Full wwPDB EM Validation Report ⓘ

May 12, 2024 – 03:05 PM EDT

PDB ID	:	8F5O
EMDB ID	:	EMD-28866
Title	:	Structure of Leishmania tarentolae IFT-A (state 1)
Authors	:	Zhou, H.; Brown, A.
Deposited on	:	2022-11-14
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:

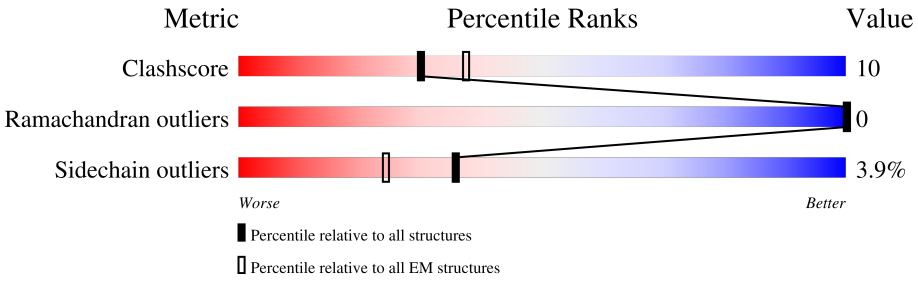
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	B	1247	68% 22% 9%
2	C	1292	68% 22% 9%
3	E	1654	47% 17% 35%
4	A	368	11% 86%
5	F	1376	31% 54% 12% 34%
6	D	1642	47% 23% 28%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 43398 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 Intraflagellar transport protein 122B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1134	8965	5674	1570	1658	63	0	0

- Molecule 2 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1179	9354	5929	1622	1735	68	0	0

- Molecule 3 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	1076	8380	5291	1451	1588	50	0	0

- Molecule 4 is a protein called NET domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	53	427	264	69	87	7	0	0

- Molecule 5 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	911	7045	4431	1231	1349	34	0	0

- Molecule 6 is a protein called TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	1180	9223	5796	1638	1738	51	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

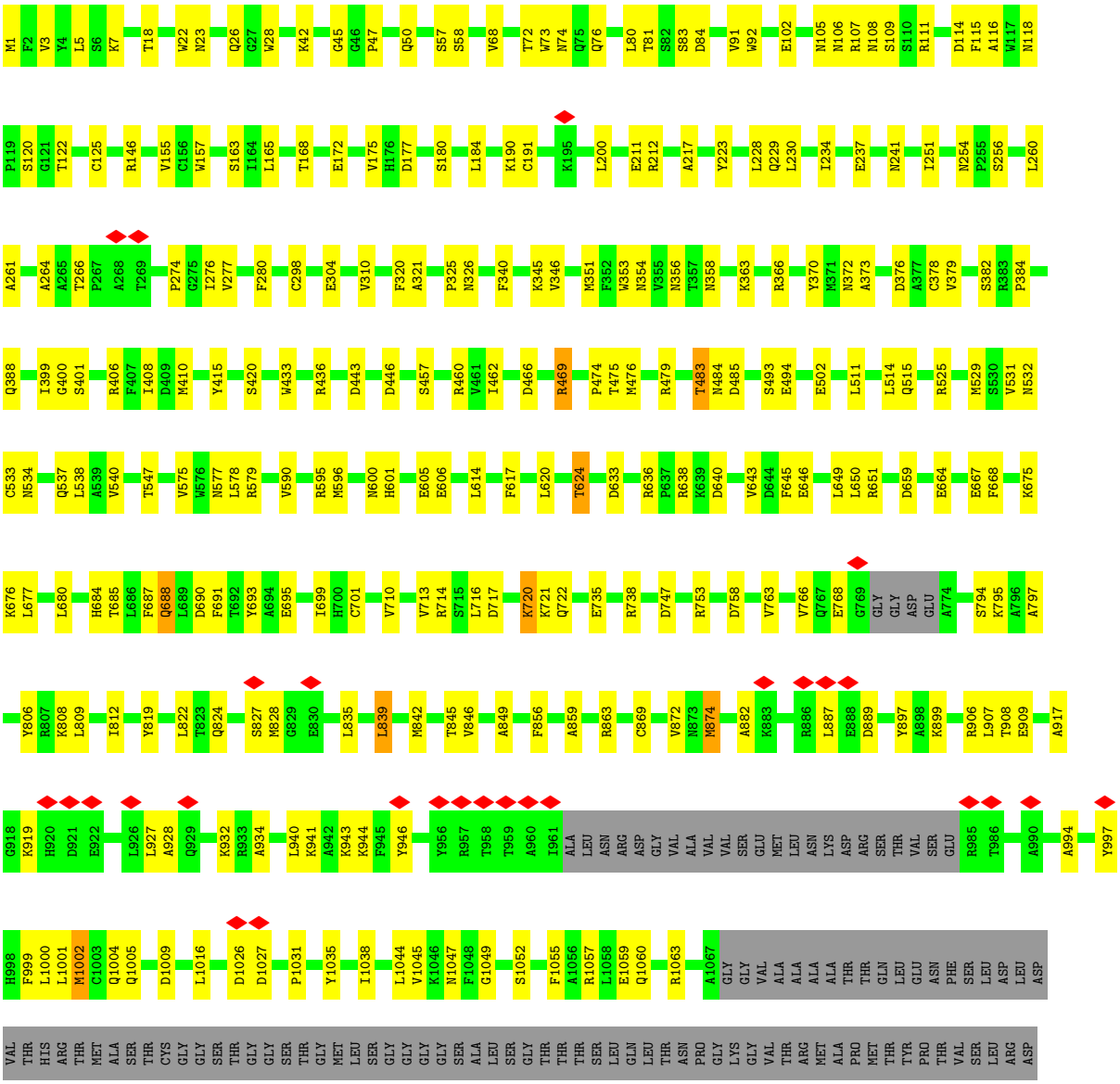
Mol	Chain	Residues	Atoms	AltConf
7	B	2	Total Zn 2 2	0
7	C	2	Total Zn 2 2	0

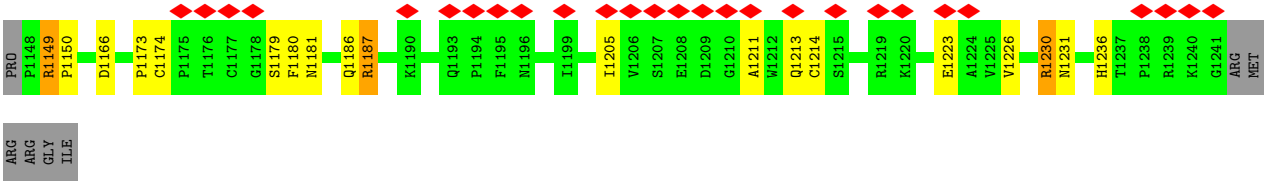
3 Residue-property plots (i)

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

- Molecule 1: Intraflagellar transport protein 122B, putative

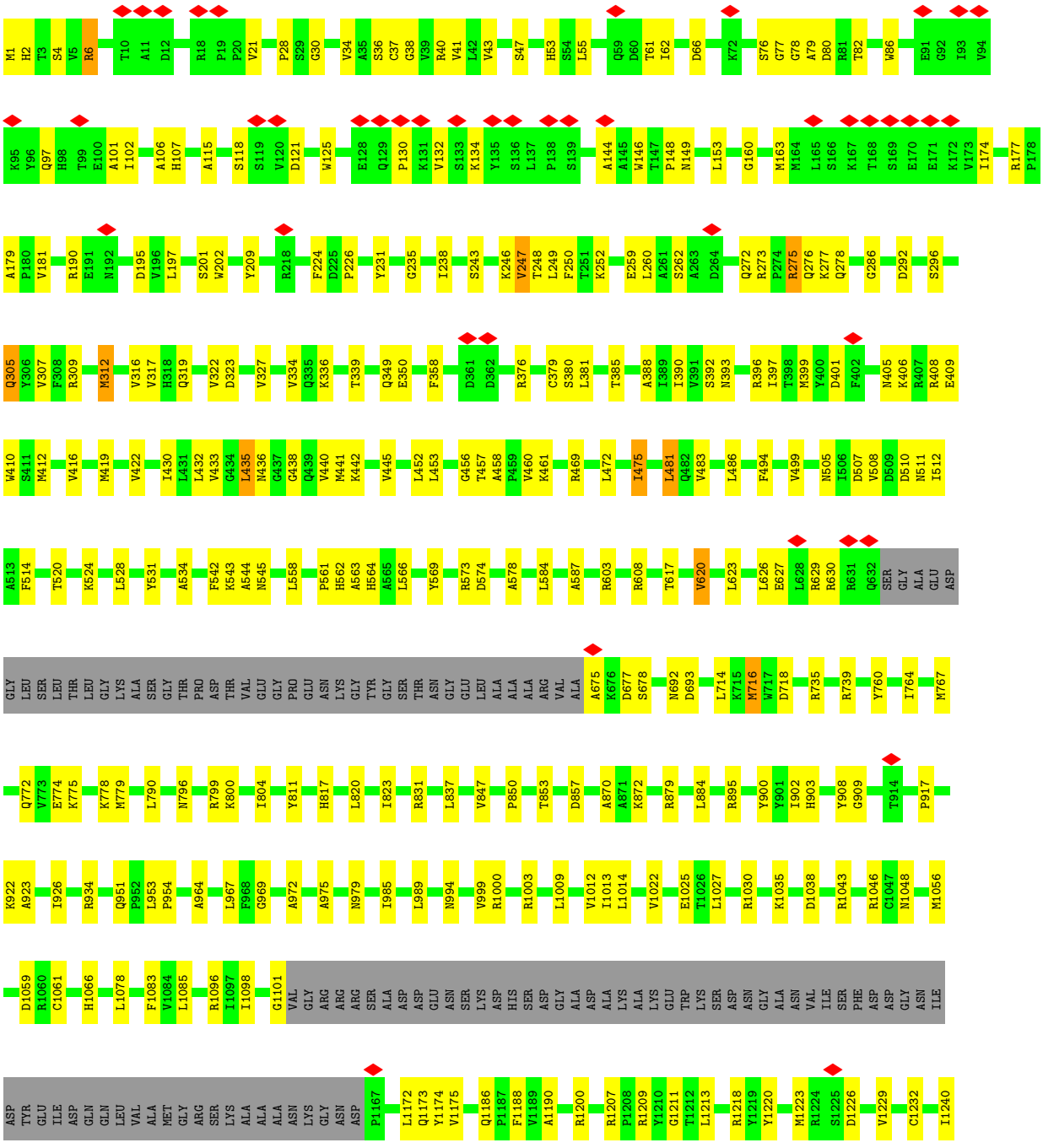
Chain B:

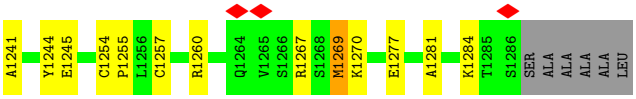




• Molecule 2: Intraflagellar transport protein 122 homolog

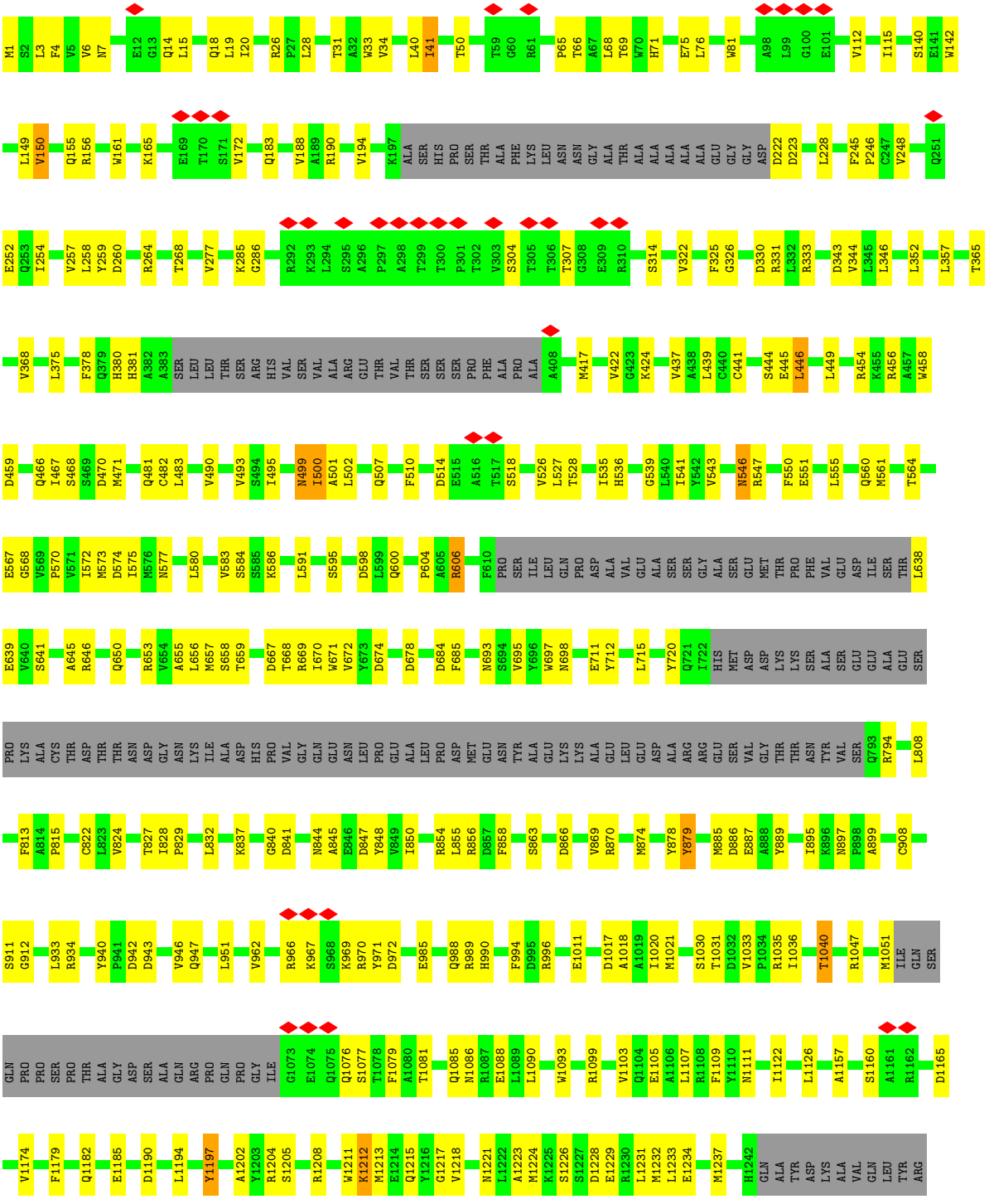
Chain C:

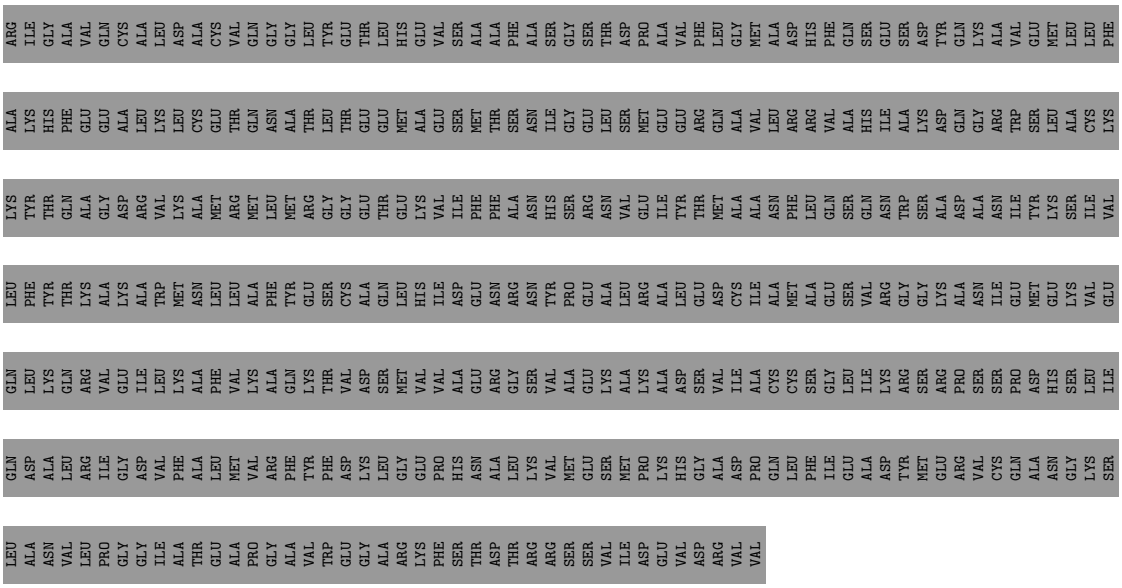




• Molecule 3: WD_REPEATS_REGION domain-containing protein

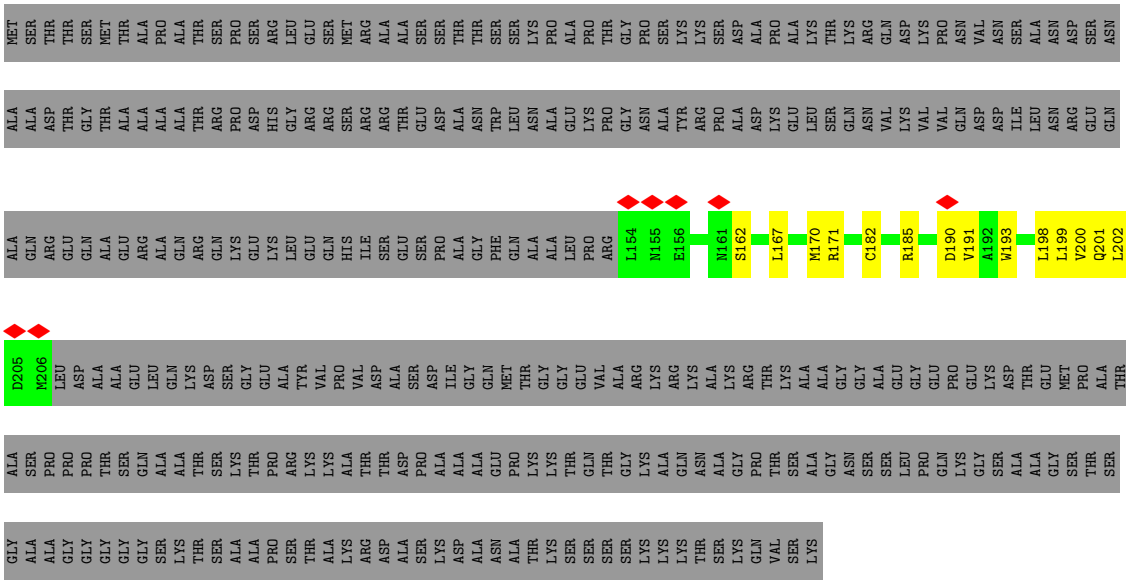
Chain E:





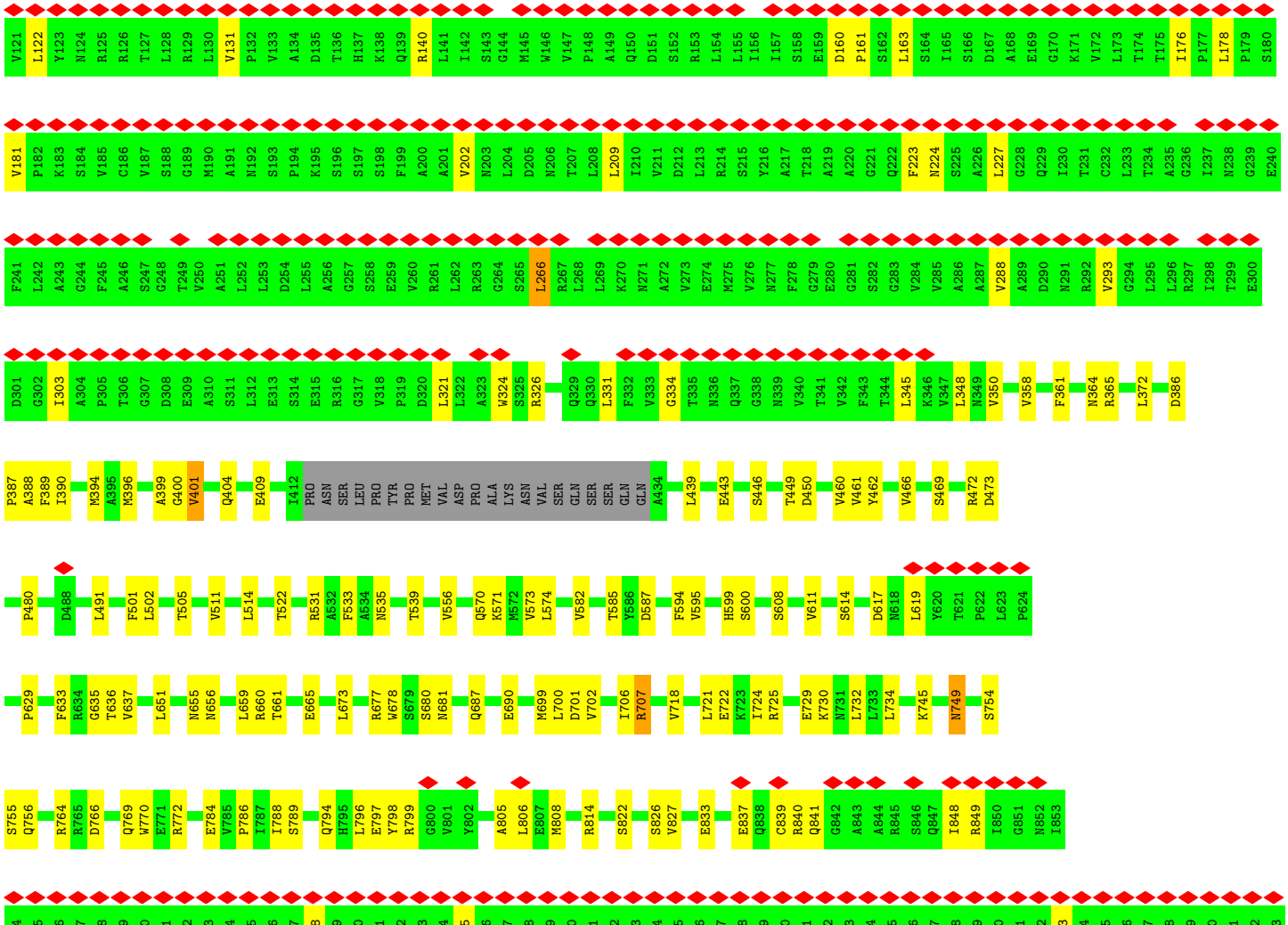
• Molecule 4: NET domain-containing protein

Chain A:



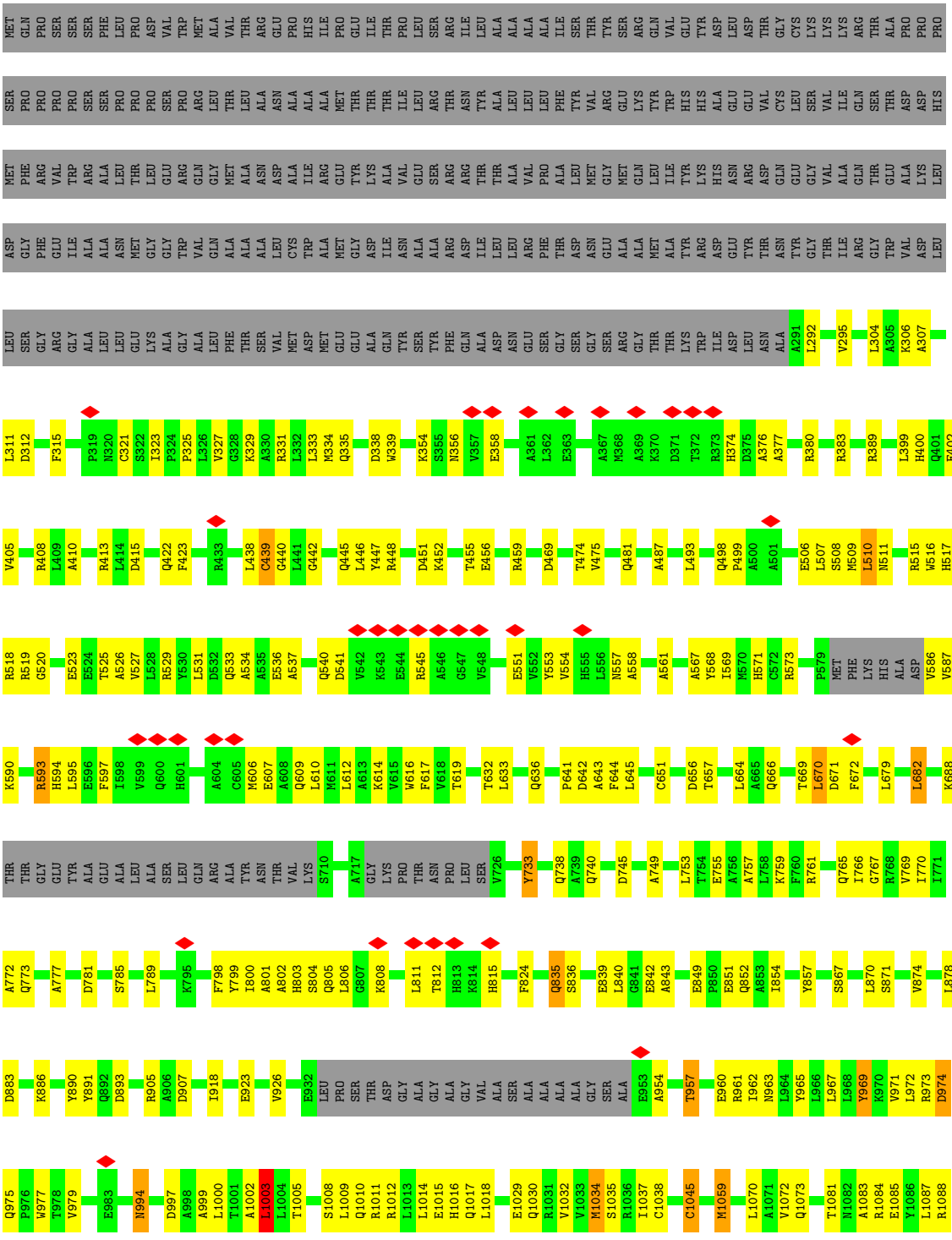
• Molecule 5: WD_REPEATS_REGION domain-containing protein

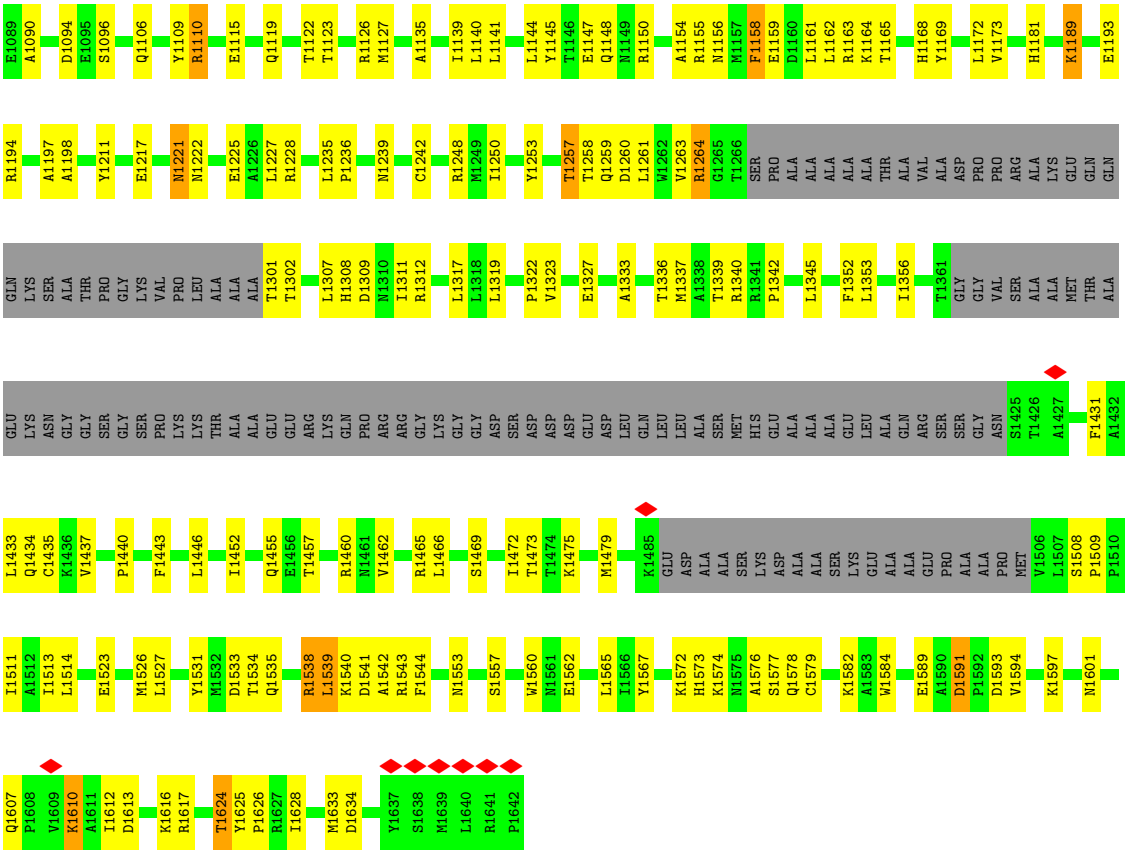
Chain F:


V121 L122 Y123 N124 R125 R126 T127 L128 R129 L130 V131 P132 V133 A134 D135 T136 H137 K138 Q139 R140 L141 I142 S143 G144 M145 W146 V147 P148 A149 Q150 D151 S152 R153 L154 L155 I156 I157 S158 E159 D160 P161 S162 L163 S164 I165 S166 D167 A168 E169 G170 K171 V172 L173 T174 T175 I176 P177 L178 P179 S180
V181 P182 K183 S184 V185 C186 V187 S188 G189 M190 A191 N192 S193 P194 K195 S196 S197 S198 F199 A200 A201 V202 N203 L204 D205 N206 T207 L208 L209 I210 V211 D212 L213 R214 S215 Y216 A217 T218 A219 A220 G221 Q222 F223 N224 S225 A226 L227 G228 Q229 I230 T231 C232 L233 T234 A235 G236 I237 N238 G239 E240
F241 L242 A243 G244 F245 A246 S247 G248 T249 V250 A251 L252 L253 D254 L255 A256 G257 S258 E259 V260 R261 L262 R263 G264 S265 L266 R267 L268 L269 K270 N271 A272 V273 E274 M275 V276 N277 F278 G279 E280 G281 S282 G283 V284 V285 A286 A287 V288 A289 D290 N291 R292 V293 G294 L295 L296 R297 I298 T299 E300
D301 G302 I303 A304 P305 T306 G307 D308 E309 A310 S311 L312 E313 S314 E315 R316 G317 V318 P319 D320 L321 L322 A323 W324 S325 R326 Q329 Q330 L331 F332 V333 G334 T335 N336 Q337 G338 N339 V340 T341 V342 F343 T344 L345 K346 V347 L348 N349 V350 V358 F361 N364 R365 L372 D386
P387 A388 F389 I390 M394 A396 M396 A399 G400 V401 Q404 E409 I412 PRO ASN SER LEU PRO TYR PRO MET VAL ASP PRO ALA LYS ASN VAL SER GLN SER SER GLN GLN A434 L439 E443 S446 T449 D450 V460 V461 Y462 V466 S469 R472 D473
P480 D488 L491 F501 L502 T505 V511 L514 T522 R531 A532 F533 A534 N535 T539 V556 Q570 K571 M572 V573 L574 V582 T585 Y586 D587 F594 V595 H599 S600 S608 V611 S614 D617 N618 L619 Y620 T621 P622 L623 P624
P629 F633 R634 G635 T636 V637 L651 N655 N656 L659 R660 T661 E665 L673 R677 W678 S679 S680 N681 Q687 E690 M699 L700 D701 V702 I706 R707 V718 L721 E722 K723 I724 R725 E729 K730 N731 L732 L733 L734 K745 N749 S754
S755 Q756 R764 R765 D766 Q769 W770 E771 R772 E784 V785 P786 I787 I788 S789 Q794 H795 L796 E797 Y798 R799 G800 V801 Y802 A805 L806 E807 M808 R814 S822 S826 V827 E833 E837 Q838 C839 R840 Q841 G842 A843 A844 R845 S846 Q847 I848 R849 I850 G851 N852 I853
A854 D855 A856 M857 K858 T859 V860 K861 E862 S863 S864 E865 V866 S867 F868 V869 K870 E871 C872 A873 K874 L875 C876 E877 E878 N879 Q880 K881 H882 E883 E884 A885 A886 Q887 L888 Y889 E890 K891 A892 G893 D894 I895 E896 R897 A898 A899 T900 I901 Y902 I903 E904 R905 C906 K907 N908 L909 K910 A911 A912 E913
R914 L915 L916 P917 F918 I919 K920 S921 R922 N923 I924 I925 G926 I927 Y928 A929 R930 G931 K932 GLU ALA GLU GLY ALA PHE VAL GLU ALA GLU LYS ALA PHE ALA GLN ALA GLU ASP TRP ASP ASN ALA VAL ARG LEU ARG ILE GLU LYS LEU ASN ASP LEU HIS GLY ALA TYR VAL ILE VAL ARG
GLN THR ARG SER ALA ASN ALA ALA ALA LEU VAL ALA ALA LYS LYS CYS THR ALA GLN LYS GLU TYR GLY THR ALA VAL GLU PHE LEU VAL LEU ALA LYS SER LEU ASP GLU ALA PHE GLU LEU ALA LYS THR HIS ASP CYS MET PHE ASN PHE GLU SER ALA LEU LEU ASN GLN VAL GLN LEU
LYS ASP GLY ILE ALA PRO LEU SER ASN GLN ALA ALA ASP PHE THR MET ILE ALA GLU TYR TYR ASP ASN ASP GLY LYS ALA GLY GLN ALA GLY MET TYR TYR HIS ILE SER GLY HIS TYR ALA LYS ALA LEU ASN LYS TYR LEU GLU SER GLY GLN PRO GLU ASP ILE GLU LYS ALA VAL GLU
VAL VAL GLY LYS ALA HIS SER ASP SER LEU THR ASN LYS PHE ILE ASP TYR LEU MET GLY GLU THR ASP GLY GLU PRO LYS ASP PRO SER TYR ILE PHE LYS LEU TYR LEU ALA MET GLY SER TYR GLU LYS ALA ALA LYS THR SER VAL ILE ILE SER ALA LYS GLU GLN GLU ILE GLY
ASN TYR LYS SER ALA HIS LYS THR LEU VAL GLU ALA TYR ARG ILE LEU GLN GLN ARG ASN MET HIS VAL SER ASN ASP LEU ARG ARG ALA LEU MET LEU LEU HIS SER TYR ILE ILE VAL LYS ASP LEU LEU LYS ILE MET LYS ASP ASP ASP THR ALA CYS ARG MET MET LEU LEU ARG VAL
SER ARG ASN ILE GLN LYS PHE PRO LYS HIS THR THR VAL THR THR THR VAL SER LEU CYS GLN LYS SER ASN ASP PHE LYS LYS SER ALA PHE GLU TYR ALA CYS TYR LEU ILE GLN ASN GLU LYS HIS ARG ALA GLU MET SER ARG LYS LYS ILE GLU LEU ARG VAL
ARG ARG HIS SER LYS ASP ASP ALA VAL ASP PRO VAL GLU PRO MET LEU PRO CYS PRO TYR CYS ASP ALA PRO VAL ALA GLU THR GLU LEU ASP CYS GLY ALA CYS LYS ASN THR ILE PRO PHE CYS ILE VAL THR GLY LYS HIS ILE VAL LYS SER ARG TYR THR SER THR ILE CYS

• Molecule 6: TPR_REGION domain-containing protein

Chain D:




