82
1	F	1212/1438 (84%)	1191 (98%)	21 (2%)	60	82
All	All	7272/8628 (84%)	7145 (98%)	127 (2%)	62	82

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	507	ARG
1	A	591	PHE
1	A	649	LEU
1	A	661	LYS
1	A	721	ASP
1	A	857	ASP
1	A	874	ASP
1	A	918	ASP
1	A	995	ASP
1	A	1068	ASP
1	A	1152	ASP
1	A	1170	ASP
1	A	1219	ASP
1	A	1232	ARG
1	A	1278	ASP
1	A	1296	PHE
1	A	1308	ASP
1	A	1330	ARG
1	A	1338	TYR
1	A	1347	ASP
1	A	1378	TRP
1	B	507	ARG
1	B	591	PHE
1	B	649	LEU
1	B	661	LYS
1	B	721	ASP
1	B	857	ASP

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Mol	Chain	Res	Type
1	B	874	ASP
1	B	918	ASP
1	B	995	ASP
1	B	1068	ASP
1	B	1152	ASP
1	B	1170	ASP
1	B	1219	ASP
1	B	1232	ARG
1	B	1278	ASP
1	B	1296	PHE
1	B	1308	ASP
1	B	1330	ARG
1	B	1338	TYR
1	B	1347	ASP
1	B	1378	TRP
1	C	455	SER
1	C	507	ARG
1	C	591	PHE
1	C	649	LEU
1	C	661	LYS
1	C	721	ASP
1	C	857	ASP
1	C	874	ASP
1	C	918	ASP
1	C	995	ASP
1	C	1068	ASP
1	C	1152	ASP
1	C	1170	ASP
1	C	1219	ASP
1	C	1232	ARG
1	C	1278	ASP
1	C	1296	PHE
1	C	1308	ASP
1	C	1330	ARG
1	C	1338	TYR
1	C	1347	ASP
1	C	1378	TRP
1	D	507	ARG
1	D	591	PHE
1	D	649	LEU
1	D	661	LYS
1	D	721	ASP

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Mol	Chain	Res	Type
1	D	857	ASP
1	D	874	ASP
1	D	918	ASP
1	D	995	ASP
1	D	1068	ASP
1	D	1152	ASP
1	D	1170	ASP
1	D	1219	ASP
1	D	1232	ARG
1	D	1278	ASP
1	D	1296	PHE
1	D	1308	ASP
1	D	1330	ARG
1	D	1338	TYR
1	D	1347	ASP
1	D	1378	TRP
1	E	507	ARG
1	E	591	PHE
1	E	649	LEU
1	E	661	LYS
1	E	721	ASP
1	E	857	ASP
1	E	874	ASP
1	E	918	ASP
1	E	995	ASP
1	E	1068	ASP
1	E	1152	ASP
1	E	1170	ASP
1	E	1219	ASP
1	E	1232	ARG
1	E	1278	ASP
1	E	1296	PHE
1	E	1308	ASP
1	E	1330	ARG
1	E	1338	TYR
1	E	1347	ASP
1	E	1378	TRP
1	F	507	ARG
1	F	591	PHE
1	F	649	LEU
1	F	661	LYS
1	F	721	ASP

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Mol	Chain	Res	Type
1	F	857	ASP
1	F	874	ASP
1	F	918	ASP
1	F	995	ASP
1	F	1068	ASP
1	F	1152	ASP
1	F	1170	ASP
1	F	1219	ASP
1	F	1232	ARG
1	F	1278	ASP
1	F	1296	PHE
1	F	1308	ASP
1	F	1330	ARG
1	F	1338	TYR
1	F	1347	ASP
1	F	1378	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	GLN
1	A	806	ASN
1	A	1050	HIS
1	B	806	ASN
1	B	1050	HIS
1	C	279	HIS
1	C	366	ASN
1	C	806	ASN
1	C	1050	HIS
1	D	806	ASN
1	D	1050	HIS
1	E	277	GLN
1	E	806	ASN
1	E	1050	HIS
1	F	242	GLN
1	F	279	HIS
1	F	806	ASN
1	F	1050	HIS

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

There are no chain breaks in this entry.

