Full wwPDB EM Validation Report

Mar 4, 2024 – 02:52 PM EST

PDB ID	:	8EZQ
EMDB ID	:	EMD-28748
Title	:	Cryo-EM structure of the S. cerevisiae guanine nucleotide exchange factor Gea2
Authors	:	Duan, H.D.; Li, H.
Deposited on	:	2022-11-01
Resolution	:	3.70 Å(reported)

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

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

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

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

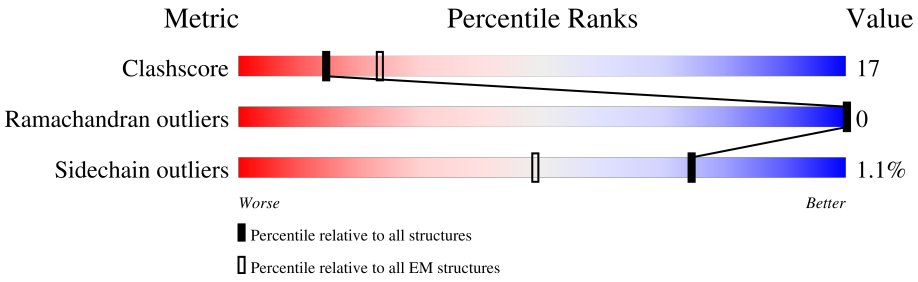
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1483	57% 29% 14%
1	B	1483	57% 29% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 20456 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 ARF guanine-nucleotide exchange factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1273	Total	C	N	O	S	0	0
			10223	6555	1667	1964	37		
1	B	1272	Total	C	N	O	S	0	0
			10233	6569	1666	1961	37		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP P39993
A	-22	HIS	-	expression tag	UNP P39993
A	-21	HIS	-	expression tag	UNP P39993
A	-20	HIS	-	expression tag	UNP P39993
A	-19	HIS	-	expression tag	UNP P39993
A	-18	HIS	-	expression tag	UNP P39993
A	-17	HIS	-	expression tag	UNP P39993
A	-16	SER	-	expression tag	UNP P39993
A	-15	SER	-	expression tag	UNP P39993
A	-14	GLY	-	expression tag	UNP P39993
A	-13	VAL	-	expression tag	UNP P39993
A	-12	ASP	-	expression tag	UNP P39993
A	-11	LEU	-	expression tag	UNP P39993
A	-10	GLY	-	expression tag	UNP P39993
A	-9	THR	-	expression tag	UNP P39993
A	-8	GLU	-	expression tag	UNP P39993
A	-7	ASN	-	expression tag	UNP P39993
A	-6	LEU	-	expression tag	UNP P39993
A	-5	TYR	-	expression tag	UNP P39993
A	-4	PHE	-	expression tag	UNP P39993
A	-3	GLN	-	expression tag	UNP P39993
A	-2	SER	-	expression tag	UNP P39993
A	-1	ASN	-	expression tag	UNP P39993
A	0	ALA	-	expression tag	UNP P39993
B	-23	MET	-	initiating methionine	UNP P39993
B	-22	HIS	-	expression tag	UNP P39993

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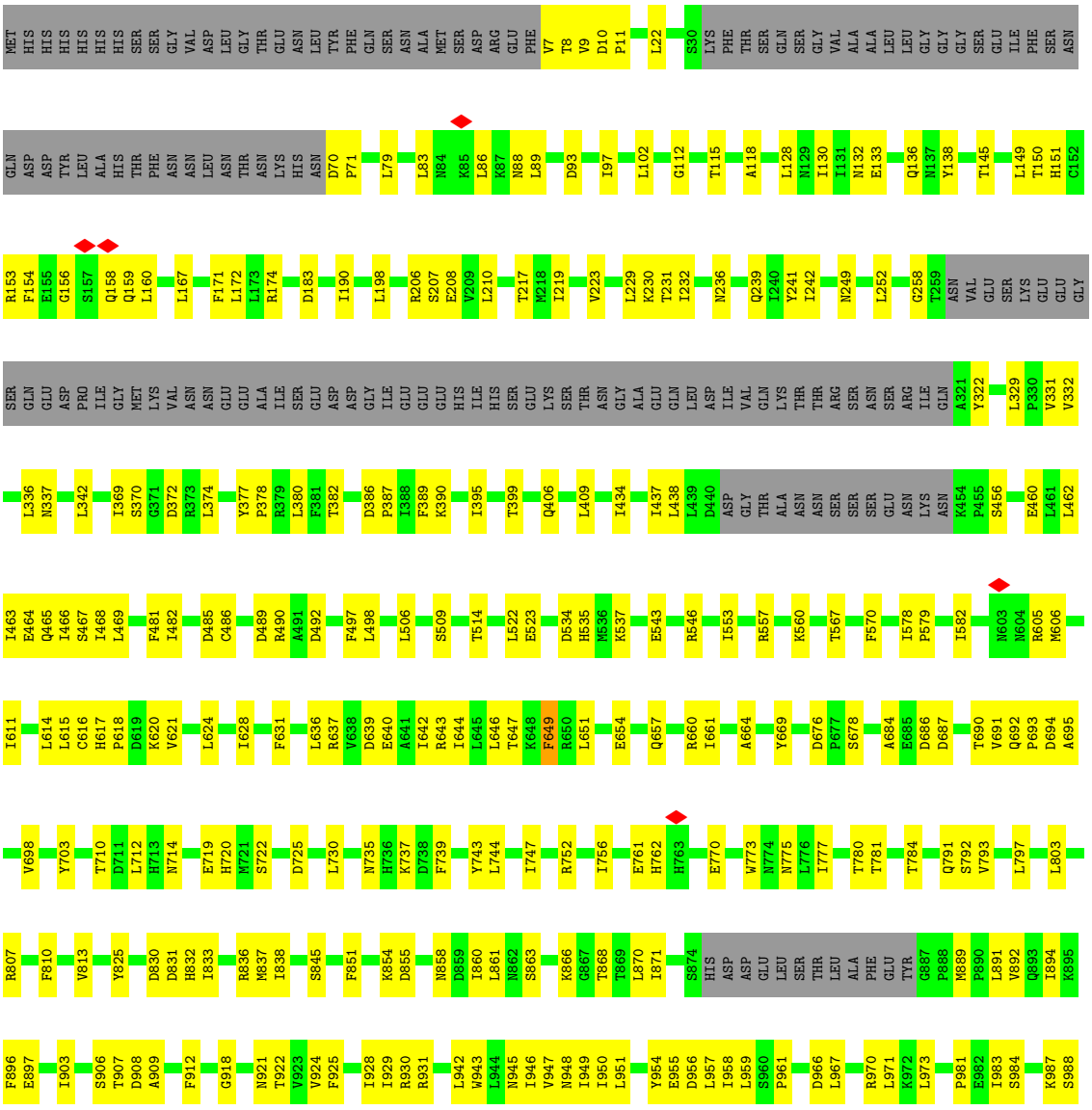
Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	HIS	-	expression tag	UNP P39993
B	-20	HIS	-	expression tag	UNP P39993
B	-19	HIS	-	expression tag	UNP P39993
B	-18	HIS	-	expression tag	UNP P39993
B	-17	HIS	-	expression tag	UNP P39993
B	-16	SER	-	expression tag	UNP P39993
B	-15	SER	-	expression tag	UNP P39993
B	-14	GLY	-	expression tag	UNP P39993
B	-13	VAL	-	expression tag	UNP P39993
B	-12	ASP	-	expression tag	UNP P39993
B	-11	LEU	-	expression tag	UNP P39993
B	-10	GLY	-	expression tag	UNP P39993
B	-9	THR	-	expression tag	UNP P39993
B	-8	GLU	-	expression tag	UNP P39993
B	-7	ASN	-	expression tag	UNP P39993
B	-6	LEU	-	expression tag	UNP P39993
B	-5	TYR	-	expression tag	UNP P39993
B	-4	PHE	-	expression tag	UNP P39993
B	-3	GLN	-	expression tag	UNP P39993
B	-2	SER	-	expression tag	UNP P39993
B	-1	ASN	-	expression tag	UNP P39993
B	0	ALA	-	expression tag	UNP P39993

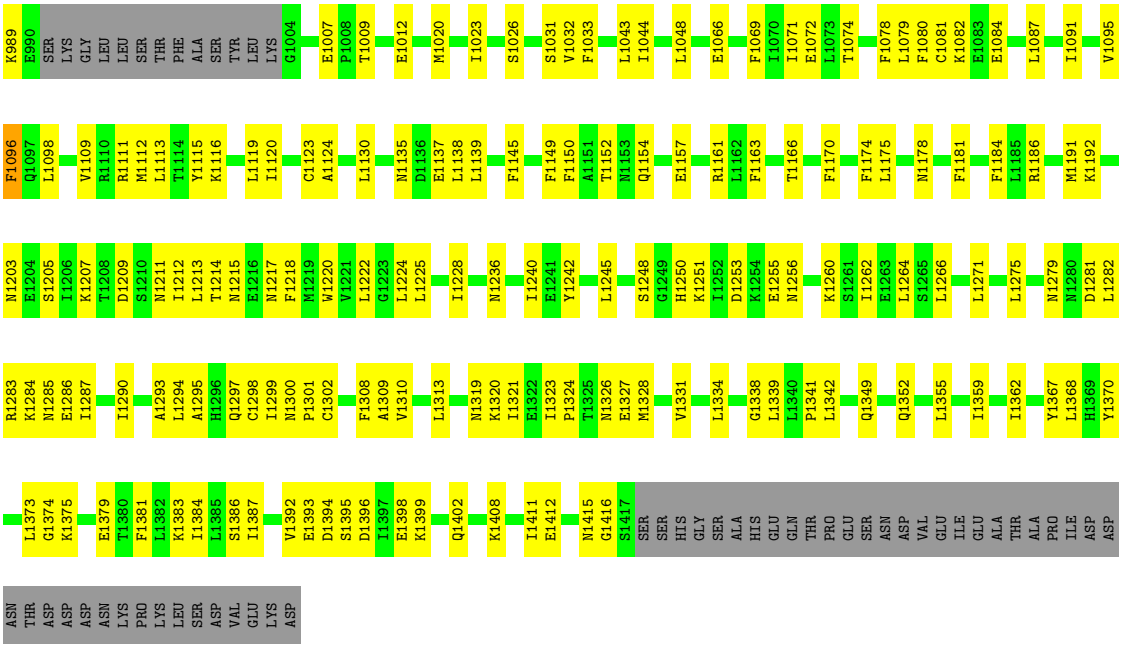
3 Residue-property plots (i)

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: ARF guanine-nucleotide exchange factor 2

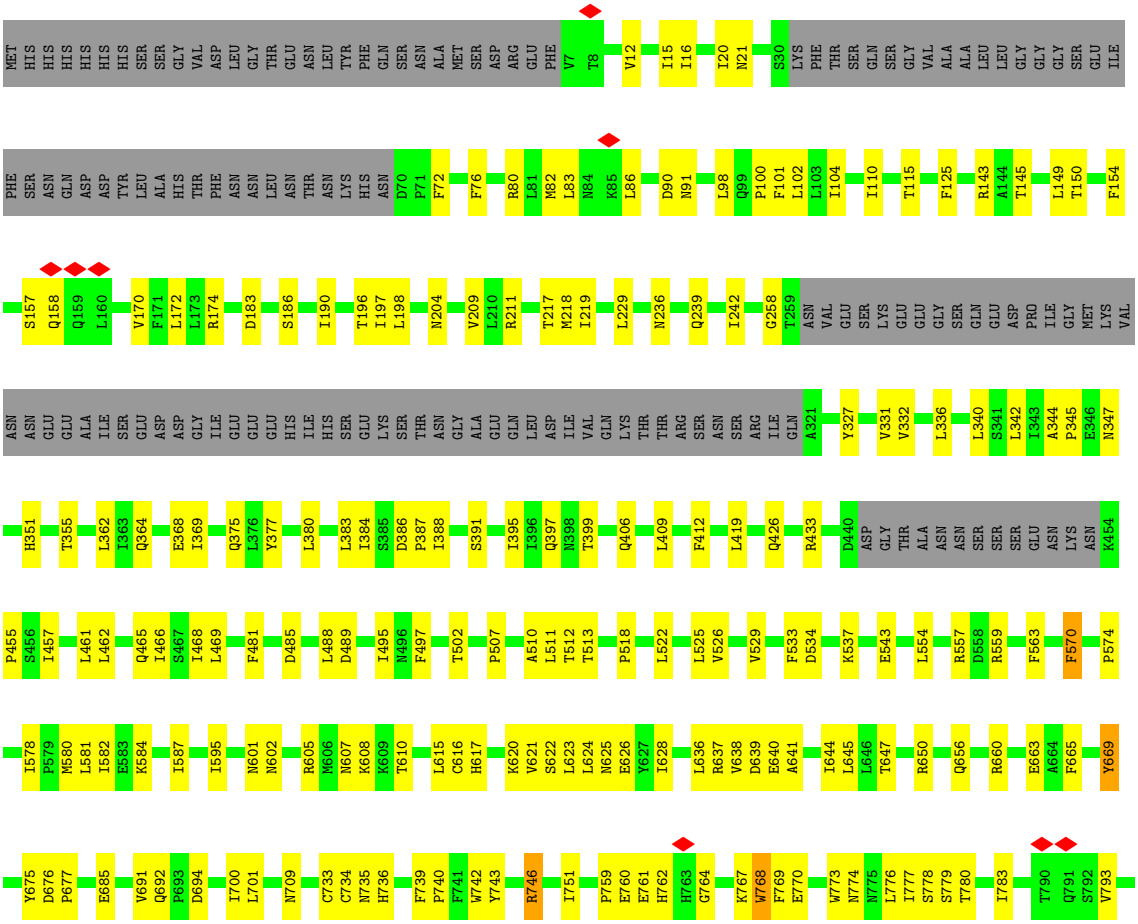
Chain A:

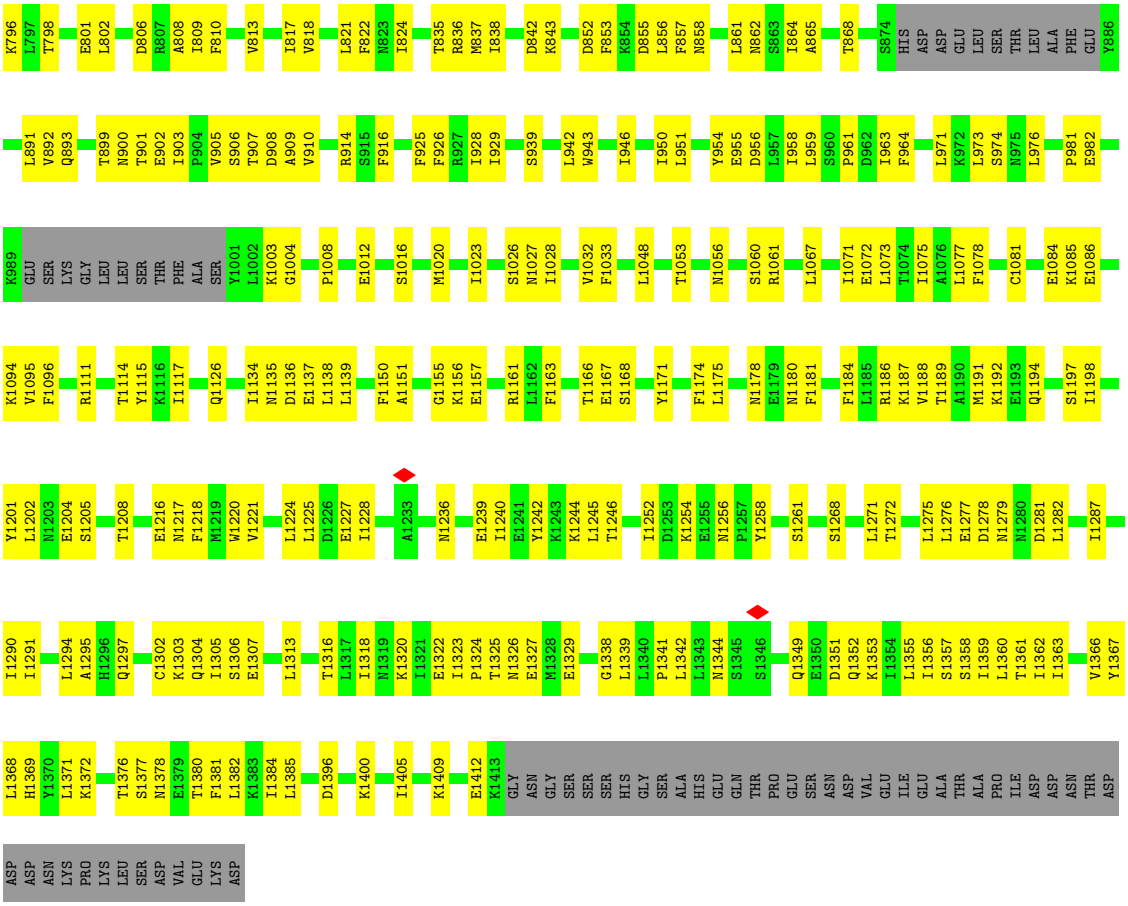




• Molecule 1: ARF guanine-nucleotide exchange factor 2

Chain B:




K796 L797 T798 E801 L802 D806 R807 A808 I809 F810 V813 I817 V818 L821 F822 N823 I824 T835 R836 M837 I838 D842 K843 D852 F853 K854 D855 L856 F857 N858 L861 N862 S863 I864 A865 T868 S874 HIS ASP ASP GLU LEU SER THR LEU ALA PHE GLU Y886
L891 V892 Q893 T899 N900 T901 E902 I903 P904 V905 S906 T907 D908 A909 V910 R914 S915 F916 F925 F926 R927 I928 I929 S939 L942 W943 I946 I950 L951 Y954 E955 D956 L957 I958 L959 S960 P961 D962 I963 F964 L971 K972 L973 S974 N975 L976 P981 E982
K989 GLU SER LYS GLY LEU LEU SER THR PHE ALA SER Y1001 L1002 K1003 G1004 P1008 E1012 S1016 M1020 I1023 S1026 N1027 I1028 V1032 F1033 L1048 T1053 N1056 S1060 R1061 L1067 I1071 E1072 L1073 T1074 I1075 A1076 L1077 F1078 C1081 E1084 K1085 E1086
K1094 V1095 F1096 R1111 T1114 Y1115 K1116 I1117 Q1126 I1134 N1135 D1136 E1137 L1138 L1139 F1150 A1151 G1155 K1156 E1157 R1161 L1162 F1163 T1166 E1167 S1168 Y1171 F1174 L1175 N1178 E1179 N1180 F1181 F1184 L1185 R1186 K1187 V1188 T1189 A1190 M1191 K1192 E1193 Q1194 S1197 I1198
Y1201 L1202 N1203 E1204 S1205 T1208 E1216 N1217 F1218 M1219 W1220 V1221 L1224 L1225 D1226 E1227 I1228 A1233 N1236 E1239 I1240 E1241 Y1242 K1243 K1244 L1245 T1246 I1252 D1253 K1254 E1255 N1256 P1257 Y1258 S1261 S1268 L1271 T1272 L1275 L1276 E1277 D1278 N1279 N1280 D1281 L1282 I1287
I1290 I1291 L1294 A1295 H1296 Q1297 C1302 K1303 Q1304 I1305 S1306 E1307 L1313 T1316 L1317 I1318 N1319 K1320 I1321 E1322 I1323 P1324 T1325 N1326 E1327 M1328 E1329 G1338 L1339 L1340 P1341 L1342 L1343 N1344 S1345 S1346 Q1349 E1350 D1351 Q1352 K1353 H1354 L1355 I1356 S1357 S1358 I1359 L1360 T1361 I1362 I1363 V1366 Y1367
L1368 H1369 Y1370 L1371 K1372 T1376 S1377 N1378 E1379 T1380 F1381 L1382 K1383 I1384 L1385 D1396 K1400 I1405 K1409 E1412 K1413 GLY ASN GLY SER SER SER HIS GLY SER ALA HIS GLU GLN THR PRO GLU SER ASN ASP VAL GLU ILE GLU ALA THR ALA PRO ILE ASP ASP ASN THR ASP
ASP ASP ASN LYS PRO LYS LEU SER ASP VAL GLU LYS ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	435876	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 ($e^-/Å^2$)	69	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.193	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	423.936, 423.936, 423.936	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/10392	0.45	0/14039
1	B	0.27	0/10404	0.47	0/14056
All	All	0.27	0/20796	0.46	0/28095

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10223	0	10417	357	0
1	B	10233	0	10436	363	0
All	All	20456	0	20853	710	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 17.

