Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 07:35 AM JST

PDB ID	:	3JBR
EMDB ID	:	EMD-6475
Title	:	Cryo-EM structure of the rabbit voltage-gated calcium channel Cav1.1 complex at 4.2 angstrom
Authors	:	Wu, J.P.; Yan, Z.; Yan, N.
Deposited on	:	2015-09-29
Resolution	:	4.20 Å(reported)
Based on initial model	:	1T0J

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:

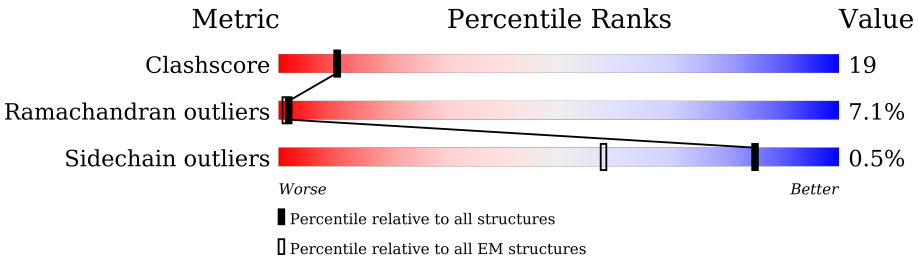
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1873	23% 47% 17% · 35%
2	B	356	79% 56% 23% 21%
3	E	222	8% 58% 5% 38%
4	F	1106	· 46% 29% · 21%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16467 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1224	7601	4843	1330	1400	28	0	0

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	281	2210	1405	385	411	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLY	-	expression tag	UNP Q8VGC3
B	15	HIS	-	expression tag	UNP Q8VGC3
B	16	MET	-	expression tag	UNP Q8VGC3
B	201	MET	-	linker	UNP Q8VGC3

- Molecule 3 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	138	688	410	138	140	0	0

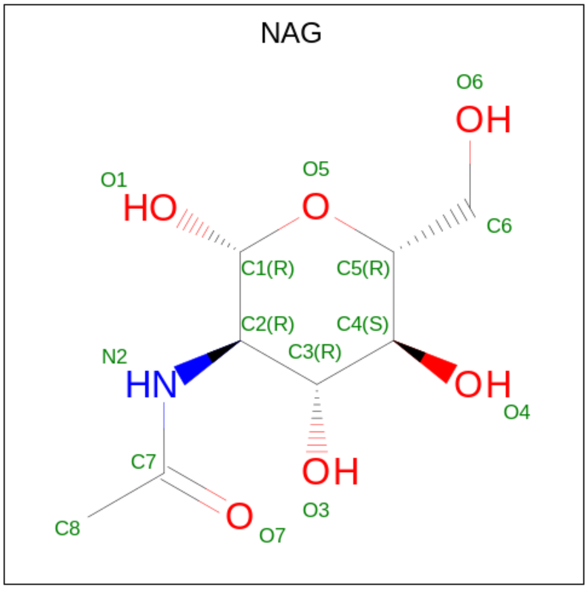
- Molecule 4 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	872	5735	3570	1042	1108	15	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
5	A	1	1	1	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	F	1	14	8	1	5	0
6	F	1	14	8	1	5	0
6	F	1	14	8	1	5	0
6	F	1	14	8	1	5	0
6	F	1	14	8	1	5	0
6	F	1	14	8	1	5	0
6	F	1	14	8	1	5	0
6	F	1	14	8	1	5	0
6	F	1	14	8	1	5	0
6	F	1	14	8	1	5	0

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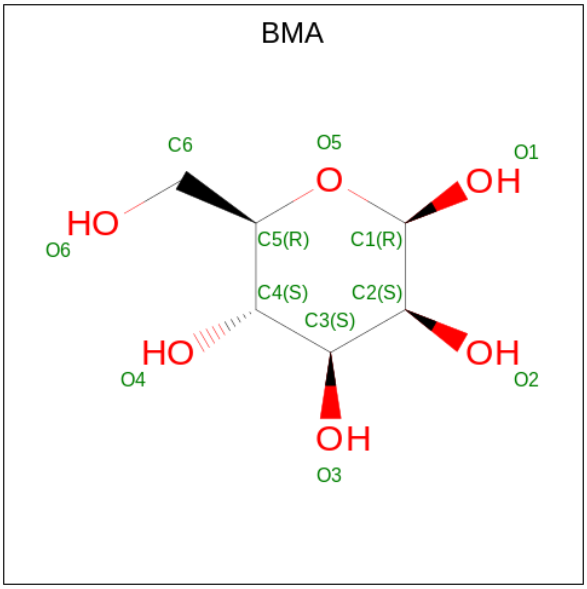
Mol	Chain	Residues	Atoms	AltConf
6	F	1	Total C N O 14 8 1 5	0
6	F	1	Total C N O 14 8 1 5	0
6	F	1	Total C N O 14 8 1 5	0
6	F	1	Total C N O 14 8 1 5	0
6	F	1	Total C N O 14 8 1 5	0

- Molecule 7 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



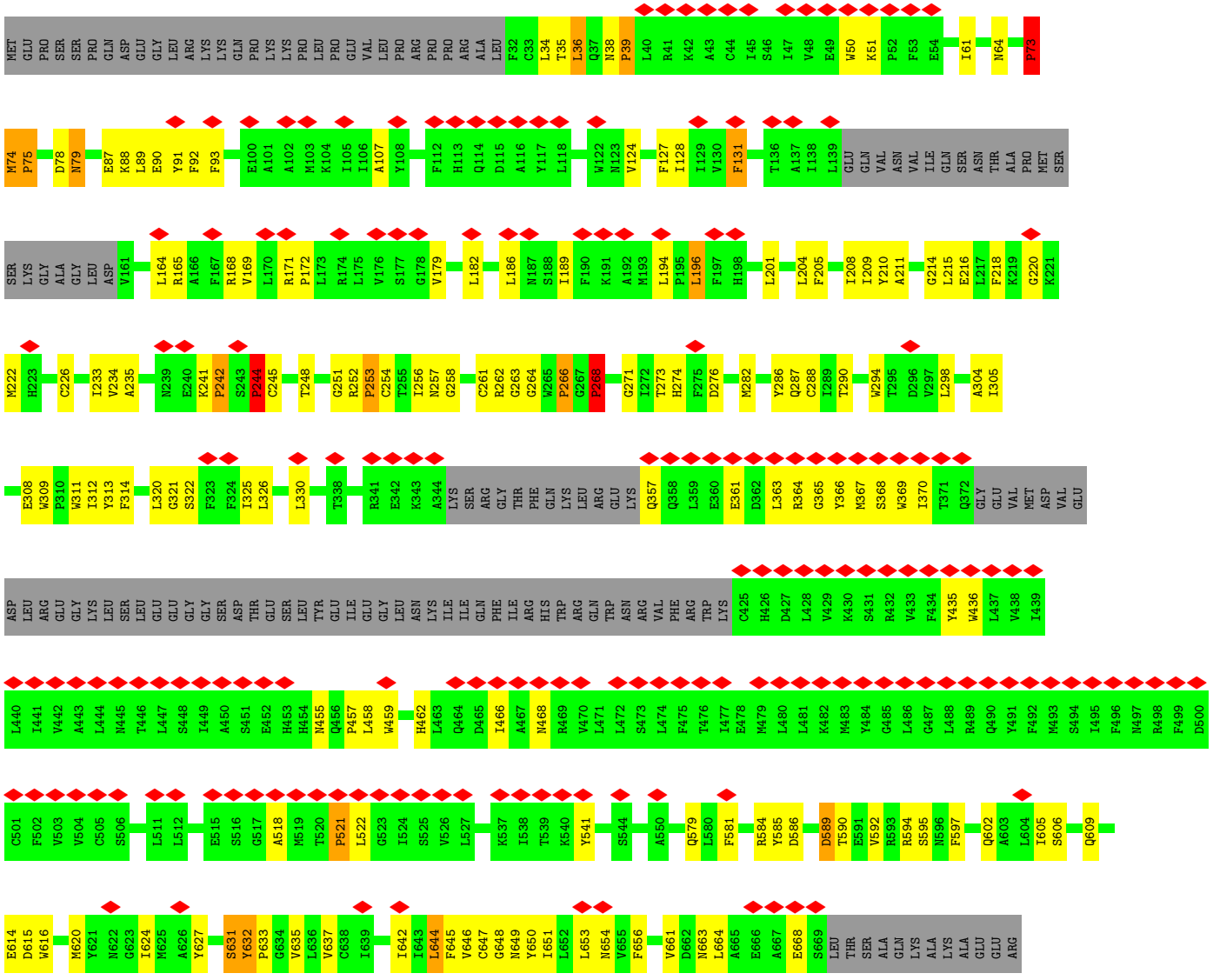
Mol	Chain	Residues	Atoms	AltConf
7	F	1	Total C O 11 6 5	0
7	F	1	Total C O 11 6 5	0

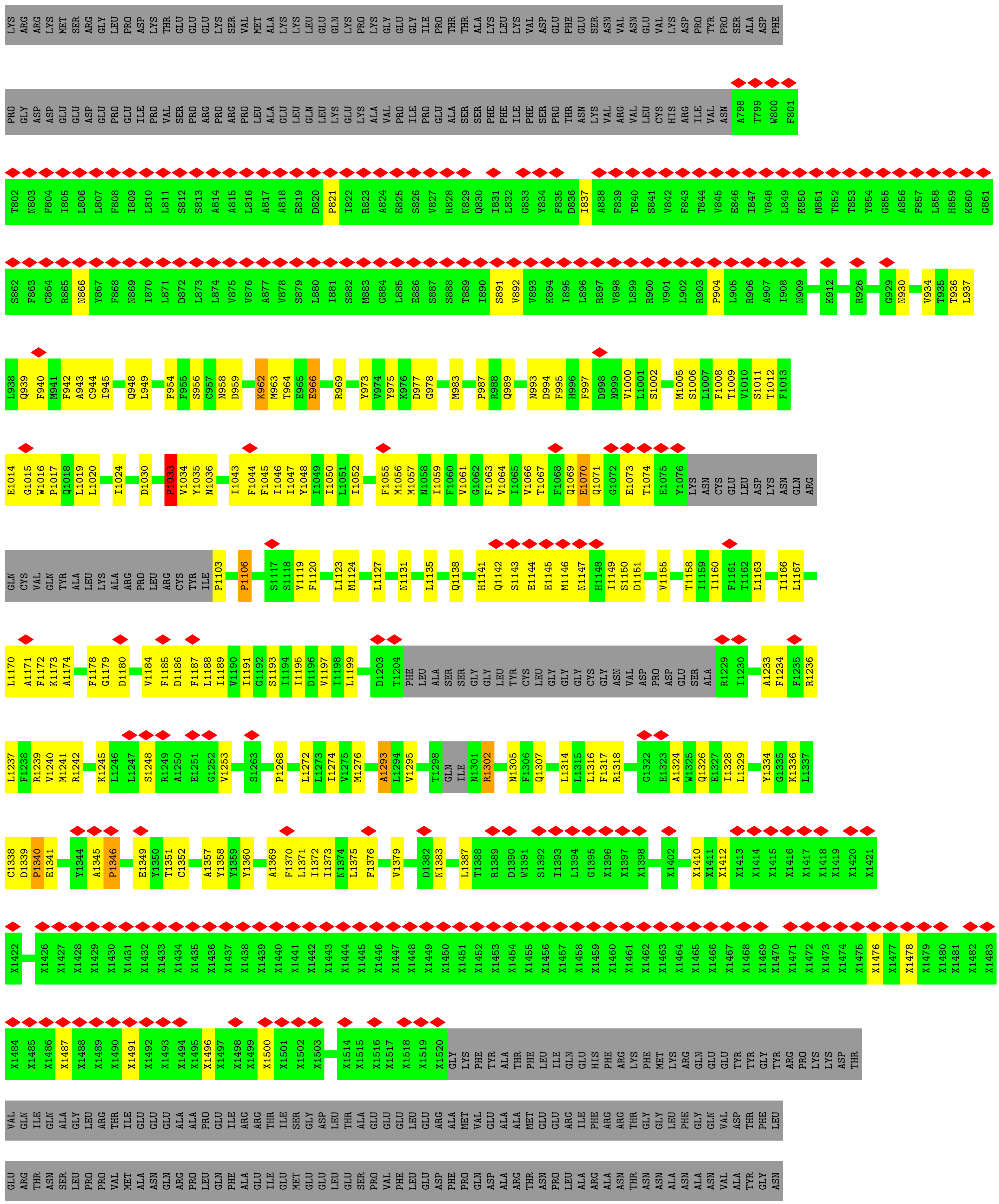
3 Residue-property plots (i)

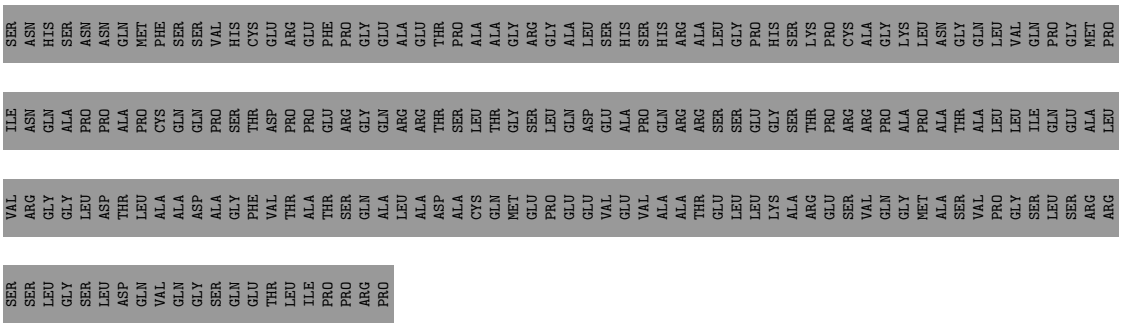
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Voltage-dependent L-type calcium channel subunit alpha-1S