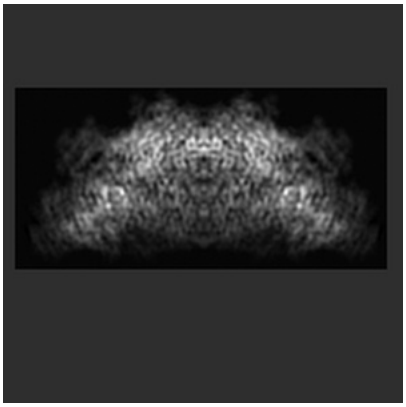
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16492. These allow visual inspection of the internal detail of the map and identification of artifacts.

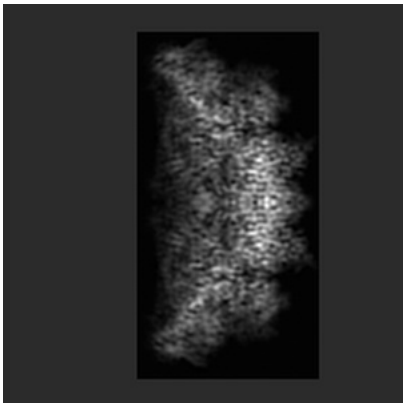
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

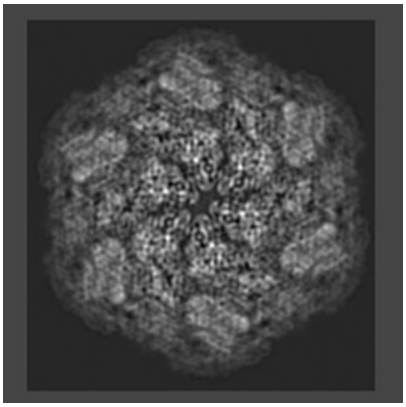
6.1.1 Primary map



X



Y



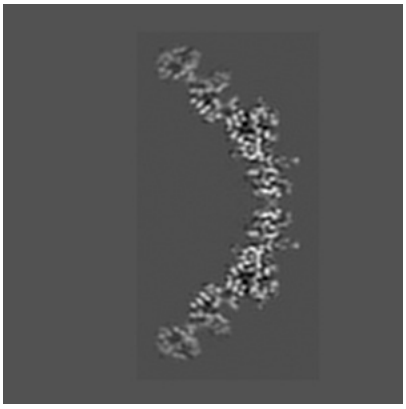
Z

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

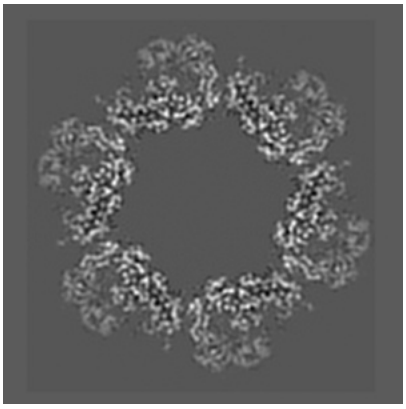
6.2 Central slices

6.2.1 Primary map

X Index: 100



Y Index: 100

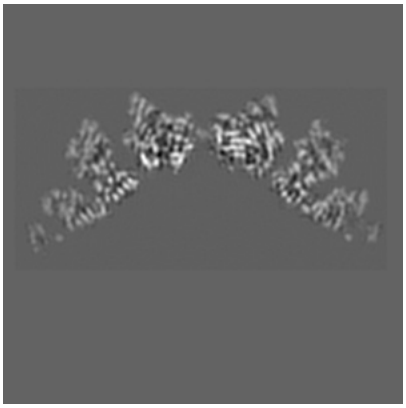


Z Index: 100

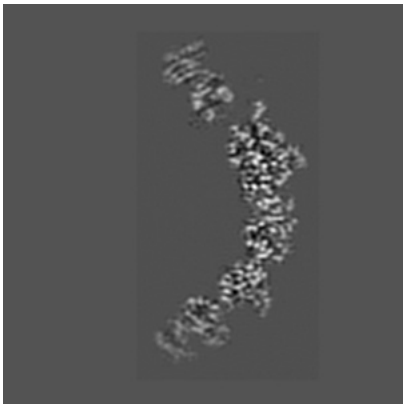
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