E1089 A1090 D1094 E1095 S1096 Q1106 Y1109 R1110 E1115 Q1119 T1122 T1123 R1126 M1127 A1135 I1139 L1140 L1141 L1144 Y1145 T1146 E1147 Q1148 N1149 R1150 A1154 R1155 N1156 M1157 F1158 E1159 D1160 L1161 L1162 R1163 K1164 T1165 H1168 Y1169 L1172 V1173 H1181 K1189 E1193
R1194 A1197 A1198 Y1211 E1217 N1221 N1222 E1225 A1226 L1227 R1228 L1235 P1236 N1239 C1242 R1248 M1249 I1250 Y1253 T1257 T1258 Q1259 D1260 L1261 W1262 V1263 R1264 G1265 T1266 SER PRO ALA ALA ALA ALA ALA THR ALA VAL ALA ASP PRO PRO ARG ALA LYS GLU GLN GLN
GLN LYS SER ALA THR PRO GLY LYS VAL PRO LEU ALA ALA ALA T1301 T1302 L1307 H1308 D1309 N1310 I1311 R1312 L1317 L1318 L1319 P1322 V1323 E1327 A1333 T1336 M1337 A1338 T1339 R1340 R1341 P1342 L1345 F1382 L1353 I1386 T1361 GLY GLY VAL SER ALA ALA MET THR ALA
GLU LYS ASN GLY GLY SER GLY SER PRO LYS LYS THR ALA ALA GLU GLU ARG LYS GLN PRO ARG ARG GLY LYS GLY GLY ASP SER ASP ASP ASP GLU ASP LEU GLN LEU LEU ALA ALA SER MET HIS GLU ALA ALA ALA GLU LEU ALA GLN ARG SER SER GLY ASN S1425 T1426 A1427 F1431 A1432
L1433 Q1434 C1435 K1436 V1437 P1440 F1443 L1446 I1452 Q1455 E1456 T1457 R1460 N1461 V1462 R1465 L1466 S1469 I1472 T1473 T1474 K1475 M1479 K1485 GLU ASP ALA ALA SER LYS ASP ALA ALA SER LYS GLU ALA ALA GLU PRO ALA ALA PRO MET V1506 L1507 S1508 P1509 P1510
I1511 A1512 I1513 L1514 E1523 M1526 L1527 Y1531 M1532 D1533 T1534 Q1535 R1538 L1539 K1540 D1541 A1542 R1543 F1544 N1553 S1557 W1560 N1561 E1562 L1565 I1566 Y1567 K1572 H1573 K1574 N1575 A1576 S1577 Q1578 C1579 K1582 A1583 W1584 E1589 A1590 D1591 P1592 D1593 V1594 K1597 N1601
Q1607 P1608 V1609 K1610 A1611 I1612 D1613 K1616 R1617 T1624 Y1625 P1626 R1627 I1628 M1633 D1634 Y1637 S1638 M1639 L1640 R1641 P1642

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	239280	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 ($e^-/Å^2$)	57.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	86.420	Depositor
Minimum map value	-36.983	Depositor
Average map value	0.020	Depositor
Map value standard deviation	1.359	Depositor
Recommended contour level	9.0	Depositor
Map size (Å)	514.6, 514.6, 514.6	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.28	0/9156	0.51	0/12403
2	C	0.28	0/9548	0.52	0/12921
3	E	0.29	0/8546	0.52	0/11608
4	A	0.25	0/432	0.56	0/584
5	F	0.28	0/7173	0.51	0/9746
6	D	0.30	0/9377	0.54	1/12718 (0.0%)
All	All	0.29	0/44232	0.52	1/59980 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1003	LEU	CA-CB-CG	5.09	127.02	115.30