Chain A:

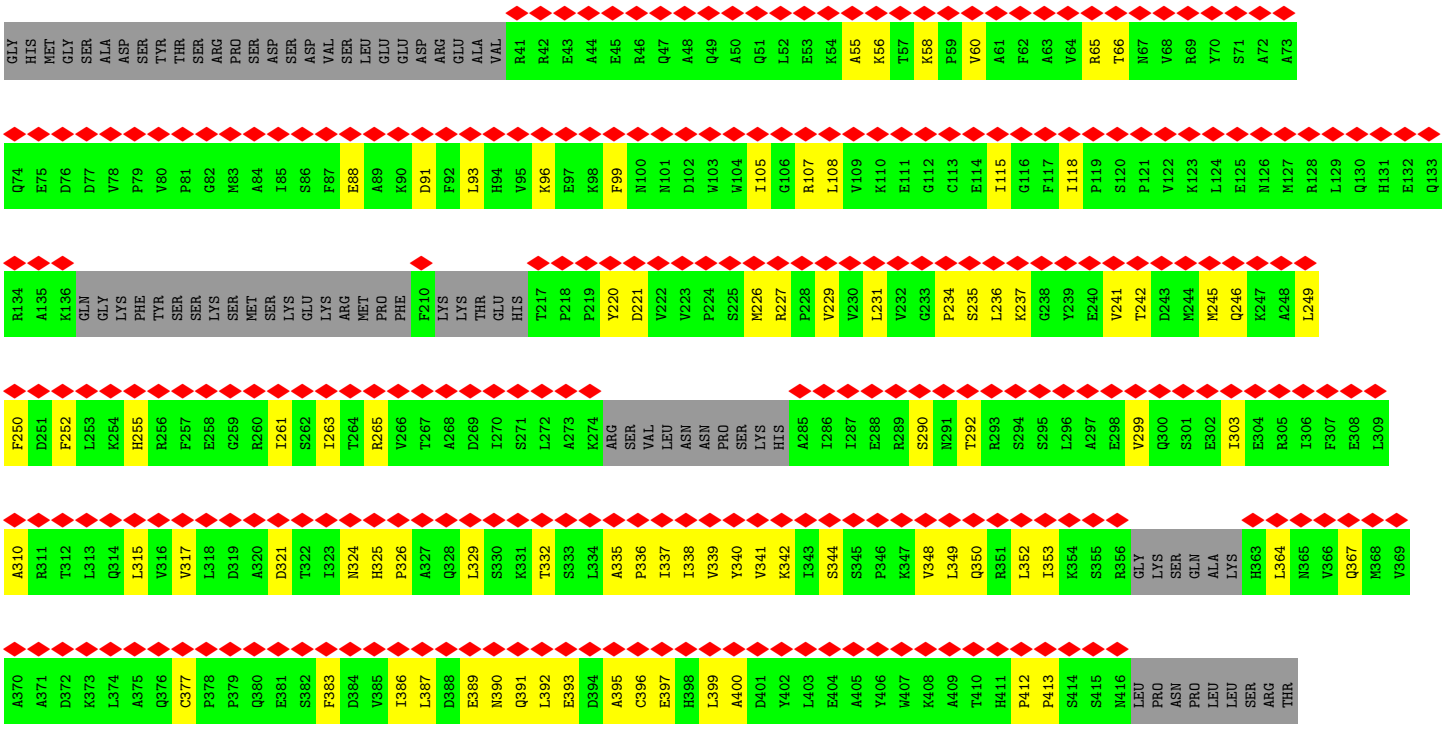



LYS ARG ARG LYS MET SER ARG GLY LEU PRO ASP LYS THR GLU GLU GLU LYS SER VAL MET ALA LYS LYS LEU GLU GLN LYS PRO LYS GLY GLU GLY ILE PRO THR THR ALA LYS LEU LYS VAL ASP GLU PHE GLU SER ASN VAL ASN GLU VAL LYS ASP PRO TYR PRO SER ALA ASP PHE
PRO GLY ASP ASP GLU GLU ASP GLU PRO GLU ILE PRO VAL SER PRO ARG PRO ARG PRO LEU ALA GLU LEU GLN LEU LYS GLU LYS ALA VAL PRO ILE PRO GLU ALA SER SER PHE PHE ILE PHE SER PRO THR ASN LYS VAL ARG VAL LEU CYS HIS ARG ILE VAL ASN A798 T799 W800 F801
T802 N803 F804 I805 L806 L807 F808 I809 L810 L811 S812 S813 A814 A815 L816 A817 A818 E819 D820 P821 I822 R823 A824 E825 S826 V827 R828 N829 Q830 I831 L832 G833 Y834 F835 D836 I837 A838 F839 T840 S841 V842 F843 T844 V845 E846 I847 V848 L849 K850 M851 T852 T853 Y854 G855 A856 F857 L858 H859 K860 G861
S862 F863 C864 R865 N866 Y867 F868 N869 I870 L871 D872 L873 L874 V875 V876 A877 V878 S879 L880 I881 S882 M883 G884 L885 E886 S887 S888 T889 I890 S891 V892 V893 K894 I895 L896 R897 V898 L899 R900 V901 L902 R903 P904 L905 R906 A907 I908 N909 K912 R926 G929 N930 V934 T935 T936 L937
L938 Q939 F940 M941 F942 A943 C944 I945 Q948 L949 F954 F955 S956 C957 N958 D959 K962 M963 T964 E965 E966 R969 Y973 V974 Y975 K976 D977 G978 M983 P987 R988 Q989 N993 D994 F995 H996 F997 D998 N999 V1000 L1001 S1002 M1005 S1006 L1007 F1008 T1009 V1010 S1011 T1012 F1013
E1014 G1015 W1016 P1017 Q1018 L1019 L1020 I1024 D1030 P1033 V1034 Y1035 N1036 I1043 F1044 F1045 I1046 I1047 Y1048 I1049 I1050 L1051 I1052 F1055 M1056 M1057 N1058 I1059 F1060 V1061 G1062 F1063 V1064 I1065 V1066 T1067 F1068 Q1069 E1070 Q1071 G1072 E1073 T1074 E1075 Y1076 LYS ASN CYS GLU LEU ASP LYS ASN GLN ARG
GLN CYS VAL GLN TYR ALA LEU LYS ALA ARG PRO LEU ARG CYS TYR ILE P1103 P1106 S1117 S1118 Y1119 F1120 L1123 M1124 L1127 N1131 L1135 Q1138 H1141 Q1142 S1143 E1144 E1145 M1146 N1147 H1148 I1149 S1150 D1151 V1155 T1158 I1159 I1160 F1161 T1162 L1163 I1166 L1167
L1170 A1171 F1172 K1173 A1174 F1178 G1179 D1180 V1184 F1185 D1186 F1187 L1188 I1189 V1190 I1191 G1192 S1193 I1194 I1195 D1196 V1197 I1198 L1199 D1203 T1204 PHE LEU ALA SER SER GLY GLY LEU TYR CYS LEU GLY GLY CYS GLY ASN VAL ASP PRO ASP GLU SER ALA R1229 I1230 A1233 F1234 F1235 R1236
L1237 F1238 R1239 V1240 M1241 R1242 K1245 L1246 L1247 S1248 R1249 A1250 E1251 G1252 V1253 S1263 P1268 L1272 L1273 I1274 V1275 M1276 A1293 L1294 V1295 T1298 GLN ILE N1301 R1302 N1305 F1306 Q1307 L1314 L1315 L1316 F1317 R1318 G1322 E1323 A1324 W1325 Q1326 E1327 I1328 L1329 Y1334 G1335 K1336 L1337
C1338 D1339 P1340 E1341 Y1344 A1345 P1346 E1349 Y1350 T1351 C1352 A1357 Y1358 Y1359 Y1360 A1369 F1370 L1371 I1372 I1373 N1374 L1375 F1376 V1379 D1382 N1383 L1387 T1388 R1389 D1390 W1391 S1392 I1393 L1394 G1395 X1396 X1397 X1398 X1402 X1410 X1411 X1412 X1413 X1414 X1415 X1416 X1417 X1418 X1419 X1420 X1421
X1422 X1426 X1427 X1428 X1429 X1430 X1431 X1432 X1433 X1434 X1435 X1436 X1437 X1438 X1439 X1440 X1441 X1442 X1443 X1444 X1445 X1446 X1447 X1448 X1449 X1450 X1451 X1452 X1453 X1454 X1455 X1456 X1457 X1458 X1459 X1460 X1461 X1462 X1463 X1464 X1465 X1466 X1467 X1468 X1469 X1470 X1471 X1472 X1473 X1474 X1475 X1476 X1477 X1478 X1479 X1480 X1481 X1482 X1483
X1484 X1485 X1486 X1487 X1488 X1489 X1490 X1491 X1492 X1493 X1494 X1495 X1496 X1497 X1498 X1499 X1500 X1501 X1502 X1503 X1514 X1515 X1516 X1517 X1518 X1519 X1520 GLY LYS PHE TYR ALA THR PHE LEU ILE GLN GLU HIS PHE ARG LYS PHE MET LYS ARG GLN GLU GLU TYR TYR GLY TYR ARG PRO LYS LYS ASP THR
VAL GLN ILE GLN ALA GLY LEU ARG THR ILE GLU GLU GLU ALA ALA PRO GLU ILE ARG ARG THR ILE SER GLY ASP LEU THR ALA GLU GLU GLU LEU GLU ARG ALA MET VAL GLU ALA ALA MET GLU GLU ARG ILE PHE ARG ARG THR GLY GLY LEU PHE GLY GLN VAL ASP THR PHE LEU
GLU ARG THR ASN SER LEU PRO PRO VAL MET ALA ASN GLN ARG PRO LEU GLN PHE ALA GLU ILE GLU MET GLU GLU LEU GLU SER PRO VAL PHE LEU GLU ASP PHE PRO GLN ASP ALA ALA ARG THR ASN PRO LEU ALA ARG ALA ASN THR ASN ASN ALA ASN ALA ASN VAL ALA TYR GLY ASN



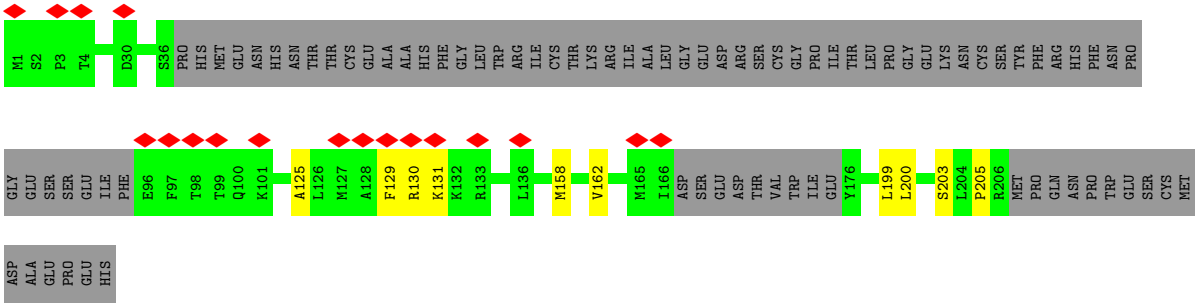
• Molecule 2: Voltage-dependent L-type calcium channel subunit beta-2

Chain B:



• Molecule 3: Voltage-dependent calcium channel gamma-1 subunit

Chain E:



• Molecule 4: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain F:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	353372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	2.0	Depositor
Maximum defocus (nm)	3.3	Depositor
Magnification	Not provided	
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.079	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, BMA

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	0.45	0/7080	0.57	19/9723 (0.2%)
2	B	0.22	0/2252	0.40	0/3051
3	E	0.31	0/685	0.45	0/950
4	F	0.48	1/4603 (0.0%)	0.67	14/6265 (0.2%)
All	All	0.43	1/14620 (0.0%)	0.58	33/19989 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	627	PRO	N-CD	5.04	1.54	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	987	PRO	N-CA-CB	6.39	110.96	103.30
1	A	1346	PRO	N-CA-CB	6.35	110.92	103.30
1	A	457	PRO	N-CA-CB	6.34	110.91	103.30
1	A	73	PRO	N-CA-CB	6.10	110.62	103.30
1	A	253	PRO	N-CA-CB	6.10	110.62	103.30
1	A	242	PRO	N-CA-CB	6.08	110.60	103.30
4	F	135	PRO	N-CA-CB	6.07	110.59	103.30
4	F	553	PRO	N-CA-CB	6.01	110.51	103.30
1	A	1103	PRO	N-CA-CB	5.99	110.49	103.30
1	A	75	PRO	N-CA-CB	5.98	110.48	103.30
4	F	1059	PRO	N-CA-CB	5.95	110.44	103.30
4	F	171	PRO	N-CA-CB	5.95	110.44	103.30
4	F	653	PRO	N-CA-CB	5.94	110.42	103.30
1	A	821	PRO	N-CA-CB	5.93	110.42	103.30
4	F	142	PRO	N-CA-CB	5.93	110.42	103.30
4	F	1053	PRO	N-CA-CB	5.91	110.39	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1340	PRO	N-CA-CB	5.85	110.31	103.30
4	F	1046	PRO	N-CA-CB	5.84	110.30	103.30
4	F	1044	PRO	N-CA-CB	5.82	110.28	103.30
4	F	485	LEU	CA-CB-CG	-5.81	101.94	115.30
4	F	1028	PRO	N-CA-CB	5.80	110.26	103.30
1	A	904	PRO	N-CA-CB	5.80	110.26	103.30
4	F	626	LEU	C-N-CD	5.78	140.53	128.40
1	A	1268	PRO	N-CA-CB	5.74	110.19	103.30
4	F	74	PRO	N-CA-CB	5.74	110.19	103.30
1	A	521	PRO	N-CA-CB	5.71	110.15	103.30
1	A	268	PRO	N-CA-CB	5.69	110.13	103.30
1	A	1106	PRO	N-CA-CB	5.67	110.10	103.30
1	A	39	PRO	N-CA-CB	5.59	110.01	103.30
1	A	266	PRO	N-CA-CB	5.53	109.93	103.30
4	F	309	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	1033	PRO	N-CA-CB	5.10	109.42	103.30
1	A	244	PRO	N-CA-CB	5.04	109.35	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7601	0	5495	201	0
2	B	2210	0	2208	65	0
3	E	688	0	336	4	0
4	F	5735	0	4413	281	0
5	A	1	0	0	0	0
6	F	210	0	195	11	0
7	F	22	0	20	2	0
All	All	16467	0	12667	542	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 19.