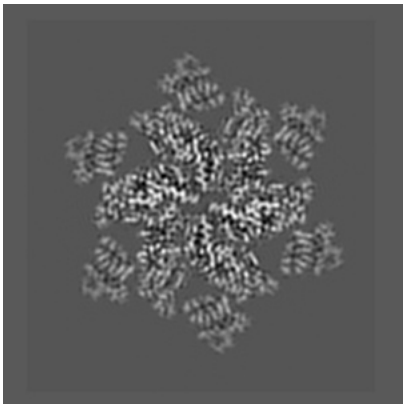
6.3.1 Primary map



X Index: 99



Y Index: 92

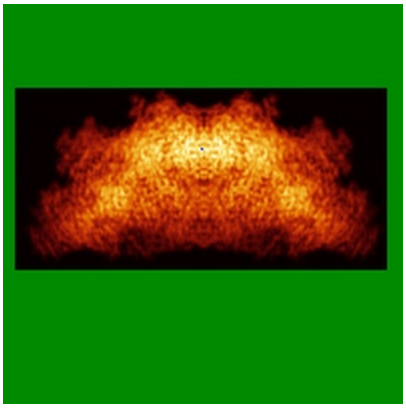


Z Index: 127

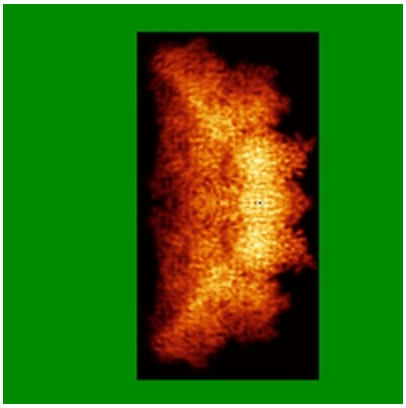
The images above show the largest variance slices of the map in three orthogonal directions.

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

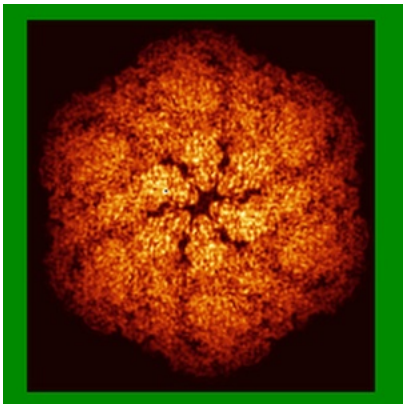
6.4.1 Primary map



X



Y

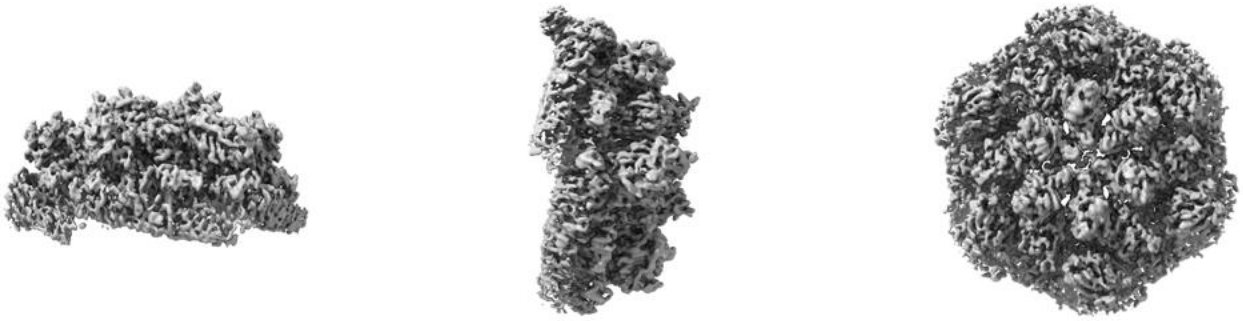


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.45621. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

