



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:26 AM UTC

PDB ID : 8ASV / pdb_00008asv
EMDB ID : EMD-15622
Title : Cryo-EM structure of yeast Elongator complex
Authors : Jaciuk, M.; Scherf, D.; Kaszuba, K.; Gaik, M.; Koscielniak, A.; Krutyholowa, R.; Rawski, M.; Indyka, P.; Biela, A.; Dobosz, D.; Lin, T.-Y.; Abbassi, N.; Hammermeister, A.; Chramiec-Glabik, A.; Kosinski, J.; Schaffrath, R.; Glatt, S.
Deposited on : 2022-08-21
Resolution : 4.35 Å(reported)
Based on initial models : 6QK7, 4A8J

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

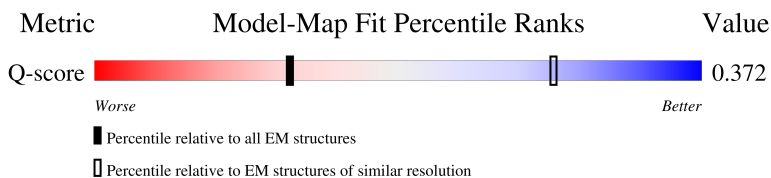
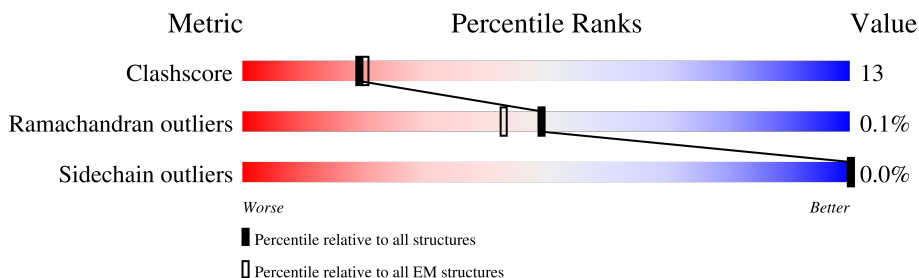
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.35 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3796 (3.85 - 4.85)

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 $\leq 5\%$. 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	1349	
1	D	1349	
2	B	788	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
3	C	557	
4	E	309	
4	H	309	
5	F	273	
5	I	273	
6	G	456	
6	J	456	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 35789 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 Elongator complex protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1235	Total	C	N	O	S	0	0
			9844	6248	1632	1925	39		
1	D	343	Total	C	N	O	S	0	0
			2769	1738	487	536	8		

- Molecule 2 is a protein called Elongator complex protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	786	Total	C	N	O	S	0	0
			6286	4000	1063	1196	27		

- Molecule 3 is a protein called Elongator complex protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	464	Total	C	N	O	S	0	0
			3730	2353	658	698	21		

- Molecule 4 is a protein called Elongator complex protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	232	Total	C	N	O	S	0	0
			1871	1196	307	361	7		
4	H	231	Total	C	N	O	S	0	0
			1865	1193	306	359	7		

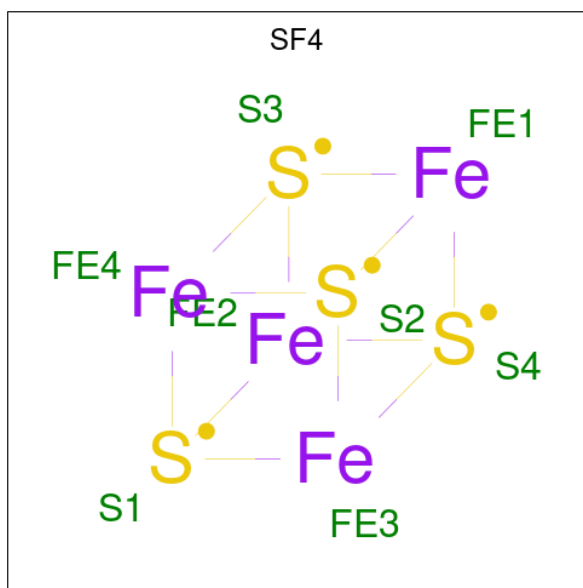
- Molecule 5 is a protein called Elongator complex protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	269	Total	C	N	O	S	0	0
			2129	1352	359	411	7		
5	I	269	Total	C	N	O	S	0	0
			2129	1352	359	411	7		

- Molecule 6 is a protein called Elongator complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	296	Total	C	N	O	S	0	0
			2346	1500	404	432	10		
6	J	353	Total	C	N	O	S	0	0
			2812	1788	488	526	10		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

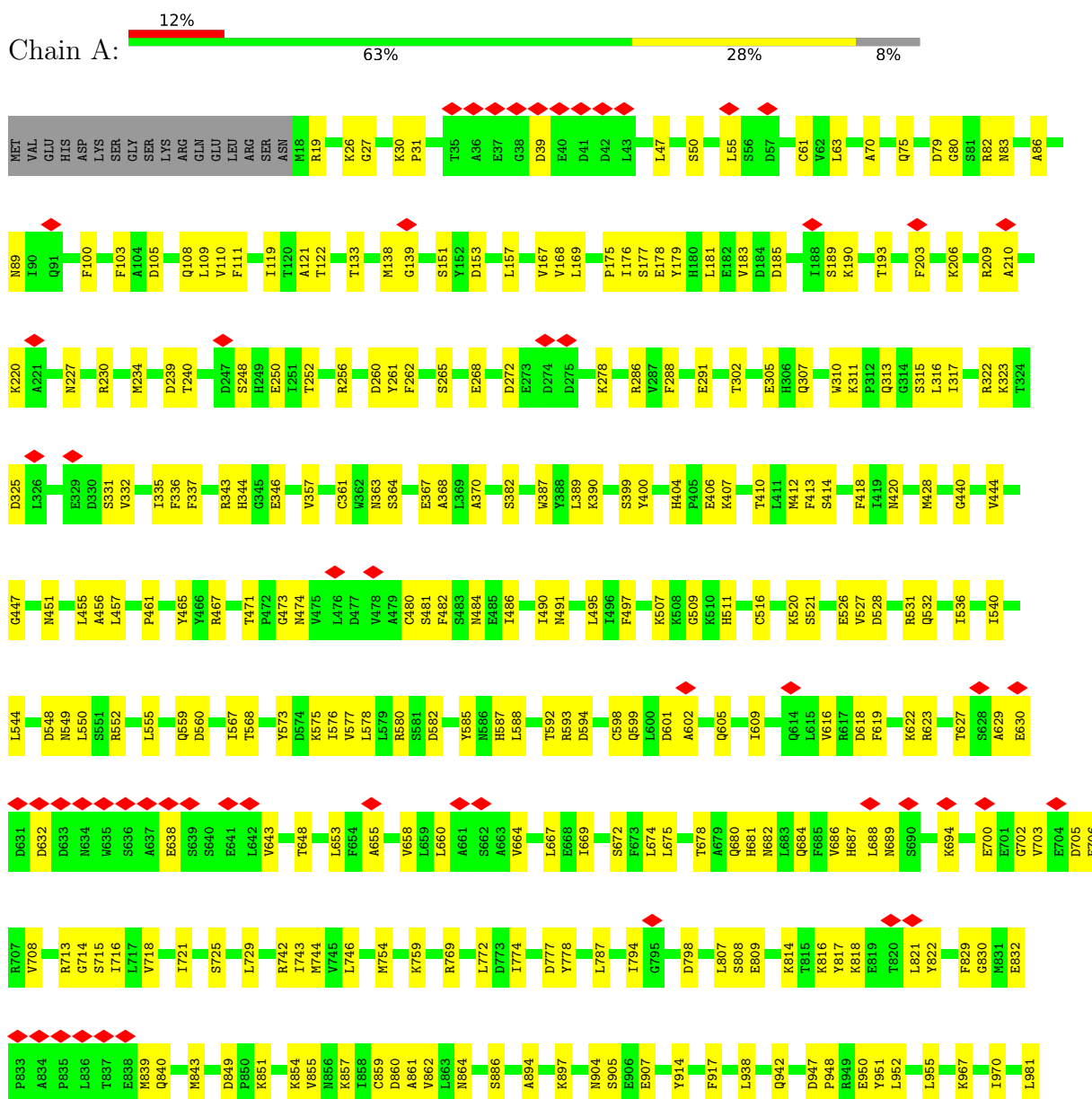


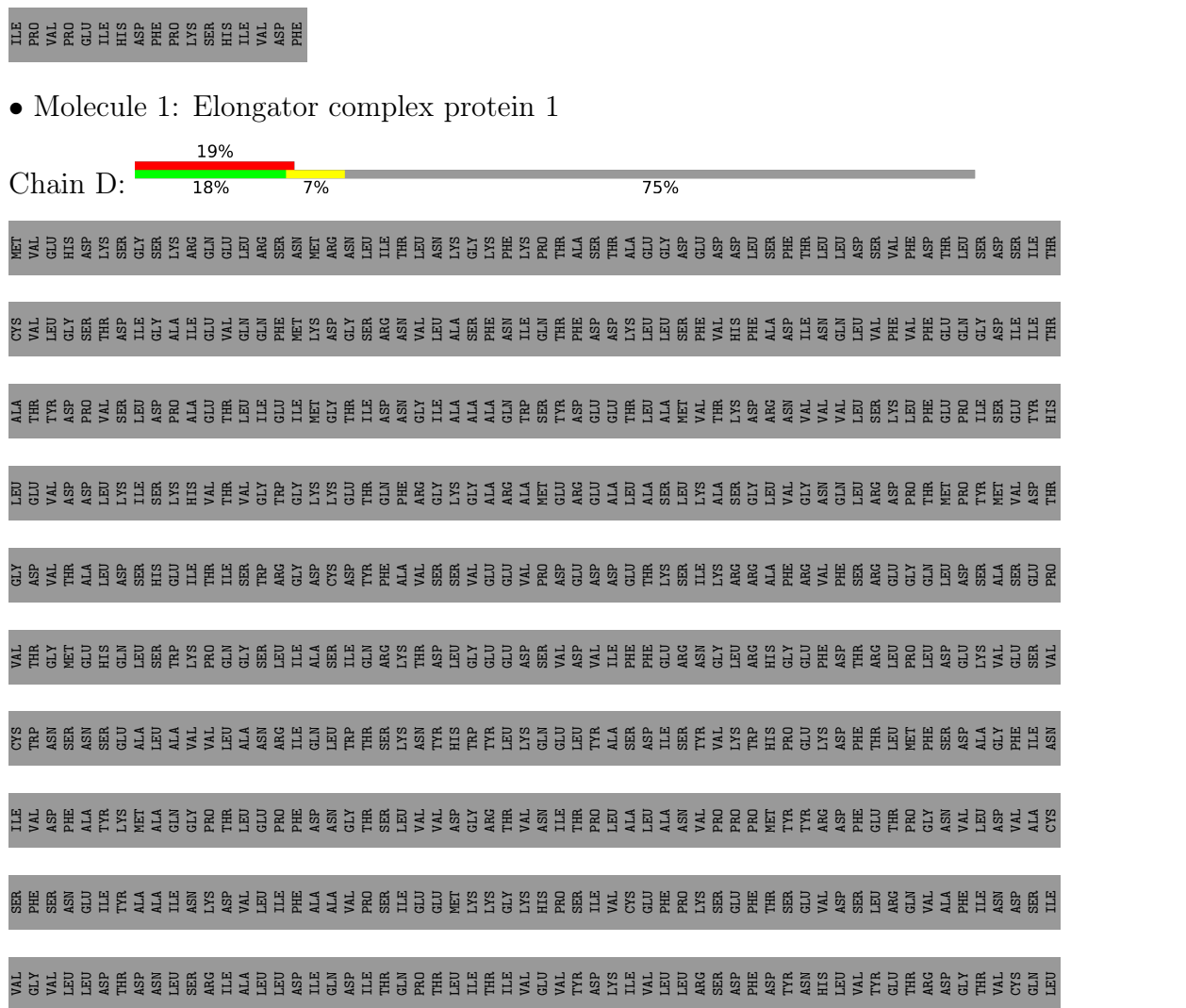
Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	Fe	S	0
			8	4	4	

3 Residue-property plots

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.

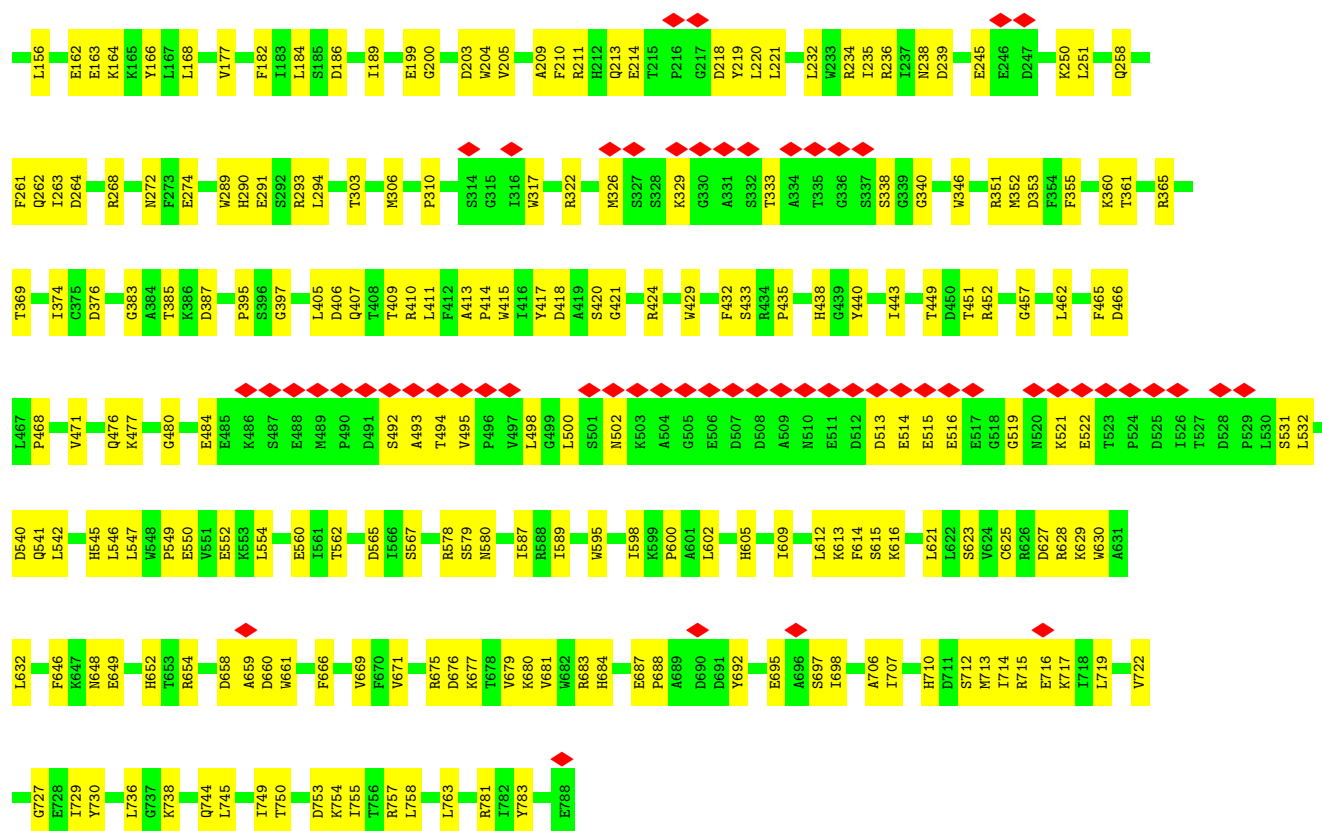
• Molecule 1: Elongator complex protein 1





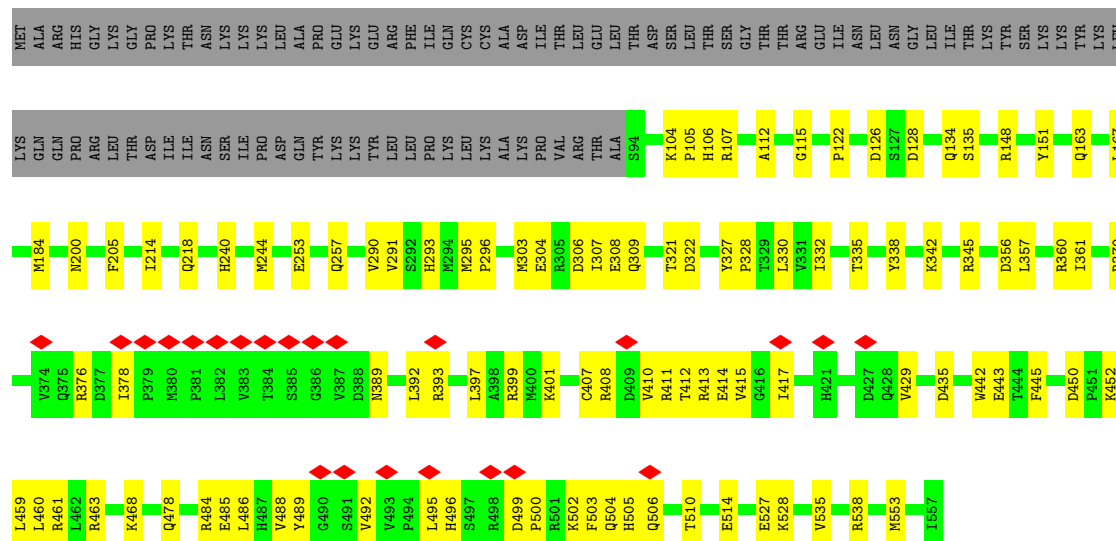
E1337	K1270	S1209	G1148	S1081	Q1021
I1338	P1271	F1210	E1149	V1082	M1022
H1339	D1272	F1211	G1150	E1083	V1023
D1340	A1273	T1212	F1151	E1084	I1024
F1341	V1274	R1213	G1152	E1085	Y1025
P1342	R1275	Y1214	I1153	L1086	M1026
K1343	V1276	T1215	I1154	L1087	I1027
S1344	E1277	A1155	E1155	S1088	Y1028
H1345	E1278	G1216	E1156	I1087	I1E
I1346	N1284	K1217	L1157	S1089	A1029
V1347	H1285	T1218	L1158	L1090	K1030
D1348	H1286	G1219	C1161	I1091	H1031
PHE	E1287	R1220	K1162	F1092	L1032
	Q1288	T1221	G1163	E1093	S1033
	A1289	A1222	G1164	H1094	S1034
	H1290	K1223	I1165	R1095	M1035
		T1224	I1166	Y1096	Q1036
	K1294	G1225	N1166	V1097	M1037
N1295	A1226	A1226	S1167	D1098	Y1038
F1296	S1227	Q1168	Q1168	A1099	T1039
V1297	R1228	L1169	L1170	A1100	D1040
	R1229	R1171	R1171	D1101	A1041
L1300	T1230	L1172	L1172	I1102	A1042
D1301	A1231	R1173	R1173	Q1103	V1043
L1302	K1232	E1174	L1104	L1104	A1044
L1303	A1305	L1175	E1105	E1105	Y1045
K1304	N1233	R1176	Y1106	Y1106	E1046
A1305	K1234	A1177	L1107	L1107	M1047
N1306	R1235	K1178	D1108	D1108	L1048
V1307	R1236	K1179	N1109	N1109	G1049
K1308	E1237	E1180	V1110	V1110	K1050
E1309	E1238	E1181	K1111	K1111	L1051
I1310	K1239	E1182	E1112	E1112	K1052
Y1311	R1240	P1183	A1113	E1053	E1053
S1312	R1241	Y1184	V1114	V1114	A1054
I1313	A1242	A1185	A1115	A1115	M1055
S1314	R1243	F1186	L1116	L1116	G1056
E1315	G1244	Y1187	K1119	K1119	A1057
K1316	K1245	G1188	A1120	A1120	Y1058
D1317	K1246	Q1189	A1126	A1126	Q1059
R1318	G1247	E1190	A1130	A1130	S1060
E1319	T1248	T1191	I1131	I1131	A1061
R1320	I1249	E1192	K1132	K1132	K1062
V1321	Y1250	Q1193	A1133	A1133	R1063
N1322	E1251	D1194	K1134	K1134	W1064
E1323	E1252	L1195	K1135	K1135	R1065
N1324	A1253	D1196	D1136	D1136	E1066
G1325	Y1254	V1197	E1137	E1137	A1067
E1326	L1255	S1198	L1138	L1138	Y1016
E1327	V1256	V1199	L1139	L1139	M1068
Y1328	V1259	A1200	E1140	E1140	S1069
Y1329	G1260	P1201	V1142	V1142	I1070
I1330	R1261	S1202	V1143	V1143	A1071
P1331	L1262	T1203	D1144	D1144	Y1072
E1332	I1263	T1204	P1145	P1145	Q1073
I1333	E1264	S1205	G1146	G1146	K1074
P1334	R1265	L1266	Q1207	Q1207	F1075
V1335	L1266	N1267	E1208	E1208	P1076
P1336	N1267	Q1268			E1077
	Q1268				E1078
					F1080