All (710) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:LEU:HD12	1:A:649:PHE:CE1	1.86	1.11
1:B:1325:THR:HG22	1:B:1326:ASN:H	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:TYR:CE1	1:A:838:ILE:HD11	1.94	1.02
1:A:615:LEU:CD1	1:A:649:PHE:CE1	2.43	1.01
1:B:1302:CYS:SG	1:B:1304:GLN:NE2	2.34	1.00
1:A:1236:ASN:OD1	1:A:1302:CYS:SG	2.24	0.95
1:A:615:LEU:HD12	1:A:649:PHE:HE1	1.29	0.95
1:B:842:ASP:OD1	1:B:928:ILE:HG12	1.68	0.93
1:A:615:LEU:CD1	1:A:649:PHE:CZ	2.50	0.93
1:A:624:LEU:HD11	1:A:661:ILE:HD13	1.53	0.91
1:A:831:ASP:OD1	1:A:832:HIS:N	2.05	0.90
1:B:1325:THR:HG22	1:B:1326:ASN:N	1.86	0.90
1:A:643:ARG:O	1:A:647:THR:HG23	1.71	0.89
1:A:615:LEU:HD13	1:A:649:PHE:CZ	2.06	0.89
1:A:615:LEU:HD13	1:A:649:PHE:HZ	1.34	0.89
1:B:518:PRO:O	1:B:522:LEU:HD13	1.73	0.89
1:B:83:LEU:HA	1:B:86:LEU:HD12	1.52	0.89
1:B:636:LEU:HD11	1:B:641:ALA:HB2	1.54	0.89
1:B:1204:GLU:O	1:B:1208:THR:HG23	1.73	0.89
1:A:1282:LEU:HD12	1:A:1287:ILE:CD1	2.04	0.88
1:B:857:PHE:HE1	1:B:861:LEU:HD11	1.38	0.87
1:B:12:VAL:HG13	1:B:83:LEU:HD12	1.56	0.87
1:A:1044:ILE:HD11	1:A:1087:LEU:HD11	1.56	0.86
1:B:522:LEU:HD21	1:B:824:ILE:HG12	1.54	0.86
1:A:1084:GLU:HG3	1:A:1087:LEU:HD23	1.57	0.84
1:B:1367:TYR:HE1	1:B:1382:LEU:CD2	1.90	0.83
1:A:128:LEU:CD2	1:B:369:ILE:CD1	2.56	0.83
1:A:838:ILE:CG2	1:A:924:VAL:HG21	2.09	0.82
1:A:112:GLY:H	1:A:160:LEU:HD21	1.44	0.82
1:B:1325:THR:CG2	1:B:1326:ASN:H	1.92	0.82
1:B:83:LEU:HD13	1:B:86:LEU:HD12	1.62	0.81
1:B:1359:ILE:O	1:B:1362:ILE:HG12	1.81	0.81
1:B:857:PHE:CE1	1:B:861:LEU:CD1	2.65	0.80
1:B:857:PHE:CE1	1:B:861:LEU:HD11	2.15	0.80
1:A:654:GLU:HB2	1:A:657:GLN:OE1	1.80	0.80
1:B:842:ASP:OD1	1:B:928:ILE:CG1	2.30	0.80
1:B:1359:ILE:O	1:B:1362:ILE:CG1	2.30	0.80
1:B:1291:ILE:HG22	1:B:1338:GLY:HA2	1.65	0.78
1:A:128:LEU:CD2	1:B:369:ILE:HD13	2.14	0.78
1:A:1260:LYS:O	1:A:1264:LEU:HG	1.84	0.78
1:B:926:PHE:CZ	1:B:1028:ILE:HD12	2.18	0.78
1:A:1044:ILE:HD11	1:A:1087:LEU:HD21	1.66	0.78
1:B:691:VAL:HG12	1:B:691:VAL:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1294:LEU:HD13	1:B:1313:LEU:HG	1.66	0.77
1:B:857:PHE:CD1	1:B:861:LEU:HD13	2.19	0.77
1:B:1189:THR:HG22	1:B:1198:ILE:HG21	1.66	0.76
1:A:128:LEU:HD21	1:B:369:ILE:CD1	2.15	0.76
1:B:1352:GLN:HA	1:B:1355:LEU:HB3	1.66	0.76
1:A:481:PHE:CE1	1:A:485:ASP:OD2	2.39	0.76
1:A:838:ILE:HG22	1:A:924:VAL:HG21	1.65	0.76
1:B:1303:LYS:NZ	1:B:1307:GLU:HG3	2.01	0.76
1:B:1302:CYS:SG	1:B:1305:ILE:HD12	2.25	0.75
1:A:1281:ASP:O	1:A:1282:LEU:HG	1.86	0.75
1:A:615:LEU:CD1	1:A:649:PHE:HE1	1.89	0.75
1:B:489:ASP:HA	1:B:605:ARG:HH12	1.50	0.75
1:B:1175:LEU:HA	1:B:1178:ASN:HD21	1.52	0.75
1:A:894:ILE:HB	1:A:903:ILE:HB	1.68	0.75
1:B:617:HIS:O	1:B:621:VAL:N	2.20	0.75
1:B:939:SER:OG	1:B:942:LEU:HG	1.87	0.75
1:B:1245:LEU:HD21	1:B:1252:ILE:HG12	1.69	0.74
1:A:1084:GLU:HG3	1:A:1087:LEU:CD2	2.17	0.74
1:A:1214:THR:HG22	1:A:1215:ASN:N	2.00	0.74
1:B:1356:ILE:HG22	1:B:1360:LEU:HD23	1.69	0.74
1:A:958:ILE:HB	1:A:1020:MET:SD	2.27	0.74
1:B:395:ILE:HG23	1:B:399:THR:HG21	1.70	0.74
1:B:1184:PHE:O	1:B:1188:VAL:HG23	1.89	0.73
1:A:1044:ILE:CD1	1:A:1087:LEU:HD11	2.19	0.72
1:A:1152:THR:HG23	1:A:1154:GLN:H	1.55	0.72
1:B:906:SER:HB2	1:B:956:ASP:OD2	1.90	0.72
1:B:1339:LEU:HD11	1:B:1362:ILE:HD11	1.69	0.72
1:A:845:SER:HA	1:A:860:ILE:HD11	1.72	0.72
1:B:1174:PHE:O	1:B:1178:ASN:ND2	2.22	0.72
1:B:1294:LEU:HB3	1:B:1313:LEU:HD12	1.72	0.72
1:A:617:HIS:O	1:A:621:VAL:N	2.23	0.71
1:A:1373:LEU:HD12	1:A:1375:LYS:HG2	1.72	0.71
1:B:1367:TYR:HE1	1:B:1382:LEU:HD22	1.55	0.71
1:B:1135:ASN:OD1	1:B:1180:ASN:ND2	2.25	0.70
1:B:581:LEU:HB3	1:B:587:ILE:HD13	1.73	0.70
1:A:395:ILE:HG23	1:A:399:THR:HG21	1.74	0.70
1:A:249:ASN:ND2	1:A:337:ASN:ND2	2.40	0.70
1:A:249:ASN:ND2	1:A:337:ASN:HD21	1.90	0.69
1:A:966:ASP:O	1:A:970:ARG:HG3	1.92	0.69
1:B:1202:LEU:HD11	1:B:1224:LEU:HD23	1.74	0.69
1:B:1339:LEU:HD13	1:B:1359:ILE:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ASP:HA	1:A:605:ARG:HE	1.58	0.69
1:A:950:ILE:HD13	1:A:1033:PHE:CZ	2.27	0.68
1:A:946:ILE:HD11	1:A:1032:VAL:HG13	1.75	0.68
1:B:1381:PHE:HA	1:B:1384:ILE:HG12	1.74	0.68
1:A:624:LEU:HD11	1:A:661:ILE:CD1	2.23	0.68
1:B:1150:PHE:HA	1:B:1155:GLY:HA3	1.76	0.68
1:A:889:MET:HB2	1:A:907:THR:HG22	1.75	0.68
1:B:925:PHE:HZ	1:B:946:ILE:HG22	1.58	0.68
1:A:1339:LEU:HD22	1:A:1387:ILE:CD1	2.24	0.68
1:A:825:TYR:CD1	1:A:838:ILE:HD11	2.29	0.67
1:A:871:ILE:CD1	1:A:945:ASN:HA	2.23	0.67
1:B:1254:LYS:HG3	1:B:1256:ASN:HB2	1.76	0.67
1:A:640:GLU:O	1:A:644:ILE:HG12	1.94	0.67
1:A:1279:ASN:ND2	1:A:1281:ASP:O	2.26	0.67
1:A:1298:CYS:SG	1:A:1309:ALA:HB1	2.35	0.67
1:B:229:LEU:CD1	1:B:332:VAL:HG11	2.24	0.67
1:A:1084:GLU:HB2	1:A:1087:LEU:HB3	1.76	0.67
1:B:650:ARG:NH2	1:B:760:GLU:O	2.25	0.67
1:A:128:LEU:CD2	1:B:369:ILE:HD11	2.23	0.67
1:A:950:ILE:CD1	1:A:1033:PHE:CZ	2.77	0.67
1:B:1302:CYS:SG	1:B:1305:ILE:HG13	2.35	0.67
1:A:1297:GLN:O	1:A:1300:ASN:ND2	2.23	0.66
1:A:1342:LEU:HD22	1:A:1359:ILE:HD12	1.76	0.66
1:B:190:ILE:HG23	1:B:331:VAL:HG21	1.76	0.66
1:B:1225:LEU:HD13	1:B:1272:THR:HG22	1.76	0.66
1:A:1392:VAL:HG22	1:A:1393:GLU:N	2.10	0.66
1:B:862:ASN:ND2	1:B:942:LEU:CD2	2.58	0.66
1:B:892:VAL:HG12	1:B:893:GLN:N	2.11	0.66
1:B:774:ASN:HA	1:B:777:ILE:HG22	1.77	0.66
1:B:821:LEU:HD22	1:B:837:MET:HE1	1.78	0.66
1:A:636:LEU:HB3	1:A:640:GLU:HB2	1.78	0.65
1:A:1225:LEU:HD11	1:A:1271:LEU:HD23	1.79	0.65
1:B:862:ASN:ND2	1:B:942:LEU:HD21	2.12	0.65
1:A:1120:ILE:HG21	1:A:1130:LEU:HD13	1.78	0.64
1:B:1303:LYS:O	1:B:1307:GLU:HG2	1.96	0.64
1:A:570:PHE:CD1	1:A:606:MET:HE3	2.33	0.64
1:A:1323:ILE:HG21	1:A:1370:TYR:HE2	1.61	0.64
1:A:249:ASN:HD21	1:A:337:ASN:ND2	1.96	0.64
1:A:838:ILE:HG21	1:A:924:VAL:HG21	1.78	0.64
1:B:958:ILE:HG22	1:B:1023:ILE:HG12	1.80	0.64
1:A:730:LEU:HD11	1:A:744:LEU:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:THR:HG22	1:A:1215:ASN:H	1.61	0.64
1:B:1302:CYS:SG	1:B:1305:ILE:CD1	2.86	0.63
1:B:1302:CYS:SG	1:B:1305:ILE:CG1	2.87	0.63
1:A:481:PHE:HE1	1:A:485:ASP:OD2	1.80	0.63
1:A:710:THR:O	1:A:714:ASN:ND2	2.31	0.63
1:B:1339:LEU:HD11	1:B:1362:ILE:CD1	2.29	0.63
1:B:857:PHE:CE1	1:B:861:LEU:HD13	2.34	0.62
1:B:905:VAL:HG23	1:B:906:SER:N	2.14	0.62
1:B:1339:LEU:CD1	1:B:1362:ILE:HD11	2.28	0.62
1:B:1359:ILE:C	1:B:1362:ILE:HG12	2.19	0.62
1:B:647:THR:HG23	1:B:779:SER:OG	2.00	0.62
1:B:1359:ILE:HA	1:B:1362:ILE:HG12	1.81	0.62
1:A:943:TRP:CZ3	1:A:1043:LEU:HD13	2.34	0.62
1:A:128:LEU:HD23	1:B:369:ILE:HD11	1.82	0.62
1:A:406:GLN:NE2	1:B:21:ASN:OD1	2.33	0.62
1:A:1044:ILE:HD11	1:A:1087:LEU:CD1	2.28	0.62
1:B:580:MET:SD	1:B:584:LYS:NZ	2.73	0.62
1:B:1359:ILE:O	1:B:1362:ILE:HG13	1.99	0.62
1:A:1209:ASP:O	1:A:1211:ASN:ND2	2.33	0.61
1:B:905:VAL:HG11	1:B:1008:PRO:HG2	1.81	0.61
1:A:987:LYS:HG2	1:A:989:LYS:H	1.65	0.61
1:A:486:CYS:HB3	1:A:553:ILE:HG22	1.83	0.61
1:A:1323:ILE:N	1:A:1324:PRO:HD3	2.15	0.61
1:B:82:MET:O	1:B:86:LEU:HG	2.00	0.61
1:B:1136:ASP:OD1	1:B:1137:GLU:N	2.33	0.61
1:B:1362:ILE:O	1:B:1366:VAL:HG12	1.99	0.61
1:A:646:LEU:HD22	1:A:651:LEU:HD21	1.82	0.61
1:A:1282:LEU:HD12	1:A:1287:ILE:HD11	1.82	0.61
1:B:340:LEU:HB2	1:B:388:ILE:HD11	1.82	0.61
1:B:485:ASP:HB3	1:B:557:ARG:HE	1.66	0.61
1:B:1078:PHE:CZ	1:B:1084:GLU:HB3	2.35	0.61
1:A:1240:ILE:HD11	1:A:1301:PRO:HB2	1.83	0.61
1:B:409:LEU:HD11	1:B:462:LEU:HD23	1.81	0.61
1:A:156:GLY:HA2	1:A:160:LEU:HD23	1.83	0.60
1:B:364:GLN:NE2	1:B:368:GLU:OE2	2.33	0.60
1:A:570:PHE:CD1	1:A:606:MET:CE	2.84	0.60
1:A:1282:LEU:HD12	1:A:1287:ILE:HD12	1.81	0.60
1:B:858:ASN:HA	1:B:942:LEU:HD11	1.83	0.60
1:A:490:ARG:O	1:A:605:ARG:NH2	2.34	0.60
1:A:1091:ILE:HG22	1:A:1119:LEU:HD11	1.84	0.60
1:B:616:CYS:O	1:B:617:HIS:ND1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:SER:HG	1:B:158:GLN:H	1.50	0.60
1:A:1323:ILE:HG21	1:A:1370:TYR:CE2	2.36	0.60
1:A:1111:ARG:NH2	1:A:1115:TYR:OH	2.35	0.59
1:B:1359:ILE:HA	1:B:1362:ILE:CD1	2.32	0.59
1:B:892:VAL:HG11	1:B:1008:PRO:HD3	1.83	0.59
1:A:1298:CYS:SG	1:A:1313:LEU:HD12	2.42	0.59
1:A:167:LEU:HD22	1:B:209:VAL:HG13	1.85	0.59
1:A:482:ILE:HD13	1:A:797:LEU:HD11	1.84	0.59
1:A:1236:ASN:CG	1:A:1302:CYS:SG	2.81	0.59
1:B:767:LYS:HA	1:B:770:GLU:HB2	1.83	0.59
1:A:1324:PRO:HD2	1:A:1326:ASN:OD1	2.03	0.59
1:B:1367:TYR:CE1	1:B:1382:LEU:HD22	2.35	0.59
1:A:854:LYS:O	1:A:858:ASN:ND2	2.35	0.58
1:A:1081:CYS:SG	1:A:1084:GLU:HG2	2.42	0.58
1:B:1325:THR:CG2	1:B:1326:ASN:N	2.57	0.58
1:A:611:ILE:O	1:A:615:LEU:HG	2.02	0.58
1:B:906:SER:CB	1:B:956:ASP:OD2	2.50	0.58
1:A:1310:VAL:HG22	1:A:1362:ILE:HD11	1.86	0.58
1:B:502:THR:HG22	1:B:525:LEU:HD21	1.86	0.58
1:A:1392:VAL:HG22	1:A:1393:GLU:H	1.67	0.58
1:A:684:ALA:HB1	1:A:690:THR:HG21	1.83	0.58
1:A:912:PHE:HE2	1:A:922:THR:HG21	1.69	0.58
1:A:482:ILE:HD13	1:A:797:LEU:CD1	2.34	0.58
1:B:901:THR:HG22	1:B:903:ILE:HG12	1.85	0.58
1:B:1056:ASN:O	1:B:1060:SER:OG	2.20	0.58
1:B:559:ARG:NH2	1:B:584:LYS:O	2.36	0.57
1:A:523:GLU:OE2	1:A:836:ARG:NH1	2.37	0.57
1:A:942:LEU:O	1:A:946:ILE:HG22	2.04	0.57
1:A:1023:ILE:O	1:A:1026:SER:OG	2.21	0.57
1:A:1373:LEU:CD1	1:A:1375:LYS:HG2	2.34	0.57
1:A:1225:LEU:HD13	1:A:1228:ILE:HD12	1.86	0.57
1:A:370:SER:HB2	1:A:374:LEU:HB2	1.87	0.57
1:A:691:VAL:HG21	1:A:743:TYR:CZ	2.40	0.57
1:A:1214:THR:CG2	1:A:1215:ASN:N	2.67	0.57
1:B:1072:GLU:HA	1:B:1115:TYR:HE2	1.69	0.57
1:A:719:GLU:O	1:A:720:HIS:ND1	2.38	0.57
1:A:730:LEU:HD11	1:A:744:LEU:HD11	1.86	0.57
1:A:1255:GLU:HG3	1:A:1256:ASN:H	1.69	0.57
1:B:174:ARG:HD2	1:B:217:THR:HG22	1.85	0.57
1:B:691:VAL:HG22	1:B:740:PRO:HG2	1.85	0.57
1:B:1368:LEU:HD12	1:B:1405:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1194:GLN:O	1:B:1197:SER:OG	2.21	0.57
1:A:892:VAL:HA	1:A:983:ILE:O	2.05	0.57
1:A:1081:CYS:SG	1:A:1082:LYS:N	2.78	0.57
1:B:242:ILE:HD12	1:B:644:ILE:HD11	1.87	0.57
1:B:406:GLN:HB2	1:B:461:LEU:HD11	1.87	0.57
1:A:967:LEU:HD12	1:A:967:LEU:O	2.05	0.56
1:B:1053:THR:HG22	1:B:1053:THR:O	2.04	0.56
1:A:252:LEU:HD13	1:A:342:LEU:HD21	1.87	0.56
1:A:637:ARG:O	1:A:639:ASP:N	2.36	0.56
1:A:691:VAL:HG22	1:A:693:PRO:HD3	1.86	0.56
1:B:764:GLY:H	1:B:767:LYS:HG2	1.71	0.56
1:B:905:VAL:HG23	1:B:906:SER:H	1.68	0.56
1:A:336:LEU:HD12	1:A:380:LEU:HD23	1.88	0.56
1:A:1281:ASP:O	1:A:1282:LEU:CG	2.52	0.56
1:A:773:TRP:O	1:A:777:ILE:HG22	2.05	0.56
1:B:1138:LEU:O	1:B:1187:LYS:NZ	2.34	0.56
1:B:1166:THR:HG22	1:B:1175:LEU:HD13	1.88	0.56
1:B:1072:GLU:OE1	1:B:1115:TYR:OH	2.24	0.56
1:B:1277:GLU:HB2	1:B:1320:LYS:HE3	1.86	0.56
1:A:1072:GLU:OE1	1:A:1115:TYR:OH	2.22	0.56
1:A:722:SER:OG	1:A:725:ASP:OD1	2.24	0.56
1:B:625:ASN:OD1	1:B:626:GLU:N	2.38	0.56
1:A:198:LEU:HD21	1:A:342:LEU:HD11	1.88	0.56
1:A:230:LYS:HD3	1:A:370:SER:HA	1.87	0.56
1:A:845:SER:HA	1:A:860:ILE:CD1	2.35	0.55
1:B:488:LEU:O	1:B:605:ARG:NH1	2.39	0.55
1:B:1191:MET:SD	1:B:1192:LYS:N	2.78	0.55
1:A:897:GLU:HB2	1:A:988:SER:HA	1.88	0.55
1:B:1008:PRO:HB3	1:B:1012:GLU:OE1	2.07	0.55
1:A:669:TYR:HD2	1:A:698:VAL:HG21	1.72	0.55
1:B:336:LEU:HD12	1:B:380:LEU:HD22	1.89	0.55
1:A:1294:LEU:HB3	1:A:1313:LEU:HG	1.89	0.55
1:B:397:GLN:HE22	1:B:768:TRP:HE1	1.54	0.55