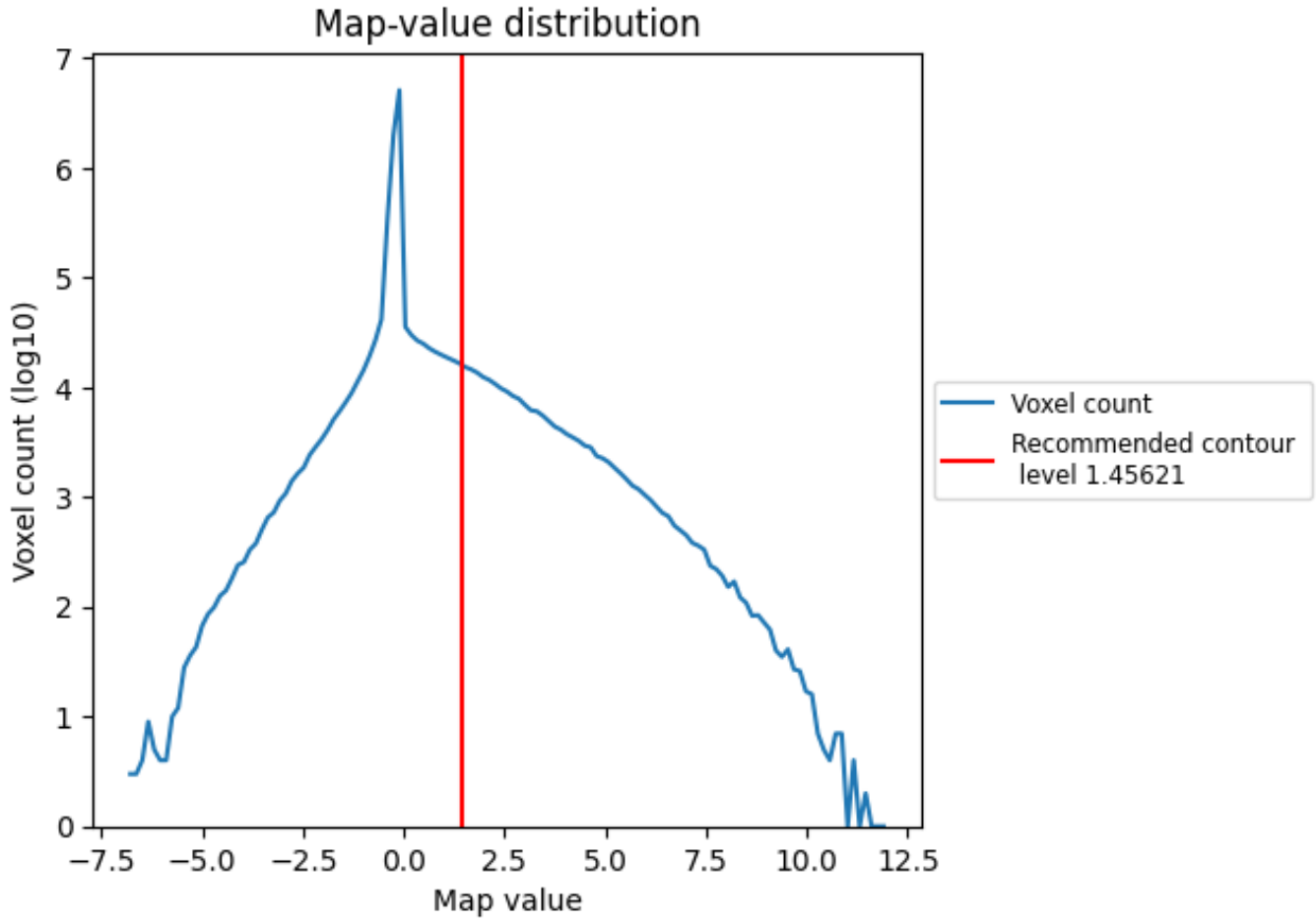
6.6 Mask visualisation (i)