MET	VAL
E3	
Q17	
T18	
Q19	
V20	
S21	
D22	
I23	
H24	
K25	
V26	
Z27	
K28	
W41	
D42	
E45	
P46	
N47	
N48	
K49	
K56	
R66	
F67	
D70	
S71	
D72	
F88	
T89	
D90	
H93	
T106	
I107	
L116	
I117	
C121	
T125	
W129	
R130	
Q131	
F138	
A141	



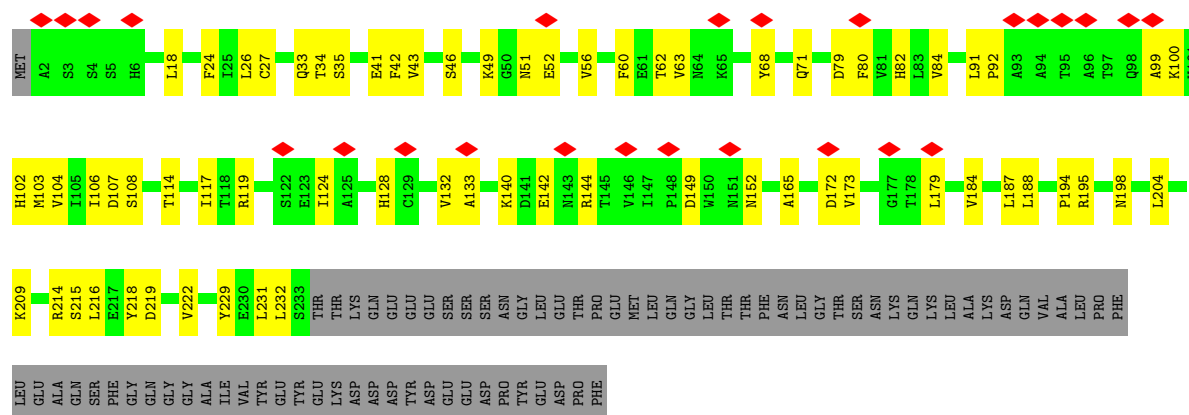
• Molecule 3: Elongator complex protein 3

Chain C: 64% 19% 17%

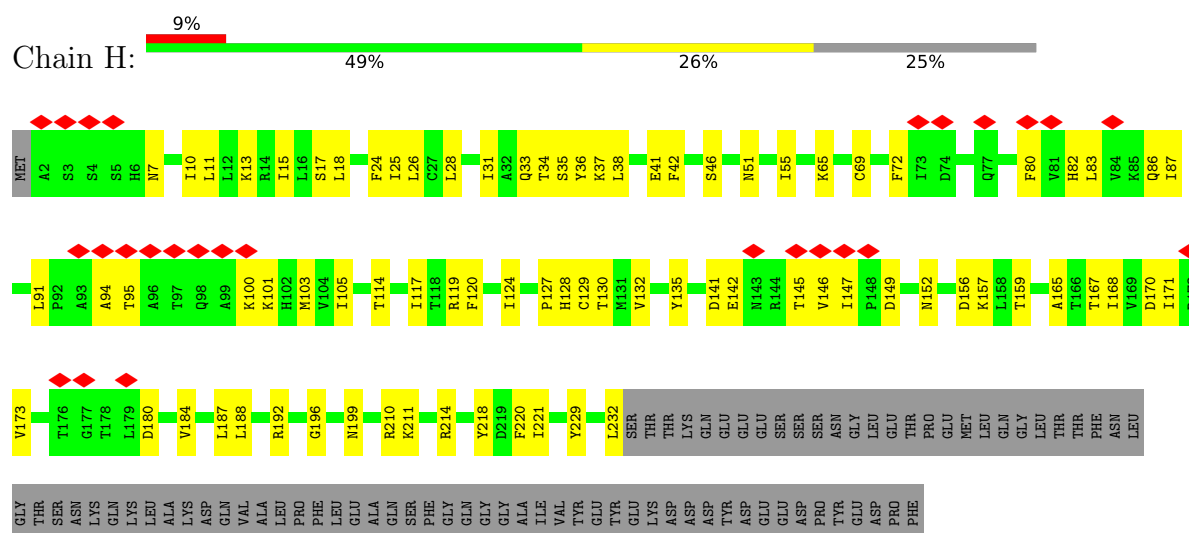


• Molecule 4: Elongator complex protein 5

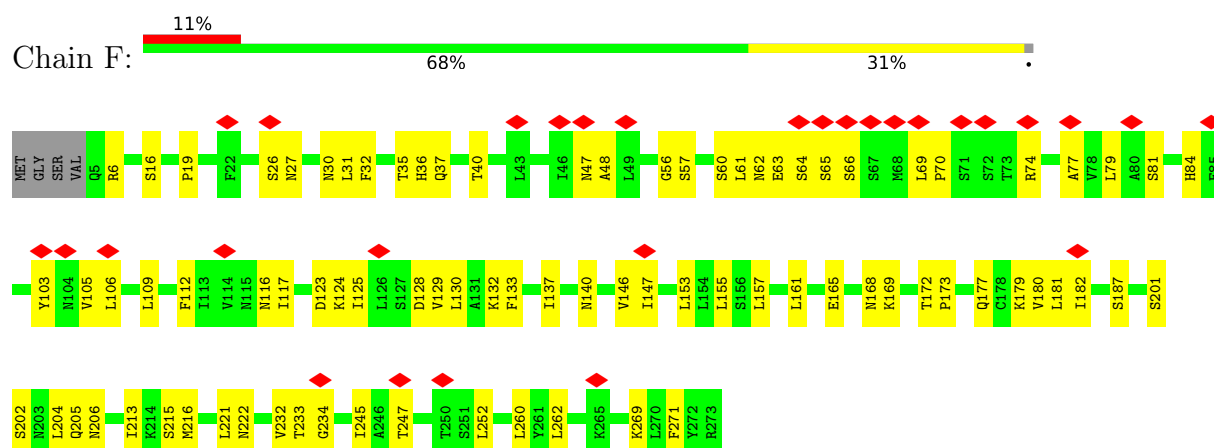
Chain E: 8% 53% 22% 25%



• Molecule 4: Elongator complex protein 5

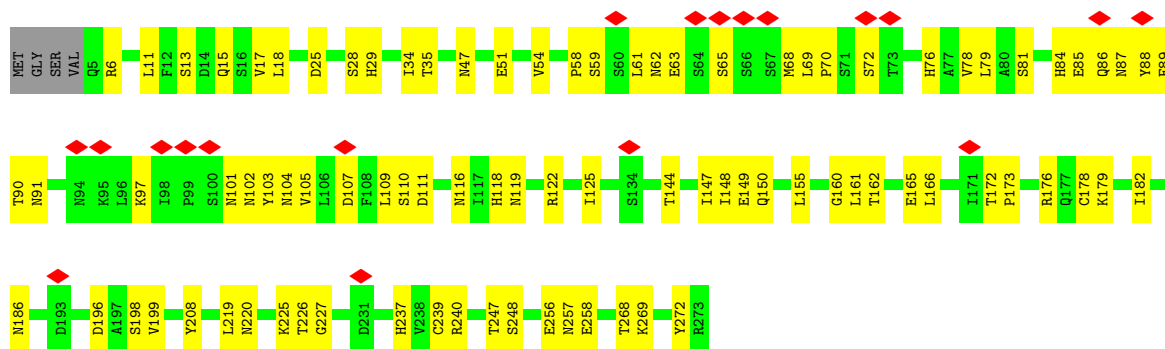


• Molecule 5: Elongator complex protein 6

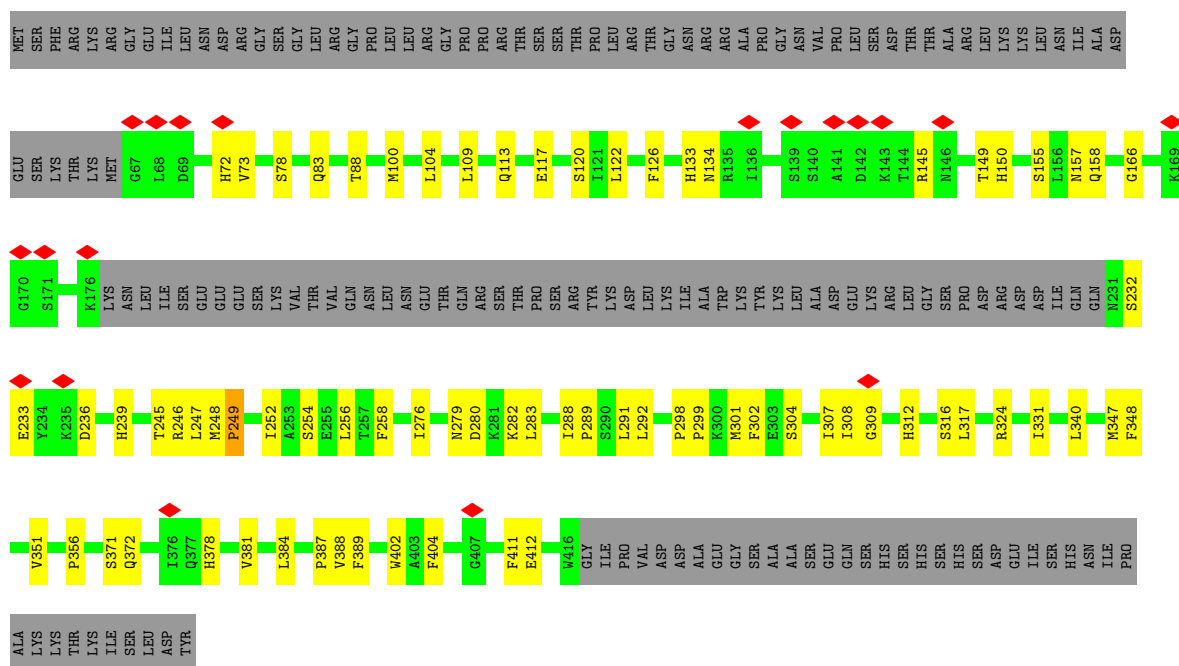


• Molecule 5: Elongator complex protein 6

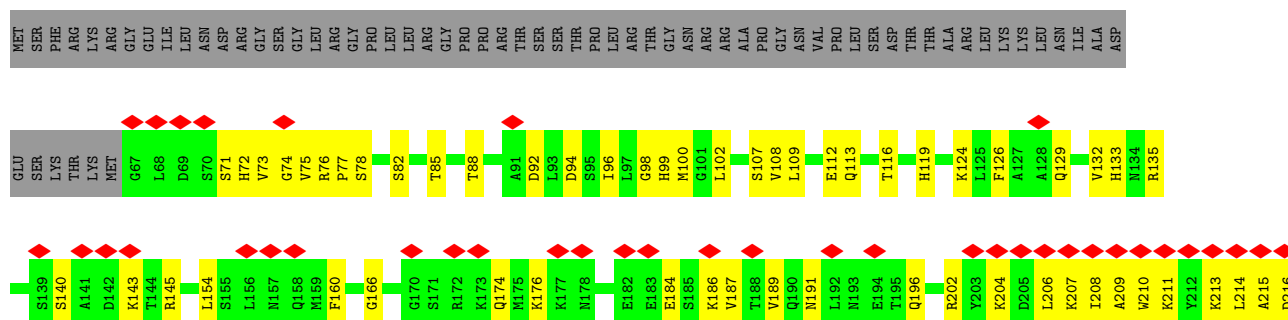


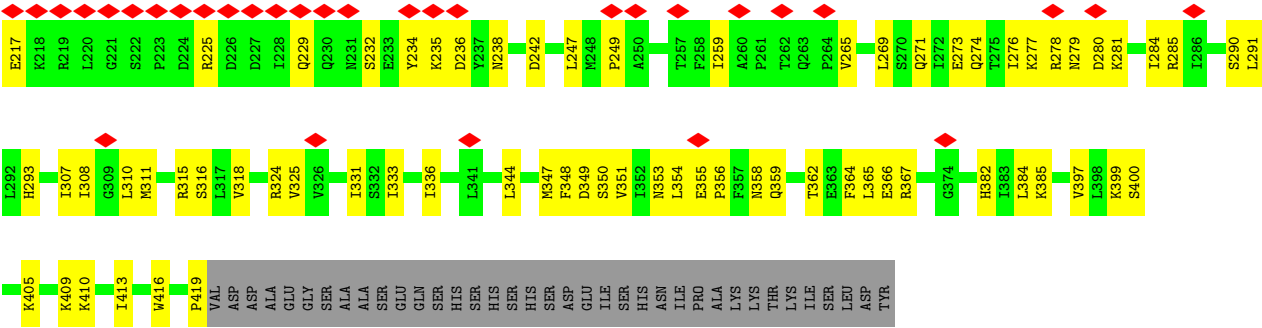


• Molecule 6: Elongator complex protein 4



• Molecule 6: Elongator complex protein 4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12514	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0169	Depositor
Map size (Å)	361.2, 361.2, 361.2	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	0.14	0/10022	0.41	0/13572
1	D	0.14	0/2814	0.41	0/3787
2	B	0.13	0/6434	0.41	0/8717
3	C	0.16	0/3811	0.43	0/5149
4	E	0.14	0/1909	0.42	0/2595
4	H	0.14	0/1903	0.39	0/2587
5	F	0.13	0/2174	0.42	0/2954
5	I	0.14	0/2174	0.42	0/2954
6	G	0.16	0/2396	0.44	0/3239
6	J	0.15	0/2870	0.46	1/3879 (0.0%)
All	All	0.14	0/36507	0.42	1/49433 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	75	VAL	N-CA-C	-5.42	107.08	111.91