1:B:1359:ILE:CA	1:B:1362:ILE:HG12	2.37	0.55
1:B:170:VAL:HG12	1:B:217:THR:HG21	1.88	0.55
1:B:1287:ILE:HA	1:B:1290:ILE:HG12	1.88	0.55
1:A:624:LEU:CD2	1:A:664:ALA:CB	2.84	0.55
1:B:1294:LEU:HD22	1:B:1313:LEU:HB2	1.88	0.55
1:B:1316:THR:HG22	1:B:1320:LYS:HZ3	1.71	0.55
1:B:1409:LYS:HD2	1:B:1412:GLU:HB2	1.88	0.55
1:B:926:PHE:CZ	1:B:1028:ILE:CD1	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LEU:HD12	1:B:554:LEU:H	1.72	0.54
1:B:607:ASN:O	1:B:610:THR:OG1	2.25	0.54
1:A:691:VAL:HG11	1:A:743:TYR:CE1	2.43	0.54
1:A:830:ASP:HB3	1:A:833:ILE:HG22	1.88	0.54
1:A:855:ASP:OD1	1:A:855:ASP:N	2.40	0.54
1:A:1044:ILE:HD12	1:A:1091:ILE:HD11	1.87	0.54
1:B:892:VAL:CG1	1:B:893:GLN:N	2.71	0.54
1:B:1281:ASP:OD1	1:B:1282:LEU:N	2.39	0.54
1:A:1087:LEU:O	1:A:1091:ILE:HG12	2.08	0.54
1:B:1302:CYS:HB3	1:B:1305:ILE:HB	1.89	0.54
1:A:1214:THR:CG2	1:A:1215:ASN:H	2.21	0.54
1:B:507:PRO:HA	1:B:510:ALA:HB3	1.89	0.54
1:B:855:ASP:N	1:B:855:ASP:OD1	2.39	0.54
1:B:764:GLY:H	1:B:767:LYS:CG	2.21	0.54
1:B:534:ASP:HA	1:B:537:LYS:HE3	1.89	0.54
1:A:780:THR:HG22	1:A:781:THR:H	1.73	0.53
1:B:1303:LYS:HZ3	1:B:1307:GLU:HG3	1.71	0.53
1:B:1323:ILE:HG23	1:B:1329:GLU:HA	1.89	0.53
1:A:207:SER:OG	1:A:208:GLU:N	2.41	0.53
1:A:925:PHE:O	1:A:929:ILE:HG12	2.09	0.53
1:A:954:TYR:HE1	1:A:961:PRO:HG3	1.74	0.53
1:A:637:ARG:HG2	1:A:747:ILE:HD11	1.90	0.53
1:B:615:LEU:HD22	1:B:624:LEU:HB3	1.90	0.53
1:A:1044:ILE:HD11	1:A:1087:LEU:CD2	2.36	0.53
1:A:183:ASP:OD1	1:A:183:ASP:O	2.27	0.53
1:A:871:ILE:HD11	1:A:945:ASN:HA	1.89	0.53
1:B:1295:ALA:HB1	1:B:1342:LEU:HD21	1.91	0.53
1:B:636:LEU:HD12	1:B:637:ARG:O	2.09	0.53
1:B:1189:THR:OG1	1:B:1227:GLU:OE1	2.23	0.53
1:A:871:ILE:HG12	1:A:871:ILE:O	2.08	0.53
1:B:622:SER:HA	1:B:625:ASN:ND2	2.24	0.53
1:A:88:ASN:OD1	1:A:89:LEU:N	2.41	0.53
1:A:1374:GLY:O	1:A:1375:LYS:HG2	2.09	0.53
1:A:1374:GLY:O	1:A:1375:LYS:HD3	2.08	0.53
1:A:1178:ASN:O	1:A:1181:PHE:N	2.42	0.52
1:A:1124:ALA:HB1	1:A:1170:PHE:HD2	1.74	0.52
1:B:12:VAL:CG1	1:B:83:LEU:HD12	2.35	0.52
1:B:624:LEU:O	1:B:628:ILE:HG12	2.09	0.52
1:A:232:ILE:O	1:A:377:TYR:OH	2.25	0.52
1:A:896:PHE:HE1	1:A:903:ILE:HD13	1.74	0.52
1:A:1412:GLU:HA	1:A:1415:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:HD23	1:B:369:ILE:CD1	2.33	0.52
1:A:386:ASP:HB3	1:A:387:PRO:HD3	1.91	0.52
1:A:951:LEU:O	1:A:955:GLU:HG2	2.10	0.52
1:A:1319:ASN:O	1:A:1320:LYS:HB2	2.09	0.52
1:B:150:THR:HG23	1:B:196:THR:HG21	1.91	0.52
1:A:930:ARG:HG2	1:A:1031:SER:HA	1.92	0.52
1:B:102:LEU:HD21	1:B:145:THR:HG22	1.90	0.52
1:B:963:ILE:HG21	1:B:1073:LEU:HD13	1.92	0.52
1:B:974:SER:O	1:B:1111:ARG:NH2	2.42	0.52
1:A:871:ILE:HD11	1:A:948:ASN:HB2	1.91	0.52
1:B:926:PHE:HZ	1:B:1028:ILE:HD12	1.70	0.52
1:B:1258:TYR:O	1:B:1261:SER:OG	2.21	0.52
1:B:1294:LEU:HD13	1:B:1313:LEU:CG	2.39	0.52
1:A:1135:ASN:HA	1:A:1139:LEU:HD23	1.91	0.52
1:B:83:LEU:HD13	1:B:86:LEU:CD1	2.38	0.52
1:B:533:PHE:HD2	1:B:843:LYS:HD2	1.74	0.52
1:B:1362:ILE:HG13	1:B:1363:ILE:N	2.25	0.52
1:A:492:ASP:OD1	1:A:560:LYS:NZ	2.35	0.52
1:B:197:ILE:HG22	1:B:218:MET:HG2	1.92	0.52
1:B:1242:TYR:O	1:B:1246:THR:HG23	2.10	0.52
1:B:1302:CYS:O	1:B:1306:SER:N	2.27	0.52
1:B:204:ASN:OD1	1:B:211:ARG:NH1	2.43	0.52
1:B:336:LEU:HB3	1:B:383:LEU:HD23	1.92	0.52
1:B:608:LYS:HG3	1:B:759:PRO:HB2	1.91	0.51
1:B:675:TYR:HB2	1:B:692:GLN:HB3	1.91	0.51
1:A:694:ASP:OD1	1:A:695:ALA:N	2.38	0.51
1:A:928:ILE:HG12	1:A:931:ARG:HH22	1.75	0.51
1:A:1084:GLU:CG	1:A:1087:LEU:HD23	2.35	0.51
1:A:1293:ALA:O	1:A:1297:GLN:NE2	2.43	0.51
1:B:1217:ASN:HA	1:B:1220:TRP:CE3	2.44	0.51
1:A:7:VAL:HG23	1:A:8:THR:HG23	1.91	0.51
1:A:981:PRO:HG2	1:A:984:SER:HB3	1.93	0.51
1:A:1078:PHE:HA	1:A:1081:CYS:HB3	1.92	0.51
1:B:637:ARG:NH2	1:B:639:ASP:OD2	2.43	0.51
1:B:1071:ILE:HD12	1:B:1095:VAL:HG12	1.92	0.51
1:B:1134:ILE:O	1:B:1138:LEU:HB2	2.11	0.51
1:B:1341:PRO:O	1:B:1344:ASN:ND2	2.40	0.51
1:A:150:THR:O	1:A:151:HIS:ND1	2.43	0.51
1:B:229:LEU:HD12	1:B:332:VAL:HG11	1.91	0.51
1:A:11:PRO:HB3	1:A:130:ILE:HD12	1.92	0.51
1:B:229:LEU:HD12	1:B:332:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASP:N	1:A:10:ASP:OD1	2.44	0.51
1:A:617:HIS:CG	1:A:618:PRO:HD2	2.46	0.51
1:B:383:LEU:HD12	1:B:387:PRO:HG2	1.93	0.51
1:B:901:THR:HG22	1:B:902:GLU:N	2.25	0.51
1:B:336:LEU:CD1	1:B:384:ILE:HD11	2.41	0.51
1:B:595:ILE:HG23	1:B:623:LEU:HD13	1.93	0.51
1:B:976:LEU:H	1:B:976:LEU:HD12	1.76	0.51
1:A:1163:PHE:O	1:A:1166:THR:OG1	2.21	0.51
1:A:242:ILE:HG21	1:A:640:GLU:HB3	1.93	0.51
1:B:344:ALA:HB3	1:B:347:ASN:HB2	1.93	0.51
1:B:481:PHE:HE1	1:B:557:ARG:CZ	2.23	0.51
1:B:518:PRO:O	1:B:522:LEU:CD1	2.54	0.51
1:B:857:PHE:CD1	1:B:861:LEU:CD1	2.87	0.50
1:B:891:LEU:HD11	1:B:956:ASP:OD1	2.12	0.50
1:B:1033:PHE:CZ	1:B:1073:LEU:HD21	2.47	0.50
1:A:628:ILE:HA	1:A:631:PHE:HD2	1.76	0.50
1:B:481:PHE:HE1	1:B:557:ARG:NH2	2.10	0.50
1:B:973:LEU:HD21	1:B:1114:THR:HG21	1.93	0.50
1:A:1222:LEU:HD11	1:A:1290:ILE:HD13	1.93	0.50
1:B:466:ILE:O	1:B:469:LEU:HB3	2.11	0.50
1:B:533:PHE:CD2	1:B:843:LYS:HD2	2.47	0.50
1:B:636:LEU:CD1	1:B:641:ALA:HB2	2.33	0.50
1:B:1359:ILE:HA	1:B:1362:ILE:CG1	2.42	0.50
1:B:406:GLN:HA	1:B:461:LEU:HD21	1.93	0.50
1:B:198:LEU:HD21	1:B:342:LEU:HD11	1.93	0.50
1:B:691:VAL:O	1:B:691:VAL:CG1	2.56	0.50
1:B:1205:SER:O	1:B:1208:THR:OG1	2.25	0.50
1:A:174:ARG:HB2	1:A:217:THR:HG23	1.94	0.50
1:A:951:LEU:HD13	1:A:1066:GLU:OE2	2.12	0.50
1:A:1242:TYR:HA	1:A:1245:LEU:HB2	1.94	0.50
1:B:380:LEU:O	1:B:384:ILE:HG12	2.12	0.49
1:B:865:ALA:O	1:B:868:THR:HG22	2.12	0.49
1:B:1023:ILE:O	1:B:1026:SER:OG	2.26	0.49
1:B:1163:PHE:O	1:B:1166:THR:OG1	2.21	0.49
1:B:1376:THR:HG22	1:B:1376:THR:O	2.12	0.49
1:B:761:GLU:O	1:B:762:HIS:ND1	2.45	0.49
1:A:534:ASP:OD1	1:A:537:LYS:NZ	2.46	0.49
1:A:954:TYR:HA	1:A:959:LEU:HB3	1.94	0.49
1:A:1007:GLU:OE1	1:A:1007:GLU:N	2.46	0.49
1:A:1071:ILE:HD11	1:A:1098:LEU:HD12	1.93	0.49
1:A:1323:ILE:N	1:A:1324:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLY:N	1:A:160:LEU:HD21	2.21	0.49
1:A:1379:GLU:O	1:A:1383:LYS:HG2	2.12	0.49
1:A:1393:GLU:O	1:A:1394:ASP:CG	2.50	0.49
1:B:1134:ILE:HA	1:B:1138:LEU:HD13	1.93	0.49
1:A:654:GLU:OE1	1:A:657:GLN:NE2	2.43	0.49
1:B:636:LEU:HD13	1:B:641:ALA:N	2.28	0.49
1:A:950:ILE:HD11	1:A:1033:PHE:CZ	2.47	0.49
1:B:336:LEU:HD13	1:B:384:ILE:HD11	1.95	0.49
1:A:102:LEU:HD21	1:A:145:THR:HG22	1.94	0.49
1:A:456:SER:OG	1:A:514:THR:N	2.45	0.49
1:A:465:GLN:O	1:A:468:ILE:HG22	2.13	0.49
1:A:1279:ASN:ND2	1:A:1281:ASP:OD1	2.46	0.49
1:A:1349:GLN:HB3	1:A:1352:GLN:HB2	1.95	0.49
1:B:426:GLN:HG3	1:B:776:LEU:HD21	1.94	0.49
1:B:1126:GLN:N	1:B:1171:TYR:OH	2.45	0.49
1:A:730:LEU:HD11	1:A:744:LEU:HD13	1.94	0.48
1:A:1295:ALA:O	1:A:1299:ILE:HG13	2.12	0.48
1:B:157:SER:OG	1:B:158:GLN:OE1	2.31	0.48
1:B:1184:PHE:HA	1:B:1187:LYS:HE2	1.94	0.48
1:B:1378:ASN:HB3	1:B:1381:PHE:CD2	2.47	0.48
1:A:1145:PHE:HB3	1:A:1150:PHE:HE1	1.77	0.48
1:B:1138:LEU:HD23	1:B:1184:PHE:CG	2.48	0.48
1:A:543:GLU:HA	1:A:546:ARG:HD2	1.94	0.48
1:A:712:LEU:HD21	1:A:752:ARG:HG2	1.95	0.48
1:A:855:ASP:HA	1:A:858:ASN:HD21	1.77	0.48
1:A:918:GLY:HA2	1:A:921:ASN:ND2	2.28	0.48
1:A:1213:LEU:HD11	1:A:1275:LEU:HD21	1.95	0.48
1:B:1380:THR:O	1:B:1384:ILE:HG23	2.13	0.48
1:A:506:LEU:O	1:A:509:SER:OG	2.22	0.48
1:A:639:ASP:HB3	1:A:747:ILE:HD12	1.95	0.48
1:A:1396:ASP:HA	1:A:1399:LYS:HG2	1.96	0.48
1:B:143:ARG:CZ	1:B:186:SER:HB3	2.44	0.48
1:B:1349:GLN:O	1:B:1351:ASP:N	2.42	0.48
1:A:947:VAL:O	1:A:950:ILE:HG22	2.14	0.48
1:A:1266:LEU:HD22	1:A:1308:PHE:HD2	1.79	0.48
1:B:16:ILE:HD11	1:B:80:ARG:HH11	1.79	0.48
1:B:801:GLU:OE1	1:B:801:GLU:N	2.38	0.48
1:B:1186:ARG:O	1:B:1189:THR:OG1	2.31	0.48
1:A:1323:ILE:HD13	1:A:1328:MET:SD	2.54	0.48
1:B:660:ARG:O	1:B:663:GLU:HG3	2.13	0.48
1:B:926:PHE:HD1	1:B:929:ILE:HD11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ARG:HG3	1:A:743:TYR:CE1	2.49	0.48
1:A:1326:ASN:O	1:A:1327:GLU:C	2.51	0.48
1:B:90:ASP:OD1	1:B:91:ASN:N	2.46	0.48
1:A:861:LEU:HB3	1:A:942:LEU:HD11	1.96	0.48
1:A:687:ASP:HA	1:A:691:VAL:HG12	1.95	0.47
1:B:638:VAL:HG22	1:B:669:TYR:HE2	1.79	0.47
1:B:1114:THR:O	1:B:1117:ILE:HG22	2.14	0.47
1:A:1253:ASP:OD1	1:A:1253:ASP:N	2.46	0.47
1:B:1357:SER:HA	1:B:1360:LEU:HD21	1.97	0.47
1:A:690:THR:OG1	1:A:691:VAL:N	2.47	0.47
1:A:691:VAL:HG21	1:A:743:TYR:CE1	2.49	0.47
1:A:1096:PHE:CE2	1:A:1116:LYS:HD2	2.49	0.47
1:B:636:LEU:HD11	1:B:641:ALA:CB	2.35	0.47
1:B:982:GLU:HG3	1:B:1061:ARG:HH11	1.80	0.47
1:B:1239:GLU:HA	1:B:1242:TYR:HB2	1.96	0.47
1:A:1374:GLY:O	1:A:1375:LYS:CG	2.63	0.47
1:B:636:LEU:CD1	1:B:637:ARG:O	2.62	0.47
1:B:637:ARG:HH21	1:B:746:ARG:HB3	1.79	0.47
1:B:638:VAL:HG21	1:B:701:LEU:HD23	1.95	0.47
1:B:910:VAL:O	1:B:914:ARG:HG2	2.14	0.47
1:A:676:ASP:OD2	1:A:678:SER:OG	2.23	0.47
1:A:1205:SER:HB3	1:A:1212:ILE:HD13	1.95	0.47
1:A:460:GLU:HG3	1:A:514:THR:HG21	1.95	0.47
1:A:1071:ILE:HD12	1:A:1095:VAL:HG12	1.96	0.47
1:B:768:TRP:CG	1:B:769:PHE:N	2.82	0.47
1:A:522:LEU:HD11	1:A:837:MET:SD	2.54	0.47
1:A:686:ASP:O	1:A:690:THR:OG1	2.30	0.47
1:A:1374:GLY:O	1:A:1375:LYS:CD	2.63	0.47
1:A:1392:VAL:CG2	1:A:1393:GLU:N	2.77	0.47
1:B:734:CYS:SG	1:B:735:ASN:N	2.87	0.47
1:B:950:ILE:HD11	1:B:1032:VAL:HG11	1.97	0.47
1:B:858:ASN:OD1	1:B:942:LEU:HD11	2.15	0.47
1:A:946:ILE:HA	1:A:949:ILE:HG22	1.96	0.47
1:B:383:LEU:O	1:B:388:ILE:HG12	2.15	0.47
1:B:1135:ASN:O	1:B:1139:LEU:HB2	2.15	0.47
1:B:1294:LEU:O	1:B:1297:GLN:HG3	2.14	0.47
1:B:1353:LYS:HD2	1:B:1353:LYS:N	2.28	0.47
1:A:958:ILE:CB	1:A:1020:MET:SD	3.00	0.47
1:A:8:THR:OG1	1:A:9:VAL:N	2.48	0.46
1:A:1084:GLU:CB	1:A:1087:LEU:HB3	2.43	0.46
1:B:340:LEU:HD13	1:B:388:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASP:HB3	1:B:387:PRO:HD3	1.96	0.46
1:B:778:SER:O	1:B:780:THR:N	2.48	0.46
1:B:798:THR:OG1	1:B:801:GLU:OE1	2.20	0.46
1:A:784:THR:O	1:A:784:THR:OG1	2.28	0.46
1:A:973:LEU:HB3	1:A:1111:ARG:HH12	1.79	0.46
1:A:1157:GLU:O	1:A:1161:ARG:HG2	2.16	0.46
1:A:1262:ILE:O	1:A:1266:LEU:HG	2.16	0.46
1:A:791:GLN:HG2	1:A:792:SER:H	1.80	0.46
1:A:1339:LEU:HD22	1:A:1387:ILE:HD11	1.94	0.46
1:A:1384:ILE:HA	1:A:1387:ILE:HD12	1.97	0.46
1:B:644:ILE:O	1:B:647:THR:HG22	2.14	0.46
1:B:899:THR:OG1	1:B:900:ASN:N	2.49	0.46
1:B:813:VAL:HG13	1:B:817:ILE:HD12	1.98	0.46
1:A:891:LEU:HD11	1:A:981:PRO:HA	1.98	0.46
1:B:1382:LEU:O	1:B:1385:LEU:HG	2.15	0.46
1:A:1044:ILE:HD11	1:A:1087:LEU:CG	2.46	0.46
1:B:336:LEU:HD23	1:B:336:LEU:HA	1.78	0.46
1:A:83:LEU:HA	1:A:86:LEU:HD12	1.98	0.46
1:A:438:LEU:HD21	1:A:463:ILE:HD13	1.98	0.46
1:A:1331:VAL:O	1:A:1334:LEU:HG	2.16	0.46
1:A:236:ASN:ND2	1:A:239:GLN:OE1	2.48	0.46
1:A:382:THR:HG23	1:A:781:THR:HG22	1.98	0.46
1:A:1149:PHE:O	1:A:1152:THR:HG22	2.16	0.46
1:A:1326:ASN:HD22	1:A:1327:GLU:CD	2.19	0.46
1:B:694:ASP:N	1:B:694:ASP:OD1	2.49	0.46
1:B:858:ASN:O	1:B:862:ASN:ND2	2.35	0.46
1:B:891:LEU:HD13	1:B:1061:ARG:HH12	1.81	0.46
1:B:1278:ASP:OD1	1:B:1279:ASN:N	2.39	0.46
1:A:971:LEU:HB3	1:A:973:LEU:HD21	1.97	0.45
1:B:383:LEU:O	1:B:387:PRO:HD2	2.16	0.45
1:A:1298:CYS:SG	1:A:1309:ALA:CB	3.04	0.45
1:A:128:LEU:HD21	1:B:369:ILE:HD11	1.90	0.45