All (542) 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)
4:F:607:ARG:HA	4:F:627:PRO:HD3	1.21	1.14
4:F:607:ARG:HA	4:F:627:PRO:CD	1.84	1.07
4:F:626:LEU:O	4:F:628:THR:N	2.02	0.92
4:F:248:GLN:HE21	4:F:447:GLN:HG2	1.37	0.89
4:F:606:ASN:O	4:F:627:PRO:HD2	1.73	0.88
1:A:256:ILE:H	1:A:257:ASN:HA	1.39	0.87
1:A:1274:ILE:HA	1:A:1371:LEU:HD21	1.58	0.86
4:F:75:ASN:CB	4:F:630:SER:O	2.23	0.85
4:F:1008:VAL:HG12	4:F:1009:GLU:H	1.45	0.81
1:A:1373:ILE:HA	1:A:1376:PHE:HD2	1.43	0.81
4:F:601:TYR:HA	4:F:1017:ILE:HG21	1.64	0.79
4:F:238:TYR:HE1	4:F:243:ARG:HD2	1.48	0.77
1:A:367:MET:SD	2:B:352:LEU:HD23	2.24	0.77
4:F:523:VAL:HG12	4:F:524:LEU:HG	1.67	0.77
4:F:626:LEU:O	4:F:628:THR:HG22	1.85	0.75
4:F:169:HIS:HB3	4:F:216:LEU:HB2	1.69	0.75
4:F:570:ASN:HD21	4:F:594:VAL:HG21	1.52	0.75
1:A:983:MET:HG3	4:F:235:ILE:HD12	1.67	0.75
4:F:302:ASP:HB2	4:F:306:PHE:HE1	1.52	0.74
4:F:509:CYS:SG	4:F:561:LEU:N	2.60	0.74
4:F:346:LEU:O	4:F:353:ARG:NH1	2.22	0.73
2:B:226:MET:H	2:B:310:ALA:HB1	1.53	0.72
1:A:1070:GLU:HA	1:A:1070:GLU:OE2	1.88	0.72
1:A:1067:THR:HA	1:A:1070:GLU:HB2	1.71	0.71
1:A:1233:ALA:HA	1:A:1236:ARG:HE	1.56	0.71
4:F:182:LEU:HD23	4:F:185:LEU:HD12	1.72	0.71
4:F:437:VAL:HA	4:F:469:PHE:HE2	1.55	0.71
4:F:73:GLU:O	4:F:632:TYR:N	2.24	0.71
2:B:99:PHE:HB2	2:B:105:ILE:HG13	1.72	0.70
4:F:607:ARG:CA	4:F:627:PRO:HD3	2.11	0.70
4:F:238:TYR:CE1	4:F:243:ARG:HD2	2.27	0.70
2:B:325:HIS:NE2	2:B:377:CYS:SG	2.65	0.70
4:F:461:VAL:HG22	4:F:484:GLN:HA	1.73	0.69
4:F:502:LEU:O	4:F:622:LEU:HB3	1.92	0.69
4:F:883:UNK:HA	4:F:892:UNK:HA	1.75	0.69
2:B:231:LEU:O	2:B:246:GLN:NE2	2.25	0.69
4:F:345:GLN:O	4:F:348:ASN:ND2	2.26	0.69
4:F:356:CYS:SG	4:F:357:ASN:N	2.61	0.69
1:A:201:LEU:O	1:A:205:PHE:N	2.25	0.69
4:F:184:GLU:HA	4:F:187:TRP:NE1	2.08	0.68
4:F:606:ASN:O	4:F:627:PRO:CD	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:343:PHE:HE1	4:F:384:VAL:HG11	1.56	0.68
4:F:1009:GLU:O	4:F:1011:LEU:N	2.26	0.68
4:F:573:LYS:HA	4:F:576:ILE:HD12	1.76	0.68
4:F:212:SER:OG	4:F:213:ALA:N	2.25	0.67
4:F:1004:ARG:NH1	4:F:1035:ILE:O	2.28	0.67
1:A:365:GLY:O	1:A:368:SER:OG	2.11	0.67
4:F:500:LYS:HG2	4:F:501:ARG:O	1.94	0.67
2:B:229:VAL:HG22	2:B:337:ILE:HB	1.76	0.67
2:B:389:GLU:HB2	2:B:395:ALA:HB2	1.77	0.67
1:A:165:ARG:HB3	1:A:579:GLN:HE21	1.60	0.66
4:F:520:ASN:ND2	4:F:560:THR:O	2.29	0.66
4:F:502:LEU:HD12	4:F:512:GLY:HA3	1.78	0.66
4:F:516:ALA:HB3	4:F:1007:HIS:HE1	1.61	0.65
4:F:184:GLU:HA	4:F:187:TRP:HE1	1.60	0.65
1:A:1373:ILE:HA	1:A:1376:PHE:CD2	2.30	0.65
4:F:210:PHE:HB3	4:F:217:ALA:HB3	1.79	0.65
4:F:343:PHE:CE1	4:F:384:VAL:HG11	2.31	0.64
4:F:516:ALA:HB3	4:F:1007:HIS:CE1	2.32	0.64
4:F:1036:GLN:O	4:F:1038:GLU:N	2.30	0.64
4:F:225:TRP:NE1	4:F:236:ASP:OD1	2.31	0.64
4:F:335:TYR:OH	4:F:369:GLU:O	2.05	0.64
1:A:309:TRP:HA	1:A:311:TRP:CD1	2.32	0.64
1:A:644:LEU:O	1:A:648:GLY:N	2.28	0.64
4:F:242:ARG:HH11	4:F:425:THR:HG23	1.61	0.64
4:F:257:LEU:HB3	4:F:360:ILE:HG22	1.79	0.64
4:F:680:UNK:O	4:F:682:UNK:N	2.31	0.63
1:A:1034:VAL:O	1:A:1036:ASN:N	2.31	0.63
1:A:165:ARG:HB3	1:A:579:GLN:NE2	2.14	0.63
4:F:282:LEU:HB3	4:F:317:LYS:HZ3	1.64	0.62
1:A:90:GLU:HB3	1:A:171:ARG:HH12	1.63	0.62
1:A:1172:PHE:O	1:A:1174:ALA:N	2.33	0.62
4:F:999:CYS:HB2	4:F:1019:ILE:H	1.63	0.62
4:F:585:SER:HB2	4:F:611:TRP:HH2	1.63	0.62
4:F:449:THR:HG22	4:F:463:THR:H	1.64	0.62
4:F:98:ALA:HB1	4:F:199:ARG:HE	1.63	0.62
1:A:211:ALA:O	1:A:215:LEU:N	2.33	0.62
1:A:369:TRP:HZ3	2:B:392:LEU:HA	1.65	0.62
4:F:417:SER:OG	4:F:418:ILE:N	2.33	0.62
4:F:196:LYS:HD3	4:F:219:TYR:HB2	1.81	0.62
4:F:132:ASP:N	4:F:140:SER:O	2.33	0.61
2:B:234:PRO:HD2	2:B:242:THR:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:LYS:H	2:B:324:ASN:HD21	1.46	0.61
2:B:341:VAL:HG22	2:B:387:LEU:HD12	1.82	0.61
4:F:95:ARG:NH2	4:F:204:SER:O	2.32	0.61
4:F:311:GLN:HA	4:F:316:ASN:HD22	1.65	0.61
4:F:606:ASN:ND2	6:F:1211:NAG:O7	2.32	0.61
1:A:1370:PHE:HA	1:A:1373:ILE:HD12	1.82	0.61
3:E:200:LEU:O	3:E:203:SER:OG	2.16	0.61
4:F:500:LYS:HZ2	4:F:502:LEU:HD13	1.65	0.61
2:B:56:LYS:HA	2:B:115:ILE:HG13	1.83	0.60
2:B:60:VAL:HA	2:B:96:LYS:HD3	1.83	0.60
4:F:607:ARG:HA	4:F:627:PRO:HD2	1.79	0.60
1:A:309:TRP:O	1:A:312:ILE:HG22	2.01	0.60
4:F:379:ASN:HD21	4:F:382:LYS:HA	1.66	0.60
4:F:1005:ILE:HG22	4:F:1007:HIS:H	1.65	0.60
4:F:500:LYS:HE3	4:F:502:LEU:HB2	1.84	0.60
1:A:645:PHE:O	1:A:649:ASN:N	2.31	0.60
1:A:584:ARG:O	1:A:586:ASP:N	2.31	0.60
4:F:911:UNK:O	4:F:915:UNK:N	2.35	0.60
1:A:288:CYS:HA	1:A:294:TRP:HB3	1.83	0.60
4:F:188:THR:HG23	4:F:189:SER:H	1.67	0.60
1:A:131:PHE:CD1	1:A:164:LEU:HB3	2.37	0.59
4:F:297:ASN:C	4:F:299:ASN:H	2.04	0.59
4:F:263:SER:O	4:F:265:SER:N	2.36	0.59
1:A:995:PHE:HB3	1:A:1006:SER:HB2	1.85	0.59
4:F:402:GLN:NE2	4:F:1063:PHE:O	2.36	0.59
1:A:602:GLN:O	1:A:605:ILE:HG13	2.02	0.59
1:A:131:PHE:HA	1:A:164:LEU:HD22	1.85	0.59
1:A:973:TYR:HE1	4:F:235:ILE:HG21	1.67	0.59
2:B:252:PHE:HA	2:B:255:HIS:CD2	2.37	0.59
4:F:570:ASN:O	4:F:572:ILE:N	2.33	0.59
2:B:231:LEU:HA	2:B:339:VAL:HB	1.83	0.59
4:F:242:ARG:NH1	4:F:421:ILE:O	2.36	0.58
4:F:298:SER:N	4:F:332:ILE:O	2.37	0.58
1:A:944:CYS:O	1:A:948:GLN:HG2	2.04	0.58
1:A:1070:GLU:O	1:A:1074:THR:N	2.35	0.58
4:F:1008:VAL:HG11	4:F:1013:ASN:HD22	1.67	0.58
1:A:1237:LEU:O	1:A:1241:MET:HG2	2.04	0.58
2:B:390:ASN:OD1	2:B:391:GLN:N	2.35	0.58
4:F:463:THR:HG22	4:F:482:LYS:HA	1.85	0.58
2:B:290:SER:OG	2:B:292:THR:OG1	2.19	0.58
4:F:256:MET:HG3	4:F:285:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1496:UNK:O	1:A:1500:UNK:N	2.36	0.57
4:F:372:GLN:HA	4:F:375:PHE:CD2	2.39	0.57
4:F:359:ILE:HB	4:F:385:ARG:HB2	1.86	0.57
4:F:210:PHE:CD2	4:F:479:THR:HG22	2.40	0.57
1:A:592:VAL:O	1:A:594:ARG:N	2.36	0.57
4:F:470:ASN:HD22	4:F:473:GLY:H	1.53	0.57
4:F:614:VAL:HG12	4:F:616:GLY:H	1.70	0.57
2:B:88:GLU:N	2:B:91:ASP:OD2	2.37	0.57
4:F:569:GLU:OE2	4:F:571:ASP:N	2.36	0.57
2:B:265:ARG:NH2	2:B:321:ASP:OD2	2.38	0.57
6:F:1209:NAG:HO4	7:F:1217:BMA:HO2	1.51	0.57
1:A:363:LEU:HA	2:B:348:VAL:HG13	1.87	0.56
4:F:497:GLU:N	4:F:497:GLU:OE1	2.38	0.56
1:A:322:SER:O	1:A:326:LEU:HG	2.04	0.56
1:A:1067:THR:O	1:A:1071:GLN:N	2.34	0.56
2:B:241:VAL:O	2:B:245:MET:HG3	2.05	0.56
2:B:341:VAL:HA	2:B:387:LEU:HB2	1.87	0.56
4:F:131:ASP:HA	4:F:141:GLU:HA	1.86	0.56
4:F:662:UNK:O	4:F:666:UNK:N	2.38	0.56
6:F:1203:NAG:O4	6:F:1204:NAG:O7	2.19	0.56
2:B:299:VAL:O	2:B:303:ILE:HG12	2.04	0.56
4:F:206:LEU:O	4:F:220:TYR:OH	2.24	0.56
4:F:322:ASP:HA	4:F:325:ASN:ND2	2.20	0.56
4:F:589:THR:HG21	4:F:610:THR:HA	1.88	0.56
4:F:1004:ARG:HG2	4:F:1014:THR:HG22	1.87	0.56
1:A:216:GLU:O	1:A:220:GLY:N	2.35	0.56
1:A:233:ILE:O	1:A:235:ALA:N	2.38	0.56
2:B:261:ILE:HA	2:B:315:LEU:HB2	1.88	0.56
1:A:1043:ILE:HG22	1:A:1047:ILE:HD11	1.89	0.55
4:F:210:PHE:HE1	4:F:212:SER:HB2	1.71	0.55
1:A:1064:VAL:O	1:A:1067:THR:OG1	2.15	0.55
1:A:975:TYR:HE1	1:A:983:MET:HB3	1.71	0.55
4:F:243:ARG:HH12	4:F:455:ALA:H	1.55	0.55
2:B:350:GLN:HA	2:B:364:LEU:HD11	1.89	0.55
4:F:307:GLN:O	4:F:308:HIS:ND1	2.40	0.55
4:F:63:TYR:O	4:F:67:GLN:N	2.40	0.55
2:B:353:ILE:HD13	2:B:367:GLN:OE1	2.07	0.55
1:A:34:LEU:O	1:A:36:LEU:N	2.40	0.55
4:F:264:GLY:N	4:F:331:GLY:O	2.36	0.55
4:F:336:LYS:HA	4:F:339:PHE:CD2	2.41	0.55
1:A:218:PHE:O	1:A:222:MET:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:MET:HA	1:A:1127:LEU:HD12	1.88	0.54
4:F:308:HIS:HB2	4:F:309:LEU:HG	1.89	0.54
2:B:387:LEU:HD21	2:B:399:LEU:HB2	1.89	0.54
4:F:298:SER:HB2	4:F:332:ILE:HG13	1.90	0.54
4:F:375:PHE:O	4:F:379:ASN:N	2.32	0.54
1:A:1158:THR:HG21	1:A:1197:VAL:HG21	1.90	0.54
1:A:1239:ARG:HG3	1:A:1242:ARG:CZ	2.38	0.54
4:F:259:LEU:HB3	4:F:296:PHE:HE1	1.72	0.54
4:F:602:ILE:HG22	4:F:603:ASP:O	2.08	0.54
1:A:1055:PHE:O	1:A:1059:ILE:HG13	2.08	0.54
2:B:252:PHE:CZ	2:B:396:CYS:HB3	2.43	0.54
1:A:322:SER:O	1:A:325:ILE:HG13	2.08	0.54
1:A:656:PHE:CE2	1:A:1057:MET:HG3	2.44	0.53
4:F:182:LEU:HA	4:F:185:LEU:HD12	1.89	0.53
4:F:248:GLN:NE2	4:F:447:GLN:HG2	2.17	0.53
4:F:505:ARG:N	4:F:509:CYS:O	2.29	0.53
4:F:62:ILE:O	4:F:66:TYR:N	2.39	0.53
4:F:1008:VAL:HG12	4:F:1009:GLU:N	2.20	0.53
4:F:530:GLN:HB2	4:F:531:PRO:HD3	1.91	0.53