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	9844	0	9769	260	0
1	D	2769	0	2757	74	0
2	B	6286	0	6167	169	0
3	C	3730	0	3693	72	0
4	E	1871	0	1872	44	0
4	H	1865	0	1867	52	0
5	F	2129	0	2108	54	0
5	I	2129	0	2108	70	0
6	G	2346	0	2398	53	0
6	J	2812	0	2870	85	0
7	C	8	0	0	0	0
All	All	35789	0	35609	905	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (905) 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:D:1322:ASN:HB3	1:D:1328:TYR:HB3	1.61	0.82
1:A:497:PHE:HB2	1:A:516:CYS:HB3	1.63	0.81
6:J:186:LYS:HG3	6:J:187:VAL:HG23	1.62	0.80
1:A:1293:GLN:HA	1:A:1296:PHE:HD2	1.46	0.80
1:A:428:MET:HE1	1:A:718:VAL:HG13	1.64	0.79
1:A:185:ASP:O	1:A:286:ARG:NH2	2.17	0.78
1:A:703:VAL:HG21	1:A:708:VAL:H	1.49	0.78
6:J:78:SER:H	6:J:82:SER:HA	1.50	0.77
1:D:1262:LEU:HA	1:D:1265:ARG:HH12	1.50	0.77
2:B:477:LYS:NZ	2:B:519:GLY:O	2.18	0.76
1:A:203:PHE:HB3	1:A:209:ARG:HH21	1.49	0.76
6:G:72:HIS:O	6:G:145:ARG:NH1	2.18	0.75
1:D:1189:GLN:NE2	1:D:1192:GLU:OE2	2.20	0.75
4:H:18:LEU:HD13	4:H:103:MET:HE1	1.69	0.75
1:A:982:GLU:HG2	1:A:1013:LEU:HD21	1.69	0.73
2:B:449:THR:HG22	2:B:452:ARG:HB2	1.71	0.73
6:J:108:VAL:HA	6:J:350:SER:HB2	1.69	0.73
5:I:111:ASP:O	5:I:116:ASN:ND2	2.22	0.72
6:J:206:LEU:HG	6:J:207:LYS:HG2	1.71	0.72
1:A:474:ASN:O	1:A:491:ASN:ND2	2.23	0.72
4:H:33:GLN:HB2	4:H:173:VAL:HB	1.72	0.72
6:J:109:LEU:HD11	6:J:348:PHE:HD2	1.54	0.72
6:J:204:LYS:HB3	6:J:410:LYS:HE2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1290:HIS:ND1	1:D:1347:VAL:O	2.23	0.71
5:I:78:VAL:HG22	5:I:104:ASN:HB2	1.73	0.71
5:F:147:ILE:HG22	5:F:182:ILE:HB	1.71	0.70
2:B:387:ASP:HB2	2:B:405:LEU:HD12	1.73	0.70
5:I:34:ILE:HG12	5:I:219:LEU:HB2	1.72	0.70
5:I:6:ARG:NH2	5:I:61:LEU:O	2.24	0.70
1:A:1103:GLN:HB3	1:A:1113:ALA:HB2	1.74	0.69
1:D:1246:LYS:NZ	1:D:1251:GLU:O	2.25	0.69
6:J:126:PHE:O	6:J:285:ARG:NH1	2.25	0.69
3:C:435:ASP:HB3	3:C:442:TRP:HE1	1.57	0.69
3:C:461:ARG:NE	3:C:485:GLU:OE2	2.26	0.69
6:J:353:ASN:HB2	6:J:382:HIS:HB2	1.74	0.69
6:J:124:LYS:HG2	6:J:160:PHE:HE1	1.58	0.69
1:D:1254:TYR:OH	1:D:1261:ARG:NH1	2.27	0.68
1:A:1282:ARG:HH22	1:D:1043:VAL:HG22	1.57	0.68
2:B:19:GLN:OE1	2:B:66:ARG:NH2	2.26	0.68
2:B:681:VAL:HG23	2:B:695:GLU:HB3	1.74	0.68
6:J:174:GLN:O	6:J:202:ARG:NH1	2.26	0.68
1:A:1018:SER:HA	1:A:1021:GLN:HB2	1.76	0.68
4:E:187:LEU:HD13	4:E:194:PRO:HG3	1.74	0.67
4:H:95:THR:HA	4:H:127:PRO:HB2	1.76	0.67
2:B:236:ARG:NH2	2:B:272:ASN:OD1	2.27	0.67
1:A:1287:GLU:HA	1:A:1290:HIS:CE1	2.28	0.67
1:A:715:SER:HB3	1:A:729:LEU:HD13	1.76	0.67
5:I:81:SER:HB2	5:I:89:PHE:HZ	1.60	0.67
6:G:291:LEU:HD23	6:G:292:LEU:HG	1.75	0.67
2:B:541:GLN:HA	2:B:545:HIS:HD2	1.60	0.66
1:D:1167:SER:O	1:D:1176:ARG:NH1	2.27	0.66
4:E:92:PRO:HB2	4:E:128:HIS:HB3	1.77	0.66
4:E:198:ASN:O	5:I:240:ARG:NH1	2.28	0.66
2:B:605:HIS:NE2	2:B:623:SER:OG	2.27	0.66
5:I:13:SER:O	5:I:15:GLN:NE2	2.29	0.66
6:G:100:MET:H	6:G:100:MET:HE2	1.61	0.66
6:G:282:LYS:O	6:G:324:ARG:NH1	2.28	0.66
4:H:51:ASN:HD21	4:H:100:LYS:HB2	1.59	0.66
6:G:145:ARG:NH2	6:G:236:ASP:OD2	2.29	0.66
1:A:1140:GLU:HA	1:A:1144:ASP:HB3	1.76	0.66
6:J:100:MET:HE2	6:J:100:MET:H	1.60	0.66
1:A:672:SER:HA	1:A:688:LEU:HB2	1.76	0.66
1:D:1304:LYS:NZ	1:D:1340:ASP:OD1	2.29	0.66
5:I:35:THR:OG1	5:I:220:ASN:OD1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:HB2	1:A:119:ILE:HB	1.76	0.65
5:I:58:PRO:HG2	5:I:62:ASN:HB2	1.77	0.65
6:J:355:GLU:HB2	6:J:382:HIS:HE1	1.62	0.65
1:A:680:GLN:O	1:A:713:ARG:NH1	2.29	0.65
5:I:72:SER:OG	5:I:101:ASN:ND2	2.30	0.65
5:I:76:HIS:HB3	5:I:144:THR:HG22	1.77	0.65
6:J:211:LYS:NZ	6:J:217:GLU:OE1	2.30	0.65
2:B:560:GLU:OE2	2:B:578:ARG:NH2	2.30	0.65
6:G:73:VAL:HG22	6:G:133:HIS:HB3	1.79	0.65
1:A:317:ILE:O	1:A:336:PHE:HA	1.97	0.65
3:C:492:VAL:O	3:C:505:HIS:ND1	2.26	0.65
2:B:47:ASN:HA	2:B:424:ARG:HH21	1.62	0.65
4:E:56:VAL:HA	4:E:71:GLN:HB2	1.78	0.65
2:B:707:ILE:HG22	2:B:722:VAL:HG12	1.78	0.65
5:F:137:ILE:HD13	5:F:177:GLN:HB3	1.79	0.65
4:E:33:GLN:HB2	4:E:173:VAL:HB	1.79	0.64
2:B:397:GLY:HA3	2:B:763:LEU:HB2	1.80	0.64
1:A:904:ASN:OD1	1:A:905:SER:N	2.31	0.64
1:A:993:VAL:HG23	1:A:997:VAL:HB	1.80	0.64
1:A:1148:GLY:HA2	1:A:1151:PHE:CE1	2.32	0.64
1:A:109:LEU:HB2	1:A:121:ALA:HB3	1.78	0.64
2:B:220:LEU:HD21	2:B:232:LEU:HD22	1.80	0.64
4:H:13:LYS:O	4:H:17:SER:N	2.26	0.64
1:A:480:CYS:SG	1:A:481:SER:N	2.71	0.64
1:A:1122:ARG:HG3	1:A:1125:ILE:HB	1.80	0.64
5:I:54:VAL:HG11	5:I:70:PRO:HB3	1.80	0.64
1:A:536:ILE:HB	1:A:540:ILE:HB	1.80	0.63
2:B:744:GLN:NE2	2:B:745:LEU:O	2.32	0.63
1:D:1114:VAL:HG13	1:D:1126:ALA:HB1	1.80	0.63
6:J:362:THR:HA	6:J:365:LEU:HB2	1.79	0.63
1:A:674:LEU:HB3	1:A:686:VAL:HB	1.79	0.63
3:C:393:ARG:NH2	3:C:412:THR:OG1	2.30	0.63
2:B:130:ARG:NH1	2:B:186:ASP:O	2.31	0.63
4:H:187:LEU:HB3	4:H:192:ARG:HB2	1.80	0.63
1:A:461:PRO:HD3	3:C:442:TRP:CD1	2.32	0.63
2:B:22:ASP:OD2	2:B:67:PHE:N	2.31	0.63
6:G:288:ILE:HG21	6:G:291:LEU:HD12	1.80	0.63
1:A:1073:GLN:HG2	1:A:1074:LYS:HG2	1.81	0.63
1:A:418:PHE:O	1:A:420:ASN:ND2	2.32	0.63
1:A:703:VAL:HA	1:A:830:GLY:HA3	1.80	0.63
1:A:1096:TYR:O	1:A:1100:ALA:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:NZ	1:A:31:PRO:O	2.29	0.62
1:A:592:THR:OG1	1:A:594:ASP:OD1	2.17	0.62
2:B:116:LEU:HA	2:B:129:TRP:O	2.00	0.62
6:G:252:ILE:HG13	6:G:254:SER:H	1.64	0.62
6:J:280:ASP:O	6:J:324:ARG:NH1	2.31	0.62
6:J:284:ILE:HB	6:J:325:VAL:HG12	1.82	0.62
1:D:1254:TYR:HH	1:D:1261:ARG:NH1	1.98	0.62
4:H:34:THR:HG22	4:H:35:SER:H	1.65	0.62
1:A:457:LEU:HD13	1:A:507:LYS:HD3	1.80	0.62
1:A:26:LYS:NZ	1:A:27:GLY:O	2.33	0.62
1:A:316:LEU:HB3	1:A:336:PHE:HB3	1.82	0.62
3:C:122:PRO:HD2	3:C:135:SER:HA	1.80	0.62
3:C:106:HIS:O	3:C:134:GLN:NE2	2.32	0.62
4:E:41:GLU:OE1	4:E:229:TYR:OH	2.14	0.62
2:B:587:ILE:HB	2:B:602:LEU:HD12	1.82	0.61
1:A:440:GLY:O	1:A:455:LEU:N	2.32	0.61
5:F:247:THR:HG21	5:F:252:LEU:HD12	1.81	0.61
6:J:85:THR:HG21	6:J:99:HIS:HB3	1.81	0.61
2:B:515:GLU:HB3	2:B:531:SER:HA	1.83	0.61
6:J:100:MET:HG3	6:J:210:TRP:HA	1.82	0.61
2:B:211:ARG:NH2	2:B:214:GLU:OE2	2.34	0.61
3:C:456:LEU:HD21	3:C:459:LEU:HD23	1.82	0.61
1:A:577:VAL:HG12	1:A:578:LEU:HD12	1.83	0.61
1:A:1047:MET:HB3	1:D:1286:ARG:HH21	1.66	0.61
5:I:162:THR:OG1	5:I:165:GLU:OE1	2.18	0.61
3:C:443:GLU:OE2	3:C:463:ARG:NH1	2.30	0.61
4:H:7:ASN:HB3	4:H:10:ILE:HB	1.82	0.60
2:B:494:THR:HG23	2:B:495:VAL:HG23	1.83	0.60
6:G:291:LEU:HB3	6:G:331:ILE:HG22	1.83	0.60
1:D:1190:GLU:HB2	1:D:1228:ARG:HH12	1.65	0.60
1:A:305:GLU:OE2	1:A:322:ARG:NH2	2.35	0.60
1:D:1218:THR:OG1	1:D:1228:ARG:NH1	2.34	0.60
5:F:62:ASN:OD1	5:F:269:LYS:NZ	2.34	0.60
2:B:421:GLY:HA2	2:B:522:GLU:HB3	1.82	0.60
4:E:140:LYS:NZ	5:I:198:SER:O	2.33	0.60
6:G:316:SER:HB2	5:I:110:SER:HA	1.82	0.60
6:J:112:GLU:OE1	6:J:119:HIS:ND1	2.34	0.60
6:J:208:ILE:HD12	6:J:238:ASN:HD22	1.67	0.60
4:H:146:VAL:O	4:H:152:ASN:ND2	2.35	0.60
6:J:100:MET:HE1	6:J:213:LYS:HB2	1.84	0.60
3:C:399:ARG:HH12	5:I:227:GLY:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:THR:OG1	2:B:374:ILE:O	2.15	0.59
6:J:269:LEU:O	6:J:273:GLU:HG2	2.01	0.59
1:A:31:PRO:HA	1:A:82:ARG:HH22	1.67	0.59
1:A:655:ALA:HB3	1:A:658:VAL:HB	1.83	0.59
5:F:216:MET:HG3	5:F:245:ILE:HG12	1.84	0.59
2:B:26:VAL:HG23	2:B:27:LYS:HG3	1.83	0.59
6:G:299:PRO:HA	6:G:302:PHE:HD2	1.68	0.59
1:A:490:ILE:HG22	1:A:495:LEU:HG	1.84	0.59
2:B:671:VAL:HG22	2:B:681:VAL:HG12	1.85	0.59
3:C:452:LYS:HB3	3:C:453:LYS:HE2	1.85	0.59
1:A:183:VAL:HG13	1:A:268:GLU:HB3	1.84	0.59
1:A:681:HIS:CE1	1:A:714:GLY:H	2.21	0.59
4:E:62:THR:O	5:I:176:ARG:NH2	2.36	0.59
1:D:1284:ASN:OD1	1:D:1286:ARG:NH2	2.36	0.59
4:H:42:PHE:O	4:H:46:SER:HB3	2.03	0.59
5:I:85:GLU:HG2	5:I:88:TYR:H	1.65	0.59
3:C:303:MET:SD	3:C:303:MET:N	2.76	0.59
2:B:727:GLY:O	2:B:750:THR:OG1	2.21	0.58
3:C:257:GLN:NE2	3:C:295:MET:SD	2.76	0.58
1:D:1103:GLN:OE1	1:D:1109:ASN:ND2	2.36	0.58
6:G:109:LEU:HD13	6:G:348:PHE:HE2	1.68	0.58
3:C:240:HIS:O	3:C:244:MET:HG3	2.04	0.58
3:C:253:GLU:HG3	3:C:291:VAL:HB	1.86	0.58
1:A:814:LYS:HD2	1:A:818:LYS:HE3	1.84	0.58
1:A:1090:LEU:HD22	1:A:1095:ARG:HD2	1.86	0.58
5:I:84:HIS:HB2	5:I:89:PHE:CE1	2.38	0.58
2:B:262:GLN:NE2	2:B:264:ASP:O	2.31	0.58
2:B:658:ASP:OD2	2:B:757:ARG:NH2	2.35	0.58
5:F:70:PRO:O	5:F:74:ARG:NH1	2.36	0.58
5:F:202:SER:O	5:F:206:ASN:HB2	2.03	0.58
6:G:412:GLU:N	6:G:412:GLU:OE1	2.36	0.58
2:B:659:ALA:HA	2:B:707:ILE:HD11	1.86	0.58
6:G:371:SER:O	6:G:372:GLN:NE2	2.37	0.58
5:I:25:ASP:O	5:I:179:LYS:NZ	2.32	0.57
6:J:211:LYS:NZ	6:J:216:ASP:OD2	2.37	0.57
1:A:859:CYS:SG	1:A:886:SER:OG	2.62	0.57
6:J:315:ARG:NH1	6:J:347:MET:O	2.30	0.57
2:B:121:CYS:HB3	2:B:125:THR:HG22	1.87	0.57
5:F:232:VAL:HG22	5:F:271:PHE:HZ	1.69	0.57
1:A:914:TYR:HA	1:A:917:PHE:HD2	1.68	0.57
2:B:351:ARG:NH1	2:B:352:MET:SD	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1173:ARG:HD2	1:D:1255:LEU:HD22	1.87	0.57
5:F:179:LYS:HG2	5:F:180:VAL:HG23	1.87	0.57
6:J:279:ASN:O	6:J:324:ARG:NH2	2.31	0.57
1:A:618:ASP:OD1	1:A:619:PHE:N	2.38	0.57
6:J:382:HIS:NE2	6:J:400:SER:OG	2.38	0.57
2:B:484:GLU:N	2:B:484:GLU:OE2	2.37	0.57
1:D:1239:ARG:HD3	1:D:1250:TYR:HA	1.86	0.57
6:G:347:MET:HA	6:G:347:MET:HE2	1.85	0.57
6:J:129:GLN:HE22	6:J:238:ASN:HD21	1.50	0.57
4:H:10:ILE:HA	4:H:13:LYS:HE3	1.85	0.56
1:A:331:SER:OG	1:A:332:VAL:N	2.39	0.56
1:A:527:VAL:HG11	1:A:552:ARG:HH22	1.71	0.56
1:A:567:ILE:HG13	1:A:568:THR:H	1.70	0.56
1:A:575:LYS:HE2	1:A:593:ARG:HD3	1.87	0.56
2:B:477:LYS:HE2	2:B:532:LEU:HD21	1.87	0.56
3:C:399:ARG:HH12	5:I:227:GLY:N	2.03	0.56
6:J:273:GLU:OE1	6:J:277:LYS:NZ	2.37	0.56
1:A:947:ASP:HB2	1:A:950:GLU:HG2	1.86	0.56
6:J:92:ASP:OD2	6:J:413:ILE:N	2.35	0.56
4:E:209:LYS:HG3	4:E:215:SER:HB2	1.88	0.56
6:G:381:VAL:HB	6:G:402:TRP:HB2	1.85	0.56
5:I:72:SER:N	5:I:101:ASN:OD1	2.39	0.56
3:C:435:ASP:HB3	3:C:442:TRP:NE1	2.20	0.56
5:I:103:TYR:HE2	5:I:105:VAL:HB	1.70	0.56
3:C:450:ASP:HB3	3:C:455:ILE:HG12	1.88	0.56
1:A:151:SER:OG	1:A:153:ASP:OD1	2.18	0.56
1:A:343:ARG:HH22	1:A:346:GLU:HB3	1.71	0.56
2:B:164:LYS:HB3	2:B:184:LEU:HB2	1.88	0.56
6:J:176:LYS:NZ	6:J:196:GLN:OE1	2.39	0.56
6:J:349:ASP:HA	6:J:385:LYS:HD3	1.88	0.56
5:I:11:LEU:HD12	5:I:17:VAL:HG13	1.88	0.55
2:B:211:ARG:HB2	2:B:289:TRP:CE2	2.41	0.55
3:C:443:GLU:OE1	3:C:484:ARG:NH2	2.28	0.55
4:H:114:THR:HA	4:H:117:ILE:HG12	1.88	0.55
1:A:616:VAL:HA	1:A:648:THR:HA	1.89	0.55
1:A:938:LEU:O	1:A:942:GLN:HG2	2.06	0.55
1:D:1171:ARG:HH11	1:D:1331:PRO:HG2	1.71	0.55
5:F:106:LEU:HD11	5:F:132:LYS:HD3	1.89	0.55
2:B:438:HIS:HD2	2:B:500:LEU:HA	1.69	0.55
5:F:123:ASP:OD1	5:F:169:LYS:NZ	2.38	0.55
1:A:995:GLU:HA	1:A:998:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:HIS:O	2:B:28:LYS:N	2.23	0.55
3:C:415:VAL:HG21	3:C:455:ILE:HD12	1.87	0.55
5:F:74:ARG:O	5:F:140:ASN:ND2	2.24	0.55
1:A:75:GLN:NE2	1:A:83:ASN:OD1	2.40	0.55
1:A:480:CYS:SG	1:A:484:ASN:ND2	2.77	0.55
2:B:598:ILE:HG22	2:B:600:PRO:HD2	1.89	0.55
1:D:1314:SER:OG	1:D:1315:GLU:N	2.38	0.55
6:G:109:LEU:HB2	6:G:348:PHE:HD2	1.71	0.55
2:B:415:TRP:CD1	2:B:424:ARG:HD2	2.42	0.55
6:G:150:HIS:HB2	6:G:282:LYS:HD3	1.89	0.55
6:J:113:GLN:NE2	6:J:354:LEU:O	2.39	0.55
1:A:108:GLN:HE22	1:A:110:VAL:HG23	1.72	0.55
1:A:520:LYS:NZ	1:A:527:VAL:O	2.28	0.55
1:A:167:VAL:HG23	1:A:178:GLU:HG3	1.88	0.55
1:A:582:ASP:HB2	1:A:623:ARG:HH12	1.72	0.54
5:I:155:LEU:HG	5:I:166:LEU:HD22	1.88	0.54
6:J:96:ILE:HD11	6:J:214:LEU:HD23	1.89	0.54
6:J:107:SER:HB2	6:J:348:PHE:HB3	1.89	0.54
1:A:169:LEU:HD23	1:A:175:PRO:HA	1.89	0.54
6:J:100:MET:HE2	6:J:100:MET:N	2.22	0.54
1:A:481:SER:HB3	1:A:486:ILE:HB	1.89	0.54
1:A:938:LEU:HD13	1:A:955:LEU:HD12	1.90	0.54
5:F:56:GLY:HA2	5:F:69:LEU:HD12	1.88	0.54
1:A:982:GLU:HA	1:A:1013:LEU:HD11	1.88	0.54
2:B:245:GLU:HA	2:B:250:LYS:HE3	1.88	0.54
2:B:258:GLN:HE21	2:B:272:ASN:HD21	1.54	0.54
3:C:306:ASP:OD1	3:C:309:GLN:NE2	2.37	0.54
1:D:1300:LEU:HD23	1:D:1303:LEU:HD21	1.90	0.54
4:E:63:VAL:O	5:I:176:ARG:NH1	2.40	0.54
5:F:79:LEU:HB2	5:F:105:VAL:HG23	1.90	0.54
5:I:87:ASN:O	5:I:91:ASN:ND2	2.41	0.54
1:A:1015:ARG:O	1:A:1021:GLN:NE2	2.40	0.54
1:D:1139:LEU:HA	1:D:1143:VAL:HB	1.90	0.54
4:H:221:ILE:HG12	4:H:232:LEU:HB2	1.90	0.54
5:I:59:SER:HA	5:I:63:GLU:HB2	1.90	0.54
1:A:854:LYS:HG3	1:A:857:LYS:HE3	1.88	0.54
2:B:567:SER:HA	2:B:614:PHE:HD2	1.72	0.54
1:D:1179:LYS:NZ	1:D:1251:GLU:OE1	2.34	0.54
1:A:1150:GLY:O	1:A:1154:ILE:HG12	2.07	0.54
2:B:687:GLU:HB2	2:B:688:PRO:HD3	1.90	0.54
1:A:672:SER:O	1:A:672:SER:OG	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:370:ARG:HG3	3:C:411:ARG:HG3	1.89	0.54
6:J:225:ARG:NE	6:J:236:ASP:OD2	2.40	0.54
1:A:50:SER:N	1:A:400:TYR:OH	2.41	0.54
2:B:290:HIS:CG	2:B:291:GLU:H	2.26	0.54
6:G:113:GLN:HB2	6:G:356:PRO:HD2	1.89	0.54
2:B:220:LEU:HD11	2:B:232:LEU:HB3	1.90	0.54
1:D:1114:VAL:HG12	1:D:1142:VAL:HG11	1.89	0.54
5:I:81:SER:HB2	5:I:89:PHE:CZ	2.40	0.54
1:A:363:ASN:OD1	1:A:364:SER:N	2.41	0.53
1:D:1109:ASN:ND2	1:D:1112:GLU:OE2	2.41	0.53
6:G:387:PRO:O	6:G:389:PHE:N	2.42	0.53
5:I:257:ASN:ND2	5:I:272:TYR:OH	2.42	0.53
2:B:675:ARG:C	2:B:677:LYS:H	2.15	0.53
4:E:43:VAL:HG21	4:E:68:TYR:HB2	1.90	0.53
1:A:580:ARG:NH1	1:A:619:PHE:O	2.41	0.53
1:A:860:ASP:O	1:A:864:ASN:ND2	2.41	0.53
2:B:218:ASP:HA	2:B:235:ILE:O	2.08	0.53
5:F:35:THR:OG1	5:F:187:SER:OG	2.27	0.53
6:G:78:SER:OG	6:G:83:GLN:N	2.41	0.53
6:G:133:HIS:CE1	6:G:236:ASP:HB3	2.44	0.53
1:A:206:LYS:HE3	3:C:115:GLY:HA2	1.91	0.53
2:B:365:ARG:NH2	2:B:540:ASP:OD1	2.42	0.53
2:B:492:SER:OG	2:B:493:ALA:N	2.38	0.53
2:B:753:ASP:OD1	2:B:754:LYS:N	2.36	0.53
3:C:408:ARG:NH1	3:C:454:ASP:OD2	2.35	0.53
3:C:500:PRO:HB2	3:C:504:GLN:H	1.73	0.53
2:B:166:TYR:HB2	2:B:182:PHE:CE1	2.44	0.53
4:E:24:PHE:HD2	4:E:165:ALA:HA	1.74	0.53
1:A:559:GLN:HG2	1:A:560:ASP:H	1.73	0.53
1:A:774:ILE:HD13	1:A:817:TYR:HD2	1.74	0.53
2:B:294:LEU:O	2:B:310:PRO:HD3	2.08	0.53
1:A:168:VAL:HG12	1:A:176:ILE:HD12	1.91	0.52