1:A:1367:TYR:OH	1:A:1381:PHE:HB2	2.16	0.45
1:B:465:GLN:O	1:B:468:ILE:HG22	2.16	0.45
1:B:647:THR:O	1:B:779:SER:OG	2.29	0.45
1:A:861:LEU:HD23	1:A:861:LEU:HA	1.82	0.45
1:B:236:ASN:OD1	1:B:239:GLN:N	2.36	0.45
1:B:522:LEU:HB3	1:B:836:ARG:HH12	1.81	0.45
1:B:700:ILE:HB	1:B:733:CYS:SG	2.56	0.45
1:B:1151:ALA:O	1:B:1156:LYS:NZ	2.29	0.45
1:A:646:LEU:HD12	1:A:756:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:PHE:CE1	1:A:1286:GLU:HB3	2.51	0.45
1:B:893:GLN:HG2	1:B:981:PRO:HG3	1.99	0.45
1:A:743:TYR:O	1:A:747:ILE:HG12	2.15	0.45
1:A:1138:LEU:HD23	1:A:1145:PHE:HE2	1.81	0.45
1:A:1323:ILE:O	1:A:1323:ILE:HG13	2.16	0.45
1:A:1415:ASN:OD1	1:A:1416:GLY:N	2.49	0.45
1:A:889:MET:SD	1:A:889:MET:N	2.89	0.45
1:B:1003:LYS:HD3	1:B:1004:GLY:N	2.32	0.45
1:A:1326:ASN:HD21	1:A:1328:MET:HG3	1.82	0.45
1:B:601:ASN:OD1	1:B:602:ASN:N	2.50	0.45
1:B:951:LEU:O	1:B:955:GLU:HG2	2.17	0.45
1:B:1157:GLU:OE2	1:B:1161:ARG:NH2	2.46	0.45
1:A:229:LEU:HD12	1:A:332:VAL:HG21	1.99	0.45
1:A:950:ILE:HD13	1:A:1033:PHE:HZ	1.78	0.45
1:B:939:SER:N	1:B:942:LEU:HD12	2.31	0.45
1:A:1203:ASN:O	1:A:1207:LYS:HG2	2.15	0.45
1:A:1412:GLU:HA	1:A:1415:ASN:HD21	1.82	0.45
1:B:908:ASP:N	1:B:908:ASP:OD1	2.50	0.45
1:A:793:VAL:HG12	1:A:793:VAL:O	2.17	0.44
1:A:958:ILE:HG13	1:A:958:ILE:O	2.17	0.44
1:B:1358:SER:O	1:B:1362:ILE:HG23	2.16	0.44
1:A:956:ASP:O	1:A:957:LEU:HB2	2.16	0.44
1:A:958:ILE:HB	1:A:1020:MET:CE	2.48	0.44
1:B:773:TRP:CZ3	1:B:776:LEU:HD23	2.52	0.44
1:B:793:VAL:HA	1:B:796:LYS:HD3	1.99	0.44
1:B:959:LEU:HD13	1:B:1028:ILE:CG2	2.47	0.44
1:A:223:VAL:HG22	1:A:369:ILE:HD11	1.98	0.44
1:A:1248:SER:HB2	1:A:1250:HIS:ND1	2.32	0.44
1:A:1394:ASP:O	1:A:1395:SER:HB3	2.17	0.44
1:B:219:ILE:HD13	1:B:362:LEU:HD23	1.99	0.44
1:B:481:PHE:CE1	1:B:557:ARG:CZ	3.00	0.44
1:B:570:PHE:CE1	1:B:574:PRO:HB3	2.53	0.44
1:B:1221:VAL:O	1:B:1225:LEU:HG	2.18	0.44
1:B:1303:LYS:HZ1	1:B:1307:GLU:HG3	1.79	0.44
1:A:730:LEU:HD13	1:A:739:PHE:HD2	1.82	0.44
1:A:761:GLU:HG3	1:A:762:HIS:ND1	2.33	0.44
1:A:1321:ILE:HD13	1:A:1370:TYR:OH	2.18	0.44
1:A:22:LEU:HD11	1:A:118:ALA:HA	1.99	0.44
1:A:624:LEU:O	1:A:628:ILE:HG12	2.17	0.44
1:A:1009:THR:O	1:A:1012:GLU:HG2	2.18	0.44
1:B:229:LEU:HD21	1:B:377:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:PHE:HD2	1:A:1175:LEU:HD22	1.83	0.44
1:B:982:GLU:HG3	1:B:1061:ARG:NH1	2.33	0.44
1:B:1138:LEU:HD23	1:B:1184:PHE:CD1	2.52	0.44
1:A:93:ASP:HA	1:A:136:GLN:HG3	1.99	0.44
1:A:611:ILE:HG22	1:A:649:PHE:HE1	1.82	0.44
1:B:1085:LYS:HG3	1:B:1086:GLU:H	1.83	0.44
1:B:1326:ASN:OD1	1:B:1327:GLU:N	2.50	0.44
1:A:390:LYS:NZ	1:A:770:GLU:OE2	2.35	0.44
1:A:909:ALA:HA	1:A:957:LEU:HD11	1.98	0.44
1:B:375:GLN:HB2	1:B:419:LEU:HD22	2.00	0.44
1:B:636:LEU:HD13	1:B:640:GLU:HB2	1.99	0.44
1:B:905:VAL:O	1:B:909:ALA:HB3	2.18	0.44
1:B:1371:LEU:HD12	1:B:1377:SER:HA	2.00	0.44
1:A:206:ARG:HG3	1:A:210:LEU:HD23	1.99	0.43
1:A:1048:LEU:HD21	1:A:1074:THR:HG21	2.00	0.43
1:A:567:THR:HG21	1:A:605:ARG:HG2	2.00	0.43
1:A:870:LEU:HD23	1:A:949:ILE:HD11	1.99	0.43
1:A:1217:ASN:HA	1:A:1220:TRP:HE3	1.83	0.43
1:B:510:ALA:O	1:B:513:THR:OG1	2.29	0.43
1:A:1398:GLU:O	1:A:1402:GLN:HG2	2.19	0.43
1:B:709:ASN:HB2	1:B:751:ILE:HD11	2.00	0.43
1:B:1016:SER:O	1:B:1020:MET:HG2	2.18	0.43
1:A:468:ILE:HD11	1:B:16:ILE:HG23	2.00	0.43
1:A:868:THR:HA	1:A:921:ASN:HD21	1.83	0.43
1:B:485:ASP:OD2	1:B:495:ILE:HG12	2.19	0.43
1:A:70:ASP:HB3	1:A:71:PRO:HD3	1.99	0.43
1:A:616:CYS:O	1:A:660:ARG:NH1	2.51	0.43
1:A:1368:LEU:HD22	1:A:1411:ILE:HD12	2.00	0.43
1:B:426:GLN:HA	1:B:776:LEU:HD21	2.01	0.43
1:B:734:CYS:C	1:B:736:HIS:H	2.21	0.43
1:B:1271:LEU:HD23	1:B:1275:LEU:HD23	2.01	0.43
1:A:535:HIS:O	1:A:803:LEU:HD21	2.18	0.43
1:A:1284:LYS:HG2	1:A:1328:MET:HB3	2.01	0.43
1:A:241:TYR:CD2	1:A:378:PRO:HB2	2.54	0.43
1:A:386:ASP:HB2	1:A:781:THR:HG21	2.01	0.43
1:A:1236:ASN:ND2	1:A:1300:ASN:HB3	2.33	0.43
1:A:1338:GLY:O	1:A:1341:PRO:HD2	2.19	0.43
1:B:20:ILE:HG13	1:B:21:ASN:N	2.33	0.43
1:B:183:ASP:HA	1:B:327:TYR:HE1	1.83	0.43
1:B:345:PRO:HD3	1:B:391:SER:HB3	2.01	0.43
1:B:656:GLN:OE1	1:B:656:GLN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:ASP:HA	1:B:809:ILE:HG22	2.00	0.43
1:B:1236:ASN:HD21	1:B:1302:CYS:N	2.16	0.43
1:B:1216:GLU:OE1	1:B:1216:GLU:N	2.52	0.43
1:A:153:ARG:HA	1:A:258:GLY:HA2	2.00	0.43
1:A:466:ILE:O	1:A:469:LEU:HB3	2.18	0.43
1:A:1186:ARG:HA	1:A:1224:LEU:HD21	2.01	0.43
1:B:1027:ASN:O	1:B:1027:ASN:ND2	2.51	0.43
1:B:1239:GLU:OE1	1:B:1302:CYS:HA	2.18	0.43
1:B:1396:ASP:O	1:B:1400:LYS:NZ	2.48	0.43
1:A:79:LEU:HD11	1:A:97:ILE:HA	2.00	0.43
1:A:1191:MET:SD	1:A:1192:LYS:N	2.92	0.43
1:B:154:PHE:CZ	1:B:258:GLY:HA2	2.54	0.43
1:B:835:THR:HA	1:B:838:ILE:HG22	1.99	0.43
1:B:954:TYR:CE1	1:B:961:PRO:HB3	2.53	0.43
1:B:1224:LEU:O	1:B:1228:ILE:HG12	2.19	0.43
1:B:1276:LEU:HD23	1:B:1320:LYS:HD2	2.00	0.43
1:B:645:LEU:HD22	1:B:665:PHE:CD1	2.54	0.42
1:B:675:TYR:HA	1:B:692:GLN:HE21	1.84	0.42
1:B:1067:LEU:O	1:B:1071:ILE:HG12	2.19	0.42
1:B:1201:TYR:O	1:B:1204:GLU:HG3	2.19	0.42
1:A:219:ILE:O	1:A:223:VAL:HG23	2.19	0.42
1:A:485:ASP:OD1	1:A:485:ASP:O	2.37	0.42
1:A:498:LEU:HD13	1:A:813:VAL:HG11	2.00	0.42
1:B:101:PHE:O	1:B:104:ILE:HG22	2.19	0.42
1:B:149:LEU:HD21	1:B:172:LEU:HD23	2.01	0.42
1:B:511:LEU:O	1:B:512:THR:OG1	2.29	0.42
1:B:1072:GLU:HA	1:B:1075:ILE:HG22	2.01	0.42
1:B:1184:PHE:HA	1:B:1187:LYS:HG2	2.01	0.42
1:A:115:THR:HG21	1:A:154:PHE:HB3	2.02	0.42
1:A:190:ILE:CG2	1:A:331:VAL:HG21	2.50	0.42
1:B:1167:GLU:HG3	1:B:1168:SER:H	1.85	0.42
1:B:1240:ILE:O	1:B:1244:LYS:HG2	2.19	0.42
1:B:1322:GLU:OE1	1:B:1324:PRO:HD2	2.20	0.42
1:A:1383:LYS:O	1:A:1386:SER:OG	2.26	0.42
1:A:1392:VAL:CG2	1:A:1393:GLU:H	2.29	0.42
1:B:838:ILE:HD12	1:B:838:ILE:HA	1.91	0.42
1:B:861:LEU:O	1:B:864:ILE:HG22	2.19	0.42
1:B:891:LEU:HD22	1:B:1061:ARG:HH12	1.84	0.42
1:A:1123:CYS:SG	1:A:1124:ALA:N	2.92	0.42
1:B:1287:ILE:O	1:B:1291:ILE:HG23	2.20	0.42
1:A:578:ILE:HD13	1:A:578:ILE:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:PHE:CD2	1:A:1175:LEU:HD22	2.54	0.42
1:B:526:VAL:HA	1:B:529:VAL:HG12	2.02	0.42
1:A:464:GLU:O	1:A:467:SER:OG	2.25	0.42
1:B:397:GLN:OE1	1:B:433:ARG:NH1	2.53	0.42
1:A:149:LEU:HD21	1:A:172:LEU:HD23	2.02	0.42
1:A:614:LEU:HD11	1:A:620:LYS:HE3	2.02	0.42
1:A:803:LEU:HD13	1:A:803:LEU:HA	1.92	0.42
1:A:807:ARG:HB2	1:A:851:PHE:CE1	2.54	0.42
1:B:15:ILE:HG12	1:B:125:PHE:CE2	2.55	0.42
1:B:574:PRO:O	1:B:578:ILE:HG12	2.20	0.42
1:B:620:LYS:HA	1:B:623:LEU:HB3	2.02	0.42
1:B:858:ASN:ND2	1:B:939:SER:HB3	2.35	0.42
1:A:372:ASP:N	1:A:372:ASP:OD1	2.51	0.42
1:A:1251:LYS:HB3	1:A:1251:LYS:HE2	1.85	0.42
1:A:579:PRO:HA	1:A:582:ILE:HG22	2.01	0.41
1:A:825:TYR:CZ	1:A:838:ILE:HD11	2.51	0.41
1:A:1138:LEU:HB3	1:A:1184:PHE:CD1	2.55	0.41
1:A:1383:LYS:O	1:A:1387:ILE:HG13	2.20	0.41
1:B:76:PHE:CE1	1:B:100:PRO:HB2	2.55	0.41
1:B:1048:LEU:HB3	1:B:1094:LYS:HG2	2.01	0.41
1:B:1294:LEU:HD22	1:B:1313:LEU:HD12	2.01	0.41
1:A:158:GLN:HG2	1:A:159:GLN:HG2	2.02	0.41
1:B:963:ILE:HG23	1:B:964:PHE:HD1	1.86	0.41
1:A:132:ASN:CG	1:A:133:GLU:H	2.24	0.41
1:A:207:SER:HB3	1:A:210:LEU:HB3	2.02	0.41
1:A:1109:VAL:O	1:A:1112:MET:HG2	2.20	0.41
1:A:1283:ARG:HB2	1:A:1285:ASN:ND2	2.35	0.41
1:A:1381:PHE:HA	1:A:1384:ILE:HG12	2.02	0.41
1:B:543:GLU:OE1	1:B:543:GLU:N	2.42	0.41
1:B:761:GLU:OE1	1:B:767:LYS:NZ	2.39	0.41
1:B:906:SER:OG	1:B:907:THR:N	2.51	0.41
1:B:98:LEU:O	1:B:102:LEU:HG	2.20	0.41
1:B:351:HIS:HB3	1:B:355:THR:HG21	2.03	0.41
1:B:578:ILE:O	1:B:582:ILE:HG12	2.20	0.41
1:B:1180:ASN:OD1	1:B:1181:PHE:N	2.53	0.41
1:A:434:ILE:HA	1:A:437:ILE:HG22	2.02	0.41
1:A:1266:LEU:HD22	1:A:1308:PHE:CD2	2.55	0.41
1:B:554:LEU:HD23	1:B:808:ALA:HB2	2.02	0.41
1:B:1077:LEU:O	1:B:1081:CYS:HB2	2.21	0.41
1:B:1357:SER:HA	1:B:1360:LEU:CD2	2.51	0.41
1:A:249:ASN:CG	1:A:337:ASN:ND2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:VAL:O	1:A:692:GLN:HG3	2.20	0.41
1:A:735:ASN:O	1:A:737:LYS:HG3	2.21	0.41
1:A:958:ILE:HG23	1:A:1023:ILE:CG2	2.51	0.41
1:A:967:LEU:HD22	1:A:1079:LEU:HD12	2.03	0.41
1:B:110:ILE:HD11	1:B:115:THR:HB	2.01	0.41
1:B:636:LEU:HD12	1:B:636:LEU:C	2.41	0.41
1:B:685:GLU:HA	1:B:742:TRP:CE2	2.55	0.41
1:A:236:ASN:HB3	1:A:239:GLN:HB2	2.03	0.41
1:A:409:LEU:HD11	1:A:462:LEU:HD23	2.02	0.41
1:A:871:ILE:CD1	1:A:948:ASN:HB2	2.50	0.41
1:B:489:ASP:HA	1:B:605:ARG:NH1	2.27	0.41
1:B:905:VAL:CG2	1:B:906:SER:N	2.83	0.41
1:B:1020:MET:HA	1:B:1023:ILE:HG22	2.02	0.41
1:B:1085:LYS:HG3	1:B:1086:GLU:OE1	2.20	0.41
1:B:1409:LYS:HZ2	1:B:1412:GLU:HB3	1.85	0.41
1:A:871:ILE:HD13	1:A:945:ASN:HA	2.00	0.41
1:B:818:VAL:HG21	1:B:856:LEU:HD11	2.02	0.41
1:B:1318:ILE:O	1:B:1369:HIS:CE1	2.74	0.41
1:A:160:LEU:HD12	1:A:160:LEU:HA	1.96	0.41
1:A:329:LEU:HA	1:A:332:VAL:HG22	2.02	0.41
1:A:570:PHE:CD1	1:A:606:MET:HE1	2.55	0.41
1:A:1113:LEU:HD13	1:A:1137:GLU:HG2	2.02	0.41
1:A:1281:ASP:C	1:A:1282:LEU:HG	2.40	0.41
1:B:676:ASP:N	1:B:677:PRO:HD2	2.35	0.41
1:B:767:LYS:HA	1:B:767:LYS:HD2	1.84	0.41
1:B:802:LEU:HD12	1:B:802:LEU:HA	1.94	0.41
1:B:852:ASP:HB3	1:B:853:PHE:H	1.68	0.41
1:B:971:LEU:HB3	1:B:973:LEU:HD23	2.03	0.41
1:B:1071:ILE:HG22	1:B:1115:TYR:CD2	2.56	0.41
1:A:112:GLY:HA2	1:A:115:THR:HG22	2.03	0.41
1:A:639:ASP:OD1	1:A:640:GLU:N	2.54	0.41
1:A:906:SER:OG	1:A:908:ASP:OD1	2.28	0.41
1:B:1242:TYR:OH	1:B:1254:LYS:HE2	2.21	0.41
1:B:1268:SER:O	1:B:1272:THR:HG23	2.21	0.41
1:A:642:ILE:O	1:A:646:LEU:HG	2.21	0.40
1:A:676:ASP:O	1:A:692:GLN:NE2	2.54	0.40
1:A:775:ASN:OD1	1:A:775:ASN:N	2.54	0.40
1:A:942:LEU:HA	1:A:942:LEU:HD12	1.81	0.40
1:A:971:LEU:O	1:A:973:LEU:HD23	2.21	0.40
1:A:1138:LEU:HD13	1:A:1184:PHE:CD2	2.56	0.40
1:A:1299:ILE:HG12	1:A:1355:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1360:LEU:HD12	1:B:1361:THR:N	2.35	0.40
1:B:1372:LYS:HD2	1:B:1372:LYS:HA	1.94	0.40
1:B:691:VAL:HG21	1:B:743:TYR:CG	2.56	0.40
1:A:961:PRO:HB3	1:A:1069:PHE:HD1	1.87	0.40
1:A:1283:ARG:HB2	1:A:1285:ASN:HD22	1.87	0.40
1:B:783:ILE:O	1:B:783:ILE:HG23	2.20	0.40
1:B:943:TRP:CE3	1:B:946:ILE:HD11	2.56	0.40
1:A:231:THR:O	1:A:231:THR:OG1	2.33	0.40
1:A:863:SER:HA	1:A:866:LYS:HG2	2.04	0.40
1:A:1408:LYS:NZ	1:A:1412:GLU:OE1	2.55	0.40
1:B:455:PRO:HB2	1:B:457:ILE:HD12	2.03	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	1261/1483 (85%)	1150 (91%)	111 (9%)	0	100	100
1	B	1260/1483 (85%)	1129 (90%)	131 (10%)	0	100	100
All	All	2521/2966 (85%)	2279 (90%)	242 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1182/1367 (86%)	1171 (99%)	11 (1%)	78 88
1	B	1183/1367 (86%)	1169 (99%)	14 (1%)	71 84
All	All	2365/2734 (86%)	2340 (99%)	25 (1%)	74 85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	TYR
1	A	171	PHE
1	A	322	TYR
1	A	389	PHE
1	A	497	PHE
1	A	557	ARG
1	A	649	PHE
1	A	703	TYR
1	A	810	PHE
1	A	1080	PHE
1	A	1096	PHE
1	B	72	PHE
1	B	412	PHE
1	B	497	PHE
1	B	563	PHE
1	B	570	PHE
1	B	669	TYR
1	B	739	PHE
1	B	746	ARG
1	B	768	TRP
1	B	810	PHE
1	B	822	PHE
1	B	916	PHE
1	B	1096	PHE
1	B	1218	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	ASN
1	A	337	ASN
1	A	602	ASN
1	A	692	GLN
1	A	858	ASN