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	B	8965	0	8873	170	0
2	C	9354	0	9301	185	0
3	E	8380	0	8309	173	0
4	A	427	0	413	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	7045	0	7054	101	0
6	D	9223	0	9265	253	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
All	All	43398	0	43215	868	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 (868) 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)
3:E:441:CYS:O	3:E:445:GLU:HB3	1.71	0.89
2:C:76:SER:HG	2:C:86:TRP:HE1	1.25	0.80
5:F:446:SER:HB3	5:F:462:TYR:HB2	1.66	0.78
2:C:197:LEU:HB3	2:C:209:TYR:O	1.84	0.76
5:F:789:SER:HB3	5:F:808:MET:HB2	1.66	0.76
3:E:499:ASN:N	3:E:499:ASN:OD1	2.22	0.73
6:D:1034:MET:SD	6:D:1034:MET:N	2.60	0.72
6:D:682:LEU:HD11	6:D:738:GLN:HB3	1.71	0.72
3:E:570:PRO:HA	3:E:584:SER:HA	1.70	0.72
2:C:4:SER:HB3	2:C:292:ASP:O	1.90	0.71
6:D:569:ILE:HD13	6:D:614:LYS:HD2	1.73	0.71
1:B:462:ILE:HD13	1:B:514:LEU:HD21	1.74	0.69
1:B:116:ALA:HB3	1:B:125:CYS:HB3	1.73	0.69
3:E:514:ASP:O	3:E:518:SER:N	2.26	0.69
6:D:1236:PRO:O	6:D:1239:ASN:ND2	2.25	0.69
6:D:1010:GLN:NE2	6:D:1030:GLN:OE1	2.27	0.68
6:D:799:TYR:O	6:D:802:ALA:HB3	1.93	0.68
3:E:1208:ARG:O	3:E:1212:LYS:NZ	2.27	0.67
5:F:321:LEU:HB3	5:F:334:GLY:O	1.95	0.67
6:D:1308:HIS:HA	6:D:1311:ILE:HD12	1.76	0.67
1:B:353:TRP:HE1	1:B:358:ASN:HA	1.60	0.67
1:B:1063:ARG:HA	1:B:1149:ARG:HH12	1.60	0.66
1:B:266:THR:O	1:B:274:PRO:HA	1.96	0.66
1:B:846:VAL:HA	2:C:430:ILE:HD11	1.78	0.66
6:D:651:CYS:HB3	6:D:656:ASP:HB2	1.78	0.66
6:D:1135:ALA:HB2	6:D:1168:HIS:HE1	1.59	0.66
6:D:1123:THR:HA	6:D:1126:ARG:HE	1.60	0.65
5:F:23:LEU:HD13	5:F:326:ARG:HH22	1.61	0.65
6:D:1591:ASP:OD2	6:D:1594:VAL:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:ND2	1:B:120:SER:OG	2.30	0.65
2:C:442:LYS:HG3	2:C:453:LEU:HD11	1.79	0.65
2:C:336:LYS:NZ	2:C:379:CYS:SG	2.70	0.65
2:C:735:ARG:HG3	2:C:739:ARG:HH22	1.62	0.64
4:A:162:SER:OG	4:A:185:ARG:NH2	2.31	0.64
3:E:656:LEU:HB2	3:E:671:TRP:HB2	1.80	0.64
2:C:41:VAL:HB	2:C:55:LEU:HB2	1.80	0.64
6:D:803:HIS:HA	6:D:806:LEU:HB3	1.79	0.64
2:C:1078:LEU:HD21	2:C:1240:ILE:HG12	1.80	0.64
3:E:20:ILE:HG22	3:E:31:THR:HG22	1.78	0.64
2:C:272:GLN:NE2	2:C:276:GLN:O	2.32	0.63
3:E:454:ARG:NH2	3:E:822:CYS:SG	2.66	0.63
6:D:632:THR:O	6:D:636:GLN:NE2	2.32	0.63
2:C:524:LYS:NZ	2:C:528:LEU:O	2.30	0.63
3:E:454:ARG:O	3:E:456:ARG:NH1	2.31	0.63
2:C:505:ASN:HB2	2:C:511:ASN:HB2	1.81	0.63
2:C:902:ILE:HD13	2:C:1257:CYS:HB3	1.81	0.63
2:C:1000:ARG:O	2:C:1000:ARG:NH1	2.31	0.63
5:F:324:TRP:O	5:F:326:ARG:NH2	2.29	0.63
1:B:646:GLU:HB3	1:B:650:LEU:HB3	1.80	0.62
6:D:1443:PHE:HB3	6:D:1465:ARG:HH22	1.64	0.62
5:F:784:GLU:HG3	5:F:788:ILE:HD11	1.80	0.62
6:D:1263:VAL:O	6:D:1340:ARG:NH2	2.32	0.62
5:F:266:LEU:HD21	5:F:303:ILE:HD12	1.82	0.62
5:F:364:ASN:OD1	5:F:365:ARG:NH1	2.32	0.62
1:B:254:ASN:ND2	1:B:256:SER:OG	2.33	0.62
3:E:26:ARG:HG3	3:E:75:GLU:HG2	1.82	0.62
5:F:223:PHE:HB3	5:F:227:LEU:HD12	1.82	0.62
6:D:1475:LYS:NZ	6:D:1508:SER:O	2.33	0.62
2:C:1207:ARG:HB3	2:C:1209:ARG:HH21	1.65	0.61
2:C:1269:MET:SD	2:C:1269:MET:N	2.70	0.61
3:E:15:LEU:HD22	3:E:446:LEU:HB2	1.82	0.61
6:D:1466:LEU:O	6:D:1469:SER:OG	2.18	0.61
1:B:433:TRP:HE1	1:B:457:SER:HB2	1.66	0.61
3:E:972:ASP:N	3:E:972:ASP:OD1	2.34	0.61
6:D:536:GLU:O	6:D:540:GLN:NE2	2.33	0.61
1:B:200:LEU:HA	1:B:223:TYR:HA	1.83	0.61
5:F:122:LEU:HB2	5:F:131:VAL:HB	1.83	0.61
1:B:532:ASN:ND2	1:B:534:ASN:OD1	2.34	0.61
6:D:1159:GLU:O	6:D:1163:ARG:N	2.33	0.61
2:C:316:VAL:HG12	2:C:327:VAL:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:ALA:HB2	1:B:812:ILE:HG21	1.83	0.61
2:C:545:ASN:OD1	2:C:562:HIS:NE2	2.33	0.61
5:F:350:VAL:HG11	5:F:389:PHE:HA	1.81	0.61
6:D:789:LEU:HD13	6:D:806:LEU:HD13	1.82	0.61
1:B:735:GLU:HB2	1:B:738:ARG:HH21	1.65	0.61
2:C:1046:ARG:NH2	2:C:1186:GLN:O	2.33	0.61
5:F:12:ALA:O	5:F:36:LYS:NZ	2.34	0.61
1:B:827:SER:OG	1:B:828:MET:SD	2.58	0.61
6:D:567:ALA:O	6:D:571:HIS:ND1	2.34	0.61
6:D:508:SER:HA	6:D:511:ASN:HD22	1.66	0.60
6:D:666:GLN:O	6:D:669:THR:OG1	2.19	0.60
1:B:74:ASN:ND2	1:B:76:GLN:OE1	2.35	0.60
6:D:537:ALA:O	6:D:541:ASP:N	2.26	0.60
6:D:1336:THR:O	6:D:1339:THR:OG1	2.17	0.60
6:D:1557:SER:HA	6:D:1560:TRP:HD1	1.66	0.60
2:C:62:ILE:HG22	2:C:78:GLY:HA3	1.84	0.60
5:F:358:VAL:HG23	5:F:372:LEU:HD21	1.83	0.60
3:E:333:ARG:HG2	3:E:344:VAL:HG22	1.83	0.60
6:D:1573:HIS:O	6:D:1601:ASN:ND2	2.34	0.60
6:D:798:PHE:O	6:D:802:ALA:N	2.33	0.59
6:D:447:TYR:OH	6:D:557:ASN:OD1	2.20	0.59
6:D:1002:ALA:O	6:D:1005:THR:OG1	2.19	0.59
6:D:1225:GLU:OE2	6:D:1228:ARG:NH1	2.34	0.59
1:B:943:LYS:HE2	1:B:1001:LEU:HD22	1.83	0.59
1:B:946:TYR:HB3	1:B:994:ALA:HA	1.83	0.59
2:C:319:GLN:O	2:C:323:ASP:HA	2.03	0.59
6:D:327:VAL:O	6:D:331:ARG:N	2.33	0.59
1:B:1:MET:N	1:B:326:ASN:OD1	2.32	0.59
2:C:148:PRO:HD2	2:C:190:ARG:HH21	1.67	0.59
3:E:190:ARG:NH1	3:E:257:VAL:O	2.36	0.59
4:A:171:ARG:HH12	6:D:1323:VAL:HG23	1.68	0.59
2:C:627:GLU:HG3	2:C:630:ARG:HH12	1.68	0.59
6:D:867:SER:O	6:D:871:SER:N	2.35	0.59
6:D:1584:TRP:HE1	6:D:1589:GLU:HG3	1.67	0.59
1:B:42:LYS:HB3	1:B:57:SER:HB3	1.84	0.59
6:D:327:VAL:HG12	6:D:331:ARG:HE	1.68	0.59
6:D:1115:GLU:OE2	6:D:1119:GLN:NE2	2.35	0.59
2:C:1098:ILE:O	2:C:1200:ARG:NH1	2.35	0.59
5:F:460:VAL:O	5:F:466:VAL:HA	2.01	0.59
6:D:1211:TYR:HE1	6:D:1248:ARG:HG3	1.68	0.58
6:D:1301:THR:OG1	6:D:1302:THR:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG13	1:B:102:GLU:HB3	1.85	0.58
3:E:829:PRO:HG2	3:E:854:ARG:HH11	1.68	0.58
1:B:83:SER:OG	1:B:84:ASP:N	2.35	0.58
3:E:365:THR:HA	3:E:378:PHE:O	2.03	0.58
1:B:633:ASP:OD2	1:B:636:ARG:NH2	2.37	0.58
2:C:406:LYS:HZ1	2:C:409:GLU:HB2	1.67	0.58
6:D:333:LEU:O	6:D:338:ASP:N	2.35	0.58
6:D:1573:HIS:HD2	6:D:1601:ASN:HA	1.69	0.58
6:D:849:GLU:OE1	6:D:852:GLN:NE2	2.37	0.58
6:D:972:LEU:HA	6:D:975:GLN:HG2	1.85	0.58
1:B:578:LEU:O	1:B:579:ARG:NH1	2.35	0.57
5:F:706:ILE:HD13	5:F:722:GLU:HG2	1.86	0.57
2:C:870:ALA:O	2:C:872:LYS:NZ	2.37	0.57
3:E:459:ASP:HB3	3:E:495:ILE:HG23	1.86	0.57
2:C:30:GLY:HA3	2:C:275:ARG:HH12	1.68	0.57
6:D:1034:MET:HA	6:D:1037:ILE:HD12	1.86	0.57
6:D:1509:PRO:HB2	6:D:1514:LEU:HD21	1.87	0.57
1:B:716:LEU:O	1:B:722:GLN:NE2	2.37	0.57
2:C:442:LYS:HE2	2:C:453:LEU:HD21	1.86	0.57
6:D:410:ALA:O	6:D:413:ARG:NH1	2.37	0.57
6:D:773:GLN:O	6:D:777:ALA:N	2.37	0.57
3:E:194:VAL:HG12	3:E:259:TYR:CZ	2.40	0.57
3:E:458:TRP:NE1	3:E:827:THR:OG1	2.36	0.57
1:B:1057:ARG:NH1	1:B:1060:GLN:OE1	2.35	0.57
2:C:179:ALA:HB3	2:C:201:SER:HB2	1.87	0.57
3:E:15:LEU:H	3:E:444:SER:HA	1.70	0.57
3:E:156:ARG:HE	3:E:183:GLN:HE21	1.53	0.57
5:F:635:GLY:HA2	5:F:651:LEU:HD12	1.85	0.57
6:D:1015:GLU:HA	6:D:1018:LEU:HD12	1.87	0.57
1:B:228:LEU:O	1:B:241:ASN:ND2	2.36	0.56
2:C:224:PHE:HB2	2:C:243:SER:H	1.70	0.56
2:C:1003:ARG:NH2	2:C:1030:ARG:O	2.38	0.56
2:C:1085:LEU:HA	2:C:1190:ALA:HB3	1.87	0.56
2:C:1223:MET:SD	2:C:1223:MET:N	2.78	0.56
5:F:396:MET:HE1	5:F:472:ARG:HH12	1.70	0.56
5:F:794:GLN:O	5:F:797:GLU:HB3	2.05	0.56
2:C:235:GLY:O	2:C:252:LYS:NZ	2.39	0.56
5:F:656:ASN:ND2	5:F:665:GLU:OE1	2.37	0.56
5:F:754:SER:OG	5:F:755:SER:N	2.38	0.56
6:D:1479:MET:HG3	6:D:1544:PHE:HE1	1.70	0.56
2:C:82:THR:HA	2:C:97:GLN:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:422:VAL:HG12	2:C:469:ARG:HH11	1.70	0.56
2:C:79:ALA:HA	2:C:101:ALA:HB1	1.87	0.56
5:F:20:VAL:HG11	5:F:59:ALA:HA	1.88	0.56
5:F:732:LEU:HD21	5:F:756:GLN:HB2	1.87	0.56
6:D:606:MET:SD	6:D:636:GLN:NE2	2.75	0.56
2:C:857:ASP:O	3:E:996:ARG:NH1	2.39	0.56
5:F:573:VAL:HG22	5:F:585:THR:HG22	1.86	0.56
6:D:1161:LEU:HA	6:D:1164:LYS:HE2	1.87	0.56
2:C:37:CYS:SG	2:C:40:ARG:NH2	2.76	0.56
2:C:796:ASN:OD1	2:C:811:TYR:OH	2.23	0.56
5:F:163:LEU:HB3	5:F:176:ILE:HB	1.88	0.56
5:F:582:VAL:HG22	5:F:595:VAL:HG12	1.87	0.56
6:D:442:GLY:O	6:D:446:LEU:N	2.38	0.56
6:D:616:TRP:O	6:D:619:THR:OG1	2.23	0.56
1:B:1186:GLN:HE21	1:B:1187:ARG:HE	1.54	0.56
6:D:334:MET:SD	6:D:335:GLN:NE2	2.79	0.56
1:B:190:LYS:NZ	1:B:237:GLU:O	2.38	0.56
2:C:520:THR:HA	2:C:534:ALA:HA	1.87	0.56
5:F:531:ARG:HH22	5:F:571:LYS:HD3	1.71	0.55
1:B:251:ILE:HB	1:B:260:LEU:HD11	1.87	0.55
2:C:349:GLN:OE1	2:C:376:ARG:NH2	2.39	0.55
2:C:416:VAL:HA	2:C:435:LEU:HA	1.87	0.55
3:E:14:GLN:N	3:E:34:VAL:O	2.34	0.55
3:E:650:GLN:OE1	3:E:653:ARG:NH2	2.40	0.55
6:D:1045:CYS:HB3	6:D:1083:ALA:HB2	1.87	0.55
1:B:606:GLU:OE2	1:B:651:ARG:NH2	2.40	0.55
1:B:819:TYR:HA	1:B:822:LEU:HB3	1.87	0.55
2:C:118:SER:OG	2:C:121:ASP:OD1	2.23	0.55
3:E:1204:ARG:HD2	3:E:1231:LEU:HD11	1.87	0.55
6:D:1455:GLN:OE1	6:D:1457:THR:N	2.39	0.55
3:E:1185:GLU:OE1	3:E:1197:TYR:OH	2.24	0.55
1:B:406:ARG:NH2	1:B:457:SER:OG	2.40	0.55
2:C:248:THR:HA	2:C:259:GLU:HA	1.87	0.55
2:C:1043:ARG:NH2	2:C:1048:ASN:OD1	2.40	0.55
3:E:1018:ALA:HA	3:E:1021:MET:HG2	1.88	0.55
6:D:800:ILE:O	6:D:804:SER:N	2.35	0.55
6:D:1475:LYS:NZ	6:D:1508:SER:OG	2.35	0.55
3:E:470:ASP:OD1	3:E:470:ASP:N	2.36	0.55
6:D:907:ASP:OD1	6:D:907:ASP:N	2.40	0.55
1:B:685:THR:O	1:B:690:ASP:N	2.37	0.55
6:D:1147:GLU:HA	6:D:1514:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:349:GLN:O	2:C:376:ARG:NE	2.39	0.54
6:D:957:THR:O	6:D:961:ARG:NH1	2.39	0.54
3:E:471:MET:HB3	3:E:483:LEU:HD11	1.90	0.54
6:D:445:GLN:HA	6:D:448:ARG:HB2	1.90	0.54
6:D:839:GLU:O	6:D:842:GLU:HB3	2.07	0.54
2:C:307:VAL:HG22	2:C:317:VAL:HG13	1.89	0.54
2:C:1013:ILE:HG22	5:F:730:LYS:HD3	1.89	0.54
3:E:547:ARG:HE	3:E:560:GLN:HA	1.71	0.54
1:B:529:MET:HG2	1:B:540:VAL:HG22	1.89	0.54
2:C:831:ARG:NH1	2:C:1277:GLU:OE2	2.40	0.54
2:C:1101:GLY:HA2	2:C:1200:ARG:HH22	1.73	0.54
3:E:260:ASP:O	3:E:264:ARG:N	2.40	0.54
3:E:711:GLU:OE1	3:E:870:ARG:NH1	2.41	0.54
3:E:886:ASP:O	5:F:798:TYR:OH	2.25	0.54
1:B:229:GLN:HG3	1:B:241:ASN:HB2	1.90	0.54
2:C:273:ARG:NH1	2:C:278:GLN:OE1	2.40	0.54
3:E:646:ARG:O	3:E:697:TRP:NE1	2.38	0.54
6:D:642:ASP:N	6:D:642:ASP:OD1	2.41	0.54
1:B:691:PHE:HB3	1:B:714:ARG:HD3	1.89	0.54
2:C:934:ARG:NH2	2:C:975:ALA:O	2.41	0.54
3:E:672:VAL:HG21	3:E:808:LEU:HD21	1.88	0.54
3:E:1020:ILE:HD12	3:E:1033:VAL:HG13	1.89	0.54
3:E:536:HIS:NE2	3:E:577:ASN:O	2.39	0.54
6:D:1084:ARG:HA	6:D:1087:LEU:HD23	1.89	0.54
2:C:160:GLY:HA2	2:C:181:VAL:HG23	1.89	0.54
2:C:510:ASP:OD1	2:C:510:ASP:N	2.40	0.54
6:D:408:ARG:NH1	6:D:554:VAL:O	2.41	0.54
1:B:165:LEU:HG	1:B:175:VAL:HG22	1.90	0.53
1:B:605:GLU:OE1	1:B:651:ARG:NH2	2.41	0.53
1:B:624:THR:HG23	1:B:643:VAL:HG23	1.89	0.53
1:B:753:ARG:NH2	1:B:758:ASP:OD2	2.40	0.53
2:C:1012:VAL:HG22	5:F:729:GLU:HA	1.89	0.53
3:E:375:LEU:HD11	3:E:439:LEU:HD11	1.90	0.53
5:F:163:LEU:HD23	5:F:176:ILE:HD12	1.89	0.53
1:B:824:GLN:NE2	1:B:827:SER:OG	2.42	0.53
2:C:28:PRO:O	2:C:275:ARG:NH2	2.40	0.53
2:C:412:MET:SD	2:C:412:MET:N	2.81	0.53
2:C:972:ALA:O	5:F:755:SER:OG	2.26	0.53
2:C:979:ASN:OD1	5:F:725:ARG:NH1	2.40	0.53
3:E:343:ASP:OD1	3:E:343:ASP:N	2.41	0.53
5:F:655:ASN:ND2	5:F:665:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:GLN:NE2	1:B:1009:ASP:OD2	2.41	0.53
6:D:824:PHE:HB3	6:D:840:LEU:HD13	1.91	0.53
3:E:547:ARG:NH1	3:E:561:MET:O	2.42	0.53
5:F:161:PRO:HB2	5:F:178:LEU:HB2	1.90	0.53
5:F:611:VAL:HG21	5:F:619:LEU:HB2	1.89	0.53
5:F:677:ARG:NH1	5:F:701:ASP:OD2	2.41	0.53
6:D:1032:VAL:O	6:D:1035:SER:OG	2.16	0.53
1:B:659:ASP:OD1	1:B:659:ASP:N	2.41	0.53
3:E:674:ASP:O	3:E:678:ASP:CA	2.57	0.53
5:F:409:GLU:HB2	5:F:439:LEU:HD11	1.90	0.53
3:E:985:GLU:OE1	3:E:988:GLN:NE2	2.42	0.53
6:D:399:LEU:HA	6:D:402:PHE:HB2	1.89	0.53
6:D:515:ARG:O	6:D:520:GLY:N	2.42	0.53
6:D:1475:LYS:HB3	6:D:1544:PHE:HZ	1.73	0.53
6:D:1540:LYS:O	6:D:1543:ARG:NH2	2.42	0.53
2:C:144:ALA:HB1	2:C:153:LEU:HD11	1.89	0.53
2:C:408:ARG:NH1	2:C:445:VAL:O	2.42	0.53
5:F:288:VAL:HG22	5:F:293:VAL:HG22	1.90	0.53
6:D:1352:PHE:HB3	6:D:1446:LEU:HD23	1.91	0.53
6:D:1533:ASP:HB3	6:D:1542:ALA:HB2	1.90	0.53
1:B:47:PRO:HA	1:B:50:GLN:HB2	1.91	0.53
6:D:1264:ARG:NE	6:D:1531:TYR:OH	2.38	0.53
1:B:310:VAL:HG13	1:B:321:ALA:HB3	1.90	0.53
1:B:493:SER:HB2	1:B:531:VAL:HG11	1.91	0.53
6:D:545:ARG:HB3	6:D:551:GLU:HB3	1.90	0.53
2:C:804:ILE:HD12	2:C:823:ILE:HD11	1.90	0.52
3:E:1157:ALA:HA	3:E:1160:SER:HB3	1.89	0.52
3:E:1208:ARG:HA	3:E:1211:TRP:CD1	2.44	0.52
2:C:34:VAL:HG22	2:C:43:VAL:HG22	1.90	0.52
3:E:572:ILE:HB	3:E:583:VAL:HB	1.91	0.52
3:E:674:ASP:O	3:E:678:ASP:HA	2.08	0.52
6:D:974:ASP:OD1	6:D:974:ASP:N	2.35	0.52
6:D:977:TRP:NE1	6:D:997:ASP:OD2	2.42	0.52
6:D:1574:LYS:O	6:D:1577:SER:OG	2.27	0.52
1:B:72:THR:HG22	1:B:81:THR:HB	1.91	0.52
1:B:906:ARG:NH2	1:B:908:THR:OG1	2.42	0.52
2:C:994:ASN:ND2	2:C:1025:GLU:OE2	2.43	0.52
2:C:1218:ARG:NH2	2:C:1220:TYR:OH	2.38	0.52
6:D:954:ALA:N	6:D:957:THR:OG1	2.43	0.52
6:D:1342:PRO:HA	6:D:1345:LEU:HD13	1.92	0.52
2:C:309:ARG:HD2	2:C:312:MET:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:693:ASP:N	2:C:693:ASP:OD1	2.41	0.52
3:E:657:MET:HG2	3:E:670:ILE:HD11	1.90	0.52
5:F:387:PRO:HA	5:F:401:VAL:HG13	1.90	0.52
5:F:350:VAL:HG12	5:F:390:ILE:HG12	1.91	0.52
6:D:589:GLU:O	6:D:593:ARG:N	2.42	0.52
1:B:372:ASN:OD1	1:B:373:ALA:N	2.41	0.52
3:E:65:PRO:HA	3:E:81:TRP:HA	1.91	0.52
3:E:466:GLN:NE2	3:E:468:SER:O	2.42	0.52
3:E:481:GLN:NE2	3:E:848:TYR:O	2.43	0.52
3:E:595:SER:OG	3:E:598:ASP:OD1	2.27	0.52
6:D:789:LEU:HD22	6:D:806:LEU:HB2	1.92	0.52
6:D:1567:TYR:HB2	6:D:1576:ALA:HB2	1.91	0.52
6:D:1462:VAL:HG22	6:D:1465:ARG:HH21	1.75	0.52
5:F:848:ILE:HG21	5:F:875:LEU:HB2	1.92	0.52
6:D:1613:ASP:OD1	6:D:1613:ASP:N	2.42	0.52
3:E:1185:GLU:OE2	3:E:1208:ARG:NH1	2.42	0.52
6:D:1148:GLN:N	6:D:1148:GLN:OE1	2.42	0.52
1:B:370:TYR:OH	1:B:372:ASN:ND2	2.36	0.52
2:C:608:ARG:HG2	2:C:623:LEU:HD23	1.91	0.52
6:D:304:LEU:HA	6:D:307:ALA:HB3	1.92	0.52
6:D:962:ILE:HD12	6:D:962:ILE:H	1.75	0.52
6:D:1534:THR:OG1	6:D:1535:GLN:NE2	2.42	0.52
1:B:23:ASN:HB2	1:B:73:TRP:CD2	2.44	0.51
2:C:505:ASN:ND2	2:C:543:LYS:O	2.43	0.51
3:E:674:ASP:O	3:E:678:ASP:N	2.43	0.51
3:E:1036:ILE:O	3:E:1040:THR:OG1	2.19	0.51
6:D:745:ASP:N	6:D:745:ASP:OD1	2.38	0.51
6:D:854:ILE:HG21	6:D:886:LYS:HZ2	1.75	0.51
6:D:1010:GLN:HG2	6:D:1034:MET:HB3	1.92	0.51
1:B:212:ARG:NH1	1:B:345:LYS:O	2.44	0.51
1:B:547:THR:HG21	1:B:575:VAL:HB	1.92	0.51
6:D:883:ASP:HB2	6:D:886:LYS:HG2	1.92	0.51
1:B:1230:ARG:NE	1:B:1231:ASN:OD1	2.43	0.51
3:E:813:PHE:O	3:E:856:ARG:NH1	2.44	0.51
3:E:869:VAL:HG13	3:E:895:ILE:HG23	1.93	0.51
5:F:202:VAL:HB	5:F:209:LEU:HB3	1.92	0.51
5:F:224:ASN:HB3	5:F:227:LEU:HG	1.92	0.51
6:D:439:CYS:SG	6:D:440:GLY:N	2.83	0.51
3:E:71:HIS:HB2	3:E:76:LEU:HB3	1.92	0.51
6:D:515:ARG:HG2	6:D:519:ARG:HD2	1.92	0.51
5:F:404:GLN:HB3	5:F:443:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1513:ILE:HD11	6:D:1526:MET:HE1	1.92	0.51
1:B:264:ALA:HB3	1:B:277:VAL:HG13	1.92	0.51
6:D:753:LEU:HD13	6:D:773:GLN:HG2	1.92	0.51
1:B:106:ASN:O	1:B:108:ASN:ND2	2.43	0.51
2:C:272:GLN:NE2	2:C:273:ARG:O	2.36	0.51
1:B:943:LYS:HZ3	1:B:944:LYS:HE3	1.76	0.51
3:E:943:ASP:O	3:E:947:GLN:NE2	2.44	0.51
3:E:1228:ASP:HB3	3:E:1231:LEU:HD23	1.92	0.51
5:F:595:VAL:HG11	5:F:673:LEU:HA	1.91	0.51
1:B:107:ARG:NH1	1:B:109:SER:OG	2.44	0.50
1:B:340:PHE:HE1	1:B:351:MET:HB2	1.76	0.50
1:B:460:ARG:HG2	1:B:474:PRO:HB3	1.93	0.50
2:C:507:ASP:HB2	2:C:544:ALA:HB2	1.92	0.50
2:C:1260:ARG:O	2:C:1267:ARG:NH2	2.45	0.50
3:E:155:GLN:O	3:E:183:GLN:NE2	2.44	0.50
3:E:507:GLN:HB3	3:E:527:LEU:HD23	1.92	0.50
5:F:745:LYS:NZ	5:F:749:ASN:OD1	2.44	0.50
6:D:1217:GLU:HB3	6:D:1222:ASN:HB3	1.92	0.50
1:B:106:ASN:ND2	1:B:108:ASN:OD1	2.45	0.50
1:B:638:ARG:NH1	1:B:640:ASP:OD2	2.44	0.50
1:B:806:TYR:HA	1:B:809:LEU:HD12	1.93	0.50
1:B:842:MET:O	1:B:845:THR:OG1	2.25	0.50
2:C:38:GLY:HA2	2:C:61:THR:HG23	1.94	0.50
2:C:923:ALA:HB2	5:F:827:VAL:HG11	1.91	0.50
6:D:498:GLN:NE2	6:D:499:PRO:O	2.44	0.50
6:D:923:GLU:HA	6:D:926:VAL:HG22	1.93	0.50
6:D:506:GLU:HA	6:D:509:MET:HG2	1.93	0.50
6:D:1123:THR:HA	6:D:1126:ARG:NE	2.26	0.50
1:B:366:ARG:NH1	1:B:384:PRO:O	2.44	0.50
2:C:617:THR:HA	2:C:620:VAL:HG12	1.94	0.50
3:E:695:VAL:HB	3:E:715:LEU:HD11	1.93	0.50
6:D:633:LEU:HD11	6:D:643:ALA:HB3	1.94	0.50
6:D:979:VAL:HG11	6:D:1072:VAL:HG22	1.92	0.50
1:B:699:ILE:HD11	2:C:714:LEU:HA	1.92	0.50
2:C:764:ILE:HD12	2:C:790:LEU:HD23	1.92	0.50
3:E:934:ARG:NH1	5:F:766:ASP:OD2	2.42	0.50
5:F:677:ARG:O	5:F:680:SER:OG	2.29	0.50
1:B:1230:ARG:NH1	4:A:190:ASP:OD1	2.44	0.50
6:D:311:LEU:HD13	6:D:329:LYS:HA	1.93	0.50
6:D:969:TYR:O	6:D:973:ARG:N	2.45	0.50
3:E:149:LEU:HB3	3:E:161:TRP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:645:ALA:HA	3:E:655:ALA:O	2.11	0.50
3:E:698:ASN:ND2	3:E:711:GLU:O	2.43	0.50
3:E:1017:ASP:N	3:E:1017:ASP:OD1	2.44	0.50
3:E:1205:SER:OG	3:E:1208:ARG:NH2	2.44	0.50
5:F:660:ARG:NH1	5:F:681:ASN:OD1	2.44	0.50
6:D:857:TYR:HB3	6:D:874:VAL:HG22	1.94	0.50
6:D:1140:LEU:O	6:D:1144:LEU:N	2.44	0.50
6:D:1257:THR:OG1	6:D:1258:THR:N	2.44	0.50
6:D:507:LEU:O	6:D:511:ASN:ND2	2.45	0.50
6:D:1460:ARG:HH12	6:D:1538:ARG:HH22	1.60	0.50
6:D:1539:LEU:HD12	6:D:1540:LYS:HD3	1.93	0.50
2:C:461:LYS:HE2	2:C:475:ILE:HD11	1.93	0.49
2:C:677:ASP:OD1	2:C:677:ASP:N	2.44	0.49
2:C:1281:ALA:HA	2:C:1284:LYS:HG2	1.92	0.49
3:E:417:MET:HA	3:E:794:ARG:HE	1.77	0.49
2:C:163:MET:HA	2:C:174:ILE:HG12	1.93	0.49
3:E:1190:ASP:N	3:E:1190:ASP:OD1	2.41	0.49
3:E:422:VAL:HG13	3:E:424:LYS:H	1.78	0.49
6:D:1333:ALA:O	6:D:1337:MET:HG2	2.12	0.49
6:D:1624:THR:O	6:D:1624:THR:OG1	2.28	0.49
5:F:599:HIS:O	5:F:599:HIS:ND1	2.41	0.49
6:D:1081:THR:HB	6:D:1084:ARG:HH21	1.76	0.49
1:B:747:ASP:OD1	1:B:747:ASP:N	2.43	0.49
2:C:675:ALA:N	2:C:678:SER:HG	2.09	0.49
3:E:260:ASP:O	3:E:264:ARG:CA	2.60	0.49
5:F:769:GLN:HB3	5:F:772:ARG:HG2	1.95	0.49
3:E:1047:ARG:HE	3:E:1093:TRP:HZ2	1.60	0.49
1:B:401:SER:HB2	2:C:561:PRO:HA	1.93	0.49
1:B:1026:ASP:HB2	1:B:1031:PRO:HG3	1.95	0.49
2:C:66:ASP:OD2	2:C:107:HIS:ND1	2.43	0.49
2:C:850:PRO:HA	2:C:853:THR:HG22	1.95	0.49
3:E:1217:GLY:O	3:E:1221:ASN:ND2	2.45	0.49
5:F:786:PRO:O	5:F:789:SER:HB2	2.12	0.49
6:D:851:GLU:HA	6:D:854:ILE:HD12	1.95	0.49
1:B:26:GLN:OE1	1:B:28:TRP:NE1	2.40	0.49
2:C:1046:ARG:HD2	2:C:1066:HIS:HB2	1.94	0.49
3:E:245:PHE:HD2	3:E:285:LYS:HZ1	1.60	0.49
5:F:659:LEU:HD13	5:F:661:THR:HG22	1.93	0.49
6:D:1070:LEU:O	6:D:1073:GLN:NE2	2.38	0.49
3:E:331:ARG:HE	3:E:344:VAL:HG11	1.77	0.49
3:E:493:VAL:HG22	3:E:502:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1077:SER:O	3:E:1081:THR:OG1	2.22	0.49
1:B:716:LEU:HD21	1:B:721:LYS:HB3	1.93	0.49
2:C:1245:GLU:OE1	3:E:1205:SER:OG	2.30	0.49
3:E:1202:ALA:HB1	3:E:1205:SER:HB2	1.95	0.49
5:F:116:LYS:HG2	5:F:140:ARG:HG3	1.94	0.49
6:D:1158:PHE:O	6:D:1161:LEU:HB3	2.13	0.49
1:B:1173:PRO:HA	1:B:1180:PHE:HA	1.95	0.48
2:C:438:GLY:O	2:C:456:GLY:N	2.46	0.48
5:F:745:LYS:NZ	5:F:745:LYS:O	2.39	0.48
1:B:649:LEU:HD21	1:B:677:LEU:HD11	1.95	0.48
1:B:863:ARG:NH2	1:B:889:ASP:OD2	2.46	0.48
1:B:917:ALA:HB1	1:B:919:LYS:HE2	1.94	0.48
6:D:1194:ARG:O	6:D:1198:ALA:N	2.46	0.48
1:B:420:SER:HB2	1:B:436:ARG:HH21	1.78	0.48
5:F:770:TRP:HE3	5:F:788:ILE:HG22	1.77	0.48
6:D:327:VAL:HB	6:D:331:ARG:HH21	1.79	0.48
1:B:1:MET:HB3	1:B:325:PRO:HA	1.93	0.48
2:C:132:VAL:HB	2:C:134:LYS:HE3	1.94	0.48
2:C:767:MET:HE1	2:C:772:GLN:H	1.79	0.48
3:E:140:SER:HA	3:E:150:VAL:O	2.12	0.48
3:E:641:SER:OG	3:E:659:THR:OG1	2.31	0.48
5:F:837:GLU:OE2	5:F:840:ARG:NH1	2.46	0.48
1:B:493:SER:OG	1:B:494:GLU:N	2.46	0.48
1:B:577:ASN:OD1	1:B:578:LEU:N	2.46	0.48
1:B:1049:GLY:HA3	1:B:1166:ASP:HB2	1.95	0.48
3:E:495:ILE:HB	3:E:500:ILE:HD12	1.96	0.48
4:A:171:ARG:NE	6:D:1319:LEU:O	2.46	0.48
5:F:903:ILE:HD13	5:F:924:ILE:HG23	1.94	0.48
6:D:509:MET:SD	6:D:509:MET:N	2.86	0.48
2:C:817:HIS:HA	2:C:820:LEU:HD12	1.95	0.48
3:E:6:VAL:HG22	3:E:449:LEU:HG	1.95	0.48
3:E:855:LEU:HB2	3:E:858:PHE:HB2	1.94	0.48
6:D:389:ARG:HH22	6:D:422:GLN:HB3	1.78	0.48
1:B:1002:MET:HA	1:B:1005:GLN:HG3	1.95	0.48
2:C:969:GLY:O	2:C:1059:ASP:N	2.45	0.48
6:D:315:PHE:HB3	6:D:325:PRO:HG2	1.94	0.48
6:D:456:GLU:HA	6:D:459:ARG:HD2	1.96	0.48
6:D:1122:THR:O	6:D:1126:ARG:HG3	2.13	0.48
2:C:80:ASP:OD2	2:C:82:THR:OG1	2.31	0.48
3:E:669:ARG:HA	3:E:684:ASP:HA	1.96	0.48