2:B:666:PHE:HZ	2:B:736:LEU:HB2	1.74	0.52
2:B:199:GLU:HG3	2:B:200:GLY:H	1.74	0.52
3:C:500:PRO:HB2	3:C:504:GLN:N	2.24	0.52
5:I:186:ASN:O	5:I:208:TYR:OH	2.19	0.52
1:A:992:ASN:O	1:A:993:VAL:C	2.51	0.52
2:B:749:ILE:O	2:B:781:ARG:NH1	2.43	0.52
6:J:366:GLU:OE2	6:J:367:ARG:NH1	2.39	0.52
3:C:253:GLU:HG2	3:C:293:HIS:CE1	2.45	0.52
4:H:38:LEU:HD21	4:H:171:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:333:ILE:HA	6:J:336:ILE:HG12	1.92	0.52
1:D:1096:TYR:HB3	1:D:1116:LEU:HD12	1.92	0.52
2:B:632:LEU:HB2	2:B:646:PHE:HB2	1.91	0.52
3:C:128:ASP:N	3:C:128:ASP:OD1	2.42	0.52
5:F:172:THR:OG1	5:F:173:PRO:HD3	2.09	0.52
2:B:156:LEU:HD22	2:B:168:LEU:HD11	1.92	0.52
2:B:131:GLN:HA	2:B:138:PHE:HA	1.92	0.52
1:D:1179:LYS:HD2	1:D:1199:VAL:HG21	1.92	0.52
5:F:31:LEU:HB3	5:F:215:SER:HA	1.91	0.52
1:A:382:SER:HB3	1:A:387:TRP:CD2	2.45	0.51
1:A:725:SER:HA	1:A:744:MET:HE3	1.92	0.51
2:B:353:ASP:HB2	2:B:369:THR:HG22	1.92	0.51
2:B:562:THR:OG1	2:B:578:ARG:N	2.44	0.51
4:E:52:GLU:OE1	4:E:52:GLU:N	2.44	0.51
6:G:100:MET:HE2	6:G:100:MET:N	2.26	0.51
3:C:495:LEU:HG	3:C:496:HIS:H	1.76	0.51
4:E:42:PHE:HE2	4:E:132:VAL:HG11	1.76	0.51
1:A:1043:VAL:O	1:A:1047:MET:HG2	2.11	0.51
1:A:952:LEU:HD23	2:B:251:LEU:HD22	1.92	0.51
2:B:234:ARG:HB3	2:B:236:ARG:HH12	1.76	0.51
4:H:31:ILE:HD11	4:H:188:LEU:HD22	1.92	0.51
1:A:981:LEU:HD12	1:A:984:LEU:HD23	1.91	0.51
1:A:1103:GLN:HG3	1:A:1109:ASN:HB2	1.93	0.51
3:C:163:GLN:O	3:C:167:LEU:HG	2.10	0.51
5:I:85:GLU:HB3	5:I:109:LEU:HD22	1.93	0.51
3:C:328:PRO:HD2	3:C:376:ARG:HD3	1.93	0.51
4:H:94:ALA:O	4:H:128:HIS:N	2.44	0.51
5:I:122:ARG:NH2	5:I:160:GLY:O	2.43	0.51
6:J:382:HIS:HD2	6:J:399:LYS:HB3	1.76	0.51
3:C:495:LEU:HB3	3:C:499:ASP:HB3	1.93	0.51
5:F:77:ALA:HB3	5:F:103:TYR:HB3	1.92	0.51
3:C:460:LEU:HD12	3:C:486:LEU:HD13	1.93	0.51
5:F:65:SER:O	5:F:66:SER:OG	2.28	0.51
1:A:664:VAL:HG12	1:A:678:THR:HA	1.92	0.50
1:D:1090:LEU:HD21	1:D:1098:ASP:HB2	1.93	0.50
4:E:106:ILE:HD12	4:E:133:ALA:HB2	1.93	0.50
6:G:155:SER:OG	6:G:157:ASN:OD1	2.29	0.50
1:A:1040:ASP:OD2	1:D:1345:HIS:N	2.44	0.50
5:F:47:ASN:OD1	5:F:48:ALA:N	2.44	0.50
1:A:311:LYS:HD3	1:A:315:SER:HB2	1.94	0.50
1:A:993:VAL:CG2	1:A:997:VAL:HB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:TYR:HA	1:A:1257:GLN:HG2	1.93	0.50
2:B:629:LYS:HG2	2:B:649:GLU:HA	1.93	0.50
5:I:28:SER:O	5:I:29:HIS:ND1	2.45	0.50
1:A:521:SER:OG	1:A:526:GLU:OE2	2.28	0.50
2:B:186:ASP:OD1	2:B:186:ASP:N	2.44	0.50
2:B:360:LYS:HG3	2:B:361:THR:HG23	1.92	0.50
2:B:660:ASP:OD1	2:B:661:TRP:N	2.43	0.50
3:C:410:VAL:O	3:C:414:GLU:HG3	2.12	0.50
5:I:147:ILE:HG12	5:I:182:ILE:HB	1.93	0.50
1:A:1266:LEU:O	1:A:1270:LYS:HG2	2.12	0.50
1:D:1273:ALA:O	1:D:1277:VAL:HG23	2.12	0.50
1:A:39:ASP:OD1	1:A:39:ASP:N	2.44	0.50
1:A:227:ASN:O	1:A:230:ARG:NE	2.36	0.50
3:C:104:LYS:HA	3:C:151:TYR:HD2	1.77	0.50
4:H:41:GLU:OE1	4:H:229:TYR:OH	2.21	0.50
1:A:307:GLN:NE2	1:A:357:VAL:O	2.44	0.50
1:A:363:ASN:HB2	1:A:368:ALA:HB3	1.92	0.50
2:B:211:ARG:NH1	2:B:293:ARG:O	2.40	0.50
1:A:456:ALA:HB2	1:A:721:ILE:HG13	1.93	0.50
2:B:385:THR:OG1	2:B:406:ASP:OD2	2.29	0.49
6:J:351:VAL:N	6:J:385:LYS:HB3	2.27	0.49
3:C:107:ARG:NH1	3:C:126:ASP:OD1	2.46	0.49
3:C:322:ASP:OD2	3:C:484:ARG:NH1	2.33	0.49
5:F:30:ASN:HA	5:F:216:MET:HE1	1.94	0.49
6:J:242:ASP:OD2	6:J:409:LYS:NZ	2.29	0.49
1:A:335:ILE:HD12	1:A:343:ARG:HH21	1.77	0.49
1:A:399:SER:HB3	1:A:414:SER:HB3	1.94	0.49
1:D:1178:LYS:HE2	1:D:1199:VAL:HG12	1.95	0.49
6:J:109:LEU:HD11	6:J:348:PHE:CD2	2.43	0.49
1:A:467:ARG:NH2	1:A:509:GLY:HA2	2.27	0.49
1:D:1187:TYR:OH	1:D:1203:GLU:O	2.30	0.49
6:J:276:ILE:HG23	6:J:284:ILE:HG13	1.94	0.49
2:B:465:PHE:HA	2:B:550:GLU:HA	1.95	0.49
5:F:130:LEU:HD22	5:F:173:PRO:HB2	1.94	0.49
6:G:298:PRO:HG2	6:G:301:MET:HG3	1.95	0.49
6:J:76:ARG:HD3	6:J:234:TYR:HA	1.94	0.49
1:A:684:GLN:HG2	1:A:708:VAL:HG22	1.93	0.49
2:B:627:ASP:OD1	2:B:627:ASP:N	2.46	0.49
1:A:1252:GLU:O	1:A:1253:GLU:HG2	2.12	0.49
1:D:1259:VAL:O	1:D:1263:ILE:HG13	2.13	0.49
1:D:1130:ALA:O	1:D:1134:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1162:LYS:O	1:D:1166:ASN:ND2	2.42	0.49
1:D:1262:LEU:HA	1:D:1265:ARG:NH1	2.25	0.49
1:D:1311:TYR:O	1:D:1333:ILE:N	2.45	0.49
5:F:232:VAL:HG11	5:F:260:LEU:HB3	1.94	0.49
4:H:141:ASP:OD1	4:H:141:ASP:N	2.46	0.49
1:A:777:ASP:HA	1:A:854:LYS:NZ	2.28	0.48
1:D:1235:ARG:HD2	1:D:1239:ARG:HD2	1.93	0.48
6:J:311:MET:HG3	6:J:344:LEU:HD12	1.94	0.48
1:A:239:ASP:OD2	1:A:302:THR:OG1	2.31	0.48
1:A:323:LYS:HD2	1:A:325:ASP:HB2	1.94	0.48
2:B:141:ALA:HB1	2:B:189:ILE:HG23	1.95	0.48
4:H:135:TYR:HE1	4:H:157:LYS:HD2	1.78	0.48
1:A:705:ASP:HB2	1:A:821:LEU:HD23	1.94	0.48
2:B:415:TRP:NE1	2:B:424:ARG:HH11	2.11	0.48
3:C:445:PHE:CE1	3:C:459:LEU:HB2	2.48	0.48
5:I:17:VAL:HG12	5:I:18:LEU:HG	1.95	0.48
3:C:332:ILE:HB	3:C:335:THR:HG23	1.95	0.48
4:E:149:ASP:OD1	4:E:152:ASN:N	2.47	0.48
5:I:118:HIS:CE1	5:I:119:ASN:HB2	2.48	0.48
2:B:712:SER:OG	2:B:713:MET:N	2.45	0.48
5:I:103:TYR:CE2	5:I:105:VAL:HB	2.49	0.48
5:I:257:ASN:OD1	5:I:258:GLU:N	2.47	0.48
6:J:166:GLY:HA2	6:J:247:LEU:HB2	1.94	0.48
1:A:1273:ALA:HB1	1:A:1296:PHE:HZ	1.78	0.48
2:B:90:ASP:HB3	2:B:93:HIS:HB2	1.96	0.48
5:F:63:GLU:HG3	5:F:64:SER:H	1.78	0.48
1:A:86:ALA:HB2	1:A:133:THR:HG21	1.95	0.48
1:A:1082:VAL:O	1:A:1085:GLU:HB3	2.13	0.48
1:A:1264:GLU:O	1:A:1268:GLN:HG3	2.13	0.48
1:A:1272:ASP:HA	1:A:1275:ARG:HE	1.77	0.48
4:H:91:LEU:HD21	4:H:129:CYS:HB2	1.94	0.48
5:I:61:LEU:HD13	5:I:268:THR:HG23	1.96	0.48
5:I:68:MET:HE3	5:I:97:LYS:HB2	1.95	0.48
1:A:389:LEU:HD23	1:A:447:GLY:HA2	1.95	0.48
1:D:1192:GLU:HB3	1:D:1214:TYR:HD1	1.78	0.48
1:A:55:LEU:HD21	1:A:406:GLU:HB3	1.96	0.48
1:A:678:THR:HG22	1:A:682:ASN:H	1.79	0.48
1:A:702:GLY:HA3	1:A:832:GLU:HG3	1.96	0.48
1:A:1128:LEU:HG	1:A:1132:LYS:HD3	1.95	0.48
3:C:407:CYS:SG	3:C:408:ARG:N	2.87	0.48
1:D:1170:ARG:NH2	1:D:1175:LEU:O	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1176:ARG:NH1	1:D:1196:ASP:OD2	2.47	0.48
1:A:47:LEU:HA	1:A:63:LEU:HA	1.96	0.48
1:A:335:ILE:HD12	1:A:343:ARG:NH2	2.29	0.48
1:A:527:VAL:HG12	1:A:528:ASP:H	1.79	0.48
2:B:654:ARG:HB2	2:B:676:ASP:N	2.29	0.48
4:H:80:PHE:HE2	4:H:119:ARG:HE	1.62	0.48
6:J:88:THR:HA	6:J:126:PHE:HE1	1.78	0.48
1:A:548:ASP:OD1	1:A:549:ASN:N	2.45	0.47
1:A:1076:PRO:HA	1:A:1079:VAL:HG23	1.96	0.47
1:D:1191:THR:HG21	1:D:1217:LYS:N	2.29	0.47
5:F:26:SER:OG	5:F:27:ASN:OD1	2.30	0.47
4:E:34:THR:HG22	4:E:35:SER:H	1.79	0.47
6:G:104:LEU:HD12	6:G:324:ARG:HA	1.96	0.47
2:B:749:ILE:HD12	2:B:783:TYR:HE2	1.79	0.47
3:C:338:TYR:OH	3:C:342:LYS:NZ	2.41	0.47
3:C:376:ARG:HG2	3:C:378:ILE:HD11	1.96	0.47
6:G:307:ILE:HD11	6:G:340:LEU:HD11	1.97	0.47
1:A:50:SER:OG	1:A:61:CYS:SG	2.72	0.47
1:A:252:THR:OG1	1:A:265:SER:OG	2.29	0.47
1:A:256:ARG:HG3	1:A:310:TRP:CE2	2.50	0.47
1:A:536:ILE:HD11	1:A:588:LEU:HG	1.96	0.47
2:B:438:HIS:CD2	2:B:500:LEU:HA	2.49	0.47
3:C:502:LYS:HA	3:C:502:LYS:HD2	1.64	0.47
5:F:124:LYS:NZ	5:F:128:ASP:OD1	2.46	0.47
5:I:86:GLN:O	5:I:90:THR:HG23	2.13	0.47
6:J:140:SER:N	6:J:143:LYS:O	2.42	0.47
1:A:19:ARG:O	1:A:390:LYS:NZ	2.40	0.47
1:A:234:MET:SD	1:A:234:MET:N	2.86	0.47
1:A:582:ASP:CG	1:A:587:HIS:H	2.22	0.47
1:A:667:LEU:HA	1:A:675:LEU:O	2.15	0.47
1:A:861:ALA:HA	1:A:864:ASN:HD21	1.80	0.47
1:D:1196:ASP:OD1	1:D:1261:ARG:NH1	2.45	0.47
6:G:117:GLU:O	6:G:120:SER:OG	2.28	0.47
5:I:89:PHE:HB3	5:I:105:VAL:HG21	1.97	0.47
1:A:19:ARG:NH2	1:A:716:ILE:HD13	2.30	0.47
1:A:706:GLU:HB2	1:A:743:ILE:HB	1.96	0.47
1:A:1072:VAL:HG21	1:A:1106:TYR:CZ	2.50	0.47
1:A:1121:TYR:HB2	1:A:1275:ARG:HH22	1.79	0.47
2:B:443:ILE:H	2:B:457:GLY:HA2	1.79	0.47
2:B:738:LYS:HA	2:B:738:LYS:HD2	1.67	0.47
3:C:553:MET:HE3	3:C:553:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:312:HIS:HE1	5:I:109:LEU:HA	1.79	0.47
4:H:103:MET:HG3	4:H:130:THR:OG1	2.14	0.47
4:H:211:LYS:HD2	4:H:211:LYS:O	2.15	0.47
6:J:72:HIS:CD2	6:J:74:GLY:H	2.33	0.47
1:A:482:PHE:HB2	1:A:585:TYR:CD2	2.49	0.47
2:B:329:LYS:H	2:B:333:THR:HG22	1.80	0.47
4:E:46:SER:OG	4:E:51:ASN:ND2	2.47	0.47
4:E:80:PHE:CE2	4:E:119:ARG:HD2	2.50	0.47
6:G:351:VAL:HB	6:G:384:LEU:HB2	1.97	0.47
5:I:101:ASN:OD1	5:I:102:ASN:N	2.48	0.47
1:A:1286:ARG:O	1:A:1290:HIS:ND1	2.44	0.47
2:B:722:VAL:CG2	2:B:730:TYR:HB2	2.45	0.47
3:C:105:PRO:HD3	3:C:151:TYR:CD2	2.50	0.47
6:G:73:VAL:O	6:G:145:ARG:NH2	2.37	0.47
5:I:69:LEU:HD13	5:I:97:LYS:HE2	1.97	0.47
6:J:291:LEU:H	6:J:331:ILE:HG22	1.79	0.47
1:A:1103:GLN:HA	1:A:1107:LEU:HD12	1.96	0.46
2:B:209:ALA:HB1	2:B:289:TRP:CD1	2.51	0.46
4:E:79:ASP:OD1	4:E:82:HIS:ND1	2.48	0.46
1:A:787:LEU:HD21	1:A:862:VAL:HA	1.97	0.46
1:A:798:ASP:OD1	1:A:798:ASP:N	2.48	0.46
1:A:1282:ARG:NH2	1:D:1043:VAL:HG22	2.28	0.46
1:D:1171:ARG:HD3	1:D:1171:ARG:HA	1.82	0.46
1:D:1192:GLU:HB3	1:D:1214:TYR:CD1	2.50	0.46
3:C:200:ASN:OD1	3:C:205:PHE:HB3	2.15	0.46
3:C:397:LEU:O	3:C:401:LYS:HG2	2.15	0.46
4:E:195:ARG:NH2	5:I:239:CYS:HA	2.31	0.46
5:F:36:HIS:O	5:F:187:SER:N	2.45	0.46
6:G:279:ASN:HB3	6:G:282:LYS:HD2	1.97	0.46
1:A:100:PHE:HA	1:A:110:VAL:O	2.16	0.46
1:A:122:THR:O	1:A:133:THR:HA	2.15	0.46
1:A:601:ASP:HB3	1:A:605:GLN:HB2	1.97	0.46
1:A:754:MET:HE1	1:A:778:TYR:HE1	1.80	0.46
2:B:615:SER:HA	2:B:661:TRP:CE2	2.51	0.46
2:B:714:ILE:O	2:B:717:LYS:HG2	2.15	0.46
1:D:1296:PHE:CD2	1:D:1341:PHE:HB2	2.51	0.46
5:F:165:GLU:O	5:F:169:LYS:HB2	2.14	0.46
1:A:544:LEU:HD13	1:A:576:ILE:HD12	1.97	0.46
1:A:706:GLU:CD	1:A:742:ARG:HB2	2.40	0.46
2:B:117:ILE:HB	2:B:129:TRP:HB2	1.96	0.46
2:B:346:TRP:NE1	2:B:355:PHE:HE1	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:654:ARG:HB3	2:B:675:ARG:HB3	1.98	0.46
1:A:189:SER:OG	1:A:190:LYS:NZ	2.49	0.46
1:A:1300:LEU:O	1:A:1304:LYS:HG2	2.15	0.46
2:B:17:GLN:HB2	2:B:20:VAL:HG13	1.97	0.46
2:B:45:GLU:HG3	2:B:46:PRO:HD2	1.97	0.46
2:B:589:ILE:HG13	2:B:598:ILE:HD12	1.97	0.46
2:B:710:HIS:HB2	2:B:719:LEU:HB2	1.98	0.46
4:H:65:LYS:HG3	4:H:72:PHE:CD1	2.50	0.46
1:A:1055:MET:O	1:A:1059:GLN:HG3	2.16	0.46
2:B:329:LYS:HB2	2:B:338:SER:HB2	1.98	0.46
3:C:356:ASP:O	3:C:360:ARG:HG2	2.16	0.46
1:A:681:HIS:O	1:A:713:ARG:NH2	2.49	0.46
2:B:616:LYS:HD2	2:B:616:LYS:HA	1.70	0.46
1:A:599:GLN:HB3	1:A:609:ILE:HD11	1.98	0.46
1:D:1168:GLN:HE21	1:D:1173:ARG:HH21	1.64	0.46
1:D:1206:THR:O	1:D:1229:ARG:NH1	2.47	0.46
6:G:304:SER:O	6:G:308:ILE:HG12	2.15	0.46
4:H:25:ILE:HG23	4:H:167:THR:HG23	1.98	0.46
4:H:101:LYS:HD2	4:H:128:HIS:ND1	2.31	0.46
1:D:1274:VAL:HG22	1:D:1341:PHE:CE1	2.51	0.46
5:F:32:PHE:HB2	5:F:182:ILE:HG12	1.97	0.46
5:F:57:SER:OG	5:F:60:SER:OG	2.33	0.46
6:G:133:HIS:CE1	6:G:239:HIS:HE1	2.34	0.46
5:I:268:THR:C	5:I:269:LYS:HD3	2.40	0.46
6:J:116:THR:OG1	6:J:356:PRO:HG3	2.16	0.46
1:A:894:ALA:HA	1:A:897:LYS:HE2	1.99	0.45
6:J:280:ASP:OD1	6:J:281:LYS:N	2.49	0.45
6:J:405:LYS:HE2	6:J:405:LYS:HB2	1.80	0.45
1:A:1252:GLU:C	1:A:1254:TYR:H	2.25	0.45
5:F:232:VAL:HG12	5:F:234:GLY:H	1.80	0.45
4:H:135:TYR:CE1	4:H:157:LYS:HD2	2.52	0.45
6:J:364:PHE:HA	6:J:367:ARG:HB2	1.98	0.45
2:B:652:HIS:CE1	2:B:680:LYS:HG3	2.52	0.45
4:E:49:LYS:HE3	4:E:51:ASN:HD21	1.82	0.45
6:G:155:SER:HB2	6:G:289:PRO:HG2	1.99	0.45
5:I:172:THR:OG1	5:I:173:PRO:HD3	2.17	0.45
1:A:444:VAL:HG21	1:A:465:TYR:CE2	2.52	0.45
1:A:653:LEU:HG	1:A:660:LEU:HD12	1.98	0.45
1:A:839:MET:HG2	1:A:840:GLN:HG2	1.99	0.45
1:A:1272:ASP:HA	1:A:1275:ARG:HH21	1.81	0.45
3:C:417:ILE:HG13	3:C:489:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:195:ARG:CZ	5:I:239:CYS:HA	2.46	0.45
5:F:37:GLN:O	5:F:40:THR:OG1	2.33	0.45
5:F:181:LEU:HD12	5:F:182:ILE:H	1.82	0.45
1:A:630:GLU:O	1:A:689:ASN:ND2	2.49	0.45
1:D:1296:PHE:CE2	1:D:1341:PHE:HB2	2.52	0.45
1:A:700:GLU:HB2	1:A:829:PHE:CD2	2.52	0.45
2:B:234:ARG:NH1	2:B:236:ARG:HD3	2.32	0.45
2:B:290:HIS:CD2	2:B:293:ARG:HB2	2.51	0.45
2:B:415:TRP:HE1	2:B:418:ASP:HA	1.82	0.45
4:H:7:ASN:O	4:H:11:LEU:N	2.39	0.45
6:J:384:LEU:HA	6:J:397:VAL:HG12	1.98	0.45
1:A:248:SER:OG	1:A:250:GLU:OE1	2.19	0.45
2:B:630:TRP:NE1	2:B:648:ASN:HD22	2.15	0.45
1:D:1277:VAL:HG13	1:D:1289:ALA:HB1	1.99	0.45
5:F:155:LEU:HD23	5:F:161:LEU:HD23	1.99	0.45
6:G:73:VAL:H	6:G:283:LEU:HD13	1.82	0.45
2:B:542:LEU:HD23	2:B:546:LEU:HD12	1.98	0.45
2:B:587:ILE:HD13	2:B:612:LEU:HD11	1.99	0.45
4:H:26:LEU:HB3	4:H:168:ILE:HD13	1.99	0.45
1:A:103:PHE:HB3	1:A:105:ASP:OD1	2.17	0.45
1:A:627:THR:HG22	1:A:638:GLU:HB2	1.98	0.45
1:A:1044:ALA:HA	1:A:1047:MET:HG2	1.99	0.45
1:A:1102:ILE:HA	1:A:1105:GLU:HG2	1.99	0.45
2:B:210:PHE:HE1	2:B:221:LEU:HD22	1.82	0.45
2:B:353:ASP:HB2	2:B:369:THR:CG2	2.47	0.45
2:B:614:PHE:CD1	2:B:621:LEU:HD13	2.51	0.45
2:B:684:HIS:HB2	2:B:692:TYR:CE2	2.52	0.45
2:B:729:ILE:HG22	2:B:745:LEU:HD23	1.99	0.45
1:D:1310:ILE:HD12	1:D:1333:ILE:HB	1.98	0.45
2:B:72:ASP:OD1	2:B:88:PHE:HB2	2.17	0.45
4:E:100:LYS:HE2	4:E:102:HIS:NE2	2.31	0.45
6:G:158:GLN:HA	6:G:258:PHE:HE2	1.81	0.45
6:J:76:ARG:HG3	6:J:77:PRO:HD2	1.99	0.45
1:A:367:GLU:N	1:A:367:GLU:OE1	2.50	0.44
1:A:1147:LEU:HD11	1:A:1280:LEU:HD12	1.98	0.44
2:B:106:THR:OG1	2:B:107:ILE:N	2.49	0.44
2:B:498:LEU:HD22	3:C:148:ARG:HH12	1.81	0.44
4:H:18:LEU:HD12	4:H:46:SER:HB2	1.99	0.44
4:H:55:ILE:HB	4:H:69:CYS:HA	1.99	0.44
5:I:196:ASP:HB2	5:I:199:VAL:HG23	1.99	0.44
5:I:256:GLU:OE1	5:I:256:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ARG:HH11	1:A:769:ARG:HG3	1.80	0.44
1:A:1028:TYR:O	1:A:1032:LEU:HG	2.18	0.44
2:B:541:GLN:HA	2:B:545:HIS:CD2	2.45	0.44
4:E:216:LEU:HB2	4:E:218:TYR:HE2	1.83	0.44
6:G:276:ILE:HD12	6:G:317:LEU:HD21	1.99	0.44
5:I:225:LYS:HD2	5:I:225:LYS:HA	1.66	0.44
6:J:129:GLN:O	6:J:132:VAL:HB	2.17	0.44
1:D:1194:ALA:HB1	1:D:1210:PHE:HB2	1.99	0.44
1:D:1270:LYS:O	1:D:1274:VAL:HG23	2.18	0.44
4:E:91:LEU:HD21	4:E:104:VAL:HG21	1.99	0.44
4:E:99:ALA:HB3	4:E:128:HIS:CD2	2.53	0.44
6:G:122:LEU:HD21	6:G:411:PHE:CG	2.53	0.44
6:G:256:LEU:HD21	6:G:258:PHE:HE1	1.82	0.44