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Mol	Chain	Res	Type
1	A	1319	ASN
1	B	1147	GLN
1	B	1178	ASN
1	B	1304	GLN
1	B	1349	GLN
1	B	1352	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

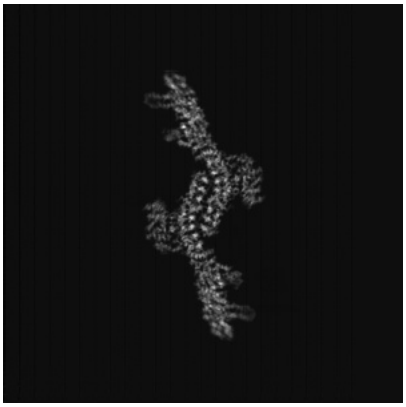
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28748. These allow visual inspection of the internal detail of the map and identification of artifacts.

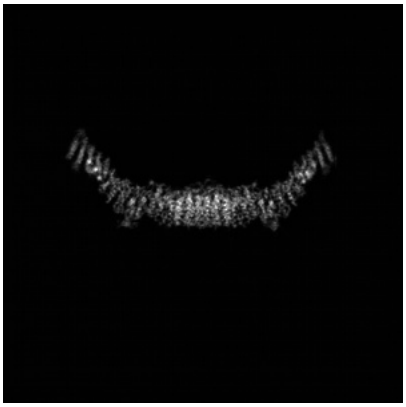
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