6:D:798:PHE:O	6:D:801:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ASN:O	1:B:358:ASN:N	2.47	0.48
2:C:926:ILE:HG13	2:C:1213:LEU:HD13	1.94	0.48
2:C:1061:CYS:HB3	2:C:1066:HIS:H	1.79	0.48
6:D:1155:ARG:NH2	6:D:1159:GLU:OE2	2.46	0.48
1:B:934:ALA:HB1	1:B:941:LYS:HE3	1.95	0.48
2:C:202:TRP:NE1	2:C:226:PRO:O	2.42	0.48
5:F:469:SER:HB3	5:F:480:PRO:HB3	1.96	0.48
6:D:766:ILE:O	6:D:769:VAL:HB	2.13	0.48
2:C:36:SER:HB2	2:C:62:ILE:HG13	1.94	0.47
2:C:385:THR:OG1	2:C:388:ALA:O	2.31	0.47
2:C:433:VAL:O	2:C:440:VAL:HA	2.14	0.47
3:E:547:ARG:CZ	3:E:561:MET:H	2.27	0.47
3:E:604:PRO:O	3:E:606:ARG:NE	2.46	0.47
3:E:658:SER:OG	3:E:667:ASP:OD2	2.27	0.47
3:E:667:ASP:OD2	3:E:669:ARG:NH1	2.46	0.47
5:F:700:LEU:HD21	5:F:734:LEU:HD23	1.95	0.47
5:F:706:ILE:HG23	5:F:718:VAL:HG13	1.96	0.47
1:B:717:ASP:OD1	1:B:717:ASP:N	2.47	0.47
3:E:539:GLY:HA3	3:E:551:GLU:O	2.14	0.47
3:E:670:ILE:HG12	3:E:695:VAL:HG11	1.95	0.47
5:F:629:PRO:HB3	5:F:637:VAL:HG11	1.95	0.47
1:B:217:ALA:HB1	1:B:230:LEU:HB3	1.96	0.47
2:C:569:TYR:HD1	2:C:574:ASP:HB3	1.79	0.47
3:E:18:GLN:HG2	3:E:19:LEU:HG	1.96	0.47
5:F:614:SER:OG	5:F:617:ASP:OD1	2.32	0.47
6:D:1264:ARG:NH2	6:D:1535:GLN:OE1	2.46	0.47
1:B:620:LEU:HD12	1:B:676:LYS:HB3	1.97	0.47
1:B:849:ALA:HB2	1:B:872:VAL:HG11	1.95	0.47
6:D:525:THR:O	6:D:529:ARG:HG2	2.15	0.47
6:D:994:ASN:HB2	6:D:1000:LEU:HD22	1.96	0.47
6:D:1181:HIS:HA	6:D:1553:ASN:OD1	2.14	0.47
6:D:1257:THR:OG1	6:D:1259:GLN:OE1	2.25	0.47
1:B:116:ALA:HB1	1:B:157:TRP:HD1	1.79	0.47
3:E:69:THR:HG1	3:E:142:TRP:HD1	1.60	0.47
6:D:767:GLY:O	6:D:770:ILE:HG12	2.15	0.47
6:D:854:ILE:HD13	6:D:886:LYS:HZ1	1.78	0.47
6:D:1567:TYR:HD1	6:D:1572:LYS:HZ1	1.63	0.47
2:C:249:LEU:HD22	2:C:260:LEU:HD11	1.96	0.47
6:D:1437:VAL:HG22	6:D:1465:ARG:HH11	1.78	0.47
6:D:1633:MET:SD	6:D:1633:MET:N	2.87	0.47
5:F:331:LEU:HD21	5:F:345:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1000:LEU:HA	6:D:1003:LEU:HD23	1.96	0.47
6:D:1011:ARG:HA	6:D:1014:LEU:HD12	1.95	0.47
1:B:191:CYS:SG	1:B:229:GLN:NE2	2.88	0.47
3:E:650:GLN:HE21	3:E:712:TYR:HB2	1.80	0.47
5:F:388:ALA:N	5:F:400:GLY:O	2.47	0.47
3:E:962:VAL:HG12	3:E:966:ARG:HG3	1.97	0.47
6:D:802:ALA:O	6:D:805:GLN:HG3	2.15	0.47
2:C:247:VAL:O	2:C:260:LEU:N	2.44	0.47
1:B:26:GLN:HB2	1:B:28:TRP:CD1	2.49	0.46
1:B:1035:TYR:HD1	1:B:1038:ILE:HD12	1.80	0.46
2:C:77:GLY:HA3	2:C:102:ILE:HD11	1.97	0.46
3:E:693:ASN:HB2	3:E:720:TYR:HE2	1.80	0.46
3:E:897:ASN:HD21	3:E:899:ALA:HB3	1.80	0.46
3:E:1107:LEU:O	3:E:1111:ASN:ND2	2.33	0.46
6:D:374:HIS:O	6:D:377:ALA:N	2.37	0.46
6:D:1250:ILE:HD11	6:D:1317:LEU:HB3	1.96	0.46
1:B:469:ARG:HA	1:B:515:GLN:HG2	1.97	0.46
2:C:718:ASP:OD1	2:C:718:ASP:N	2.48	0.46
3:E:28:LEU:HD23	3:E:41:ILE:HD11	1.97	0.46
6:D:671:ASP:OD1	6:D:672:PHE:N	2.48	0.46
6:D:1123:THR:O	6:D:1127:MET:HG3	2.15	0.46
1:B:899:LYS:O	1:B:899:LYS:NZ	2.38	0.46
2:C:438:GLY:HA2	2:C:460:VAL:HG23	1.97	0.46
2:C:895:ARG:NH2	2:C:1255:PRO:O	2.42	0.46
6:D:529:ARG:O	6:D:533:GLN:N	2.48	0.46
2:C:106:ALA:HB3	2:C:115:ALA:HB3	1.96	0.46
2:C:246:LYS:HG2	2:C:262:SER:HA	1.98	0.46
2:C:441:MET:SD	2:C:452:LEU:HA	2.55	0.46
2:C:505:ASN:OD1	2:C:508:VAL:N	2.36	0.46
3:E:541:ILE:HB	3:E:573:MET:HE1	1.98	0.46
5:F:387:PRO:HB3	5:F:399:ALA:HB1	1.97	0.46
6:D:374:HIS:O	6:D:376:ALA:N	2.48	0.46
1:B:869:CYS:HA	1:B:872:VAL:HG12	1.96	0.46
1:B:882:ALA:HA	1:B:887:LEU:HD12	1.97	0.46
2:C:573:ARG:HB3	2:C:603:ARG:HH12	1.81	0.46
2:C:1083:PHE:HD2	2:C:1190:ALA:HB2	1.80	0.46
1:B:168:THR:HG1	1:B:172:GLU:H	1.63	0.46
1:B:794:SER:OG	1:B:795:LYS:NZ	2.49	0.46
2:C:125:TRP:HZ3	2:C:130:PRO:HA	1.81	0.46
5:F:160:ASP:OD1	5:F:160:ASP:N	2.38	0.46
5:F:533:PHE:CD1	5:F:573:VAL:HB	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:645:LEU:HD21	6:D:664:LEU:HA	1.97	0.46
6:D:1094:ASP:OD1	6:D:1096:SER:OG	2.34	0.46
1:B:106:ASN:N	1:B:106:ASN:OD1	2.48	0.46
1:B:997:TYR:CZ	1:B:1000:LEU:HD23	2.51	0.46
2:C:1218:ARG:HH21	2:C:1220:TYR:HH	1.61	0.46
3:E:1:MET:O	3:E:693:ASN:ND2	2.44	0.46
3:E:470:ASP:HA	3:E:490:VAL:HG23	1.97	0.46
5:F:788:ILE:H	5:F:788:ILE:HG13	1.52	0.46
6:D:770:ILE:O	6:D:773:GLN:HB2	2.15	0.46
6:D:1462:VAL:O	6:D:1465:ARG:NH2	2.49	0.46
1:B:1231:ASN:HB3	1:B:1236:HIS:HA	1.98	0.46
2:C:774:GLU:O	2:C:778:LYS:NZ	2.44	0.46
2:C:1009:LEU:HD11	2:C:1014:LEU:HD11	1.98	0.46
2:C:1241:ALA:HB1	3:E:1204:ARG:HD3	1.97	0.46
5:F:570:GLN:HA	5:F:587:ASP:HB3	1.98	0.46
1:B:466:ASP:OD2	1:B:479:ARG:NH1	2.47	0.46
1:B:768:GLU:N	1:B:768:GLU:OE1	2.49	0.46
2:C:190:ARG:NH1	2:C:195:ASP:OD1	2.49	0.46
3:E:254:ILE:HD11	3:E:268:THR:HB	1.98	0.46
3:E:832:LEU:HD23	3:E:850:ILE:HD11	1.98	0.46
5:F:535:ASN:OD1	5:F:539:THR:N	2.45	0.46
6:D:321:CYS:O	6:D:323:ILE:N	2.43	0.46
6:D:997:ASP:OD1	6:D:1000:LEU:N	2.46	0.46
2:C:1078:LEU:HD13	2:C:1229:VAL:HG13	1.98	0.46
3:E:1223:ALA:O	3:E:1226:SER:OG	2.26	0.46
5:F:633:PHE:O	5:F:636:THR:OG1	2.32	0.46
6:D:452:LYS:HE2	6:D:481:GLN:HG2	1.96	0.46
1:B:614:LEU:HD12	1:B:624:THR:HB	1.98	0.45
1:B:684:HIS:O	1:B:688:GLN:HG3	2.16	0.45
1:B:1205:ILE:HG21	1:B:1211:ALA:HB2	1.98	0.45
5:F:449:THR:OG1	5:F:461:VAL:O	2.31	0.45
1:B:808:LYS:O	1:B:812:ILE:HG12	2.16	0.45
1:B:1004:GLN:NE2	4:A:182:CYS:O	2.49	0.45
2:C:837:LEU:HG	2:C:847:VAL:HG21	1.98	0.45
1:B:483:THR:OG1	1:B:485:ASP:OD1	2.33	0.45
2:C:43:VAL:HB	2:C:53:HIS:HB2	1.97	0.45
2:C:231:TYR:HB3	2:C:235:GLY:HA2	1.97	0.45
6:D:753:LEU:HD22	6:D:773:GLN:HG2	1.98	0.45
1:B:114:ASP:HB3	1:B:155:VAL:HG12	1.97	0.45
2:C:967:LEU:HB3	2:C:985:ILE:HD13	1.97	0.45
3:E:33:TRP:HE1	3:E:40:LEU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1229:GLU:O	3:E:1233:LEU:HB2	2.17	0.45
6:D:1634:ASP:OD1	6:D:1634:ASP:N	2.50	0.45
3:E:879:TYR:CZ	3:E:887:GLU:HB3	2.51	0.45
5:F:100:CYS:SG	5:F:101:PHE:N	2.90	0.45
5:F:473:ASP:N	5:F:473:ASP:OD1	2.47	0.45
6:D:967:LEU:O	6:D:971:VAL:HG13	2.17	0.45
1:B:664:GLU:O	1:B:667:GLU:HG3	2.16	0.45
1:B:835:LEU:HD12	1:B:835:LEU:H	1.82	0.45
2:C:149:ASN:OD1	2:C:190:ARG:NH2	2.49	0.45
2:C:401:ASP:OD1	2:C:405:ASN:N	2.50	0.45
2:C:799:ARG:HE	2:C:800:LYS:HZ3	1.65	0.45
3:E:4:PHE:CD1	3:E:449:LEU:HB3	2.52	0.45
3:E:1215:GLN:OE1	3:E:1218:VAL:N	2.43	0.45
1:B:18:THR:OG1	1:B:68:VAL:O	2.32	0.45
1:B:105:ASN:OD1	1:B:106:ASN:N	2.50	0.45
1:B:940:LEU:O	1:B:943:LYS:NZ	2.47	0.45
2:C:508:VAL:HB	2:C:511:ASN:ND2	2.31	0.45
3:E:456:ARG:HD2	3:E:824:VAL:HG22	1.99	0.45
3:E:551:GLU:HB3	3:E:555:LEU:HA	1.98	0.45
3:E:844:ASN:HD22	3:E:847:ASP:HB2	1.82	0.45
3:E:863:SER:HB3	3:E:866:ASP:HB2	1.98	0.45
6:D:755:GLU:HG2	6:D:759:LYS:HE2	1.97	0.45
6:D:1308:HIS:O	6:D:1312:ARG:HG2	2.17	0.45
2:C:1172:LEU:HD12	2:C:1173:GLN:HG3	1.99	0.45
6:D:516:TRP:HA	6:D:520:GLY:HA3	1.97	0.45
6:D:527:VAL:O	6:D:531:LEU:N	2.41	0.45
3:E:815:PRO:HD2	3:E:856:ARG:HH22	1.82	0.45
5:F:36:LYS:HD2	5:F:38:ARG:HE	1.81	0.45
6:D:451:ASP:O	6:D:455:THR:OG1	2.25	0.45
6:D:1085:GLU:HA	6:D:1088:ARG:NH2	2.32	0.45
2:C:481:LEU:HD12	2:C:499:VAL:HG11	1.98	0.45
2:C:1232:CYS:SG	2:C:1244:TYR:OH	2.64	0.45
3:E:933:LEU:HD21	3:E:951:LEU:HA	1.98	0.45
4:A:167:LEU:HA	4:A:170:MET:HG2	1.99	0.45
5:F:721:LEU:HD23	5:F:724:ILE:HD11	1.98	0.45
6:D:1106:GLN:HB3	6:D:1110:ARG:NH2	2.32	0.45
6:D:1135:ALA:O	6:D:1139:ILE:HG22	2.16	0.45
6:D:1541:ASP:HA	6:D:1544:PHE:HB3	1.98	0.45
1:B:578:LEU:HG	1:B:590:VAL:HG22	1.98	0.44
3:E:501:ALA:HA	3:E:510:PHE:HA	1.99	0.44
6:D:1038:CYS:SG	6:D:1090:ALA:HA	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:HB3	1:B:320:PHE:HB2	1.98	0.44
1:B:146:ARG:NH2	1:B:180:SER:O	2.50	0.44
1:B:378:CYS:SG	1:B:379:VAL:N	2.89	0.44
1:B:1179:SER:O	1:B:1181:ASN:ND2	2.50	0.44
3:E:536:HIS:HB2	3:E:575:ILE:HD13	1.99	0.44
5:F:36:LYS:HG3	5:F:38:ARG:HG2	1.97	0.44
6:D:812:THR:O	6:D:815:HIS:NE2	2.50	0.44
6:D:1109:TYR:CG	6:D:1140:LEU:HD11	2.53	0.44
6:D:1309:ASP:HA	6:D:1312:ARG:HG2	1.98	0.44
6:D:1531:TYR:O	6:D:1534:THR:OG1	2.28	0.44
1:B:897:TYR:OH	1:B:909:GLU:OE2	2.29	0.44
2:C:177:ARG:NH1	2:C:209:TYR:OH	2.49	0.44
3:E:1213:MET:HB2	3:E:1215:GLN:HB2	1.99	0.44
6:D:587:VAL:HA	6:D:590:LYS:HB3	1.99	0.44
6:D:769:VAL:O	6:D:772:ALA:HB3	2.18	0.44
6:D:1239:ASN:OD1	6:D:1242:CYS:N	2.50	0.44
2:C:379:CYS:HA	2:C:393:ASN:HB2	2.00	0.44
3:E:568:GLY:HA3	3:E:586:LYS:NZ	2.31	0.44
3:E:1076:GLN:HA	3:E:1079:PHE:HD2	1.83	0.44
1:B:363:LYS:NZ	1:B:400:GLY:O	2.33	0.44
2:C:884:LEU:HB3	2:C:900:TYR:CE2	2.53	0.44
6:D:1311:ILE:HD13	6:D:1339:THR:HA	1.99	0.44
1:B:408:ILE:HG22	1:B:410:MET:HG3	2.00	0.44
1:B:675:LYS:NZ	1:B:701:CYS:O	2.51	0.44
1:B:710:VAL:HA	1:B:713:VAL:HG22	2.00	0.44
1:B:1213:GLN:NE2	1:B:1214:CYS:O	2.42	0.44
2:C:319:GLN:O	2:C:323:ASP:CA	2.65	0.44
2:C:472:LEU:HB2	2:C:486:LEU:HD11	1.99	0.44
2:C:872:LYS:HA	2:C:872:LYS:HD3	1.90	0.44
3:E:258:LEU:HD23	3:E:258:LEU:HA	1.87	0.44
3:E:1020:ILE:HD11	3:E:1036:ILE:HB	1.99	0.44
6:D:590:LYS:O	6:D:590:LYS:NZ	2.40	0.44
6:D:878:LEU:HD21	6:D:890:TYR:CD2	2.53	0.44
6:D:1059:MET:SD	6:D:1059:MET:N	2.91	0.44
2:C:380:SER:N	2:C:392:SER:O	2.49	0.44
3:E:254:ILE:HD12	3:E:254:ILE:HA	1.78	0.44
6:D:354:LYS:HE3	6:D:383:ARG:HD2	2.00	0.44
6:D:413:ARG:H	6:D:413:ARG:HD2	1.83	0.44
6:D:962:ILE:HA	6:D:965:TYR:HD2	1.83	0.44
1:B:502:GLU:HB2	1:B:525:ARG:HH21	1.82	0.43
1:B:720:LYS:HB3	1:B:720:LYS:HE3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:LYS:HA	2:C:277:LYS:HD3	1.88	0.43
2:C:531:TYR:HB2	2:C:564:HIS:CD2	2.53	0.43
3:E:248:VAL:HG12	3:E:286:GLY:HA3	1.98	0.43
5:F:687:GLN:OE1	5:F:687:GLN:N	2.44	0.43
6:D:840:LEU:O	6:D:843:ALA:HB3	2.18	0.43
1:B:114:ASP:OD1	1:B:115:PHE:N	2.50	0.43
1:B:600:ASN:OD1	1:B:601:HIS:ND1	2.43	0.43
3:E:546:ASN:ND2	3:E:568:GLY:O	2.51	0.43
6:D:870:LEU:O	6:D:874:VAL:HG23	2.18	0.43
1:B:443:ASP:OD1	1:B:446:ASP:N	2.43	0.43
2:C:21:VAL:HG23	2:C:286:GLY:HA2	2.00	0.43
2:C:390:ILE:HG13	2:C:399:MET:HG3	2.00	0.43
6:D:356:ASN:HD21	6:D:358:GLU:HB3	1.83	0.43
6:D:606:MET:HA	6:D:609:GLN:HB3	2.00	0.43
6:D:1594:VAL:HA	6:D:1597:LYS:HB2	2.00	0.43
1:B:251:ILE:HA	1:B:261:ALA:O	2.19	0.43
1:B:475:THR:OG1	1:B:476:MET:N	2.51	0.43
2:C:1:MET:SD	2:C:296:SER:OG	2.71	0.43
3:E:260:ASP:O	3:E:264:ARG:HA	2.17	0.43
6:D:475:VAL:HG13	6:D:487:ALA:HA	2.00	0.43
1:B:685:THR:HB	1:B:690:ASP:HB3	1.99	0.43
3:E:330:ASP:HA	3:E:352:LEU:O	2.17	0.43
6:D:765:GLN:HA	6:D:798:PHE:CE2	2.54	0.43
2:C:917:PRO:HG2	2:C:922:LYS:HE3	2.00	0.43
2:C:1175:VAL:HG11	2:C:1188:PHE:HE1	1.84	0.43
3:E:1093:TRP:NE1	3:E:1105:GLU:OE2	2.43	0.43
3:E:1103:VAL:HG11	3:E:1126:LEU:HD21	2.01	0.43
5:F:925:ILE:HA	5:F:928:TYR:HB3	2.00	0.43
6:D:292:LEU:HA	6:D:295:VAL:HB	1.98	0.43
6:D:306:LYS:O	6:D:306:LYS:NZ	2.52	0.43
6:D:777:ALA:HB3	6:D:785:SER:HB2	2.01	0.43
6:D:1523:GLU:O	6:D:1527:LEU:HG	2.18	0.43
6:D:1579:CYS:HA	6:D:1582:LYS:HD2	2.00	0.43
1:B:22:TRP:CZ2	1:B:304:GLU:HG3	2.53	0.43
3:E:1107:LEU:HG	3:E:1122:ILE:HG21	2.00	0.43
6:D:1145:TYR:CD2	6:D:1154:ALA:HB2	2.54	0.43
1:B:928:ALA:O	1:B:932:LYS:HG2	2.19	0.43
2:C:884:LEU:HD23	2:C:884:LEU:HA	1.86	0.43
3:E:252:GLU:N	3:E:252:GLU:OE1	2.52	0.43
3:E:885:MET:HE1	3:E:908:CYS:HA	2.00	0.43
3:E:1179:PHE:O	3:E:1182:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:757:ALA:HA	6:D:766:ILE:HD11	2.00	0.43
6:D:805:GLN:HA	6:D:808:LYS:HD2	2.01	0.43
4:A:171:ARG:HH11	6:D:1322:PRO:HA	1.84	0.43
5:F:161:PRO:HD3	5:F:181:VAL:HG22	1.99	0.43
6:D:1617:ARG:O	6:D:1617:ARG:NE	2.52	0.43
3:E:246:PRO:O	3:E:285:LYS:NZ	2.50	0.43
3:E:837:LYS:HB3	3:E:840:GLY:HA3	2.01	0.43
5:F:348:LEU:HD11	5:F:386:ASP:HB3	2.01	0.43
5:F:822:SER:O	5:F:826:SER:OG	2.26	0.43
1:B:5:LEU:HD23	1:B:5:LEU:HA	1.89	0.42
1:B:376:ASP:OD1	1:B:376:ASP:N	2.52	0.42
1:B:1016:LEU:HD11	1:B:1045:VAL:HG11	2.01	0.42
2:C:569:TYR:HB3	2:C:578:ALA:HB2	1.99	0.42
5:F:574:LEU:HD23	5:F:574:LEU:HA	1.73	0.42
1:B:835:LEU:O	1:B:839:LEU:HG	2.19	0.42
2:C:381:LEU:HD13	2:C:419:MET:HB2	2.01	0.42
2:C:393:ASN:O	2:C:396:ARG:HG3	2.18	0.42
5:F:533:PHE:CG	5:F:573:VAL:HB	2.53	0.42
6:D:836:SER:HA	6:D:839:GLU:HG2	2.00	0.42
6:D:1135:ALA:HB2	6:D:1168:HIS:CE1	2.47	0.42
6:D:1193:GLU:O	6:D:1197:ALA:N	2.44	0.42
1:B:353:TRP:NE1	1:B:358:ASN:HA	2.28	0.42
1:B:532:ASN:OD1	1:B:537:GLN:N	2.39	0.42
1:B:577:ASN:ND2	1:B:614:LEU:H	2.17	0.42
2:C:350:GLU:OE2	2:C:376:ARG:NH2	2.53	0.42
2:C:909:GLY:HA3	2:C:1211:GLY:HA3	2.01	0.42
2:C:951:GLN:NE2	3:E:1031:THR:O	2.53	0.42
3:E:456:ARG:HB2	3:E:824:VAL:HG13	2.00	0.42
5:F:25:PRO:HG3	5:F:106:GLN:HE22	1.84	0.42
6:D:586:VAL:O	6:D:590:LYS:N	2.38	0.42
1:B:212:ARG:CZ	1:B:346:VAL:HA	2.50	0.42
2:C:121:ASP:OD1	2:C:121:ASP:N	2.51	0.42
2:C:1226:ASP:OD1	2:C:1226:ASP:N	2.51	0.42
3:E:165:LYS:HE3	3:E:172:VAL:HG11	2.01	0.42
4:A:199:LEU:HA	4:A:202:LEU:HG	2.00	0.42
5:F:372:LEU:HD13	5:F:372:LEU:HA	1.83	0.42
5:F:600:SER:HA	5:F:699:MET:HA	2.02	0.42
6:D:508:SER:HB2	6:D:534:ALA:HB2	2.02	0.42
1:B:80:LEU:HB3	1:B:92:TRP:HB2	2.00	0.42
1:B:614:LEU:HD12	1:B:614:LEU:HA	1.87	0.42
1:B:1027:ASP:OD1	1:B:1027:ASP:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:304:SER:HG	3:E:307:THR:HG1	1.57	0.42
3:E:357:LEU:HD12	3:E:368:VAL:HA	2.00	0.42
3:E:911:SER:OG	3:E:912:GLY:N	2.52	0.42
3:E:1011:GLU:OE2	3:E:1035:ARG:NH1	2.37	0.42
6:D:1150:ARG:O	6:D:1150:ARG:NH1	2.46	0.42
2:C:238:ILE:HG23	2:C:250:PHE:HB2	2.02	0.42
2:C:954:PRO:HB2	3:E:1099:ARG:HH11	1.84	0.42
3:E:346:LEU:HD23	3:E:346:LEU:H	1.85	0.42
6:D:1562:GLU:HA	6:D:1565:LEU:HD12	2.00	0.42
2:C:2:HIS:HE1	2:C:4:SER:HB2	1.84	0.42
3:E:1081:THR:O	3:E:1085:GLN:NE2	2.35	0.42
6:D:534:ALA:HA	6:D:537:ALA:HB3	2.02	0.42
1:B:3:VAL:HG21	1:B:280:PHE:CE1	2.54	0.42
1:B:168:THR:OG1	1:B:172:GLU:N	2.50	0.42
2:C:146:TRP:CE2	2:C:153:LEU:HD13	2.54	0.42
2:C:309:ARG:HD3	2:C:334:VAL:HG13	2.02	0.42
3:E:541:ILE:HG12	3:E:550:PHE:CD1	2.54	0.42
3:E:547:ARG:NE	3:E:560:GLN:HA	2.32	0.42
3:E:574:ASP:O	3:E:580:LEU:HA	2.20	0.42
6:D:1012:ARG:HH21	6:D:1016:HIS:CD2	2.37	0.42
6:D:1345:LEU:HD21	6:D:1452:ILE:HG13	2.02	0.42
1:B:699:ILE:HD12	1:B:699:ILE:HA	1.93	0.42
1:B:1059:GLU:OE2	1:B:1149:ARG:NH2	2.53	0.42
2:C:909:GLY:HA2	2:C:1213:LEU:HG	2.02	0.42
3:E:112:VAL:HA	3:E:115:ILE:HG12	2.01	0.42
3:E:510:PHE:HE1	3:E:526:VAL:HG23	1.85	0.42
3:E:808:LEU:HD23	3:E:808:LEU:HA	1.82	0.42
3:E:1231:LEU:HD13	3:E:1231:LEU:HA	1.86	0.42
6:D:558:ALA:HA	6:D:561:ALA:HB3	2.02	0.42
6:D:972:LEU:HB2	6:D:999:ALA:HB2	2.01	0.42
6:D:1221:ASN:N	6:D:1221:ASN:OD1	2.52	0.42
1:B:118:ASN:HD21	1:B:122:THR:H	1.67	0.42
2:C:305:GLN:NE2	2:C:339:THR:HG21	2.34	0.42
6:D:404:LEU:HD13	6:D:440:GLY:HA2	2.02	0.42
6:D:523:GLU:HB3	6:D:526:ALA:HB3	2.02	0.42
6:D:1005:THR:O	6:D:1009:LEU:HG	2.19	0.42
6:D:1573:HIS:CD2	6:D:1601:ASN:HA	2.51	0.42
1:B:1174:CYS:N	1:B:1179:SER:O	2.50	0.41
2:C:626:LEU:O	2:C:629:ARG:NH2	2.53	0.41
5:F:116:LYS:HA	5:F:140:ARG:HA	2.02	0.41
5:F:796:LEU:HD12	5:F:805:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1511:ILE:HA	6:D:1514:LEU:HD12	2.01	0.41
2:C:249:LEU:HD12	2:C:249:LEU:HA	1.90	0.41
3:E:501:ALA:HB2	3:E:535:ILE:HD12	2.02	0.41
1:B:484:ASN:OD1	1:B:484:ASN:N	2.53	0.41
1:B:596:MET:HE1	1:B:645:PHE:CD2	2.55	0.41
3:E:711:GLU:HG3	3:E:828:ILE:HD12	2.00	0.41
6:D:331:ARG:O	6:D:335:GLN:HG2	2.20	0.41
6:D:607:GLU:HA	6:D:610:LEU:HD23	2.02	0.41
6:D:777:ALA:O	6:D:781:ASP:N	2.47	0.41
3:E:1030:SER:HB2	3:E:1088:GLU:HB2	2.02	0.41
5:F:707:ARG:O	5:F:707:ARG:NH1	2.53	0.41
6:D:1235:LEU:HD12	6:D:1236:PRO:HA	2.02	0.41
3:E:467:ILE:HD12	3:E:845:ALA:HB1	2.02	0.41
5:F:502:LEU:HD12	5:F:511:VAL:HG22	2.03	0.41
5:F:799:ARG:HA	5:F:799:ARG:HD3	1.84	0.41
6:D:1433:LEU:HD22	6:D:1434:GLN:HE21	1.86	0.41
6:D:1625:TYR:HA	6:D:1626:PRO:HD3	1.94	0.41
1:B:1149:ARG:HA	1:B:1150:PRO:HD3	1.95	0.41
6:D:1353:LEU:HD23	6:D:1353:LEU:HA	1.83	0.41
6:D:510:LEU:HD13	6:D:510:LEU:HA	1.91	0.41
1:B:872:VAL:HG13	1:B:874:MET:HG2	2.01	0.41
2:C:397:ILE:HD13	2:C:410:TRP:HB2	2.03	0.41
3:E:222:ASP:HB3	3:E:223:ASP:H	1.65	0.41
3:E:638:LEU:HB3	3:E:639:GLU:H	1.61	0.41
3:E:668:THR:O	3:E:685:PHE:N	2.37	0.41
6:D:376:ALA:O	6:D:380:ARG:HG2	2.21	0.41
6:D:1189:LYS:HZ3	6:D:1189:LYS:HG2	1.79	0.41
6:D:1228:ARG:H	6:D:1228:ARG:HG3	1.68	0.41
6:D:1260:ASP:OD1	6:D:1261:LEU:N	2.41	0.41
1:B:538:LEU:HD21	1:B:540:VAL:HG23	2.03	0.41
1:B:688:GLN:HG3	1:B:688:GLN:H	1.77	0.41
1:B:763:VAL:HA	1:B:766:VAL:HG12	2.03	0.41
1:B:1049:GLY:O	1:B:1052:SER:OG	2.29	0.41
2:C:483:VAL:HG13	2:C:494:PHE:H	1.86	0.41
2:C:714:LEU:HB3	2:C:716:MET:SD	2.61	0.41
2:C:837:LEU:HD23	2:C:837:LEU:HA	1.93	0.41
2:C:964:ALA:HB1	2:C:989:LEU:HB2	2.03	0.41
2:C:1038:ASP:OD1	2:C:1038:ASP:N	2.54	0.41
3:E:528:THR:OG1	3:E:543:VAL:O	2.32	0.41
3:E:971:TYR:CE2	3:E:994:PHE:HB3	2.56	0.41
4:A:198:LEU:O	4:A:201:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:491:LEU:HA	5:F:505:THR:HA	2.02	0.41
6:D:1612:ILE:O	6:D:1616:LYS:HG2	2.21	0.41
2:C:350:GLU:HG3	2:C:376:ARG:HE	1.86	0.41
2:C:879:ARG:HH12	3:E:969:LYS:HE2	1.86	0.41
2:C:1035:LYS:HA	2:C:1035:LYS:HD2	1.86	0.41
3:E:188:VAL:HG21	3:E:228:LEU:HD23	2.02	0.41
3:E:1212:LYS:HE3	3:E:1212:LYS:HB3	1.76	0.41
6:D:405:VAL:HG13	6:D:553:TYR:HD2	1.86	0.41
6:D:1141:LEU:HD23	6:D:1141:LEU:HA	1.76	0.41
6:D:1169:TYR:O	6:D:1173:VAL:HG23	2.20	0.41
2:C:82:THR:HG22	2:C:97:GLN:HB3	2.03	0.40
2:C:903:HIS:NE2	2:C:1257:CYS:O	2.41	0.40
2:C:951:GLN:HB3	2:C:953:LEU:HD13	2.02	0.40
2:C:1270:LYS:H	2:C:1270:LYS:HG3	1.66	0.40
3:E:1051:MET:HG2	3:E:1109:PHE:HZ	1.86	0.40
5:F:501:PHE:HB2	5:F:514:LEU:HD21	2.04	0.40
6:D:740:GLN:HB2	6:D:749:ALA:HB2	2.03	0.40
6:D:960:GLU:O	6:D:963:ASN:HB2	2.21	0.40
6:D:1106:GLN:HB3	6:D:1110:ARG:CZ	2.50	0.40
1:B:45:GLY:O	1:B:50:GLN:NE2	2.37	0.40
2:C:692:ASN:OD1	2:C:693:ASP:N	2.54	0.40
3:E:940:TYR:HD2	3:E:946:VAL:HG21	1.86	0.40
6:D:415:ASP:OD1	6:D:415:ASP:N	2.53	0.40
6:D:438:LEU:HD23	6:D:438:LEU:HA	1.94	0.40
6:D:641:PRO:HD3	6:D:670:LEU:HD21	2.03	0.40
6:D:811:LEU:HG	6:D:812:THR:HG23	2.04	0.40
6:D:1440:PRO:HB3	6:D:1466:LEU:HD11	2.03	0.40
1:B:175:VAL:HG21	1:B:234:ILE:HD12	2.03	0.40
1:B:399:ILE:HG23	2:C:587:ALA:HA	2.03	0.40
2:C:6:ARG:NH1	2:C:47:SER:O	2.37	0.40
2:C:1027:LEU:HD21	5:F:556:VAL:HA	2.04	0.40
3:E:564:THR:N	3:E:567:GLU:OE1	2.44	0.40
6:D:312:ASP:OD1	6:D:329:LYS:NZ	2.45	0.40
6:D:493:LEU:HD13	6:D:493:LEU:HA	1.97	0.40
6:D:891:TYR:HD1	6:D:891:TYR:HA	1.74	0.40
6:D:1628:ILE:HD13	6:D:1628:ILE:HA	1.96	0.40
1:B:177:ASP:HB2	1:B:184:LEU:HD11	2.02	0.40
1:B:276:ILE:HD12	1:B:298:CYS:HB3	2.03	0.40
1:B:1223:GLU:HA	1:B:1226:VAL:HG12	2.03	0.40
2:C:563:ALA:HA	2:C:566:LEU:HB3	2.04	0.40
2:C:1014:LEU:HD13	2:C:1022:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:314:SER:OG	3:E:326:GLY:O	2.39	0.40
5:F:594:PHE:CZ	5:F:608:SER:HB3	2.57	0.40
5:F:764:ARG:HD3	5:F:764:ARG:HA	1.94	0.40
5:F:766:ASP:N	5:F:766:ASP:OD1	2.52	0.40
6:D:594:HIS:CE1	6:D:595:LEU:HG	2.57	0.40
6:D:761:ARG:HD2	6:D:761:ARG:HA	1.90	0.40
6:D:1162:LEU:HD23	6:D:1162:LEU:HA	1.89	0.40
6:D:1607:GLN:HB2	6:D:1610:LYS:NZ	2.36	0.40
1:B:73:TRP:CH2	1:B:80:LEU:HD12	2.57	0.40
1:B:856:PHE:HA	1:B:859:ALA:HB3	2.04	0.40
2:C:457:THR:OG1	2:C:458:ALA:N	2.55	0.40
2:C:800:LYS:HA	2:C:800:LYS:HD3	1.89	0.40
2:C:1232:CYS:SG	2:C:1254:CYS:HB2	2.61	0.40
3:E:3:LEU:HG	3:E:454:ARG:HG2	2.04	0.40
3:E:1194:LEU:HD21	3:E:1218:VAL:HG11	2.03	0.40
5:F:841:GLN:HG2	5:F:868:PHE:CD1	2.57	0.40
6:D:733:TYR:OH	6:D:753:LEU:HA	2.22	0.40
6:D:835:GLN:H	6:D:835:GLN:HG3	1.69	0.40
6:D:1591:ASP:OD2	6:D:1593:ASP:N	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	B	1126/1247 (90%)	1091 (97%)	35 (3%)	0	100	100
2	C	1173/1292 (91%)	1119 (95%)	54 (5%)	0	100	100
3	E	1064/1654 (64%)	1023 (96%)	41 (4%)	0	100	100
4	A	51/368 (14%)	45 (88%)	6 (12%)	0	100	100
5	F	907/1376 (66%)	865 (95%)	42 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	1164/1642 (71%)	1118 (96%)	46 (4%)	0	100	100
All	All	5485/7579 (72%)	5261 (96%)	224 (4%)	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	B	960/1046 (92%)	926 (96%)	34 (4%)	36	67
2	C	1014/1094 (93%)	986 (97%)	28 (3%)	43	72
3	E	903/1373 (66%)	862 (96%)	41 (4%)	27	61
4	A	50/288 (17%)	47 (94%)	3 (6%)	19	52
5	F	779/1177 (66%)	763 (98%)	16 (2%)	53	79
6	D	971/1320 (74%)	910 (94%)	61 (6%)	18	51
All	All	4677/6298 (74%)	4494 (96%)	183 (4%)	36	64