1:A:240:THR:O	1:A:302:THR:OG1	2.30	0.44
1:A:272:ASP:HB3	1:A:278:LYS:O	2.18	0.44
1:A:1290:HIS:HA	1:A:1293:GLN:HB3	1.98	0.44
2:B:449:THR:HG23	2:B:451:THR:H	1.81	0.44
1:D:1169:LEU:HD12	1:D:1306:ASN:OD1	2.16	0.44
5:I:161:LEU:HD11	5:I:165:GLU:HB2	1.98	0.44
6:J:88:THR:HA	6:J:126:PHE:CE1	2.53	0.44
6:J:135:ARG:NH2	6:J:249:PRO:O	2.41	0.44
1:A:278:LYS:HE3	1:A:278:LYS:HB2	1.72	0.44
2:B:376:ASP:N	2:B:376:ASP:OD1	2.50	0.44
2:B:715:ARG:O	2:B:716:GLU:HG3	2.18	0.44
1:D:1167:SER:HA	1:D:1170:ARG:HH22	1.82	0.44
4:E:114:THR:HA	4:E:117:ILE:HG12	1.98	0.44
5:F:232:VAL:HG22	5:F:271:PHE:CZ	2.52	0.44
6:J:154:LEU:HA	6:J:259:ILE:HB	2.00	0.44
6:J:358:ASN:OD1	6:J:359:GLN:N	2.48	0.44
1:A:179:TYR:OH	1:A:185:ASP:OD2	2.31	0.44
1:A:455:LEU:C	1:A:457:LEU:H	2.25	0.44
2:B:468:PRO:HD2	2:B:471:VAL:HG21	2.00	0.44
3:C:503:PHE:O	3:C:506:GLN:HG2	2.18	0.44
5:I:178:CYS:SG	5:I:179:LYS:N	2.91	0.44
6:J:71:SER:O	6:J:145:ARG:NE	2.48	0.44
1:A:252:THR:HG1	1:A:265:SER:HG	1.64	0.44
1:A:343:ARG:NH2	1:A:346:GLU:OE1	2.50	0.44
1:A:412:MET:HE2	1:A:412:MET:HA	2.00	0.44
2:B:414:PRO:HB3	2:B:429:TRP:NE1	2.33	0.44
2:B:565:ASP:OD2	2:B:613:LYS:HA	2.18	0.44
4:E:84:VAL:HG22	4:E:124:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:218:TYR:HB3	4:H:220:PHE:CZ	2.53	0.44
1:A:1242:ALA:HB3	1:A:1245:LYS:HA	2.00	0.44
2:B:41:TRP:CD1	2:B:42:ASP:H	2.36	0.44
2:B:609:ILE:HA	2:B:625:CYS:SG	2.58	0.44
3:C:184:MET:HE2	3:C:240:HIS:CD2	2.53	0.44
3:C:327:TYR:CD1	3:C:376:ARG:HD2	2.53	0.44
1:D:1058:TYR:HB3	1:D:1063:ARG:O	2.18	0.44
5:F:133:PHE:O	5:F:137:ILE:HG23	2.18	0.44
6:J:208:ILE:HG23	6:J:235:LYS:HA	1.99	0.44
1:A:1179:LYS:HD3	1:A:1246:LYS:O	2.17	0.43
3:C:413:ARG:O	3:C:456:LEU:N	2.51	0.43
1:D:1173:ARG:HB2	1:D:1246:LYS:HD2	2.00	0.43
1:D:1294:LYS:HA	1:D:1297:VAL:HG22	2.00	0.43
4:H:11:LEU:O	4:H:15:ILE:HD12	2.17	0.43
4:H:87:ILE:HG12	4:H:124:ILE:HD12	1.99	0.43
5:I:225:LYS:HB3	5:I:226:THR:H	1.71	0.43
6:J:290:SER:OG	6:J:293:HIS:ND1	2.51	0.43
6:J:416:TRP:HE1	6:J:419:PRO:HA	1.83	0.43
1:A:669:ILE:HG12	1:A:674:LEU:HD13	1.99	0.43
1:A:1078:GLU:O	1:A:1082:VAL:HG22	2.18	0.43
1:A:1123:TYR:CE2	1:A:1276:VAL:HG22	2.53	0.43
2:B:261:PHE:CE2	2:B:263:ILE:HA	2.53	0.43
4:E:107:ASP:OD1	4:E:108:SER:N	2.50	0.43
5:F:6:ARG:NH2	5:F:62:ASN:O	2.52	0.43
6:G:109:LEU:HB2	6:G:348:PHE:CD2	2.51	0.43
6:J:176:LYS:NZ	6:J:196:GLN:HB3	2.33	0.43
3:C:304:GLU:O	3:C:307:ILE:N	2.51	0.43
4:H:105:ILE:HG13	4:H:132:VAL:HG13	1.98	0.43
6:J:318:VAL:HG23	6:J:325:VAL:HG23	1.99	0.43
1:A:444:VAL:HG21	1:A:465:TYR:CZ	2.53	0.43
1:A:664:VAL:HA	1:A:678:THR:HA	1.99	0.43
1:A:742:ARG:NH2	3:C:429:VAL:O	2.50	0.43
2:B:238:ASN:ND2	2:B:239:ASP:OD2	2.51	0.43
2:B:476:GLN:O	2:B:480:GLY:HA2	2.18	0.43
6:G:88:THR:HG23	6:G:126:PHE:CD1	2.54	0.43
1:A:181:LEU:HD11	1:A:286:ARG:NH1	2.33	0.43
1:A:193:THR:OG1	3:C:345:ARG:NH2	2.51	0.43
2:B:411:LEU:HB3	2:B:433:SER:O	2.18	0.43
3:C:214:ILE:HG13	3:C:535:VAL:HG21	1.99	0.43
1:D:1191:THR:HG21	1:D:1217:LYS:H	1.81	0.43
6:G:378:HIS:HB2	6:G:404:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:36:TYR:CE2	4:H:37:LYS:HG2	2.53	0.43
6:J:88:THR:N	6:J:94:ASP:OD1	2.43	0.43
1:A:26:LYS:HE2	1:A:413:PHE:HZ	1.84	0.43
1:A:79:ASP:OD1	1:A:80:GLY:N	2.52	0.43
1:A:531:ARG:HE	1:A:532:GLN:HE22	1.65	0.43
2:B:417:TYR:CE2	2:B:480:GLY:HA3	2.53	0.43
2:B:513:ASP:OD1	2:B:514:GLU:N	2.51	0.43
2:B:516:GLU:HG3	2:B:532:LEU:HD23	2.00	0.43
3:C:295:MET:HG2	3:C:327:TYR:HB2	2.00	0.43
1:D:1187:TYR:OH	1:D:1206:THR:OG1	2.24	0.43
6:J:189:VAL:HG23	6:J:191:ASN:H	1.84	0.43
2:B:210:PHE:CE1	2:B:221:LEU:HD13	2.53	0.43
2:B:466:ASP:HB3	2:B:549:PRO:HG2	2.00	0.43
1:A:818:LYS:HE2	1:A:818:LYS:HB3	1.71	0.43
1:A:1066:GLU:O	1:A:1070:ILE:HG12	2.19	0.43
2:B:177:VAL:HG22	2:B:205:VAL:HG21	2.00	0.43
6:G:308:ILE:HG13	6:G:309:GLY:N	2.34	0.43
1:A:311:LYS:HE2	1:A:313:GLN:HB3	2.01	0.43
1:A:407:LYS:HD3	1:A:410:THR:HG21	2.00	0.43
1:A:451:ASN:HB3	1:A:465:TYR:HB3	2.01	0.43
2:B:415:TRP:HD1	2:B:424:ARG:HD2	1.83	0.43
2:B:628:ARG:HD2	2:B:654:ARG:C	2.43	0.43
2:B:722:VAL:HG23	2:B:730:TYR:HB2	2.01	0.43
3:C:330:LEU:HD12	3:C:378:ILE:HG12	1.99	0.43
6:G:232:SER:OG	6:G:233:GLU:N	2.51	0.43
1:A:262:PHE:CZ	1:A:288:PHE:HB2	2.53	0.43
1:A:336:PHE:HB2	1:A:344:HIS:O	2.18	0.43
1:A:694:LYS:HB2	1:A:694:LYS:HE2	1.86	0.43
1:A:967:LYS:HA	1:A:970:ILE:HD12	2.01	0.43
3:C:510:THR:O	3:C:514:GLU:HG3	2.18	0.43
1:A:1278:GLU:O	1:A:1282:ARG:HG2	2.19	0.42
1:A:1287:GLU:HA	1:A:1290:HIS:HE1	1.81	0.42
1:D:1290:HIS:C	1:D:1294:LYS:HZ2	2.27	0.42
4:E:26:LEU:HD12	4:E:27:CYS:N	2.34	0.42
6:G:166:GLY:HA2	6:G:247:LEU:HD13	2.01	0.42
6:J:72:HIS:CG	6:J:73:VAL:N	2.87	0.42
6:J:259:ILE:HG12	6:J:271:GLN:HE21	1.84	0.42
1:A:807:LEU:HG	1:A:855:VAL:HG12	2.00	0.42
1:A:1274:VAL:O	1:A:1277:VAL:HG22	2.20	0.42
3:C:478:GLN:HG3	3:C:527:GLU:HB2	2.01	0.42
6:J:265:VAL:HG21	6:J:310:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:LYS:HE3	1:A:851:LYS:HB2	1.87	0.42
1:A:948:PRO:HA	1:A:951:TYR:CE2	2.55	0.42
2:B:502:ASN:HD22	2:B:547:LEU:C	2.26	0.42
2:B:714:ILE:O	2:B:714:ILE:HG13	2.19	0.42
5:F:61:LEU:C	5:F:63:GLU:H	2.27	0.42
5:F:109:LEU:O	6:J:316:SER:HB2	2.19	0.42
4:H:28:LEU:HB2	4:H:170:ASP:CG	2.45	0.42
1:A:382:SER:HB3	1:A:387:TRP:CE2	2.55	0.42
1:A:404:HIS:CE1	1:A:407:LYS:H	2.37	0.42
1:A:759:LYS:HA	1:A:794:ILE:HD11	2.01	0.42
1:A:1029:ALA:HA	1:A:1032:LEU:HD12	2.01	0.42
2:B:411:LEU:HB3	2:B:433:SER:HB2	2.02	0.42
2:B:680:LYS:HG2	2:B:697:SER:OG	2.20	0.42
4:E:231:LEU:HG	4:E:232:LEU:N	2.34	0.42
5:F:201:SER:O	5:F:205:GLN:HG2	2.19	0.42
4:H:83:LEU:HD22	4:H:120:PHE:HE2	1.84	0.42
5:I:79:LEU:HD22	5:I:147:ILE:HB	2.01	0.42
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.83	0.42
1:A:210:ALA:O	3:C:112:ALA:HB1	2.18	0.42
1:A:622:LYS:N	1:A:643:VAL:O	2.44	0.42
1:A:716:ILE:O	1:A:729:LEU:HB2	2.19	0.42
2:B:477:LYS:NZ	2:B:522:GLU:HG2	2.34	0.42
4:E:184:VAL:O	4:E:188:LEU:HG	2.20	0.42
6:G:252:ILE:HG13	6:G:254:SER:N	2.33	0.42
4:H:196:GLY:O	4:H:199:ASN:ND2	2.52	0.42
5:I:149:GLU:HG2	5:I:150:GLN:HG3	2.01	0.42
1:A:444:VAL:HG23	1:A:451:ASN:HB2	2.01	0.42
1:A:1143:VAL:O	1:A:1147:LEU:HB2	2.19	0.42
1:A:1293:GLN:HA	1:A:1296:PHE:CD2	2.38	0.42
2:B:162:GLU:HG3	2:B:163:GLU:H	1.85	0.42
2:B:213:GLN:HG2	2:B:219:TYR:CD1	2.55	0.42
5:F:204:LEU:HD23	5:F:204:LEU:HA	1.87	0.42
4:H:156:ASP:OD1	4:H:159:THR:OG1	2.28	0.42
1:A:177:SER:OG	1:A:291:GLU:O	2.32	0.42
1:A:849:ASP:OD1	1:A:849:ASP:N	2.53	0.42
2:B:234:ARG:HB2	2:B:274:GLU:CD	2.44	0.42
2:B:413:ALA:HB3	2:B:432:PHE:CD1	2.54	0.42
4:E:117:ILE:HD13	4:E:117:ILE:HA	1.94	0.42
4:E:219:ASP:HB2	4:E:232:LEU:HD22	2.01	0.42
5:F:125:ILE:O	5:F:129:VAL:HG23	2.20	0.42
5:F:213:ILE:HD11	4:H:31:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:248:MET:HA	6:G:249:PRO:HA	1.86	0.42
4:H:82:HIS:O	4:H:86:GLN:HG2	2.19	0.42
4:H:180:ASP:O	4:H:184:VAL:HG23	2.20	0.42
1:A:361:CYS:HB2	1:A:370:ALA:HB3	2.01	0.42
1:A:816:LYS:HD3	1:A:816:LYS:HA	1.81	0.42
1:A:1127:SER:O	1:A:1131:ILE:HG12	2.20	0.42
2:B:146:ILE:HD13	2:B:146:ILE:HA	1.93	0.42
1:D:1225:GLY:C	1:D:1227:SER:H	2.28	0.42
6:J:73:VAL:HG11	6:J:133:HIS:NE2	2.35	0.42
1:A:808:SER:OG	1:A:809:GLU:N	2.53	0.42
1:A:1035:ASN:O	1:A:1037:MET:HG3	2.20	0.42
1:A:1119:LYS:HA	1:A:1119:LYS:HD2	1.77	0.42
2:B:383:GLY:O	2:B:410:ARG:NH2	2.53	0.42
2:B:395:PRO:HG3	2:B:449:THR:C	2.45	0.42
2:B:579:SER:OG	2:B:580:ASN:N	2.52	0.42
2:B:630:TRP:CE2	2:B:648:ASN:HB3	2.55	0.42
6:G:133:HIS:HE1	6:G:236:ASP:HB3	1.84	0.42
6:J:209:ALA:HA	6:J:235:LYS:HB3	2.00	0.42
6:J:274:GLN:HB3	6:J:278:ARG:NH1	2.35	0.42
1:A:598:CYS:HA	1:A:609:ILE:HG12	2.02	0.41
1:A:1134:LYS:NZ	1:D:1072:VAL:HG12	2.35	0.41
2:B:326:MET:HE3	2:B:326:MET:HB3	1.96	0.41
3:C:389:ASN:OD1	3:C:392:LEU:HD12	2.20	0.41
5:I:148:ILE:HD12	5:I:148:ILE:HA	1.95	0.41
5:I:247:THR:OG1	5:I:248:SER:N	2.53	0.41
6:J:229:GLN:H	6:J:232:SER:HB2	1.85	0.41
1:A:952:LEU:HA	2:B:251:LEU:HD13	2.02	0.41
2:B:211:ARG:HH12	2:B:294:LEU:HA	1.85	0.41
2:B:234:ARG:HH12	2:B:236:ARG:HD3	1.84	0.41
2:B:261:PHE:O	2:B:268:ARG:HG3	2.20	0.41
2:B:263:ILE:HD12	2:B:263:ILE:H	1.83	0.41
2:B:477:LYS:HG2	2:B:532:LEU:HD11	2.01	0.41
1:D:1039:THR:O	1:D:1043:VAL:HG23	2.20	0.41
6:G:280:ASP:OD1	6:G:280:ASP:N	2.50	0.41
4:H:26:LEU:HD23	4:H:168:ILE:HD12	2.02	0.41
4:H:147:ILE:O	4:H:149:ASP:N	2.48	0.41
5:I:68:MET:HE3	5:I:97:LYS:HG3	2.02	0.41
1:A:157:LEU:HD23	1:A:169:LEU:HD12	2.01	0.41
1:A:220:LYS:HE3	1:A:220:LYS:HB2	1.79	0.41
1:A:687:HIS:CE1	1:A:822:TYR:HA	2.55	0.41
1:A:1114:VAL:HG13	1:A:1142:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:TRP:NE1	2:B:418:ASP:HA	2.35	0.41
2:B:727:GLY:HA2	2:B:755:ILE:HG12	2.03	0.41
4:E:195:ARG:HA	4:E:195:ARG:HD3	1.87	0.41
5:I:220:ASN:HB2	5:I:237:HIS:HB2	2.02	0.41
2:B:420:SER:HA	2:B:521:LYS:HE3	2.02	0.41
2:B:669:VAL:HG22	2:B:683:ARG:HD3	2.02	0.41
5:F:64:SER:HB3	5:F:65:SER:H	1.71	0.41
5:F:81:SER:HB2	5:F:84:HIS:HB2	2.02	0.41
1:A:138:MET:HE3	1:A:139:GLY:H	1.86	0.41
1:A:746:LEU:HD23	1:A:746:LEU:HA	1.91	0.41
1:A:1158:LEU:O	1:A:1162:LYS:HG3	2.20	0.41
2:B:407:GLN:HB3	2:B:440:TYR:O	2.19	0.41
2:B:567:SER:HA	2:B:614:PHE:CD2	2.53	0.41
5:F:233:THR:HG23	5:F:262:LEU:HD12	2.02	0.41
5:I:122:ARG:HA	5:I:125:ILE:HD12	2.02	0.41
1:A:1013:LEU:HD23	1:A:1013:LEU:HA	1.92	0.41
2:B:500:LEU:HD23	2:B:500:LEU:H	1.86	0.41
4:H:33:GLN:HG3	4:H:171:ILE:HD12	2.02	0.41
4:H:120:PHE:O	4:H:124:ILE:HG12	2.21	0.41
1:A:260:ASP:OD1	1:A:261:TYR:N	2.53	0.41
1:A:653:LEU:HB2	1:A:664:VAL:HG21	2.03	0.41
1:A:772:LEU:HD23	1:A:772:LEU:HA	1.88	0.41
1:A:843:MET:HE2	1:A:843:MET:HB2	1.98	0.41
2:B:552:GLU:HG2	2:B:595:TRP:CD1	2.56	0.41
3:C:304:GLU:O	3:C:308:GLU:OE1	2.38	0.41
3:C:488:VAL:O	3:C:488:VAL:HG13	2.21	0.41
1:D:1021:GLN:O	1:D:1024:ILE:HG22	2.21	0.41
4:E:142:GLU:OE2	4:E:144:ARG:HB3	2.21	0.41
4:E:179:LEU:HD11	4:E:194:PRO:HG2	2.03	0.41
5:F:146:VAL:HG13	5:F:181:LEU:HD13	2.02	0.41
5:F:153:LEU:O	5:F:157:LEU:HG	2.21	0.41
5:I:65:SER:OG	5:I:68:MET:SD	2.79	0.41
6:J:98:GLY:HA2	6:J:213:LYS:HD2	2.03	0.41
6:J:307:ILE:HG13	6:J:308:ILE:N	2.35	0.41
1:A:904:ASN:HB3	1:A:907:GLU:HB2	2.03	0.41
2:B:306:MET:HE2	2:B:322:ARG:HD3	2.02	0.41
1:D:1161:CYS:O	1:D:1165:ILE:HG12	2.20	0.41
4:E:172:ASP:OD1	4:E:173:VAL:N	2.54	0.41
5:F:36:HIS:HB3	5:F:221:LEU:HB2	2.01	0.41
4:H:210:ARG:NH1	4:H:214:ARG:HB3	2.36	0.41
1:A:317:ILE:HB	1:A:337:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:ARG:NH2	6:J:184:GLU:O	2.54	0.41
2:B:182:PHE:HE2	2:B:184:LEU:HD23	1.86	0.41
2:B:203:ASP:OD1	2:B:204:TRP:N	2.49	0.41
2:B:462:LEU:O	2:B:554:LEU:HD23	2.21	0.41
2:B:679:VAL:HB	2:B:698:ILE:HG22	2.02	0.41
3:C:218:GLN:HE21	3:C:538:ARG:HD2	1.85	0.41
3:C:290:VAL:HG23	3:C:321:THR:OG1	2.21	0.41
3:C:468:LYS:HE3	3:C:468:LYS:HB2	1.78	0.41
1:D:1066:GLU:O	1:D:1070:ILE:HG12	2.20	0.41
1:D:1140:GLU:HG2	1:D:1141:GLU:N	2.36	0.41
1:D:1161:CYS:HA	1:D:1164:GLN:HG2	2.03	0.41
4:E:60:PHE:H	4:E:107:ASP:CG	2.29	0.41
4:E:204:LEU:HD12	4:E:222:VAL:HG21	2.03	0.41
4:E:214:ARG:HD2	6:J:358:ASN:HA	2.02	0.41
6:G:246:ARG:HD3	6:G:246:ARG:HA	1.87	0.41
5:I:68:MET:O	5:I:97:LYS:HB3	2.21	0.41
5:I:86:GLN:HB2	5:I:107:ASP:OD2	2.20	0.41
6:J:315:ARG:HA	6:J:318:VAL:HG12	2.03	0.41
1:A:555:LEU:O	1:A:567:ILE:HG22	2.21	0.41
1:A:1273:ALA:HA	1:A:1276:VAL:HB	2.03	0.41
2:B:317:TRP:N	2:B:317:TRP:CD1	2.89	0.41
5:F:222:ASN:OD1	4:H:192:ARG:NH2	2.54	0.41
6:G:166:GLY:N	6:G:245:THR:O	2.34	0.41
5:I:47:ASN:O	5:I:51:GLU:HG2	2.21	0.41
6:J:85:THR:HG23	6:J:102:LEU:C	2.46	0.41
1:A:444:VAL:CG2	1:A:451:ASN:HB2	2.51	0.40
1:A:550:LEU:HD22	1:A:573:TYR:HA	2.03	0.40
1:A:629:ALA:HB3	1:A:632:ASP:HA	2.04	0.40
1:A:1173:ARG:NH2	1:A:1251:GLU:OE2	2.52	0.40
2:B:706:ALA:HB3	2:B:758:LEU:HD12	2.03	0.40
3:C:296:PRO:HD2	3:C:327:TYR:O	2.20	0.40
5:F:168:ASN:O	5:F:172:THR:OG1	2.26	0.40
4:H:80:PHE:HE1	4:H:120:PHE:HB2	1.86	0.40
1:A:601:ASP:OD1	1:A:602:ALA:N	2.46	0.40
1:A:700:GLU:HB2	1:A:829:PHE:HD2	1.86	0.40
1:D:1030:LYS:HA	1:D:1030:LYS:HD2	1.92	0.40
5:F:16:SER:HB2	5:F:19:PRO:HG3	2.03	0.40
5:F:112:PHE:HA	5:F:116:ASN:HB2	2.02	0.40
1:A:471:THR:OG1	1:A:473:GLY:O	2.30	0.40
1:A:660:LEU:HD23	1:A:660:LEU:HA	1.90	0.40
1:A:1114:VAL:HA	1:A:1117:TYR:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:478:GLN:HE21	3:C:528:LYS:HB2	1.86	0.40
1:D:1088:SER:HB3	1:D:1092:PHE:CZ	2.56	0.40
4:E:18:LEU:HD11	4:E:103:MET:SD	2.62	0.40
6:G:134:ASN:HB2	6:G:149:THR:HG22	2.02	0.40
4:H:142:GLU:O	4:H:145:THR:HG22	2.21	0.40
6:J:214:LEU:HD12	6:J:215:ALA:H	1.85	0.40
1:A:70:ALA:HA	1:A:89:ASN:HA	2.04	0.40
2:B:303:THR:H	2:B:340:GLY:HA2	1.86	0.40
2:B:409:THR:C	2:B:435:PRO:HD2	2.47	0.40
3:C:357:LEU:O	3:C:361:ILE:HG12	2.21	0.40
1:D:1266:LEU:O	1:D:1270:LYS:HG3	2.21	0.40
5:F:112:PHE:CZ	5:F:117:ILE:HD11	2.56	0.40
4:H:24:PHE:HD2	4:H:165:ALA:HA	1.86	0.40
5:I:65:SER:O	5:I:68:MET:HG2	2.21	0.40
5:I:186:ASN:OD1	5:I:186:ASN:C	2.65	0.40
1:A:467:ARG:HA	1:A:511:HIS:CE1	2.57	0.40
1:A:1252:GLU:CD	1:A:1253:GLU:H	2.30	0.40
2:B:234:ARG:HB2	2:B:274:GLU:CG	2.52	0.40
4:E:92:PRO:HD3	4:E:102:HIS:CG	2.57	0.40
5:I:70:PRO:O	5:I:102:ASN:ND2	2.55	0.40
6:J:349:ASP:O	6:J:350:SER:OG	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1231/1349 (91%)	1124 (91%)	106 (9%)	1 (0%)	48	83
1	D	341/1349 (25%)	298 (87%)	43 (13%)	0	100	100
2	B	784/788 (100%)	714 (91%)	70 (9%)	0	100	100
3	C	462/557 (83%)	425 (92%)	37 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	230/309 (74%)	212 (92%)	18 (8%)	0	100	100
4	H	229/309 (74%)	216 (94%)	13 (6%)	0	100	100
5	F	267/273 (98%)	243 (91%)	24 (9%)	0	100	100
5	I	267/273 (98%)	244 (91%)	23 (9%)	0	100	100
6	G	292/456 (64%)	268 (92%)	22 (8%)	2 (1%)	18	55
6	J	351/456 (77%)	306 (87%)	45 (13%)	0	100	100
All	All	4454/6119 (73%)	4050 (91%)	401 (9%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	249	PRO
1	A	993	VAL
6	G	388	VAL