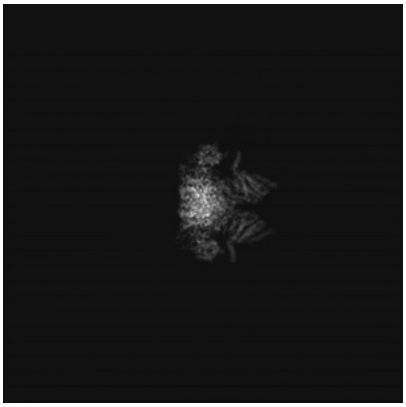
6.1.1 Primary map



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: 256

Y Index: 256

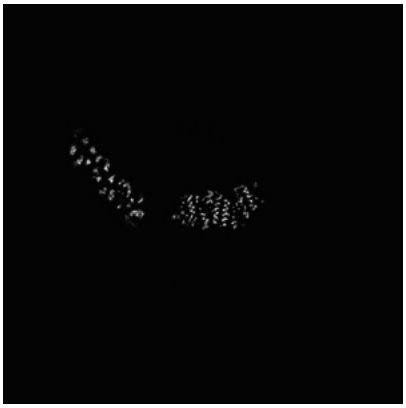
Z Index: 256

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

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 256



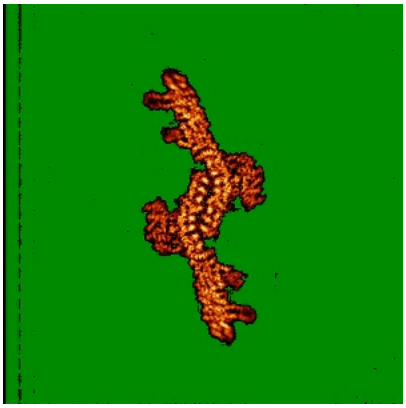
Y Index: 274

Z Index: 273

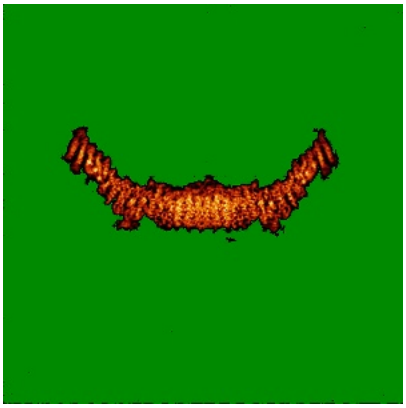
The images above show the largest variance slices of the map in three orthogonal directions.

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

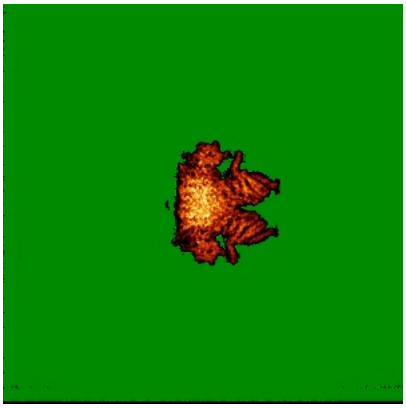
6.4.1 Primary map



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

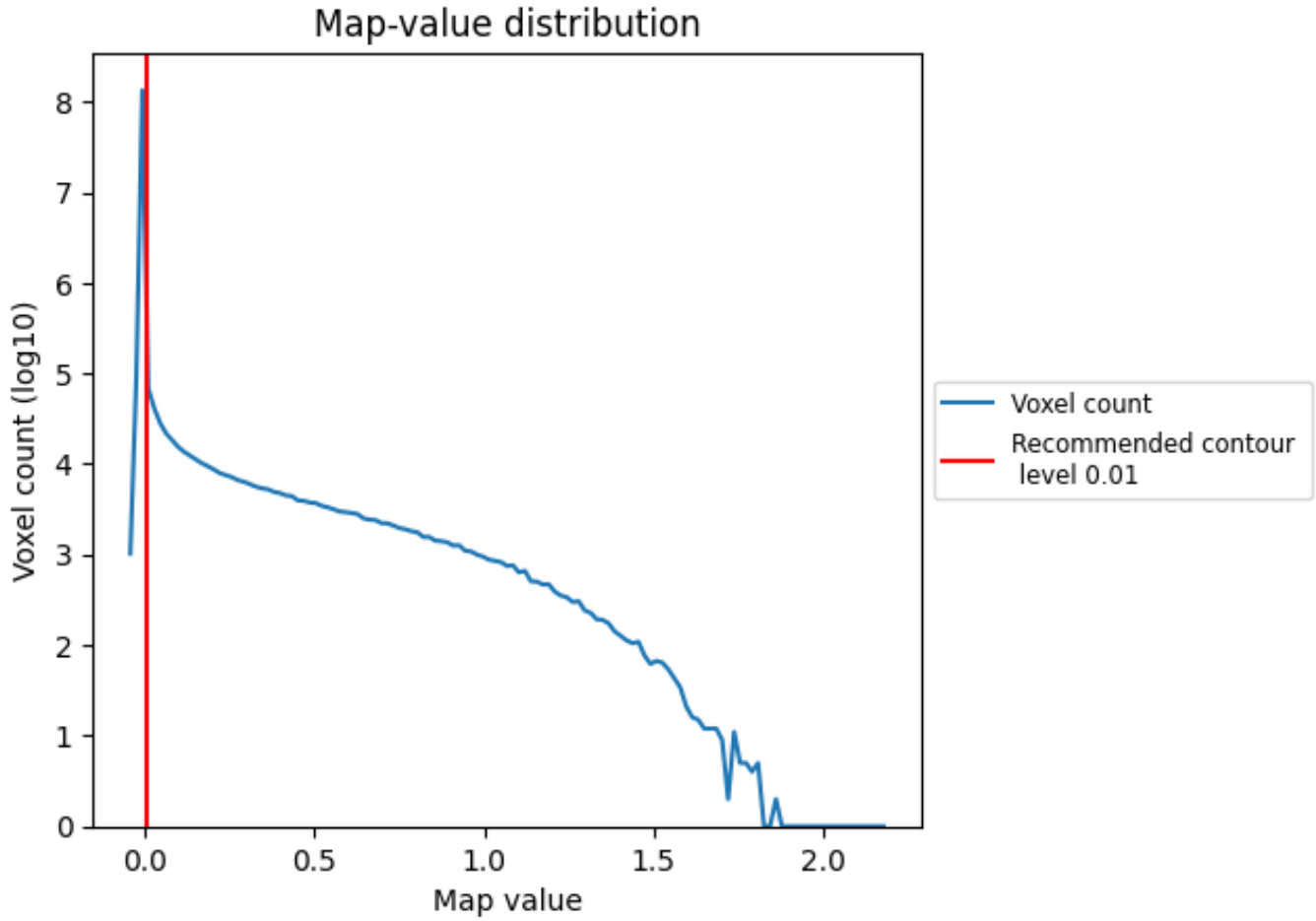
6.6 Mask visualisation (i)

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

7 Map analysis

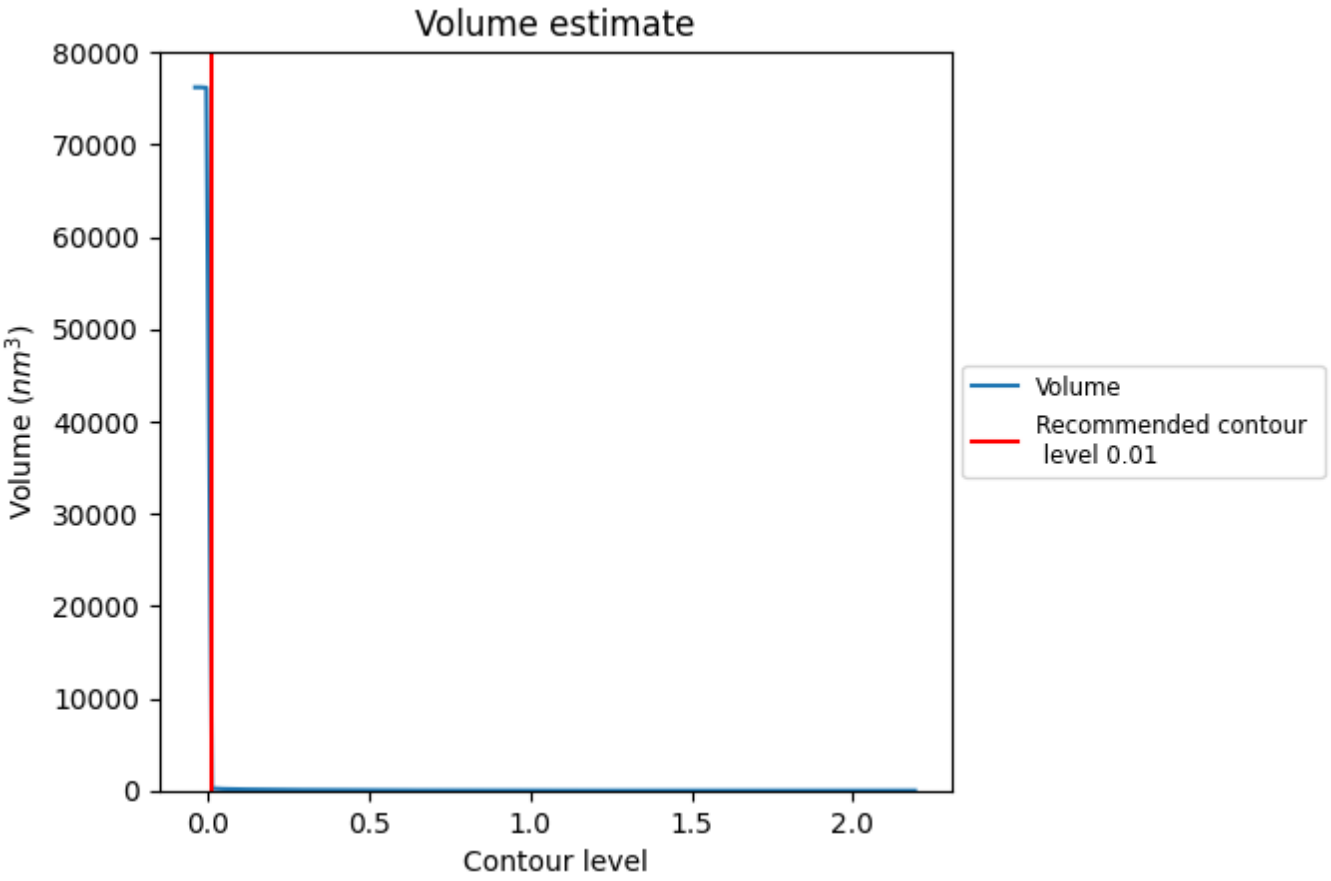
This section contains the results of statistical analysis of the map.