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	58	SER
1	B	111	ARG
1	B	163	SER
1	B	211	GLU
1	B	356	ASN
1	B	382	SER
1	B	388	GLN
1	B	415	TYR
1	B	469	ARG
1	B	483	THR
1	B	511	LEU
1	B	533	CYS
1	B	595	ARG

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Mol	Chain	Res	Type
1	B	617	PHE
1	B	624	THR
1	B	668	PHE
1	B	680	LEU
1	B	687	PHE
1	B	688	GLN
1	B	693	TYR
1	B	695	GLU
1	B	720	LYS
1	B	839	LEU
1	B	874	MET
1	B	907	LEU
1	B	927	LEU
1	B	999	PHE
1	B	1002	MET
1	B	1044	LEU
1	B	1047	ASN
1	B	1055	PHE
1	B	1149	ARG
1	B	1187	ARG
1	B	1230	ARG
2	C	6	ARG
2	C	247	VAL
2	C	275	ARG
2	C	305	GLN
2	C	312	MET
2	C	322	VAL
2	C	358	PHE
2	C	432	LEU
2	C	435	LEU
2	C	436	ASN
2	C	475	ILE
2	C	481	LEU
2	C	512	ILE
2	C	514	PHE
2	C	542	PHE
2	C	558	LEU
2	C	584	LEU
2	C	620	VAL
2	C	716	MET
2	C	760	TYR
2	C	775	LYS