5.3.2 Protein sidechains ⓘ

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	1095/1196 (92%)	1094 (100%)	1 (0%)	88	88
1	D	293/1196 (24%)	293 (100%)	0	100	100
2	B	690/692 (100%)	690 (100%)	0	100	100
3	C	406/490 (83%)	406 (100%)	0	100	100
4	E	218/285 (76%)	218 (100%)	0	100	100
4	H	217/285 (76%)	217 (100%)	0	100	100
5	F	252/255 (99%)	252 (100%)	0	100	100
5	I	252/255 (99%)	252 (100%)	0	100	100
6	G	267/408 (65%)	267 (100%)	0	100	100
6	J	320/408 (78%)	320 (100%)	0	100	100
All	All	4010/5470 (73%)	4009 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	993	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	83	ASN
1	A	293	GLN
1	A	391	GLN
1	A	420	ASN
1	A	430	GLN
1	A	484	ASN
1	A	532	GLN
1	A	634	ASN
1	A	681	HIS
1	A	752	ASN
1	A	771	ASN
1	A	864	ASN
1	A	1109	ASN
2	B	24	HIS
2	B	176	ASN
2	B	290	HIS
2	B	438	HIS
3	C	218	GLN
3	C	219	GLN
3	C	268	ASN
1	D	1103	GLN
1	D	1109	ASN
1	D	1193	GLN
1	D	1291	GLN
4	E	128	HIS
5	F	36	HIS
5	F	41	GLN
5	F	94	ASN
5	F	102	ASN
5	F	205	GLN
6	G	129	GLN
6	G	133	HIS
6	G	231	ASN
4	H	198	ASN
4	H	203	GLN