4:F:557:GLU:HB3	4:F:558:PRO:HA	1.90	0.53
2:B:235:SER:OG	2:B:236:LEU:N	2.41	0.53
4:F:414:GLU:O	4:F:423:ILE:HG21	2.08	0.53
1:A:1120:PHE:HA	1:A:1123:LEU:HD12	1.90	0.53
1:A:1146:MET:HA	1:A:1149:ILE:HD12	1.90	0.53
1:A:1186:ASP:HA	1:A:1189:ILE:HD12	1.90	0.53
4:F:76:ASN:O	4:F:78:ARG:N	2.42	0.53
1:A:1056:MET:HA	1:A:1059:ILE:HD12	1.92	0.52
4:F:614:VAL:HB	4:F:618:ASP:O	2.08	0.52
4:F:163:TYR:O	4:F:221:PRO:HD3	2.09	0.52
4:F:256:MET:HB2	4:F:291:VAL:HG22	1.90	0.52
4:F:615:ASN:ND2	6:F:1203:NAG:O5	2.42	0.52
1:A:186:LEU:O	1:A:189:ILE:HG22	2.09	0.52
4:F:411:TYR:CE2	4:F:427:GLU:HG3	2.44	0.52
4:F:500:LYS:HE2	4:F:624:LEU:HD12	1.91	0.52
4:F:503:THR:OG1	4:F:511:ASN:OD1	2.15	0.52
6:F:1203:NAG:O6	6:F:1204:NAG:O7	2.27	0.52
1:A:186:LEU:HA	1:A:189:ILE:HG22	1.90	0.52
1:A:1336:LYS:C	1:A:1351:THR:HA	2.30	0.52
1:A:298:LEU:HA	1:A:314:PHE:HE2	1.74	0.52
1:A:581:PHE:HB2	1:A:597:PHE:CD2	2.45	0.52
1:A:997:PHE:HE1	1:A:1006:SER:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:595:LYS:HA	4:F:604:LYS:HA	1.90	0.52
1:A:993:ASN:O	1:A:995:PHE:N	2.36	0.52
1:A:1187:PHE:CE2	1:A:1191:ILE:HD11	2.43	0.52
4:F:188:THR:HG23	4:F:189:SER:N	2.24	0.52
4:F:427:GLU:HB3	4:F:431:VAL:HG23	1.91	0.52
1:A:661:VAL:O	1:A:664:LEU:HG	2.09	0.52
4:F:192:ASP:O	4:F:196:LYS:HG2	2.09	0.52
4:F:293:VAL:HG23	4:F:320:LEU:HD21	1.90	0.52
4:F:391:VAL:HG12	4:F:415:ILE:HB	1.91	0.52
1:A:1014:GLU:OE2	1:A:1324:ALA:HA	2.09	0.52
1:A:1334:TYR:CE1	1:A:1352:CYS:HA	2.44	0.52
1:A:1383:ASN:O	1:A:1387:LEU:N	2.25	0.52
4:F:393:GLN:OE1	4:F:393:GLN:N	2.43	0.52
1:A:1002:SER:O	1:A:1005:MET:HB3	2.10	0.52
4:F:178:SER:HB3	4:F:181:VAL:HG23	1.90	0.52
4:F:191:LEU:HD11	4:F:195:PHE:HE2	1.74	0.52
1:A:287:GLN:O	1:A:290:THR:OG1	2.17	0.52
1:A:962:LYS:O	1:A:964:THR:N	2.43	0.52
4:F:263:SER:OG	4:F:265:SER:OG	2.14	0.52
1:A:592:VAL:C	1:A:594:ARG:H	2.12	0.51
4:F:403:TRP:O	4:F:407:GLU:HB2	2.10	0.51
1:A:954:PHE:O	1:A:956:SER:N	2.43	0.51
1:A:1369:ALA:O	1:A:1373:ILE:HG13	2.09	0.51
2:B:227:ARG:NE	2:B:335:ALA:O	2.24	0.51
1:A:581:PHE:O	1:A:585:TYR:N	2.31	0.51
1:A:651:ILE:HA	1:A:654:ASN:ND2	2.25	0.51
1:A:1131:ASN:O	1:A:1135:LEU:HG	2.10	0.51
2:B:231:LEU:HD23	2:B:249:LEU:HD13	1.93	0.51
4:F:444:LYS:HD3	4:F:469:PHE:CE1	2.45	0.51
1:A:1019:LEU:HG	1:A:1045:PHE:CZ	2.46	0.51
2:B:387:LEU:HD11	2:B:399:LEU:HD22	1.93	0.51
4:F:208:GLN:HA	4:F:481:LEU:HD23	1.92	0.51
1:A:244:PRO:HA	1:A:304:ALA:HB2	1.92	0.51
4:F:167:ALA:HB3	4:F:218:ARG:HB2	1.92	0.51
4:F:192:ASP:HB3	4:F:196:LYS:HE3	1.91	0.51
4:F:242:ARG:HE	4:F:425:THR:CG2	2.24	0.51
4:F:886:UNK:N	4:F:889:UNK:O	2.43	0.51
2:B:263:ILE:HG12	2:B:317:VAL:HB	1.93	0.51
2:B:342:LYS:HE3	2:B:344:SER:HB2	1.93	0.51
4:F:352:SER:O	4:F:354:ALA:N	2.38	0.51
4:F:570:ASN:HD22	4:F:573:LYS:HE3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:243:ARG:NH1	4:F:455:ALA:H	2.10	0.50
4:F:266:VAL:HB	4:F:270:THR:HG23	1.92	0.50
2:B:348:VAL:O	2:B:352:LEU:HG	2.11	0.50
4:F:320:LEU:O	4:F:324:VAL:HG23	2.12	0.50
1:A:124:VAL:HA	1:A:127:PHE:HD2	1.76	0.50
4:F:309:LEU:C	4:F:311:GLN:H	2.13	0.50
1:A:958:ASN:HD22	1:A:989:GLN:H	1.59	0.50
1:A:128:ILE:O	1:A:131:PHE:HB3	2.11	0.50
1:A:369:TRP:HE1	2:B:245:MET:HG2	1.77	0.50
1:A:268:PRO:C	1:A:271:GLY:H	2.15	0.49
2:B:229:VAL:HB	2:B:317:VAL:HG22	1.94	0.49
2:B:252:PHE:HE2	2:B:400:ALA:HB2	1.78	0.49
4:F:99:LEU:HB3	4:F:466:LEU:CD2	2.42	0.49
4:F:576:ILE:HD13	4:F:609:TYR:OH	2.12	0.49
4:F:580:MET:HG2	4:F:611:TRP:CZ3	2.47	0.49
1:A:1020:LEU:O	1:A:1024:ILE:HG12	2.12	0.49
2:B:66:THR:HG22	2:B:220:TYR:HE1	1.76	0.49
4:F:274:ILE:HD11	4:F:363:PHE:HB2	1.92	0.49
4:F:312:ALA:O	4:F:314:VAL:N	2.43	0.49
1:A:61:ILE:O	1:A:64:ASN:HB2	2.13	0.49
1:A:1006:SER:O	1:A:1009:THR:OG1	2.16	0.49
2:B:93:LEU:HB3	2:B:118:ILE:HD13	1.93	0.49
4:F:313:ASN:O	4:F:317:LYS:HB3	2.12	0.49
4:F:505:ARG:HG3	4:F:619:TYR:HE1	1.77	0.49
1:A:663:ASN:HD22	1:A:1061:VAL:HG12	1.78	0.49
1:A:1048:TYR:CZ	1:A:1052:ILE:HD11	2.48	0.49
1:A:942:PHE:HA	1:A:945:ILE:HD12	1.95	0.49
1:A:1163:LEU:O	1:A:1167:LEU:HG	2.13	0.49
1:A:1234:PHE:O	1:A:1237:LEU:HB3	2.13	0.49
4:F:281:MET:O	4:F:285:LEU:N	2.45	0.49
4:F:73:GLU:C	4:F:632:TYR:H	2.16	0.49
4:F:99:LEU:HB3	4:F:466:LEU:HD23	1.95	0.49
4:F:61:ASP:O	4:F:65:LYS:N	2.42	0.49
4:F:1006:PHE:CD1	4:F:1012:MET:HG3	2.48	0.49
1:A:964:THR:HA	1:A:1030:ASP:O	2.13	0.49
1:A:1043:ILE:O	1:A:1047:ILE:HG13	2.12	0.49
4:F:99:LEU:HD21	4:F:481:LEU:HG	1.94	0.49
4:F:594:VAL:HG22	4:F:595:LYS:O	2.12	0.49
1:A:89:LEU:HG	1:A:93:PHE:CE2	2.48	0.48
1:A:647:CYS:O	1:A:650:TYR:HB3	2.13	0.48
1:A:1015:GLY:HA3	1:A:1326:GLN:HE22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:LEU:HD23	2:B:108:LEU:HA	1.94	0.48
2:B:227:ARG:NH2	2:B:336:PRO:O	2.46	0.48
4:F:109:VAL:HG12	4:F:187:TRP:HB2	1.94	0.48
4:F:214:THR:OG1	4:F:215:GLY:N	2.45	0.48
4:F:261:ASP:OD2	4:F:263:SER:OG	2.30	0.48
1:A:1127:LEU:HD13	1:A:1160:ILE:HG21	1.94	0.48
4:F:259:LEU:HD23	4:F:296:PHE:CE1	2.49	0.48
1:A:290:THR:HG21	1:A:616:TRP:HZ2	1.79	0.48
1:A:597:PHE:HE1	1:A:606:SER:HB3	1.78	0.48
1:A:1019:LEU:HG	1:A:1045:PHE:HZ	1.78	0.48
1:A:1144:GLU:O	1:A:1146:MET:N	2.46	0.48
4:F:461:VAL:HG13	4:F:483:ASN:O	2.13	0.48
1:A:581:PHE:HB2	1:A:597:PHE:HD2	1.78	0.48
2:B:326:PRO:HG3	2:B:383:PHE:CZ	2.49	0.48
2:B:340:TYR:HB2	2:B:383:PHE:CD1	2.49	0.48
4:F:186:ASN:HD21	6:F:1207:NAG:H2	1.79	0.48
4:F:238:TYR:OH	4:F:243:ARG:NH2	2.36	0.48
4:F:588:LYS:O	4:F:611:TRP:NE1	2.47	0.48
4:F:609:TYR:CB	4:F:624:LEU:HA	2.43	0.48
1:A:210:TYR:OH	1:A:320:LEU:HD12	2.13	0.48
4:F:308:HIS:HA	4:F:309:LEU:HD23	1.95	0.48
4:F:494:VAL:HA	4:F:497:GLU:OE2	2.13	0.48
4:F:518:ASP:HB2	4:F:1007:HIS:CD2	2.47	0.48
4:F:609:TYR:HB2	4:F:624:LEU:HA	1.96	0.48
4:F:88:ILE:O	4:F:92:LEU:HG	2.14	0.48
4:F:299:ASN:OD1	4:F:300:ALA:N	2.46	0.48
4:F:988:ASN:HD22	6:F:1205:NAG:C7	2.27	0.48
4:F:764:UNK:O	4:F:766:UNK:N	2.46	0.48
1:A:455:ASN:O	1:A:459:TRP:N	2.41	0.47
1:A:1147:ASN:O	1:A:1150:SER:OG	2.22	0.47
4:F:218:ARG:NH2	4:F:456:LEU:HD12	2.28	0.47
1:A:131:PHE:HZ	1:A:168:ARG:HH21	1.61	0.47
1:A:179:VAL:HB	1:A:182:LEU:HD12	1.96	0.47
4:F:358:LYS:O	4:F:384:VAL:HA	2.14	0.47
4:F:460:LEU:HD23	4:F:517:ILE:HG23	1.96	0.47
1:A:1476:UNK:O	1:A:1478:UNK:N	2.48	0.47
2:B:55:ALA:HA	2:B:58:LYS:HD2	1.96	0.47
4:F:606:ASN:O	4:F:627:PRO:CG	2.62	0.47
1:A:216:GLU:HG3	1:A:1240:VAL:HG21	1.97	0.47
1:A:606:SER:O	1:A:609:GLN:HB3	2.14	0.47
4:F:248:GLN:HE22	4:F:448:TRP:C	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:506:PHE:HB2	4:F:618:ASP:HB2	1.96	0.47
1:A:79:ASN:HA	4:F:332:ILE:HA	1.97	0.47
1:A:369:TRP:CD1	2:B:245:MET:HG2	2.50	0.47
1:A:964:THR:O	1:A:966:GLU:N	2.43	0.47
2:B:250:PHE:HE1	2:B:317:VAL:HG12	1.80	0.47
1:A:1193:SER:O	1:A:1197:VAL:HG23	2.14	0.46
4:F:271:LEU:HA	4:F:274:ILE:HG22	1.97	0.46
4:F:297:ASN:ND2	4:F:330:LYS:O	2.48	0.46
4:F:673:UNK:O	4:F:677:UNK:N	2.47	0.46
1:A:61:ILE:HA	1:A:64:ASN:OD1	2.15	0.46
2:B:349:LEU:HA	2:B:352:LEU:HD12	1.98	0.46
4:F:988:ASN:ND2	6:F:1205:NAG:O7	2.48	0.46
1:A:1009:THR:O	1:A:1012:THR:OG1	2.22	0.46
1:A:1066:VAL:O	1:A:1070:GLU:N	2.42	0.46
4:F:1000:GLY:O	4:F:1001:ASN:ND2	2.48	0.46
4:F:1006:PHE:HD1	4:F:1012:MET:HG3	1.79	0.46
4:F:485:LEU:O	4:F:489:VAL:HG23	2.15	0.46
4:F:524:LEU:HD21	4:F:1033:LEU:N	2.31	0.46
1:A:369:TRP:NE1	2:B:245:MET:HG2	2.29	0.46
4:F:195:PHE:O	4:F:199:ARG:HG3	2.16	0.46
4:F:263:SER:HA	4:F:297:ASN:HD22	1.81	0.46
4:F:281:MET:SD	4:F:363:PHE:HZ	2.39	0.46
4:F:492:VAL:HG13	4:F:501:ARG:NH1	2.30	0.46
4:F:1063:PHE:HA	4:F:1064:ASP:HA	1.64	0.46
1:A:435:TYR:HA	1:A:436:TRP:HA	1.69	0.46
1:A:649:ASN:O	1:A:653:LEU:HG	2.15	0.46
2:B:107:ARG:HB3	2:B:115:ILE:HD13	1.97	0.46
1:A:131:PHE:CE1	1:A:164:LEU:HB3	2.50	0.46
1:A:210:TYR:O	1:A:214:GLY:N	2.37	0.46
1:A:363:LEU:O	1:A:367:MET:HG2	2.16	0.46
1:A:631:SER:OG	1:A:633:PRO:HD2	2.16	0.46
4:F:524:LEU:HD21	4:F:1033:LEU:H	1.81	0.46
1:A:245:CYS:O	1:A:264:GLY:HA2	2.16	0.46
1:A:958:ASN:HA	1:A:959:ASP:HA	1.68	0.46
2:B:65:ARG:N	2:B:221:ASP:O	2.31	0.46
4:F:595:LYS:HB2	6:F:1212:NAG:H83	1.98	0.46
1:A:124:VAL:O	1:A:128:ILE:HG12	2.16	0.46
1:A:326:LEU:O	1:A:330:LEU:HG	2.16	0.46