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

7 Map analysis

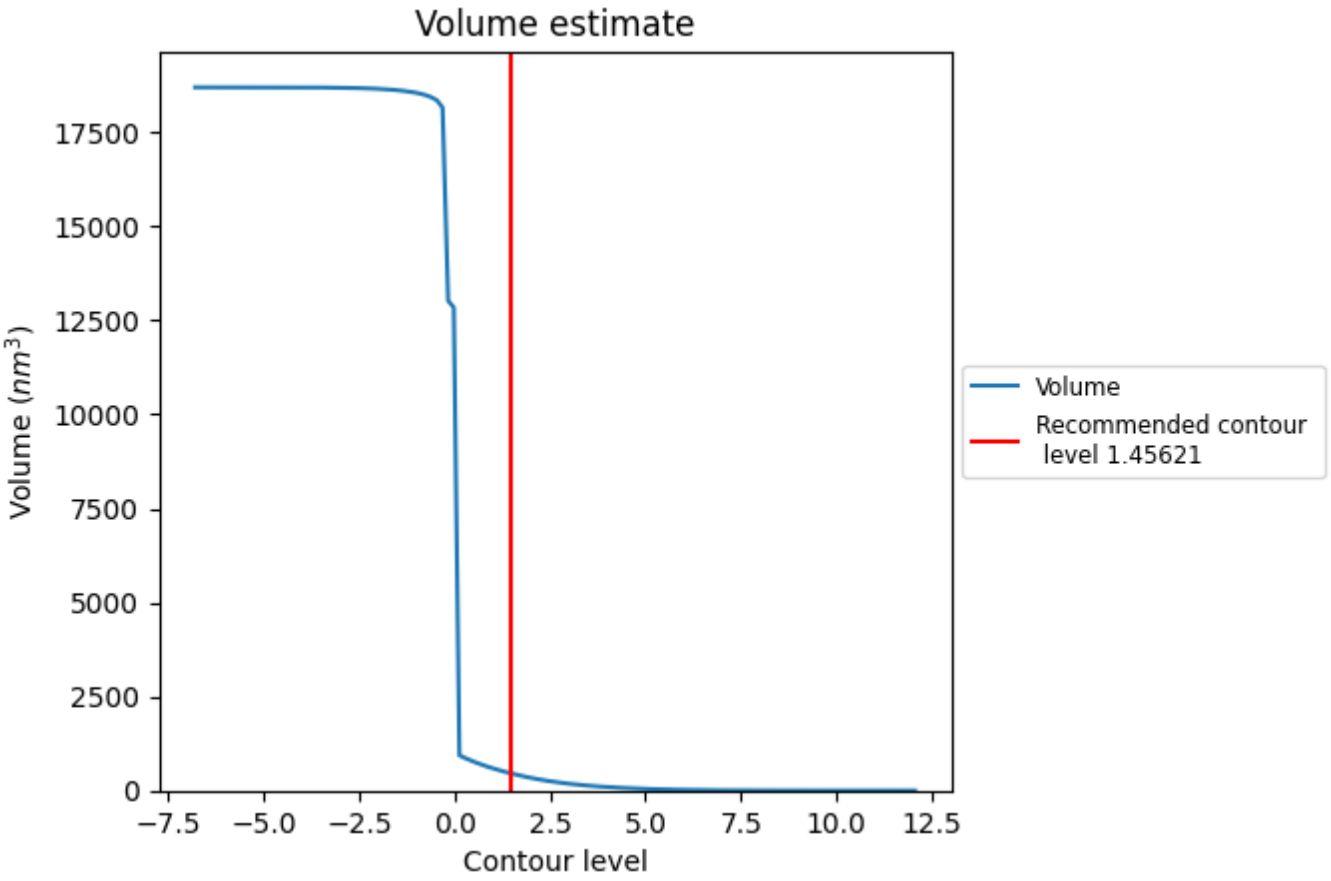
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