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Mol	Chain	Res	Type
2	C	779	MET
2	C	908	TYR
2	C	999	VAL
2	C	1056	MET
2	C	1096	ARG
2	C	1174	TYR
2	C	1269	MET
3	E	7	ASN
3	E	41	ILE
3	E	50	THR
3	E	66	THR
3	E	68	LEU
3	E	150	VAL
3	E	277	VAL
3	E	322	VAL
3	E	325	PHE
3	E	380	HIS
3	E	381	HIS
3	E	437	VAL
3	E	446	LEU
3	E	482	CYS
3	E	499	ASN
3	E	500	ILE
3	E	546	ASN
3	E	591	LEU
3	E	600	GLN
3	E	606	ARG
3	E	841	ASP
3	E	874	MET
3	E	878	TYR
3	E	879	TYR
3	E	889	TYR
3	E	942	ASP
3	E	967	LYS
3	E	970	ARG
3	E	989	ARG
3	E	990	HIS
3	E	1040	THR
3	E	1086	ASN
3	E	1090	LEU
3	E	1165	ASP
3	E	1174	VAL

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Mol	Chain	Res	Type
3	E	1197	TYR
3	E	1212	LYS
3	E	1224	MET
3	E	1232	MET
3	E	1234	GLU
3	E	1237	MET
4	A	191	VAL
4	A	193	TRP
4	A	200	VAL
5	F	266	LEU
5	F	361	PHE
5	F	394	MET
5	F	401	VAL
5	F	450	ASP
5	F	522	THR
5	F	678	TRP
5	F	690	GLU
5	F	702	VAL
5	F	707	ARG
5	F	749	ASN
5	F	806	LEU
5	F	814	ARG
5	F	833	GLU
5	F	839	CYS
5	F	849	ARG
6	D	339	TRP
6	D	400	HIS
6	D	423	PHE
6	D	439	CYS
6	D	469	ASP
6	D	474	THR
6	D	510	LEU
6	D	517	HIS
6	D	518	ARG
6	D	568	TYR
6	D	573	ARG
6	D	593	ARG
6	D	597	PHE
6	D	612	LEU
6	D	617	PHE
6	D	644	PHE
6	D	657	THR

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Mol	Chain	Res	Type
6	D	670	LEU
6	D	679	LEU
6	D	682	LEU
6	D	688	LYS
6	D	733	TYR
6	D	835	GLN
6	D	893	ASP
6	D	905	ARG
6	D	918	ILE
6	D	957	THR
6	D	969	TYR
6	D	974	ASP
6	D	994	ASN
6	D	1003	LEU
6	D	1008	SER
6	D	1017	GLN
6	D	1029	GLU
6	D	1034	MET
6	D	1045	CYS
6	D	1059	MET
6	D	1110	ARG
6	D	1156	ASN
6	D	1158	PHE
6	D	1165	THR
6	D	1172	LEU
6	D	1189	LYS
6	D	1221	ASN
6	D	1227	LEU
6	D	1253	TYR
6	D	1257	THR
6	D	1264	ARG
6	D	1307	LEU
6	D	1327	GLU
6	D	1356	ILE
6	D	1431	PHE
6	D	1435	CYS
6	D	1472	ILE
6	D	1473	THR
6	D	1538	ARG
6	D	1539	LEU
6	D	1578	GLN
6	D	1591	ASP

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Mol	Chain	Res	Type
6	D	1610	LYS
6	D	1624	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	106	ASN
1	B	108	ASN
1	B	229	GLN
1	B	824	GLN
3	E	183	GLN
3	E	600	GLN
6	D	511	ASN
6	D	540	GLN
6	D	1578	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

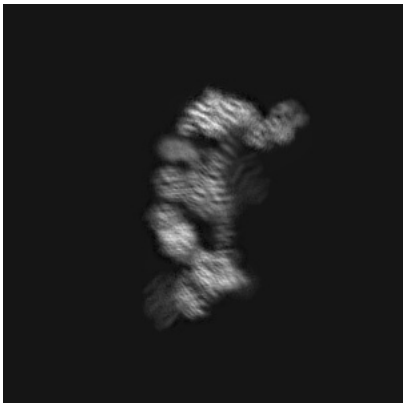
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28866. These allow visual inspection of the internal detail of the map and identification of artifacts.

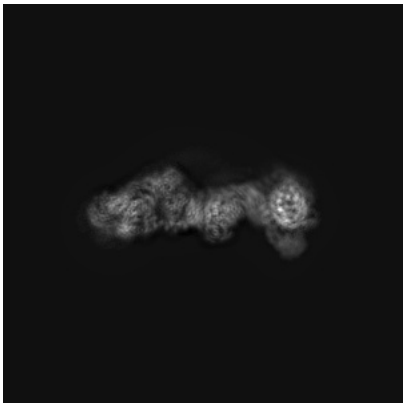
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

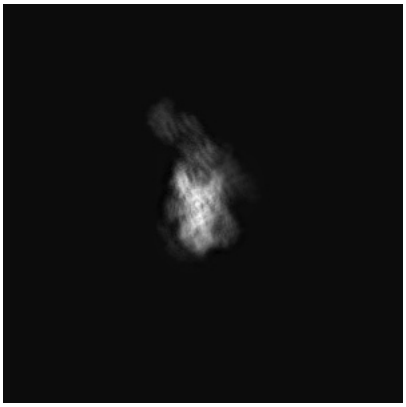
6.1.1 Primary map



X



Y

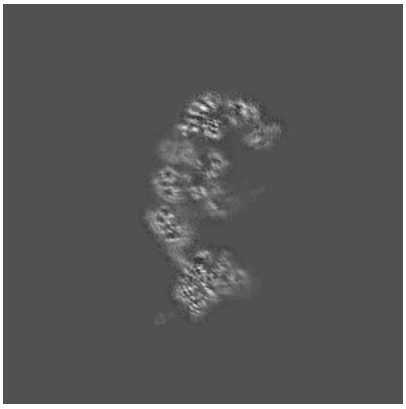


Z

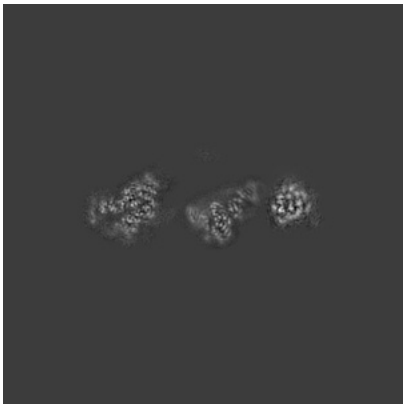
The images above show the map projected in three orthogonal directions.

6.2 Central slices

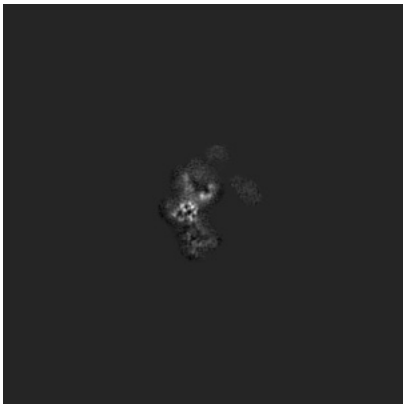
6.2.1 Primary map



X Index: 310



Y Index: 310

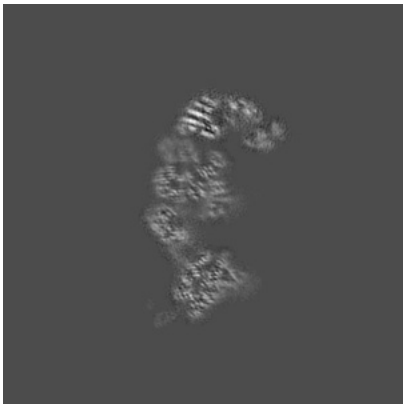


Z Index: 310

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: 305

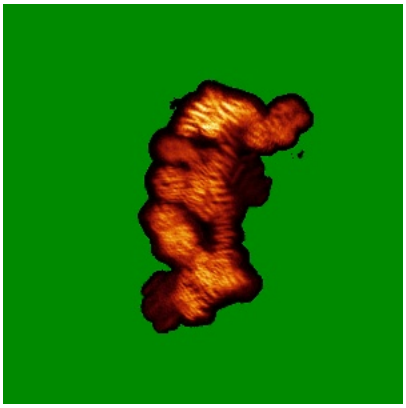
Y Index: 325

Z Index: 429

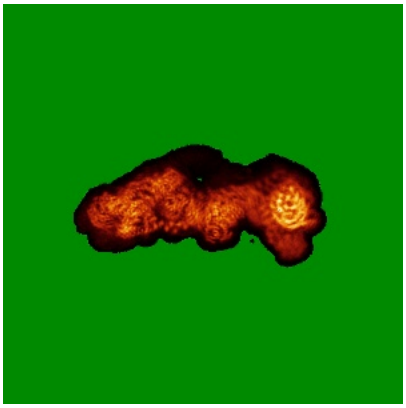
The images above show the largest variance slices of the map in three orthogonal directions.

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

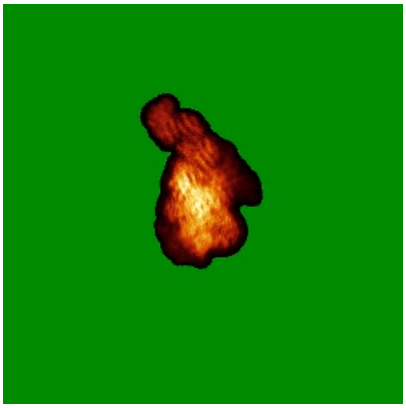
6.4.1 Primary map



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 9.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

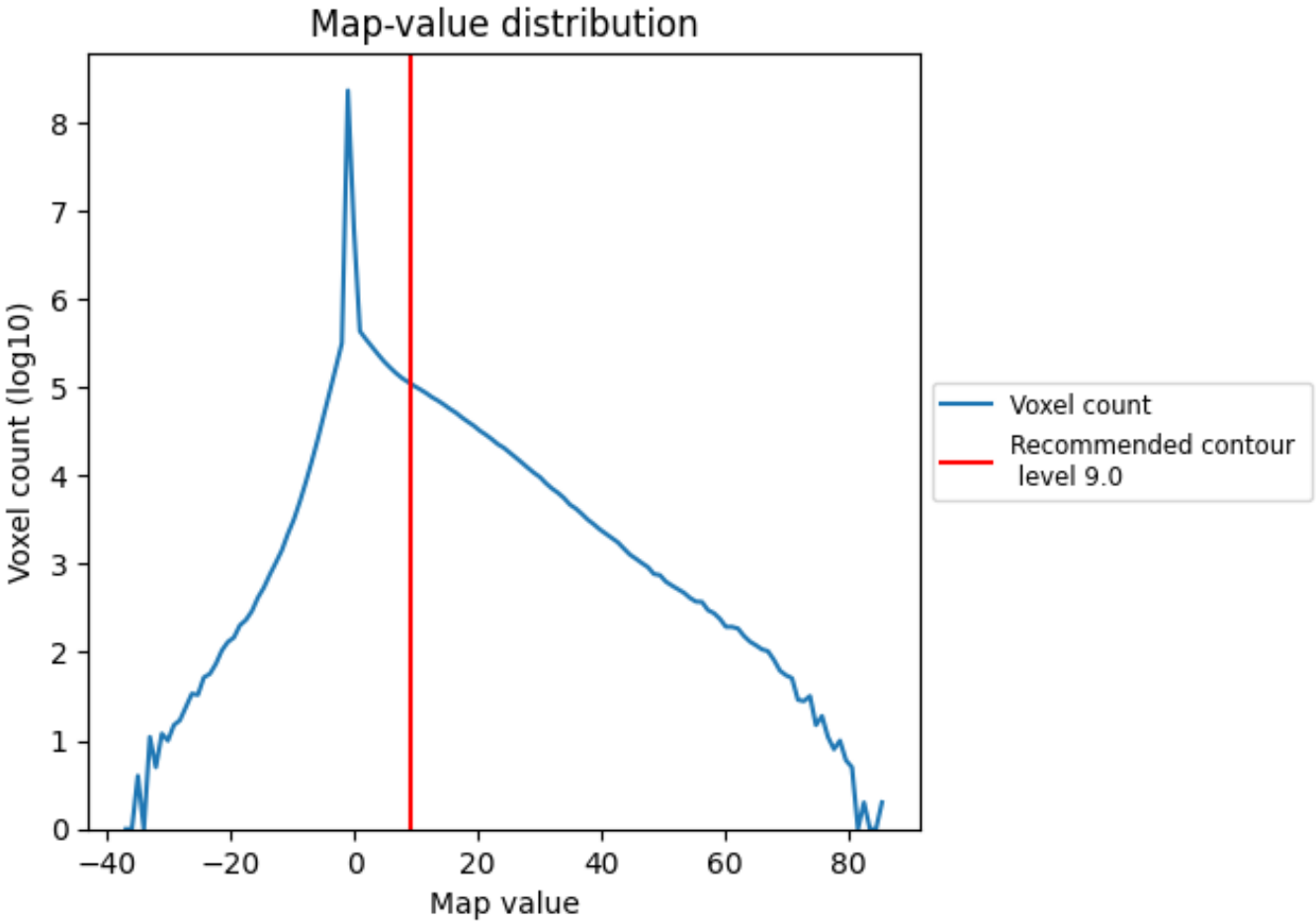
6.6 Mask visualisation (i)