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Mol	Chain	Res	Type
5	I	62	ASN
6	J	83	GLN
6	J	129	GLN
6	J	158	GLN
6	J	359	GLN
6	J	377	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
7	SF4	C	601	3	0,12,12	-	-	-		

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
7	SF4	C	601	3	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

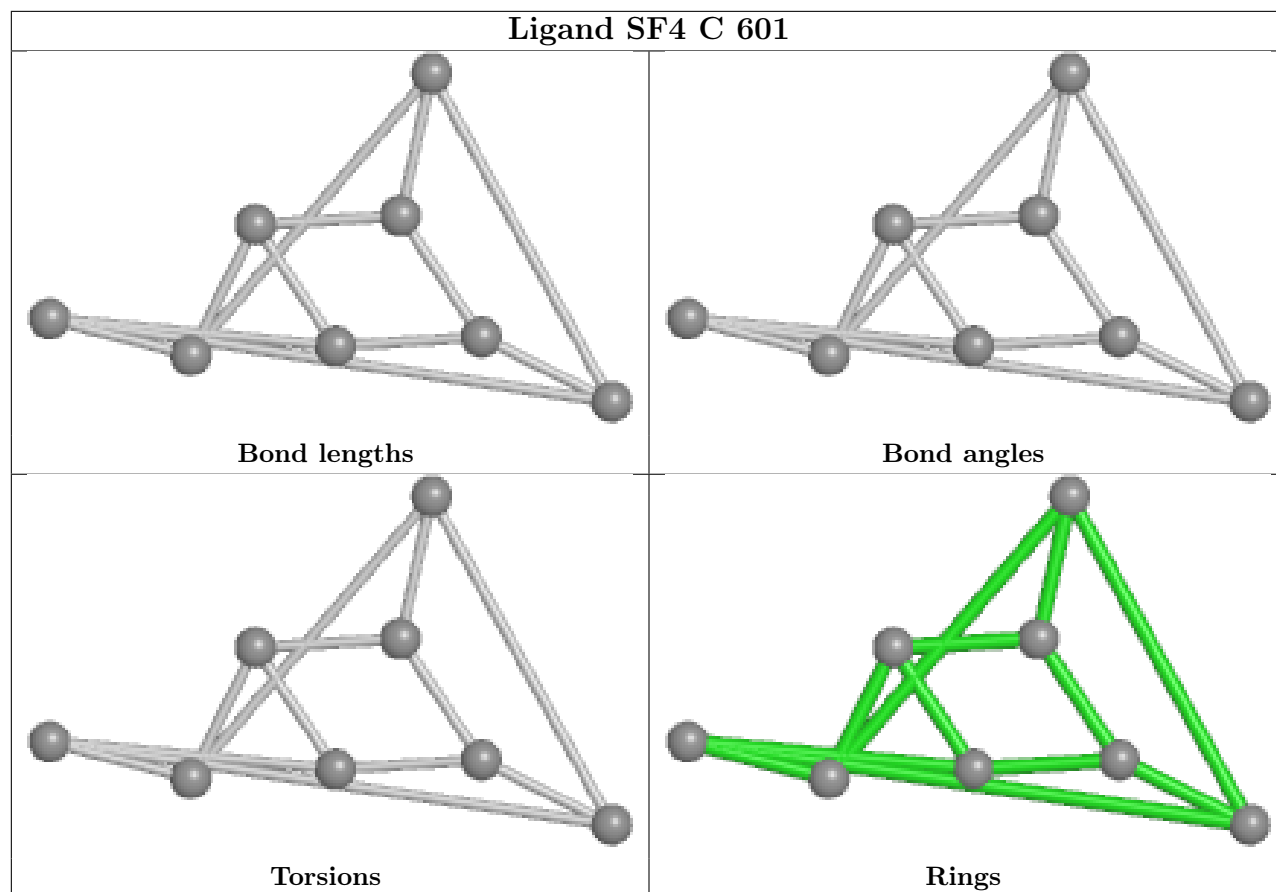
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

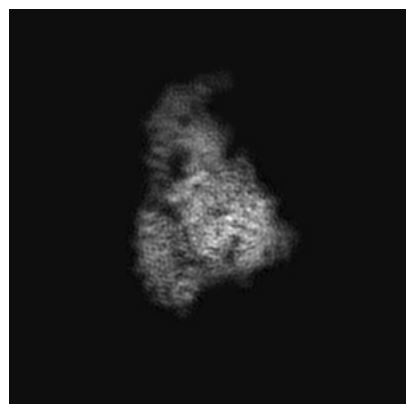
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15622. These allow visual inspection of the internal detail of the map and identification of artifacts.

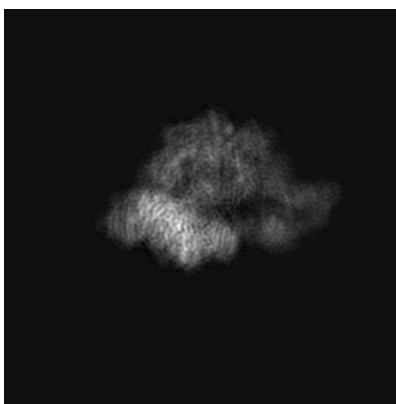
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

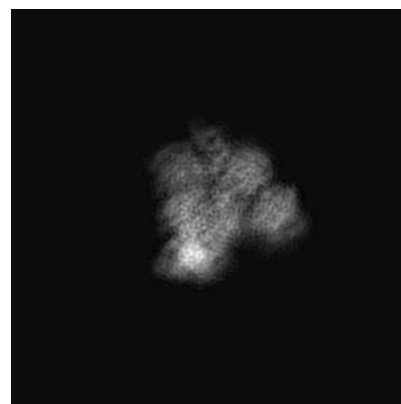
6.1.1 Primary map



X

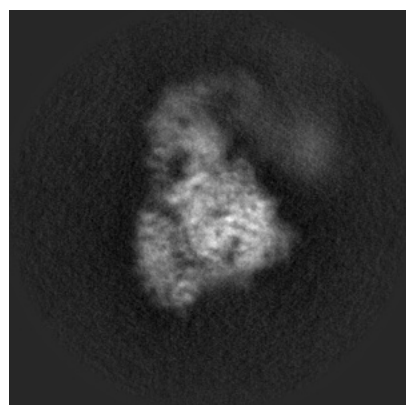


Y

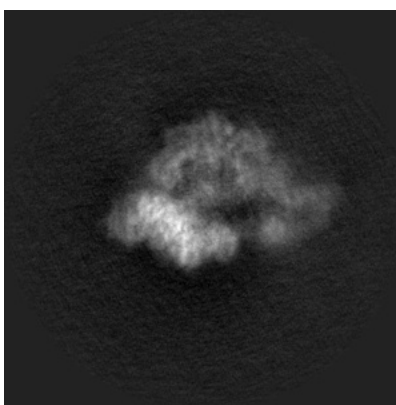


Z

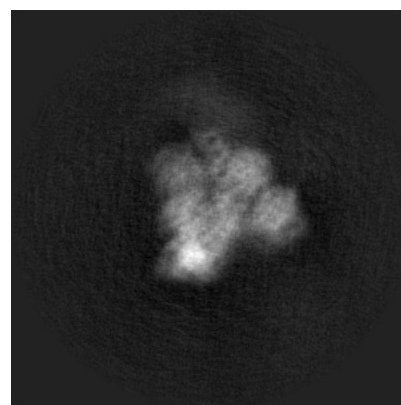
6.1.2 Raw map



X



Y

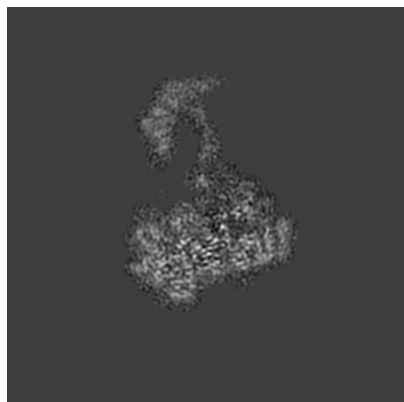


Z

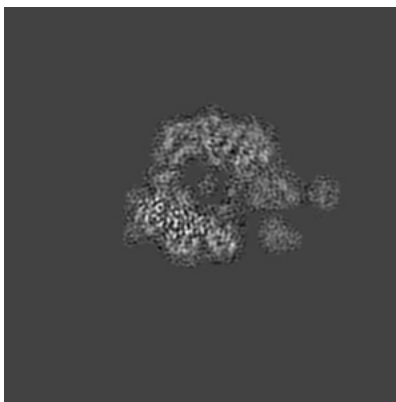
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

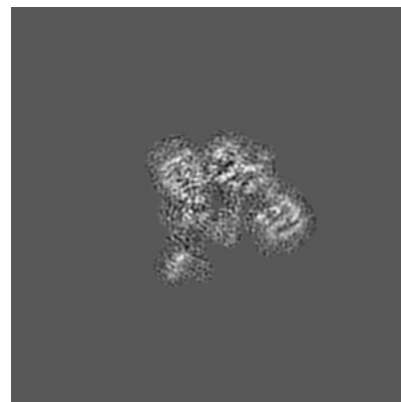
6.2.1 Primary map



X Index: 210

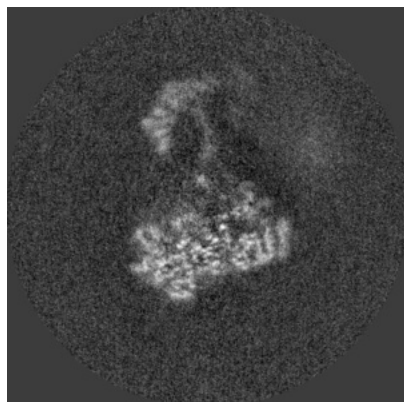


Y Index: 210

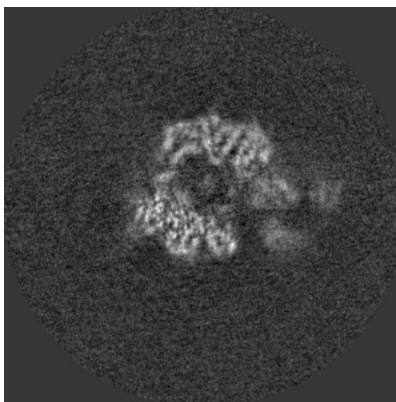


Z Index: 210

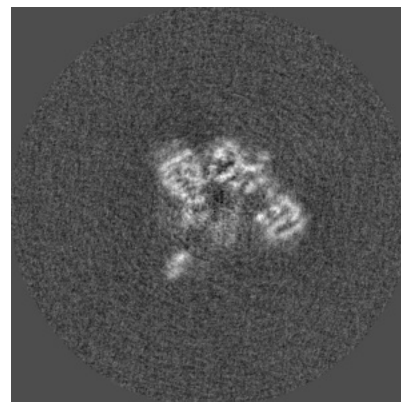
6.2.2 Raw map



X Index: 210



Y Index: 210

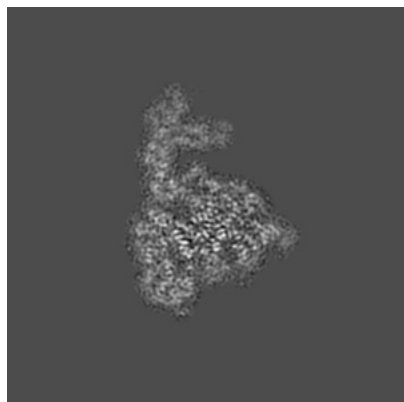


Z Index: 210

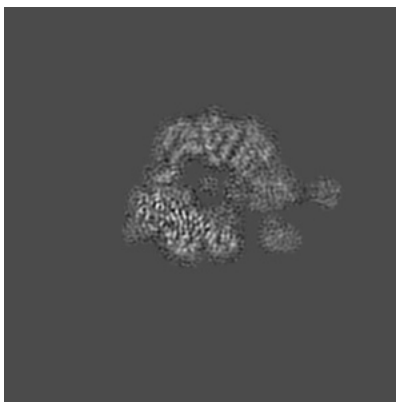
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

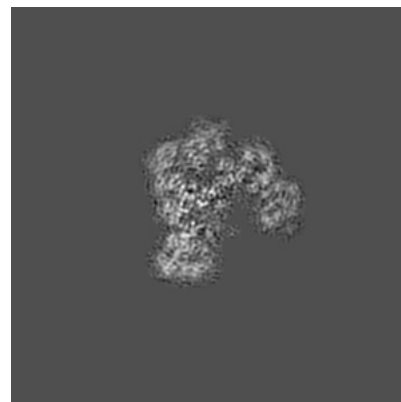
6.3.1 Primary map



X Index: 189

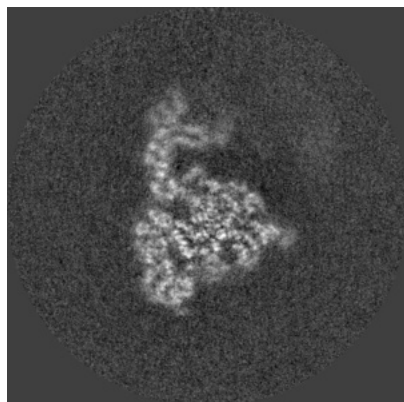


Y Index: 212

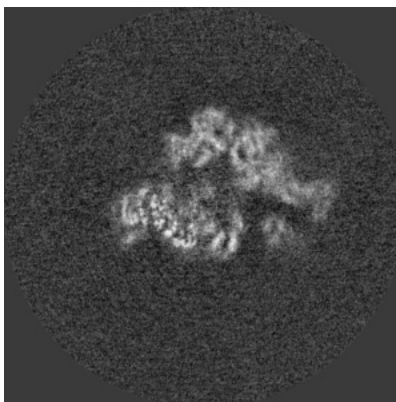


Z Index: 189

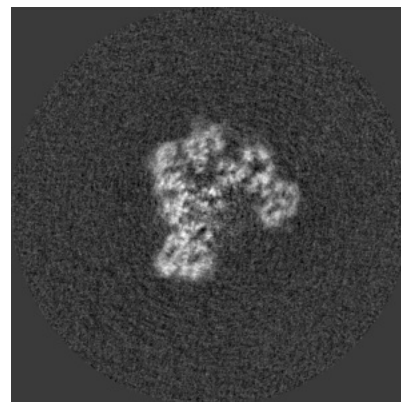
6.3.2 Raw map



X Index: 189



Y Index: 196

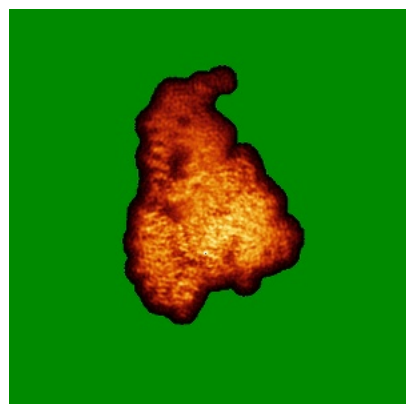


Z Index: 188

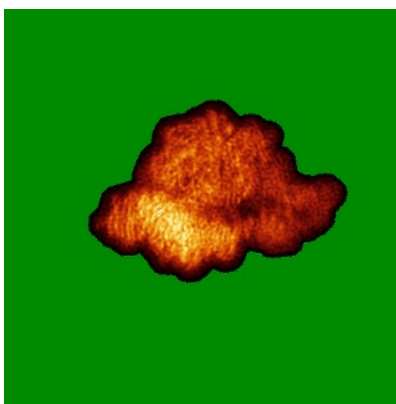
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

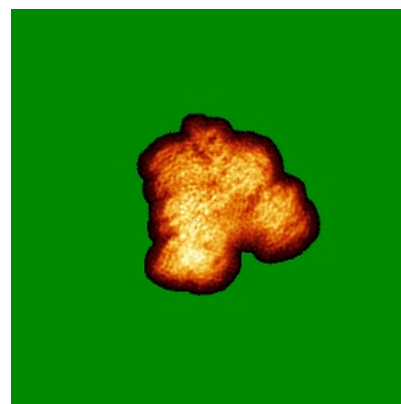
6.4.1 Primary map



X

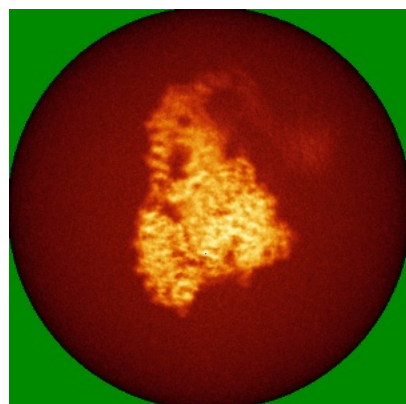


Y

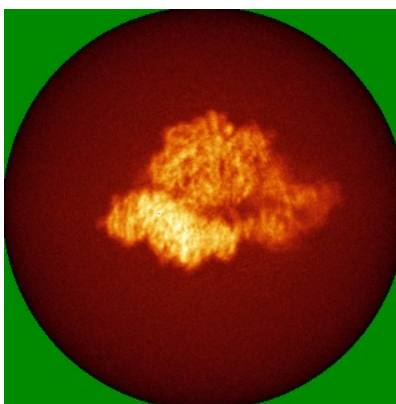


Z

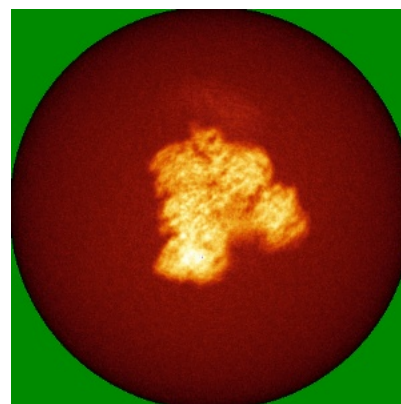
6.4.2 Raw map



X



Y

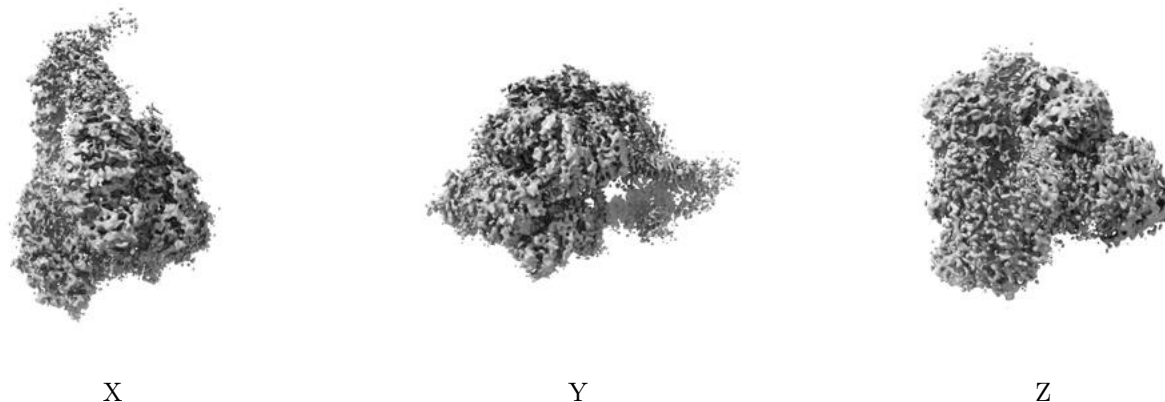


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0169. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