2:B:237:LYS:H	2:B:324:ASN:ND2	2.10	0.46
2:B:393:GLU:O	2:B:397:GLU:HG2	2.16	0.46
4:F:254:LYS:HA	4:F:357:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:254:LYS:HG2	4:F:357:ASN:HD21	1.80	0.45
4:F:512:GLY:O	4:F:514:TYR:N	2.43	0.45
4:F:617:THR:HG22	4:F:618:ASP:OD1	2.16	0.45
4:F:858:UNK:O	4:F:862:UNK:HG2	2.17	0.45
1:A:1015:GLY:HA3	1:A:1326:GLN:NE2	2.31	0.45
1:A:290:THR:HG21	1:A:616:TRP:CZ2	2.51	0.45
1:A:1151:ASP:O	1:A:1155:VAL:HG23	2.17	0.45
4:F:509:CYS:N	4:F:561:LEU:O	2.49	0.45
4:F:587:GLU:O	4:F:589:THR:HG23	2.16	0.45
1:A:614:GLU:OE2	1:A:615:ASP:HB2	2.16	0.45
1:A:1272:LEU:O	1:A:1276:MET:N	2.44	0.45
1:A:1487:UNK:O	1:A:1491:UNK:N	2.50	0.45
4:F:505:ARG:HG3	4:F:619:TYR:CE1	2.52	0.45
4:F:576:ILE:HD11	4:F:590:PHE:CZ	2.52	0.45
4:F:591:ARG:HB3	4:F:608:THR:HG22	1.99	0.45
1:A:73:PRO:HA	1:A:74:MET:HA	1.55	0.45
1:A:620:MET:O	1:A:624:ILE:HD12	2.16	0.45
1:A:1142:GLN:HA	1:A:1143:SER:HA	1.63	0.45
4:F:336:LYS:HB3	4:F:374:ILE:HD11	1.98	0.45
1:A:969:ARG:HH21	4:F:177:GLY:HA3	1.81	0.45
1:A:1057:MET:O	1:A:1061:VAL:HG23	2.17	0.45
4:F:219:TYR:O	4:F:220:TYR:CG	2.69	0.45
4:F:449:THR:CG2	4:F:463:THR:H	2.26	0.45
4:F:568:LEU:HD12	4:F:596:SER:HA	1.97	0.45
1:A:1372:ILE:HG22	1:A:1376:PHE:CE2	2.52	0.45
4:F:102:LEU:HG	4:F:199:ARG:NH2	2.32	0.45
4:F:130:LYS:N	4:F:141:GLU:O	2.49	0.45
2:B:66:THR:HG22	2:B:220:TYR:CE1	2.52	0.45
4:F:186:ASN:OD1	6:F:1207:NAG:H2	2.16	0.45
4:F:285:LEU:HD23	4:F:286:SER:O	2.17	0.45
4:F:290:PHE:N	4:F:290:PHE:CD1	2.83	0.45
1:A:204:LEU:O	1:A:208:ILE:N	2.50	0.44
1:A:1033:PRO:HA	1:A:1034:VAL:HA	1.74	0.44
4:F:224:PRO:HA	4:F:225:TRP:HA	1.60	0.44
1:A:1329:LEU:HD11	1:A:1358:TYR:CD1	2.52	0.44
2:B:329:LEU:O	2:B:332:THR:OG1	2.23	0.44
4:F:86:ARG:HG2	4:F:90:LYS:HE3	2.00	0.44
4:F:333:THR:HG22	4:F:335:TYR:HB2	1.98	0.44
1:A:930:ASN:O	1:A:934:VAL:HG23	2.17	0.44
1:A:1195:ILE:O	1:A:1199:LEU:HG	2.16	0.44
1:A:1302:ARG:O	1:A:1305:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:184:GLU:O	4:F:188:THR:HG22	2.17	0.44
2:B:65:ARG:HB3	2:B:221:ASP:HB2	2.00	0.44
4:F:509:CYS:SG	4:F:560:THR:HA	2.58	0.44
4:F:1007:HIS:CG	4:F:1008:VAL:H	2.36	0.44
1:A:664:LEU:O	1:A:668:GLU:N	2.45	0.44
1:A:1233:ALA:HB2	1:A:1236:ARG:HH21	1.83	0.44
4:F:453:LEU:HB2	4:F:557:GLU:OE2	2.18	0.44
1:A:286:TYR:O	1:A:290:THR:HG23	2.18	0.44
4:F:487:LEU:HD22	4:F:490:MET:SD	2.58	0.44
1:A:205:PHE:O	1:A:209:ILE:N	2.40	0.43
4:F:123:GLU:HA	4:F:124:VAL:HA	1.74	0.43
4:F:334:ASP:HB3	4:F:337:LYS:HB2	1.99	0.43
4:F:343:PHE:O	4:F:347:LEU:N	2.51	0.43
1:A:1123:LEU:O	1:A:1127:LEU:HG	2.17	0.43
1:A:366:TYR:HD2	2:B:348:VAL:HG11	1.82	0.43
1:A:647:CYS:O	1:A:651:ILE:HG13	2.18	0.43
4:F:462:ILE:HG13	4:F:485:LEU:HD11	2.00	0.43
1:A:631:SER:OG	1:A:632:TYR:N	2.41	0.43
1:A:942:PHE:HD1	1:A:1044:PHE:CE1	2.36	0.43
4:F:297:ASN:C	4:F:299:ASN:N	2.70	0.43
1:A:1314:LEU:O	1:A:1317:PHE:N	2.48	0.43
2:B:229:VAL:HB	2:B:317:VAL:HA	2.01	0.43
4:F:98:ALA:HB1	4:F:199:ARG:NE	2.31	0.43
4:F:117:GLU:O	4:F:119:PHE:N	2.51	0.43
4:F:196:LYS:HB3	4:F:196:LYS:HE2	1.81	0.43
2:B:55:ALA:HB1	2:B:105:ILE:HG21	2.01	0.43
4:F:600:ARG:HA	4:F:600:ARG:HD3	1.65	0.43
1:A:194:LEU:O	1:A:196:LEU:N	2.48	0.43
1:A:1185:PHE:HA	1:A:1188:LEU:HD12	2.00	0.43
2:B:353:ILE:HB	2:B:364:LEU:HD13	1.99	0.43
4:F:271:LEU:HD11	4:F:327:ILE:HG23	2.00	0.43
1:A:1046:ILE:O	1:A:1050:ILE:HG13	2.19	0.43
2:B:329:LEU:HB3	2:B:336:PRO:HG3	2.01	0.43
2:B:412:PRO:HA	2:B:413:PRO:HD3	1.92	0.43
1:A:90:GLU:HA	1:A:93:PHE:HD2	1.83	0.43
1:A:458:LEU:O	1:A:462:HIS:N	2.31	0.43
1:A:631:SER:H	1:A:635:VAL:HG23	1.83	0.43
3:E:125:ALA:O	3:E:129:PHE:N	2.52	0.43
4:F:334:ASP:O	4:F:336:LYS:N	2.51	0.43
1:A:1063:PHE:O	1:A:1067:THR:HG23	2.18	0.43
3:E:158:MET:O	3:E:162:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:465:THR:HG22	4:F:480:ASN:HB3	2.01	0.43
4:F:92:LEU:HD22	4:F:448:TRP:CH2	2.54	0.42
4:F:302:ASP:HB2	4:F:306:PHE:CE1	2.42	0.42
1:A:226:CYS:N	1:A:274:HIS:HE2	2.17	0.42
4:F:96:SER:O	4:F:100:VAL:HG23	2.19	0.42
4:F:248:GLN:NE2	4:F:448:TRP:O	2.35	0.42
4:F:461:VAL:HG13	4:F:483:ASN:C	2.39	0.42
1:A:958:ASN:ND2	1:A:989:GLN:H	2.16	0.42
1:A:1318:ARG:CZ	1:A:1328:ILE:HD11	2.49	0.42
4:F:390:SER:HB2	4:F:414:GLU:HG2	2.01	0.42
4:F:622:LEU:HD12	4:F:623:ALA:H	1.83	0.42
1:A:1008:PHE:O	1:A:1011:SER:HB3	2.19	0.42
4:F:113:HIS:O	4:F:115:TRP:N	2.39	0.42
4:F:564:LEU:HD13	4:F:574:VAL:HG22	2.01	0.42
1:A:1239:ARG:HG3	1:A:1242:ARG:NH2	2.33	0.42
2:B:326:PRO:HB3	2:B:338:ILE:HG21	2.01	0.42
4:F:335:TYR:CE2	4:F:339:PHE:HE2	2.37	0.42
4:F:596:SER:C	4:F:602:ILE:HG23	2.40	0.42
4:F:609:TYR:HB2	4:F:623:ALA:O	2.19	0.42
4:F:868:UNK:HA	4:F:869:UNK:HA	1.76	0.42
1:A:282:MET:HG2	1:A:286:TYR:CE2	2.55	0.42
4:F:86:ARG:O	4:F:90:LYS:HG3	2.20	0.42
4:F:236:ASP:OD1	4:F:238:TYR:HB3	2.19	0.42
1:A:88:LYS:O	1:A:91:TYR:HB3	2.20	0.42
1:A:1178:PHE:O	1:A:1180:ASP:N	2.53	0.42
4:F:107:GLU:OE2	4:F:444:LYS:NZ	2.53	0.42
4:F:470:ASN:HD22	4:F:473:GLY:N	2.14	0.42
4:F:485:LEU:HD23	4:F:485:LEU:HA	1.68	0.42
1:A:87:GLU:HA	1:A:90:GLU:OE1	2.20	0.42
1:A:89:LEU:O	1:A:92:PHE:HB3	2.20	0.42
1:A:210:TYR:HD2	1:A:313:TYR:CE1	2.37	0.42
4:F:359:ILE:CB	4:F:385:ARG:HB2	2.49	0.42
4:F:595:LYS:HB3	4:F:602:ILE:HG21	2.02	0.42
4:F:614:VAL:HG12	4:F:616:GLY:N	2.32	0.41
1:A:943:ALA:HB1	1:A:1000:VAL:HG13	2.02	0.41
1:A:1069:GLN:O	1:A:1073:GLU:N	2.49	0.41
4:F:248:GLN:NE2	4:F:447:GLN:O	2.53	0.41
4:F:528:ASN:O	4:F:531:PRO:HD2	2.20	0.41
1:A:357:GLN:O	1:A:361:GLU:HG2	2.19	0.41
1:A:589:ASP:HA	1:A:590:THR:HA	1.81	0.41
4:F:256:MET:SD	4:F:359:ILE:HD11	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:TRP:HA	1:A:311:TRP:NE1	2.35	0.41
1:A:321:GLY:O	1:A:325:ILE:HG23	2.20	0.41
1:A:937:LEU:HA	1:A:940:PHE:HD2	1.84	0.41
1:A:1375:LEU:O	1:A:1379:VAL:HG23	2.20	0.41
4:F:626:LEU:C	4:F:628:THR:N	2.73	0.41
1:A:1184:VAL:O	1:A:1188:LEU:HG	2.20	0.41
4:F:304:SER:O	4:F:305:CYS:SG	2.79	0.41
4:F:488:GLY:O	4:F:492:VAL:HG23	2.20	0.41
4:F:489:VAL:HA	4:F:492:VAL:HB	2.02	0.41
4:F:505:ARG:HG2	4:F:506:PHE:N	2.36	0.41
1:A:1119:TYR:O	1:A:1123:LEU:HG	2.21	0.41
1:A:1293:ALA:N	1:A:1338:CYS:O	2.54	0.41
1:A:1410:UNK:O	1:A:1412:UNK:N	2.53	0.41
4:F:85:ALA:O	4:F:89:GLU:HG3	2.21	0.41
4:F:609:TYR:CG	4:F:624:LEU:HD23	2.55	0.41
1:A:169:VAL:O	1:A:172:PRO:HD2	2.20	0.41
1:A:936:THR:O	1:A:939:GLN:HB2	2.21	0.41
4:F:356:CYS:O	4:F:358:LYS:NZ	2.51	0.41
4:F:356:CYS:O	4:F:358:LYS:HG3	2.20	0.41
4:F:411:TYR:HB3	4:F:431:VAL:HG21	2.03	0.41
1:A:595:SER:HB3	1:A:605:ILE:HD11	2.03	0.41
1:A:969:ARG:HD2	4:F:177:GLY:HA3	2.03	0.41
4:F:292:ASN:OD1	4:F:308:HIS:HB3	2.20	0.41
4:F:437:VAL:HA	4:F:469:PHE:CE2	2.43	0.41
4:F:606:ASN:C	4:F:627:PRO:HG3	2.41	0.41
1:A:1166:ILE:O	1:A:1170:LEU:HG	2.21	0.41
1:A:1372:ILE:HA	1:A:1375:LEU:HD12	2.03	0.41
4:F:335:TYR:CE2	4:F:371:ALA:HB2	2.56	0.41
4:F:444:LYS:HD3	4:F:469:PHE:HE1	1.85	0.41
4:F:505:ARG:HB3	4:F:508:LEU:O	2.20	0.41
1:A:627:TYR:CD2	1:A:637:VAL:HG21	2.56	0.41
2:B:340:TYR:HD2	2:B:386:ILE:HG12	1.86	0.41
3:E:199:LEU:O	3:E:203:SER:N	2.53	0.41
6:F:1209:NAG:O3	7:F:1217:BMA:O5	2.27	0.41
1:A:370:ILE:HD11	2:B:352:LEU:HB3	2.03	0.40
1:A:1016:TRP:N	1:A:1017:PRO:HD2	2.35	0.40
4:F:115:TRP:HA	4:F:183:ASN:OD1	2.21	0.40
4:F:175:TYR:O	4:F:177:GLY:N	2.54	0.40
4:F:460:LEU:H	4:F:460:LEU:HG	1.66	0.40
4:F:500:LYS:HZ1	4:F:502:LEU:HD22	1.86	0.40
1:A:165:ARG:O	1:A:168:ARG:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:282:LEU:HD23	4:F:282:LEU:HA	1.85	0.40
1:A:632:TYR:H	1:A:633:PRO:HD2	1.86	0.40
1:A:1245:LYS:O	1:A:1248:SER:HB2	2.21	0.40
1:A:1316:LEU:HD11	1:A:1360:TYR:OH	2.20	0.40
4:F:195:PHE:HA	4:F:198:ASN:ND2	2.37	0.40
1:A:521:PRO:HA	1:A:522:LEU:HA	1.59	0.40
1:A:642:ILE:O	1:A:646:VAL:HB	2.21	0.40
4:F:554:LYS:O	4:F:555:SER:OG	2.31	0.40
4:F:568:LEU:HD11	4:F:597:GLN:H	1.87	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	1084/1873 (58%)	936 (86%)	75 (7%)	73 (7%)	1 15
2	B	272/356 (76%)	261 (96%)	11 (4%)	0	100 100
3	E	132/222 (60%)	127 (96%)	2 (2%)	3 (2%)	5 31
4	F	617/1106 (56%)	461 (75%)	83 (14%)	73 (12%)	0 5
All	All	2105/3557 (59%)	1785 (85%)	171 (8%)	149 (7%)	2 13