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.

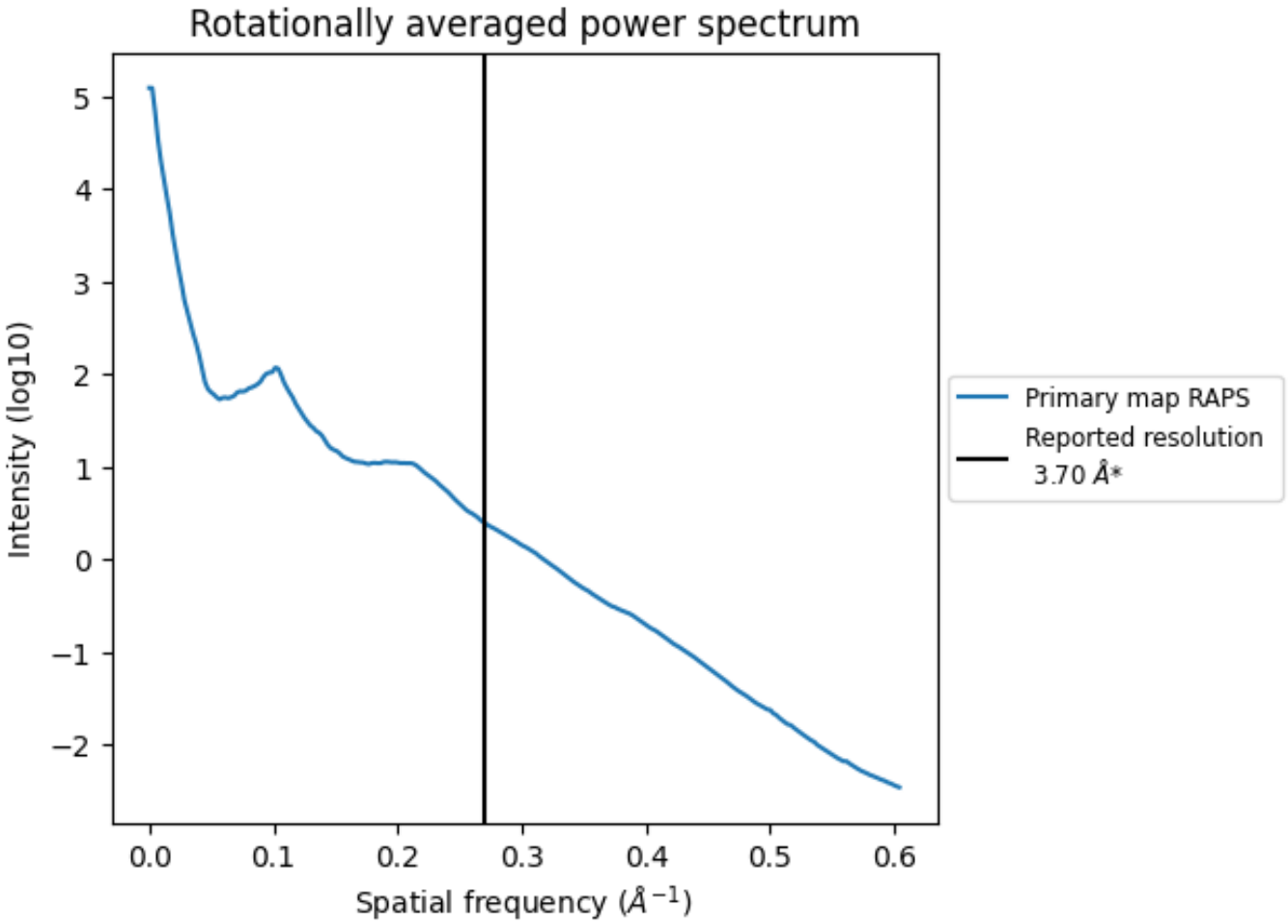
7.2 Volume estimate (i)



The volume at the recommended contour level is 12112 nm^3; this corresponds to an approximate mass of 10941 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 0.270 Å^{-1}

8 Fourier-Shell correlation (i)

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

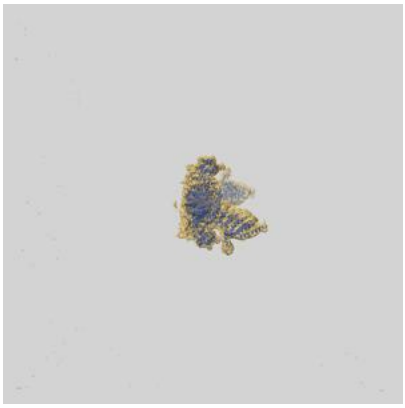
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28748 and PDB model 8EZQ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay

X

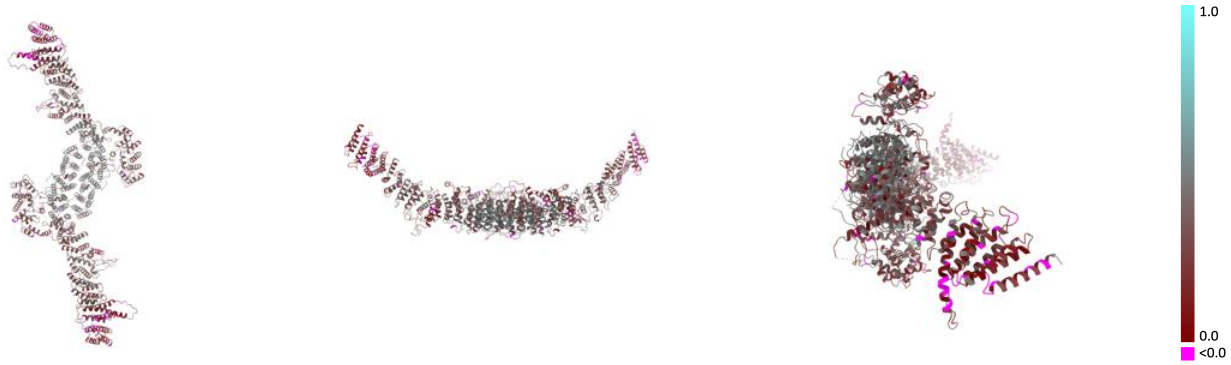
Y



Z

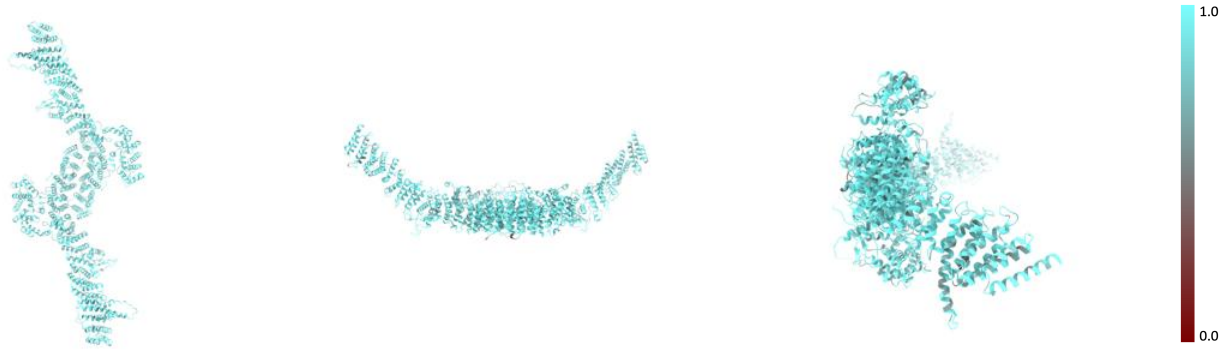
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



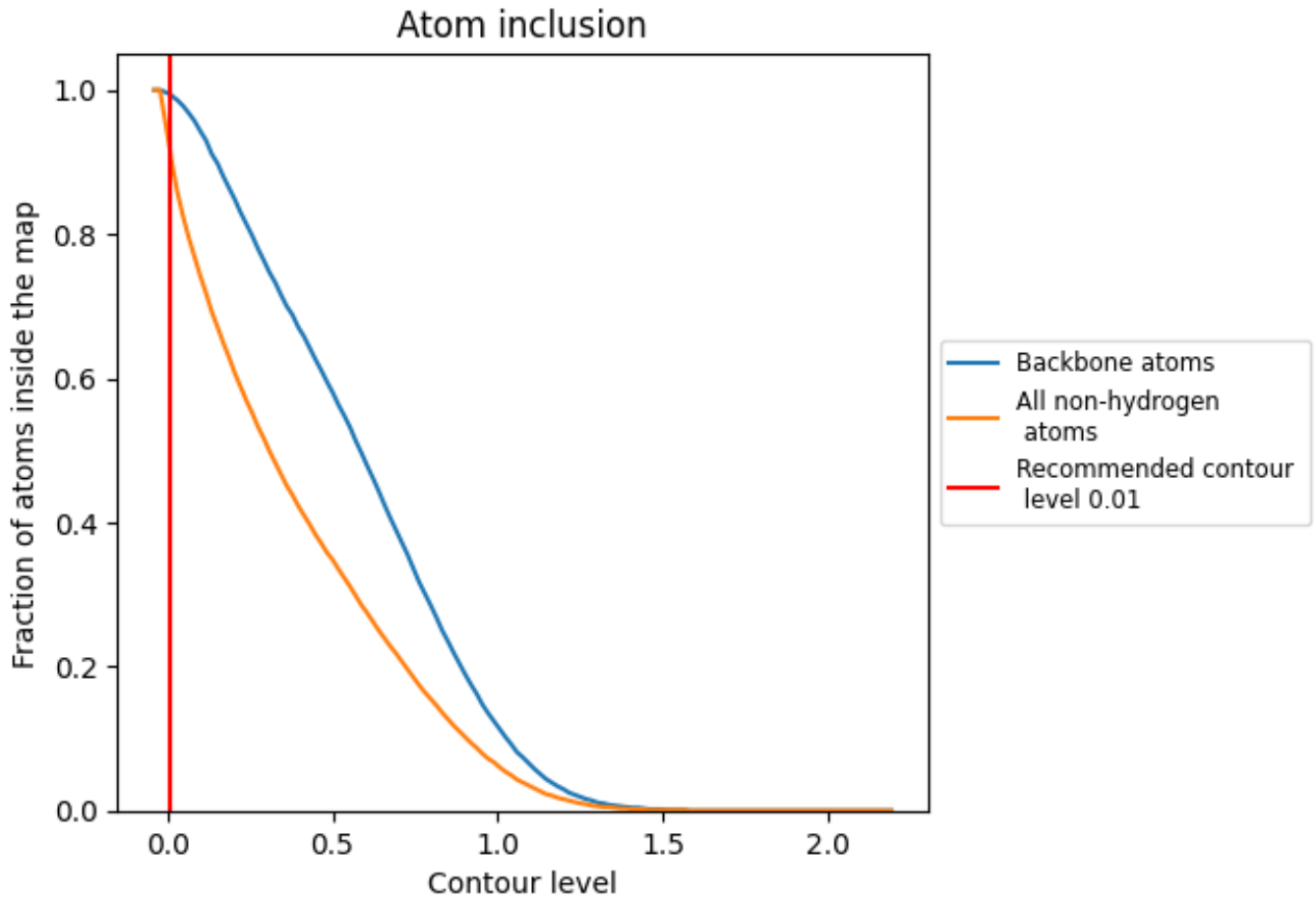
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9120	0.3290
A	0.9170	0.3370
B	0.9070	0.3200