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

7 Map analysis

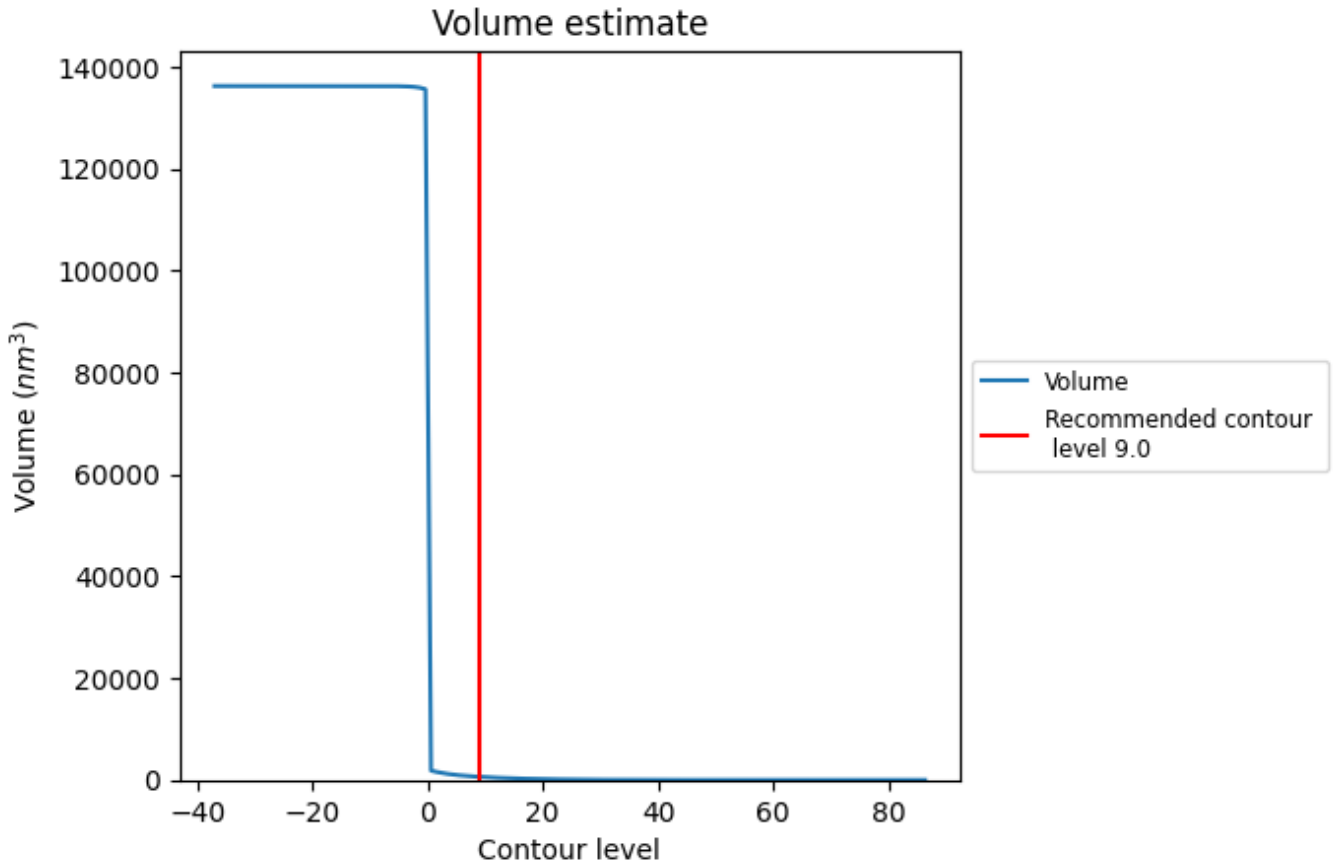
This section contains the results of statistical analysis of the map.

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.

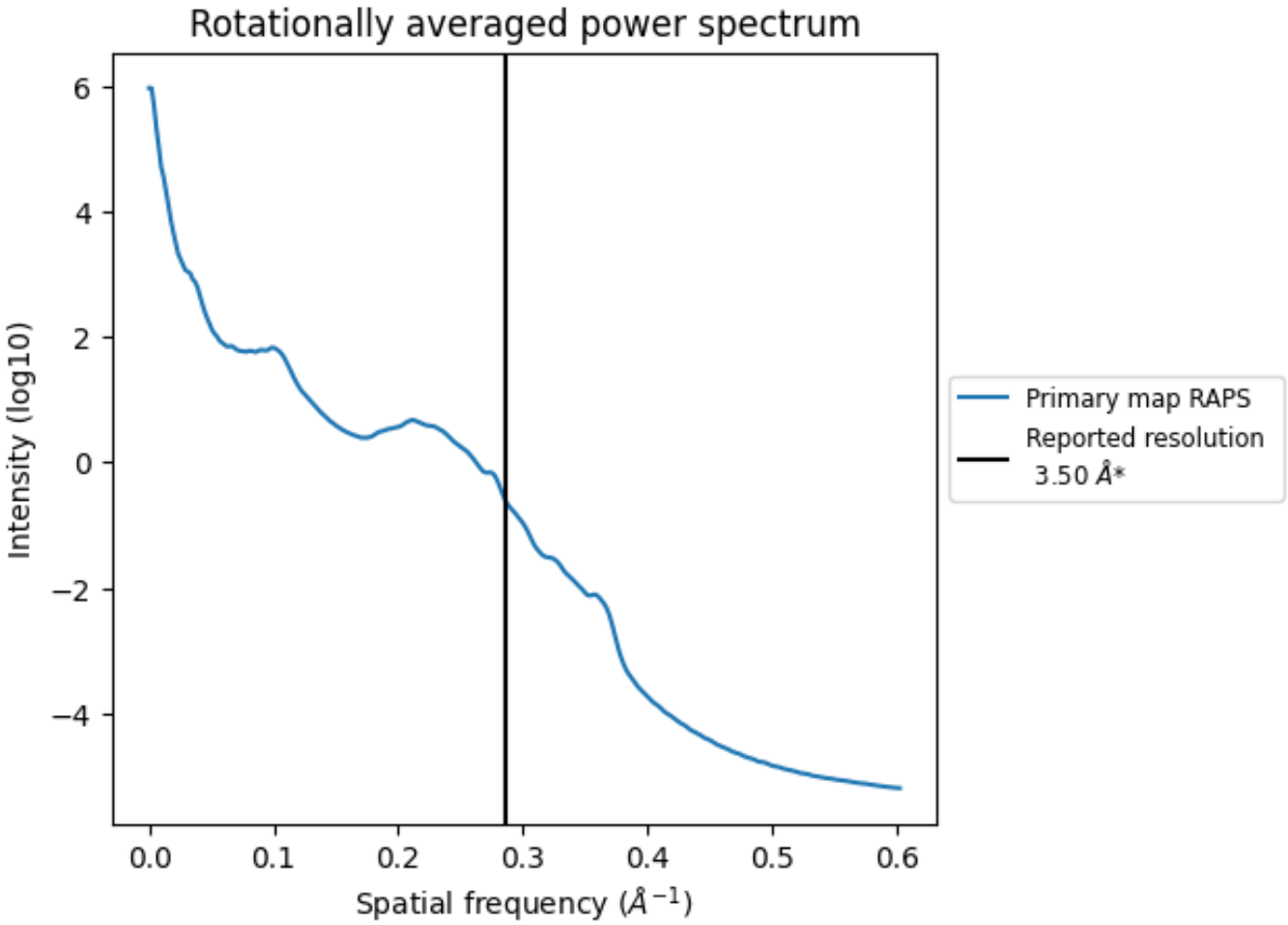
7.2 Volume estimate



The volume at the recommended contour level is 619 nm^3; this corresponds to an approximate mass of 559 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}

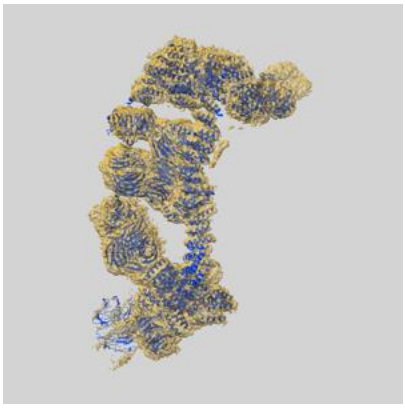
8 Fourier-Shell correlation (i)

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

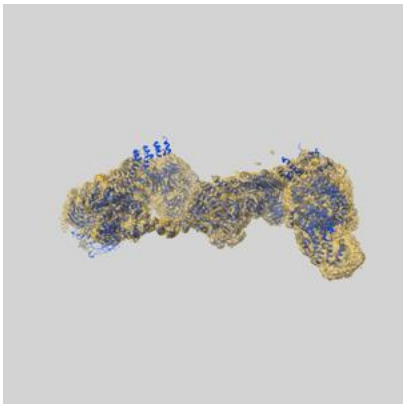
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28866 and PDB model 8F5O. Per-residue inclusion information can be found in section 3 on page 5.

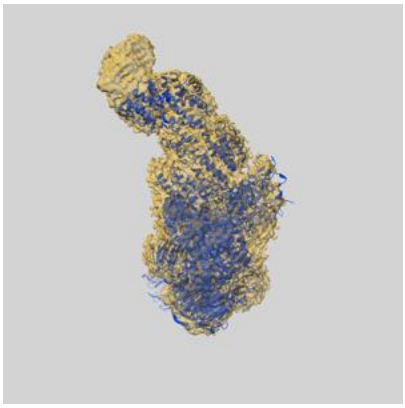
9.1 Map-model overlay



X



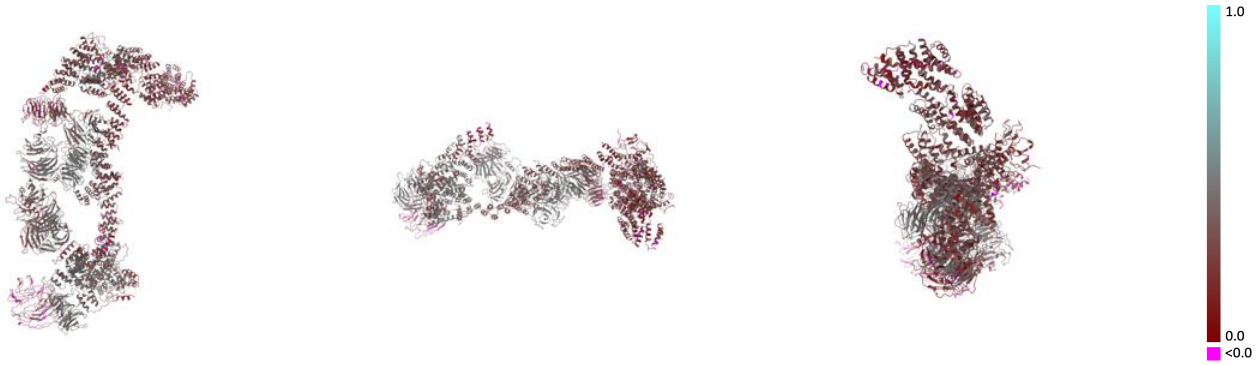
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9.0 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.

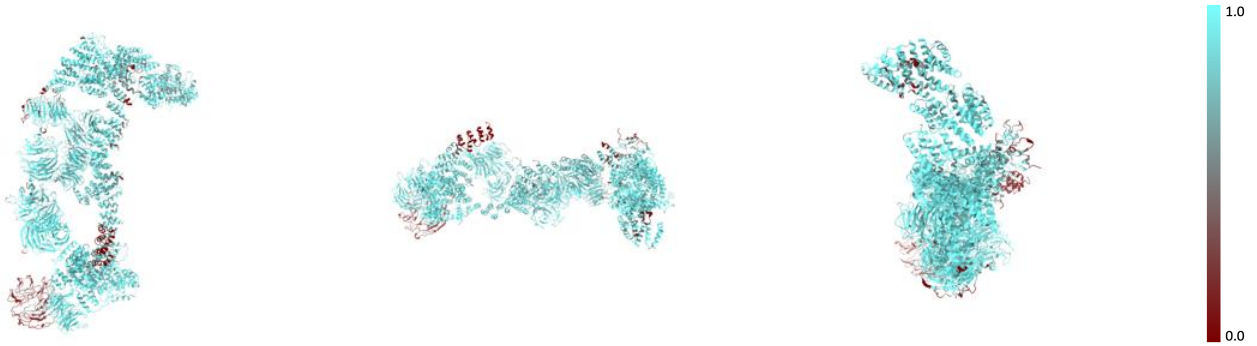
9.2 Q-score mapped to coordinate model (i)



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.

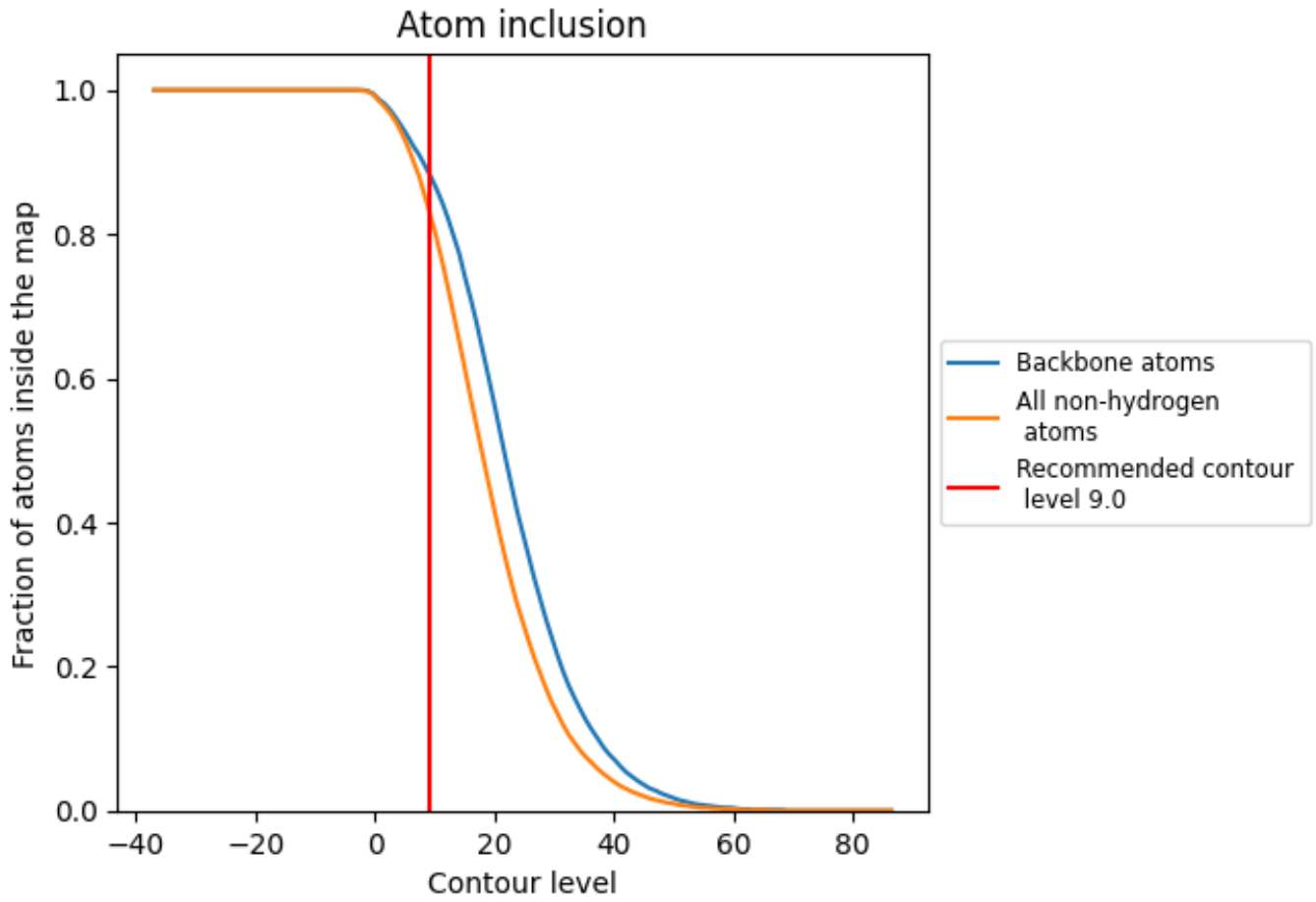
9.3 Atom inclusion mapped to coordinate model (i)



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 (9.0).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (9.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.3350
A	0.8160	0.2460
B	0.8770	0.3710
C	0.8760	0.3370
D	0.8970	0.2880
E	0.9350	0.3800
F	0.5230	0.2970