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	39	PRO
1	A	74	MET
1	A	75	PRO
1	A	242	PRO
1	A	244	PRO

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Mol	Chain	Res	Type
1	A	248	THR
1	A	253	PRO
1	A	266	PRO
1	A	268	PRO
1	A	305	ILE
1	A	518	ALA
1	A	1033	PRO
1	A	1035	TYR
1	A	1106	PRO
1	A	1295	VAL
1	A	1307	GLN
1	A	1340	PRO
1	A	1346	PRO
3	E	130	ARG
4	F	56	VAL
4	F	73	GLU
4	F	74	PRO
4	F	117	GLU
4	F	121	SER
4	F	134	ASP
4	F	142	PRO
4	F	305	CYS
4	F	351	VAL
4	F	510	PRO
4	F	618	ASP
4	F	629	TYR
4	F	630	SER
4	F	638	ILE
4	F	1008	VAL
4	F	1035	ILE
4	F	1036	GLN
4	F	1046	PRO
4	F	1053	PRO
1	A	35	THR
1	A	50	TRP
1	A	51	LYS
1	A	78	ASP
1	A	107	ALA
1	A	262	ARG
1	A	263	GLY
1	A	273	THR
1	A	276	ASP

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Mol	Chain	Res	Type
1	A	589	ASP
1	A	632	TYR
1	A	891	SER
1	A	962	LYS
1	A	963	MET
1	A	966	GLU
1	A	1138	GLN
1	A	1141	HIS
1	A	1173	LYS
3	E	205	PRO
4	F	72	VAL
4	F	77	ALA
4	F	138	ASN
4	F	141	GLU
4	F	264	GLY
4	F	308	HIS
4	F	314	VAL
4	F	347	LEU
4	F	349	TYR
4	F	356	CYS
4	F	409	LYS
4	F	441	ASP
4	F	458	LEU
4	F	470	ASN
4	F	520	ASN
4	F	522	TYR
4	F	639	GLU
4	F	1043	GLY
4	F	1062	CYS
1	A	79	ASN
1	A	131	PHE
1	A	234	VAL
1	A	251	GLY
1	A	466	ILE
1	A	468	ASN
1	A	541	TYR
1	A	631	SER
1	A	892	VAL
1	A	978	GLY
1	A	1145	GLU
1	A	1179	GLY
1	A	1293	ALA

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Mol	Chain	Res	Type
1	A	1341	GLU
1	A	1345	ALA
1	A	1357	ALA
3	E	131	LYS
4	F	118	ASP
4	F	125	VAL
4	F	164	GLN
4	F	265	SER
4	F	335	TYR
4	F	394	HIS
4	F	438	LEU
4	F	475	PHE
4	F	525	LEU
4	F	555	SER
4	F	571	ASP
4	F	1032	ARG
4	F	1037	ALA
4	F	1050	VAL
1	A	36	LEU
1	A	196	LEU
1	A	252	ARG
1	A	261	CYS
1	A	644	LEU
1	A	949	LEU
1	A	1171	ALA
1	A	1302	ARG
1	A	1349	GLU
4	F	163	TYR
4	F	251	ALA
4	F	311	GLN
4	F	330	LYS
4	F	353	ARG
4	F	557	GLU
4	F	627	PRO
4	F	1010	LYS
4	F	1047	CYS
1	A	241	LYS
1	A	254	CYS
1	A	258	GLY
1	A	308	GLU
1	A	977	ASP
1	A	994	ASP

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Mol	Chain	Res	Type
4	F	186	ASN
4	F	348	ASN
4	F	380	LYS
4	F	495	SER
4	F	1007	HIS
1	A	837	ILE
1	A	866	ASN
4	F	137	LYS
4	F	220	TYR
4	F	395	ASN
1	A	1339	ASP
4	F	310	VAL
4	F	499	ILE
1	A	1253	VAL
4	F	634	ILE
4	F	327	ILE
1	A	73	PRO

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	430/1519 (28%)	428 (100%)	2 (0%)	86 90
2	B	240/315 (76%)	240 (100%)	0	100 100
3	E	3/192 (2%)	3 (100%)	0	100 100
4	F	417/706 (59%)	414 (99%)	3 (1%)	81 86
All	All	1090/2732 (40%)	1085 (100%)	5 (0%)	85 90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	ARG
1	A	1070	GLU
4	F	359	ILE
4	F	626	LEU

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Mol	Chain	Res	Type
4	F	628	THR

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

Mol	Chain	Res	Type
1	A	579	GLN
1	A	654	ASN
1	A	663	ASN
1	A	958	ASN
1	A	1131	ASN
2	B	67	ASN
2	B	314	GLN
2	B	324	ASN
2	B	363	HIS
4	F	316	ASN
4	F	570	ASN
4	F	615	ASN
4	F	1007	HIS
4	F	1013	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	F	1213	-	14,14,15	0.30	0	17,19,21	0.37	0
7	BMA	F	1216	-	11,11,12	0.56	0	15,15,17	0.76	0
6	NAG	F	1207	-	14,14,15	0.25	0	17,19,21	0.44	0
6	NAG	F	1212	-	14,14,15	0.25	0	17,19,21	0.44	0
6	NAG	F	1208	-	14,14,15	0.29	0	17,19,21	0.44	0
6	NAG	F	1210	-	14,14,15	0.27	0	17,19,21	0.39	0
6	NAG	F	1215	-	14,14,15	0.29	0	17,19,21	0.48	0
6	NAG	F	1206	-	14,14,15	0.28	0	17,19,21	0.40	0
7	BMA	F	1217	-	11,11,12	0.63	0	15,15,17	0.70	0
6	NAG	F	1202	-	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	F	1205	-	14,14,15	0.23	0	17,19,21	0.40	0
6	NAG	F	1201	-	14,14,15	0.24	0	17,19,21	0.55	0
6	NAG	F	1209	-	14,14,15	0.27	0	17,19,21	0.39	0
6	NAG	F	1204	-	14,14,15	0.22	0	17,19,21	0.51	0
6	NAG	F	1203	-	14,14,15	0.31	0	17,19,21	0.36	0
6	NAG	F	1211	-	14,14,15	0.26	0	17,19,21	0.37	0
6	NAG	F	1214	-	14,14,15	0.31	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1213	-	-	0/6/23/26	0/1/1/1
7	BMA	F	1216	-	-	0/2/19/22	0/1/1/1
6	NAG	F	1207	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1212	-	-	1/6/23/26	0/1/1/1
6	NAG	F	1208	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1210	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1215	-	-	3/6/23/26	0/1/1/1
6	NAG	F	1206	-	-	0/6/23/26	0/1/1/1
7	BMA	F	1217	-	-	0/2/19/22	0/1/1/1
6	NAG	F	1202	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1205	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1201	-	-	3/6/23/26	0/1/1/1
6	NAG	F	1209	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1204	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1203	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1211	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1214	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1201	NAG	O5-C5-C6-O6
6	F	1205	NAG	O5-C5-C6-O6
6	F	1203	NAG	C4-C5-C6-O6
6	F	1202	NAG	O5-C5-C6-O6
6	F	1207	NAG	O5-C5-C6-O6
6	F	1209	NAG	O5-C5-C6-O6
6	F	1211	NAG	O5-C5-C6-O6
6	F	1205	NAG	C4-C5-C6-O6
6	F	1203	NAG	O5-C5-C6-O6
6	F	1202	NAG	C4-C5-C6-O6
6	F	1209	NAG	C4-C5-C6-O6
6	F	1207	NAG	C4-C5-C6-O6
6	F	1201	NAG	C4-C5-C6-O6
6	F	1214	NAG	O5-C5-C6-O6
6	F	1215	NAG	C4-C5-C6-O6
6	F	1211	NAG	C4-C5-C6-O6
6	F	1215	NAG	O5-C5-C6-O6
6	F	1214	NAG	C4-C5-C6-O6
6	F	1215	NAG	C3-C2-N2-C7
6	F	1212	NAG	O5-C5-C6-O6
6	F	1201	NAG	C3-C2-N2-C7
6	F	1209	NAG	C1-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1207	NAG	2	0
6	F	1212	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1217	BMA	2	0
6	F	1205	NAG	2	0
6	F	1209	NAG	2	0
6	F	1204	NAG	2	0
6	F	1203	NAG	3	0
6	F	1211	NAG	1	0

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.