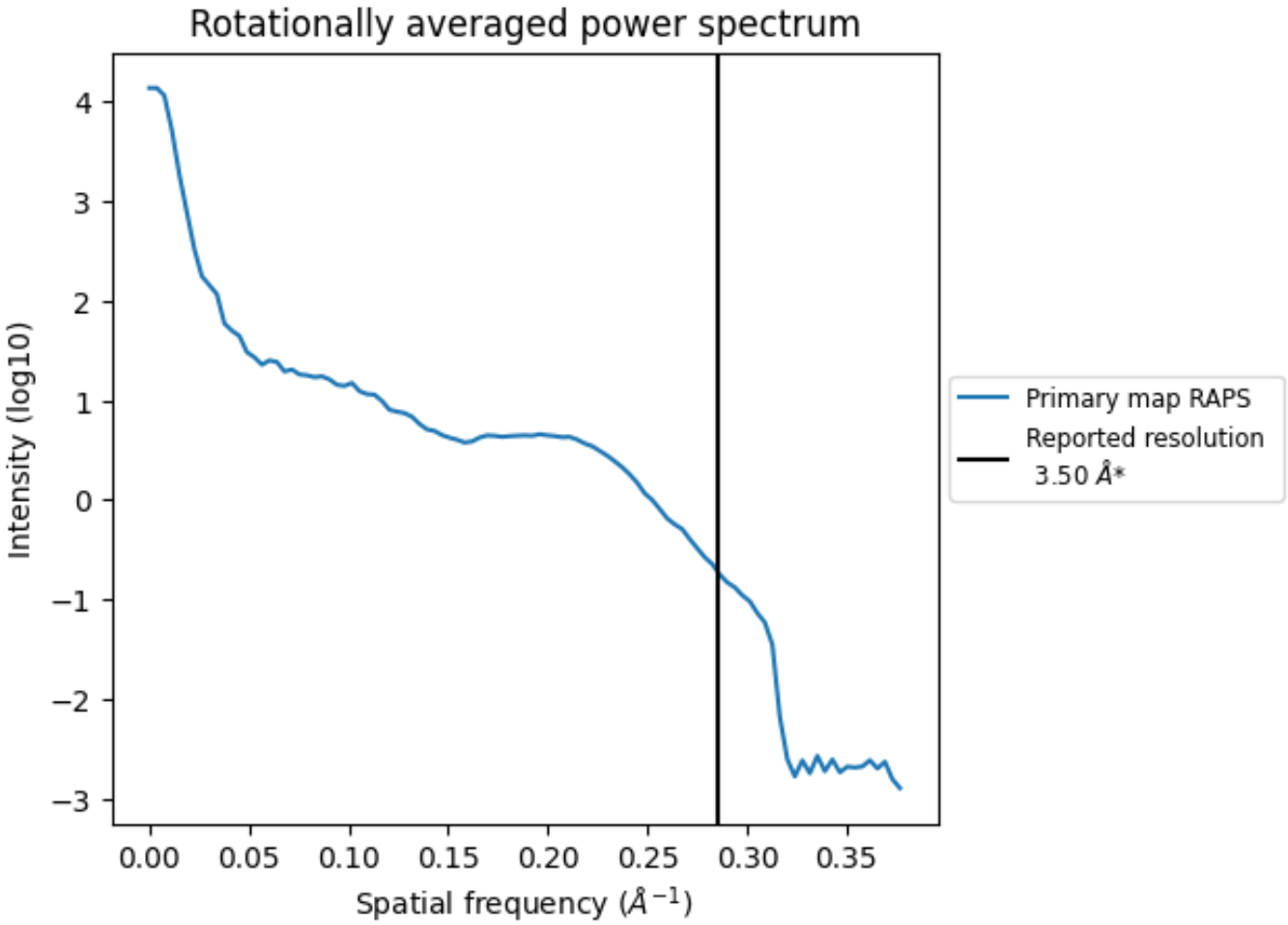
7.2 Volume estimate



The volume at the recommended contour level is 462 nm^3; this corresponds to an approximate mass of 417 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

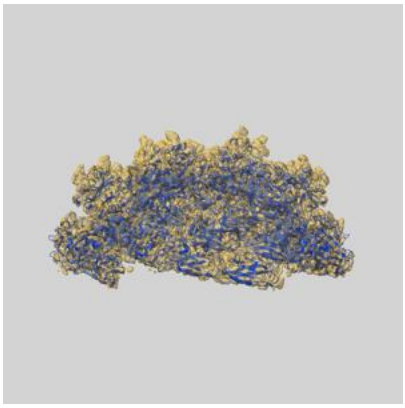
8 Fourier-Shell correlation

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

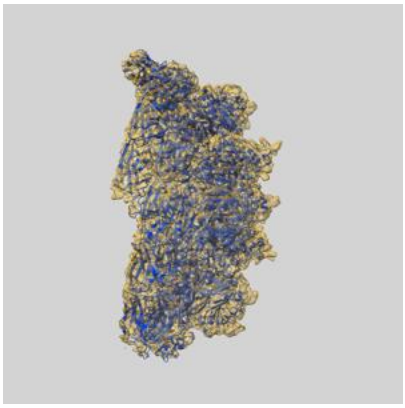
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16492 and PDB model 8C8R. Per-residue inclusion information can be found in section 3 on page 4.

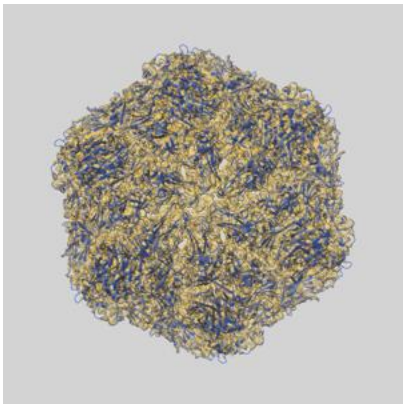
9.1 Map-model overlay



X



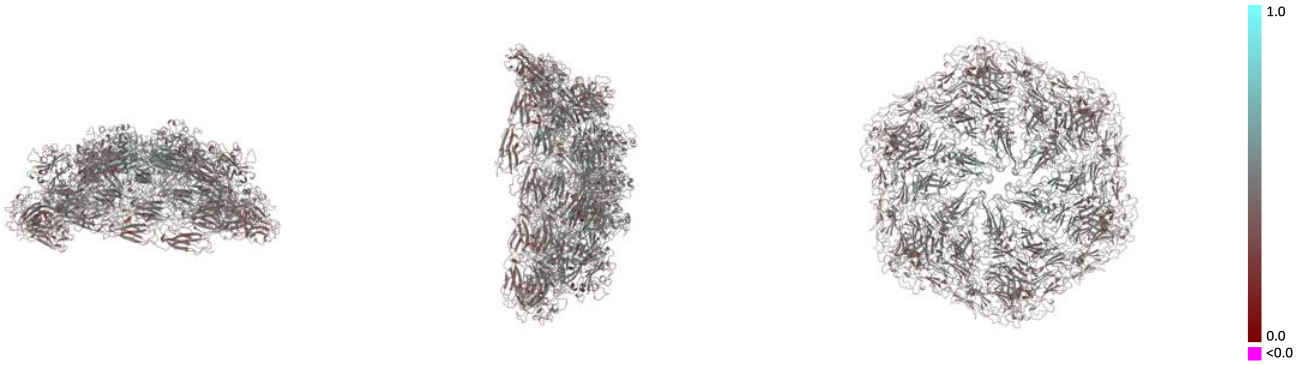
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.45621 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.

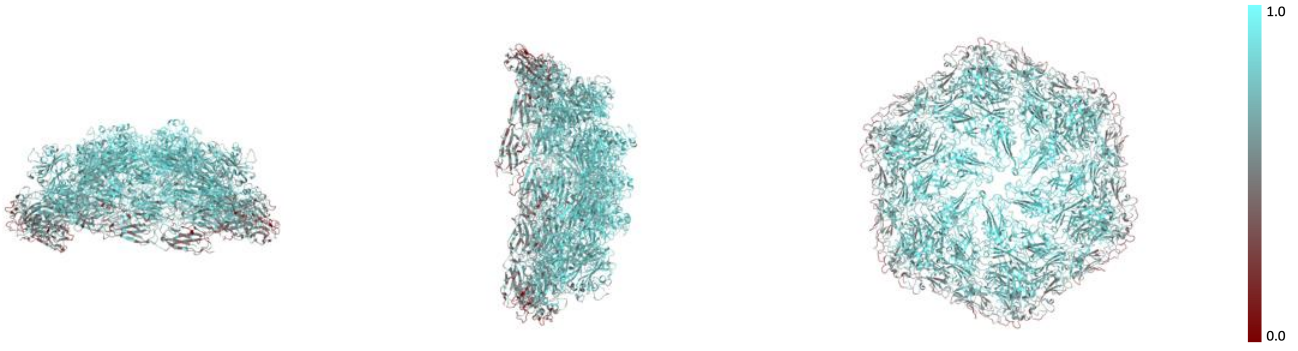
9.2 Q-score mapped to coordinate model (i)



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.