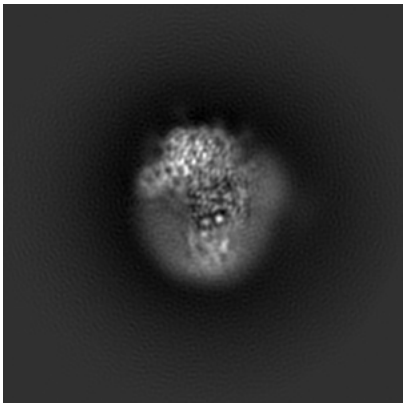
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6475. These allow visual inspection of the internal detail of the map and identification of artifacts.

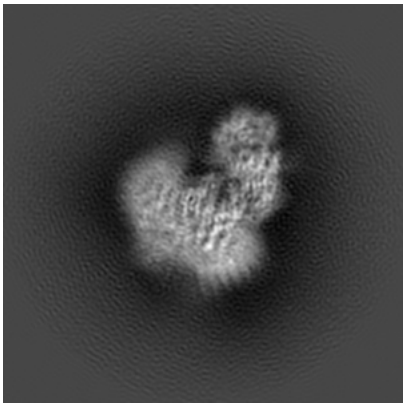
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

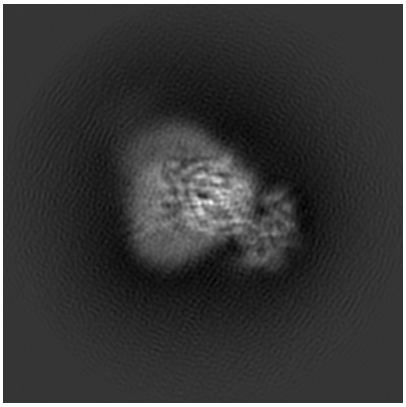
6.1.1 Primary map



X



Y

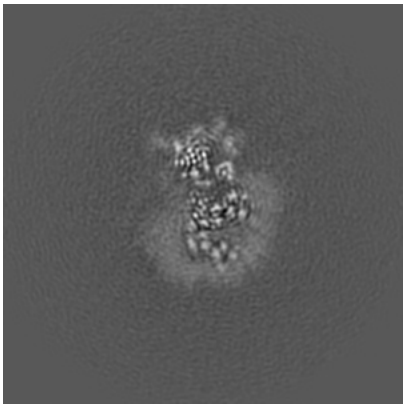


Z

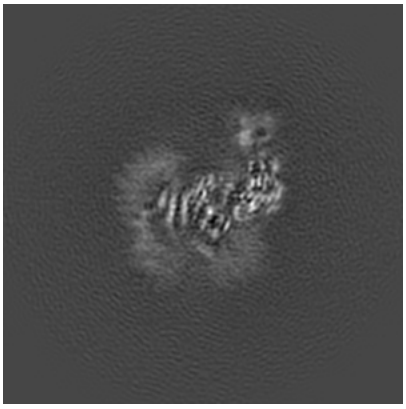
The images above show the map projected in three orthogonal directions.

6.2 Central slices

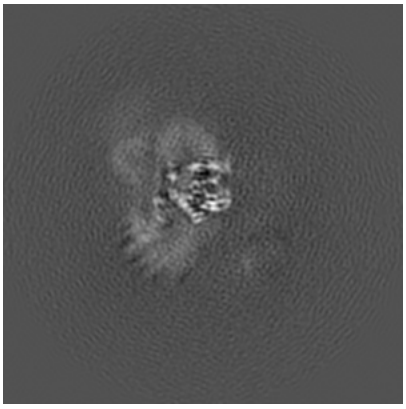
6.2.1 Primary map



X Index: 128



Y Index: 128

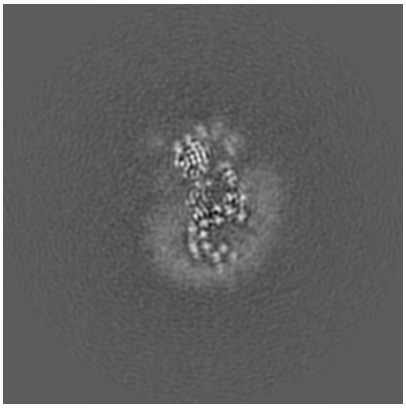


Z Index: 128

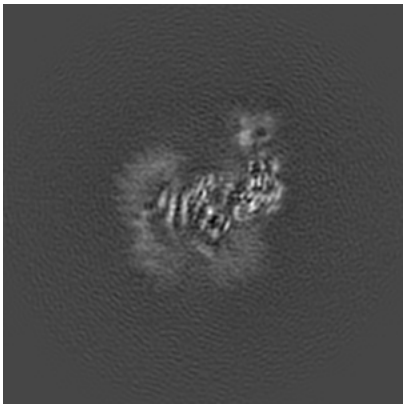
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

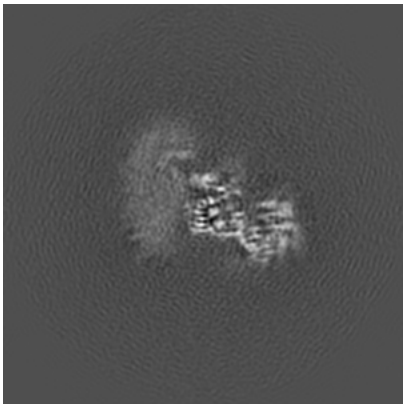
6.3.1 Primary map



X Index: 126



Y Index: 128

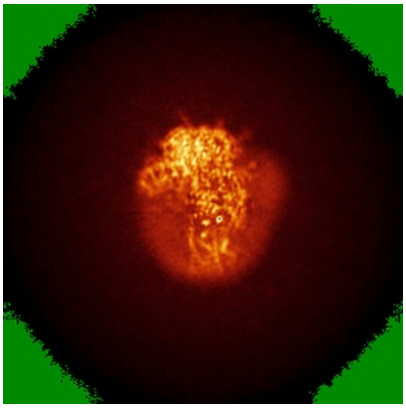


Z Index: 153

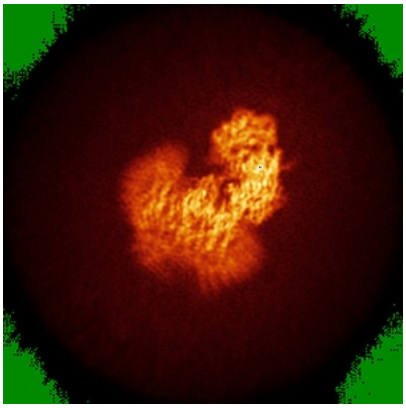
The images above show the largest variance slices of the map in three orthogonal directions.

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

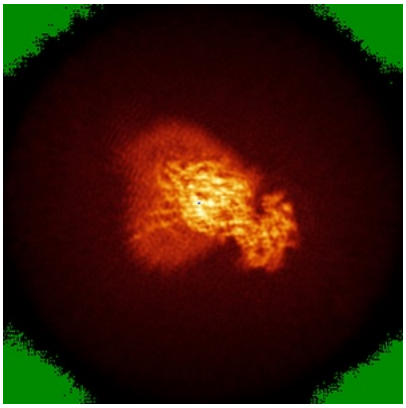
6.4.1 Primary map



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

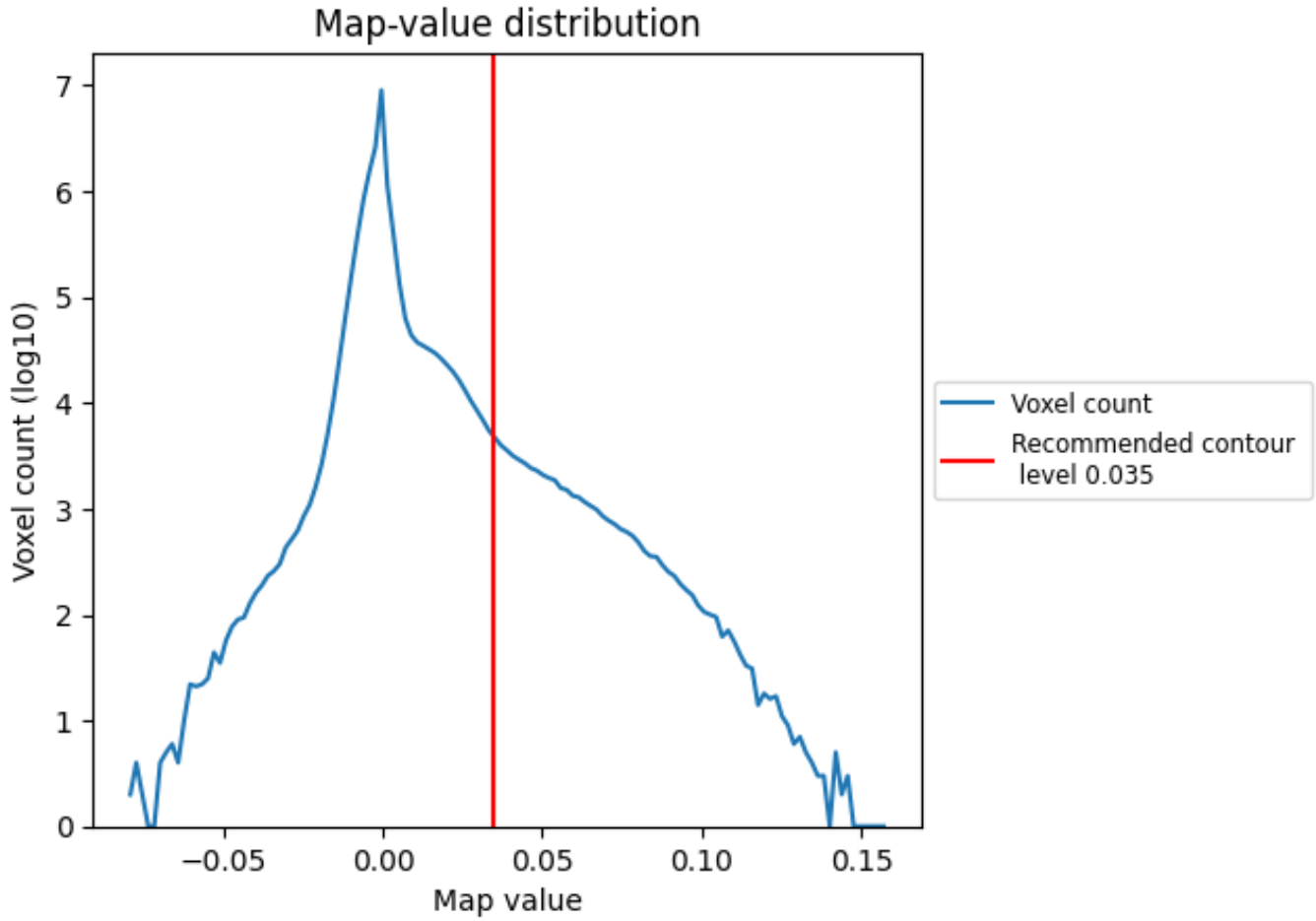
6.6 Mask visualisation (i)