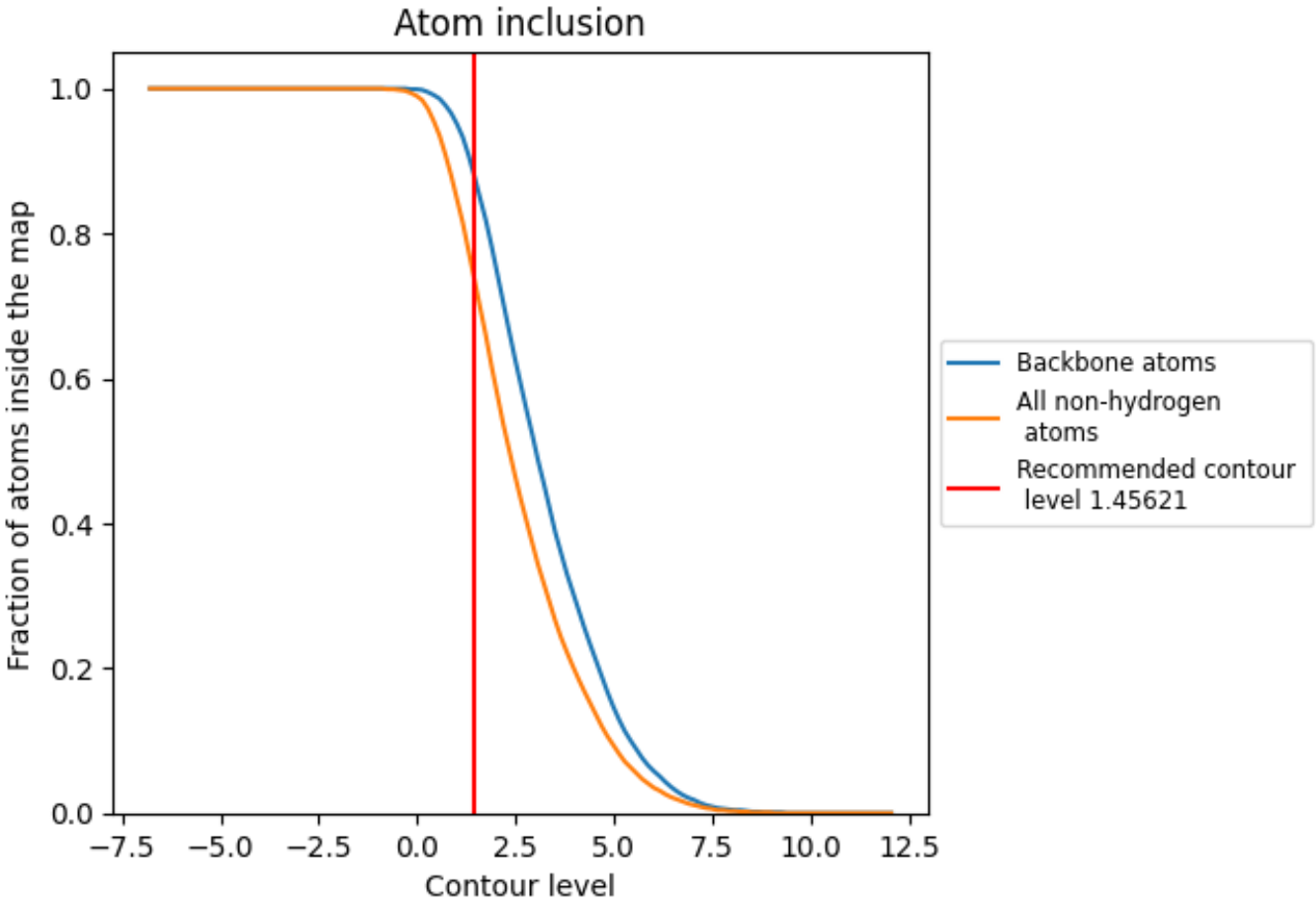
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.45621).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 74% 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 (1.45621) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.4380
A	0.7430	0.4440
B	0.7370	0.4350
C	0.7300	0.4350
D	0.7430	0.4440
E	0.7340	0.4360
F	0.7290	0.4350