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

7 Map analysis

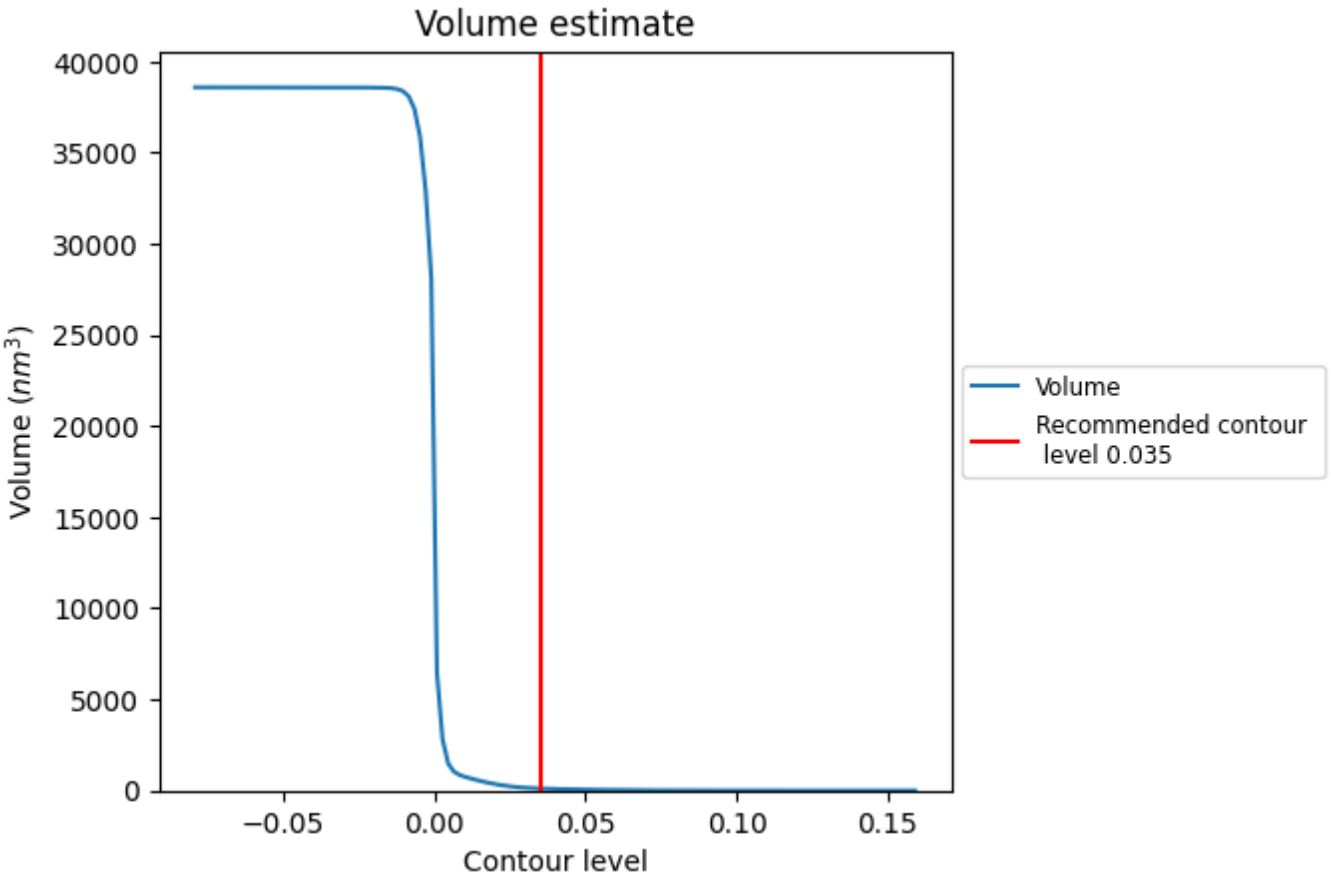
This section contains the results of statistical analysis of the map.

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.

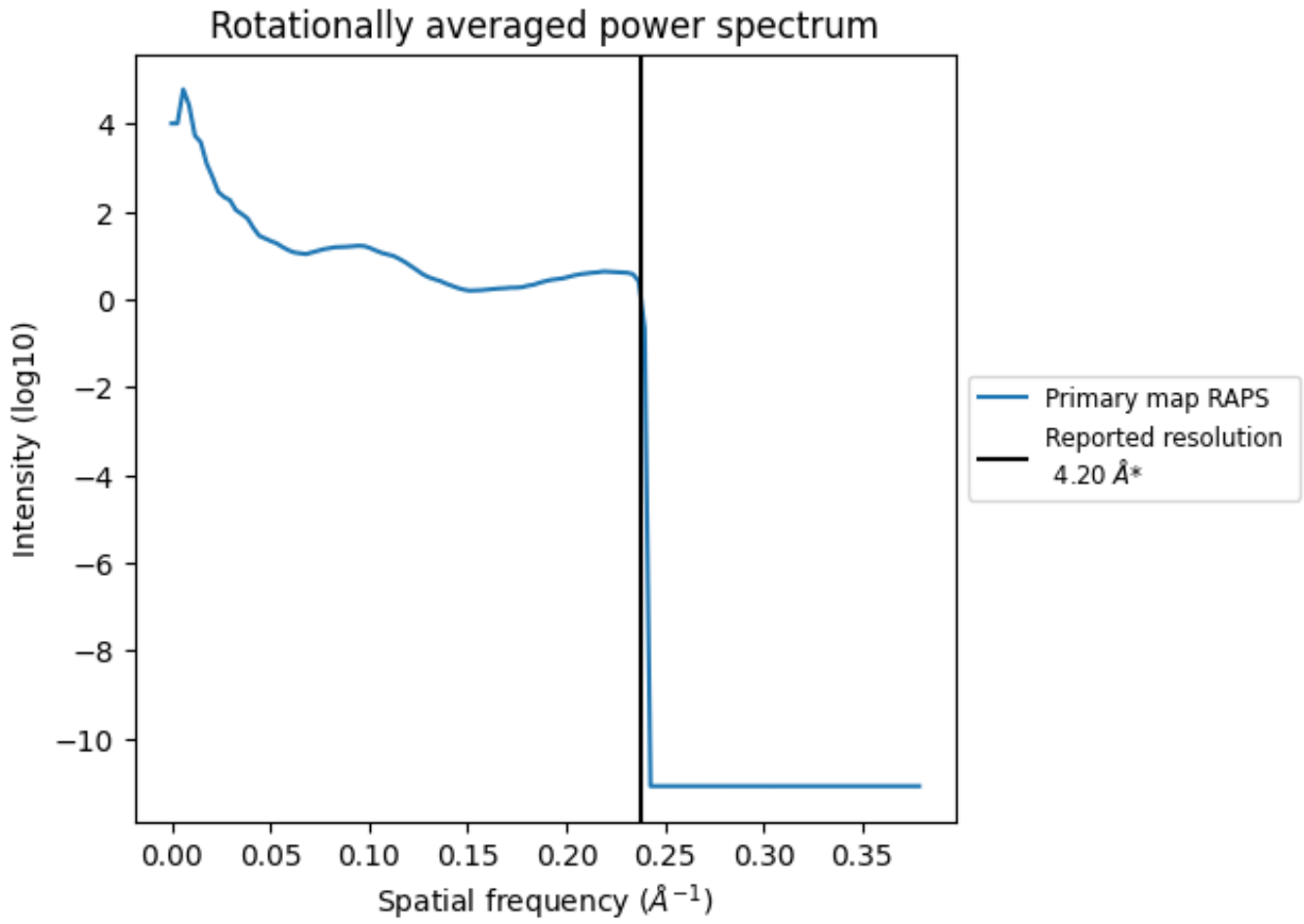
7.2 Volume estimate



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 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 0.238 Å^{-1}

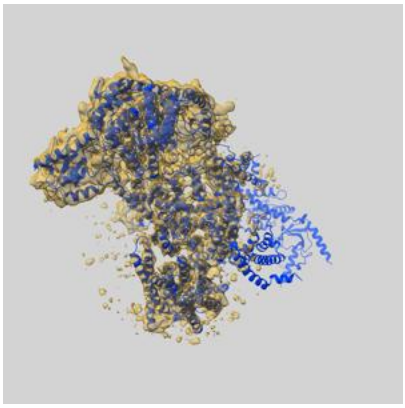
8 Fourier-Shell correlation (i)

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

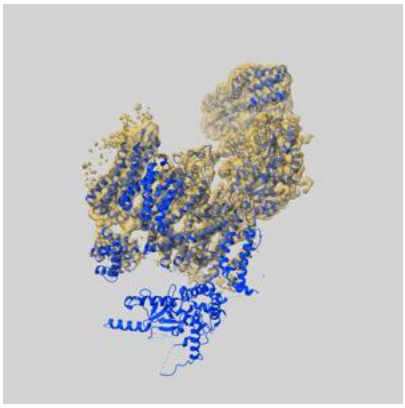
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6475 and PDB model 3JBR. Per-residue inclusion information can be found in section 3 on page 6.

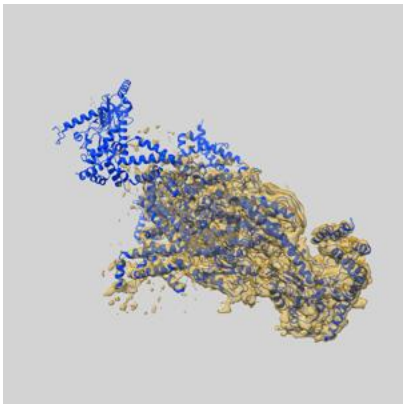
9.1 Map-model overlay



X



Y



Z

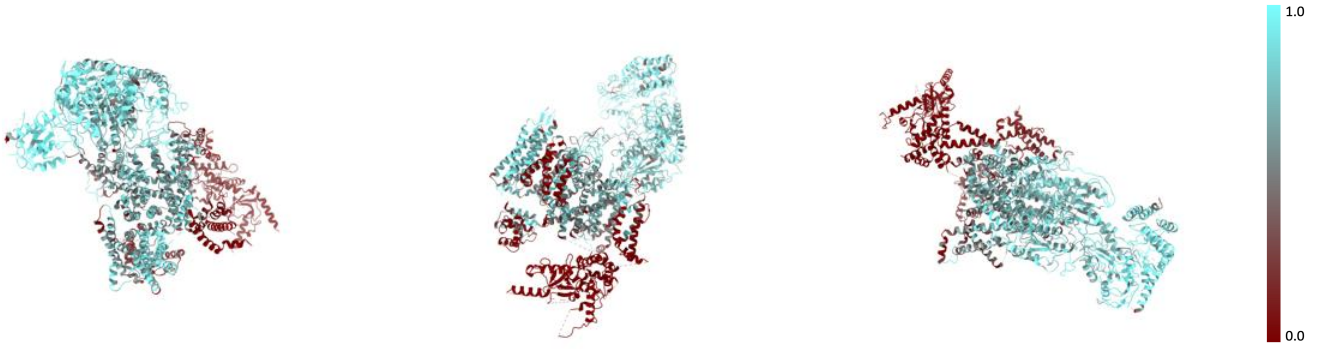
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

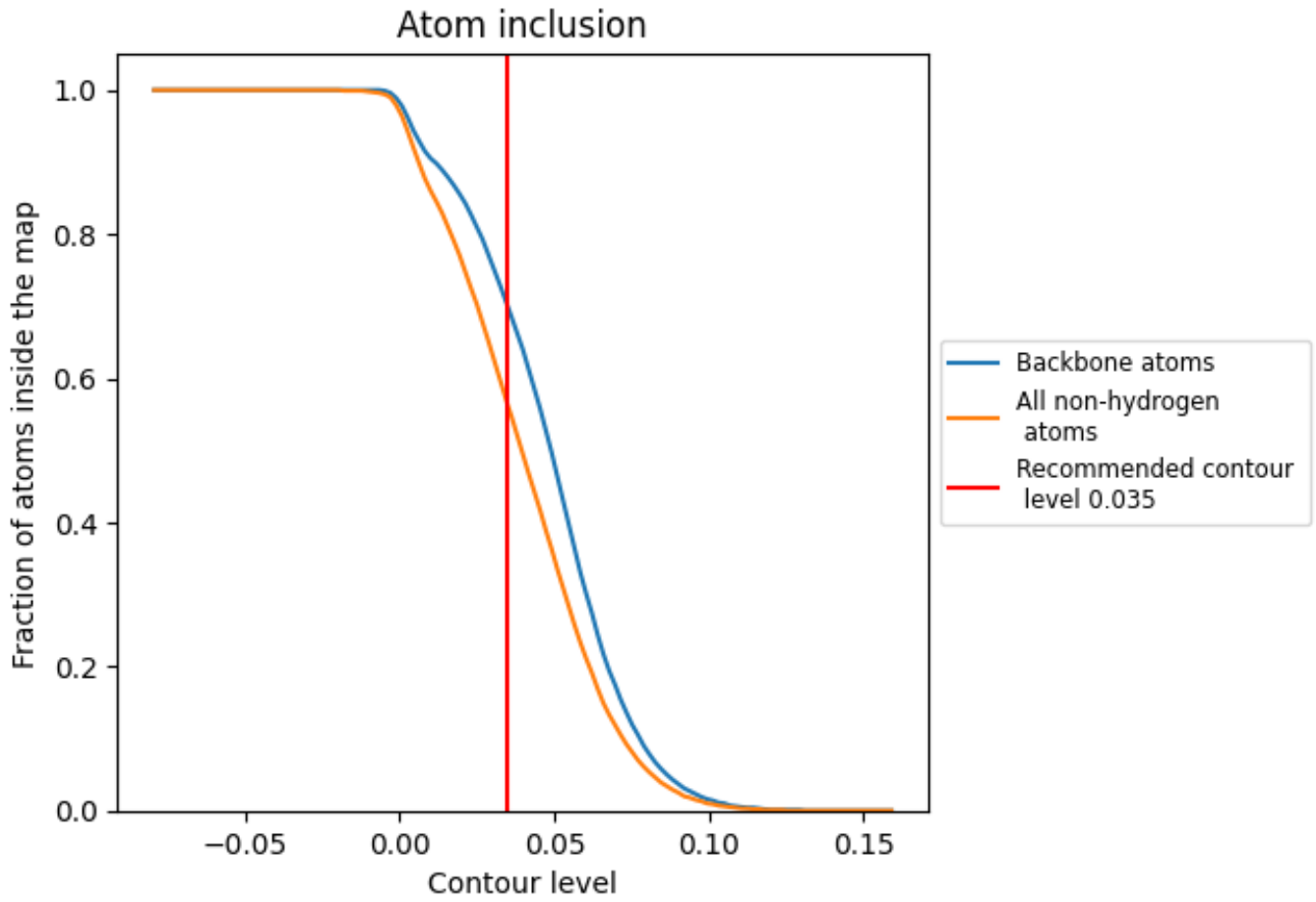
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5630	0.2980
A	0.5290	0.3090
B	0.0000	0.0640
E	0.7570	0.2800
F	0.7910	0.3730