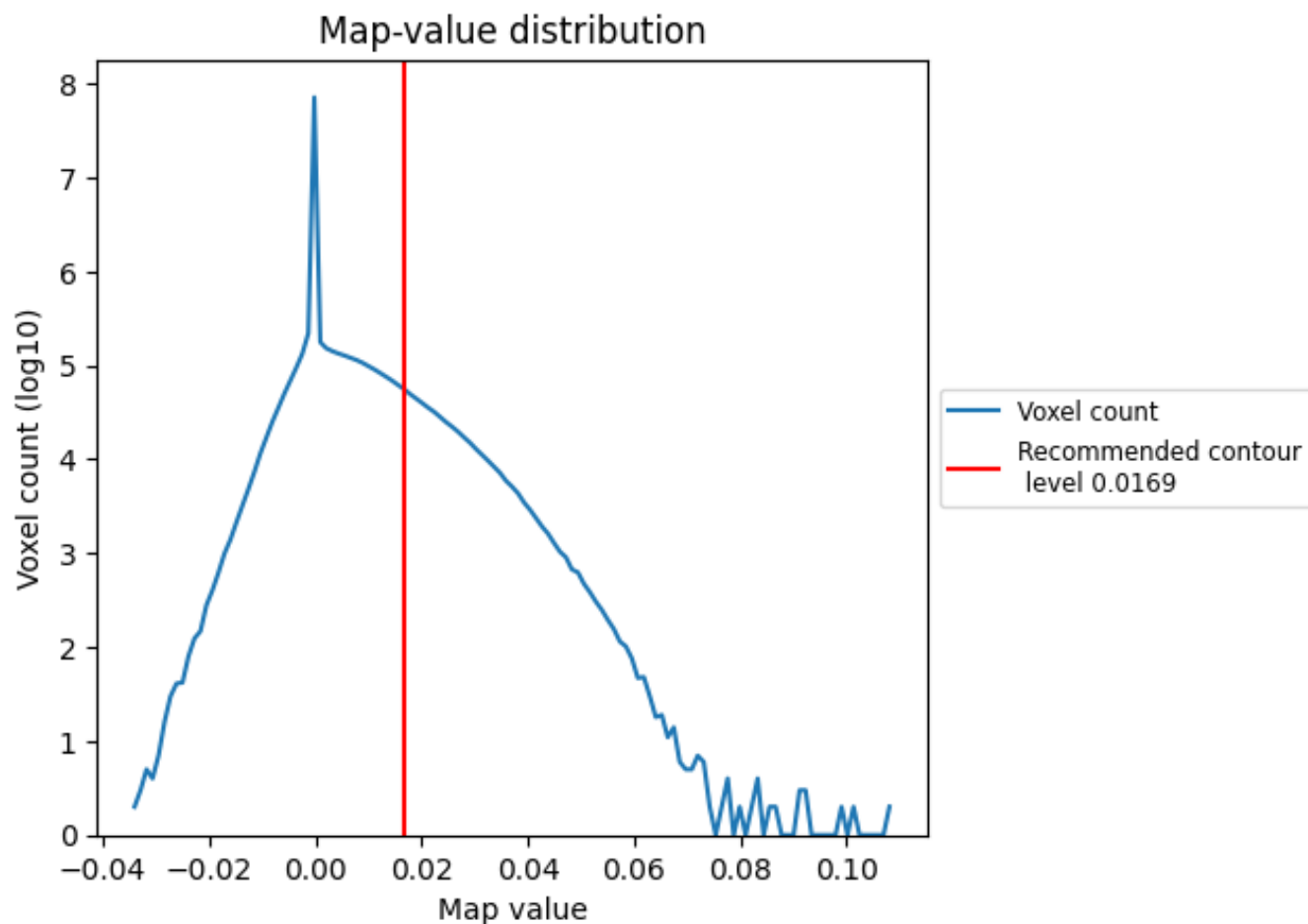
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

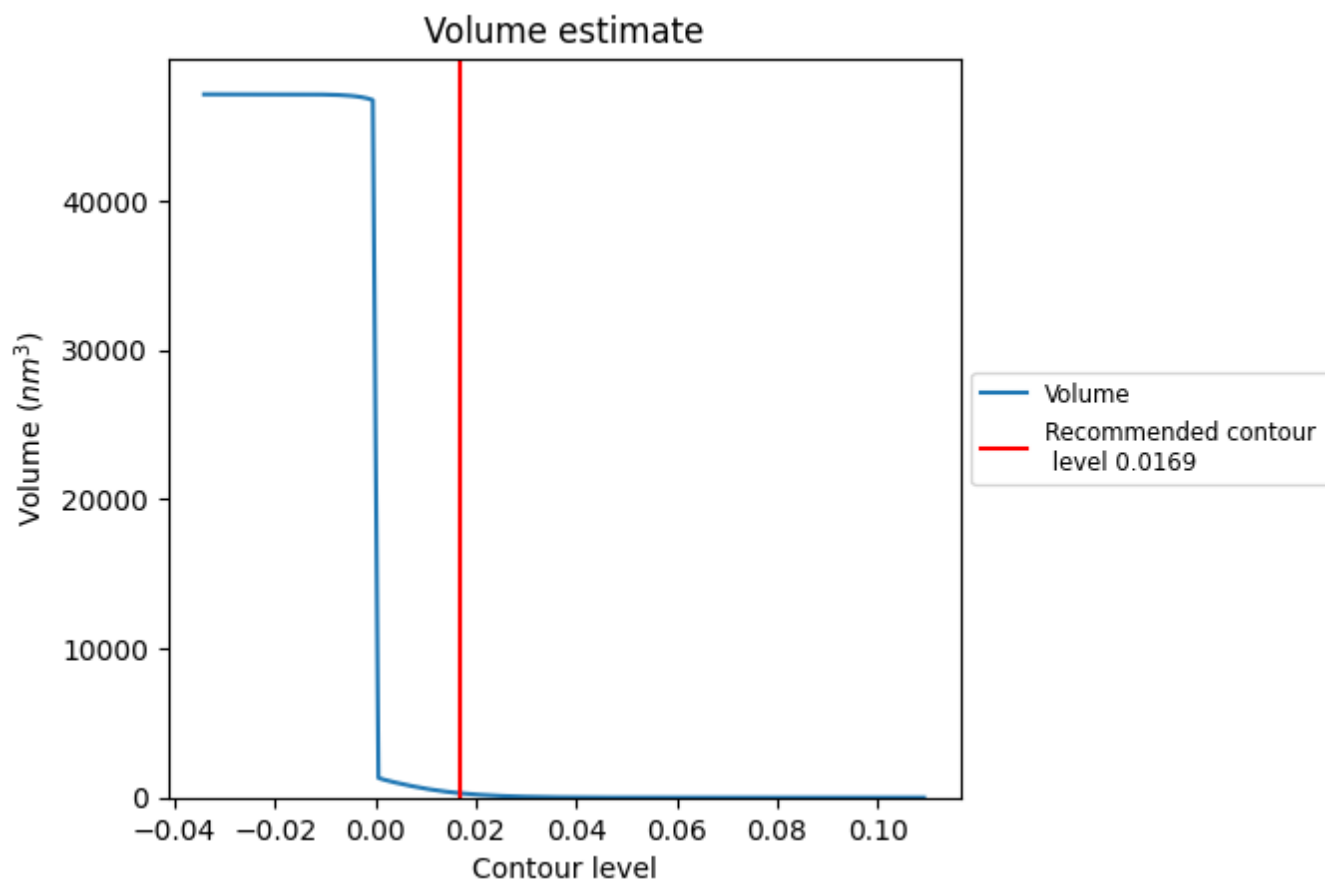
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

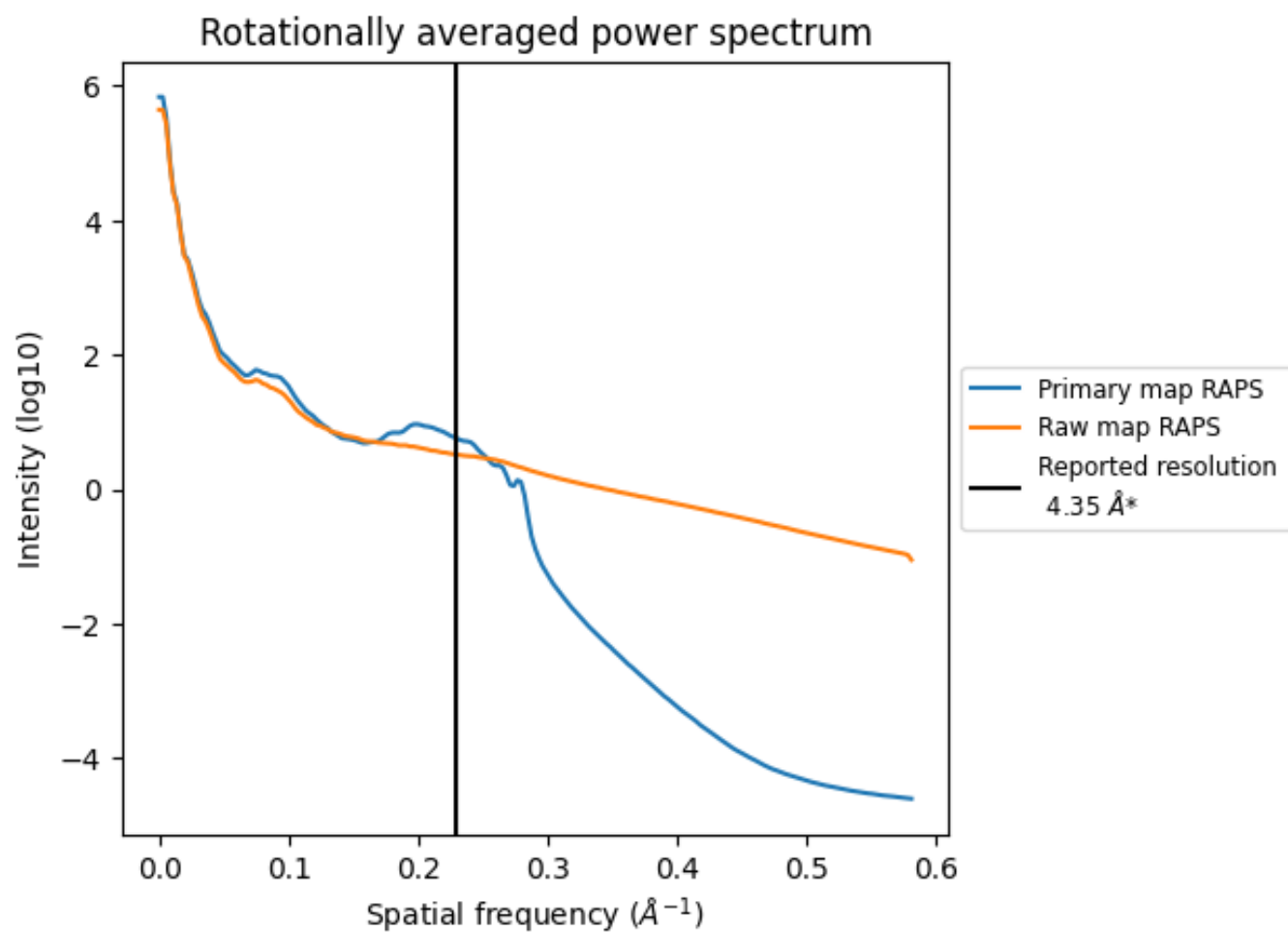
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 292 nm³; this corresponds to an approximate mass of 264 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 ⓘ

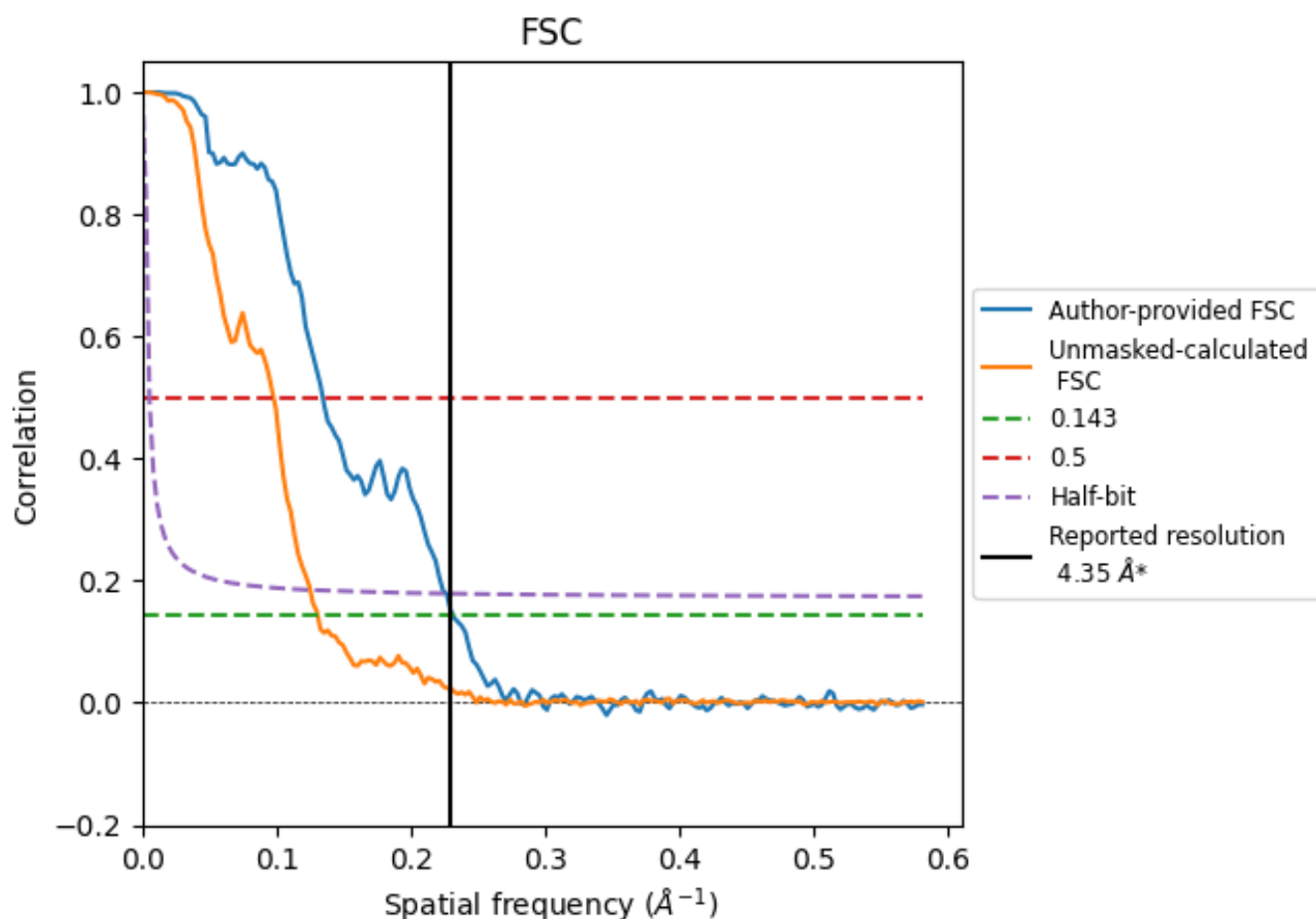


*Reported resolution corresponds to spatial frequency of 0.230 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.230 Å⁻¹

8.2 Resolution estimates [i](#)

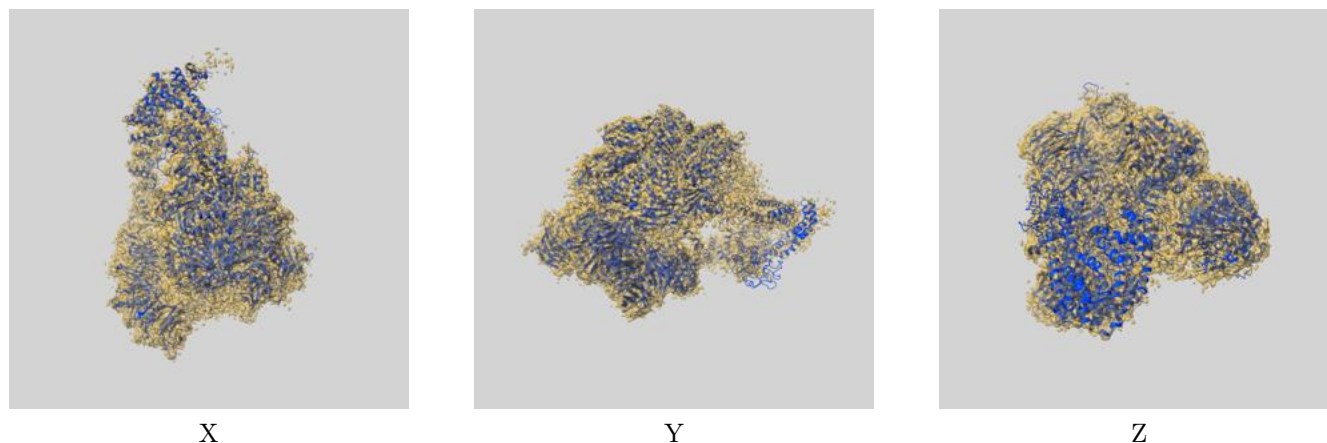
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.35	-	-
Author-provided FSC curve	4.32	7.43	4.41
Unmasked-calculated*	7.65	10.22	7.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.65 differs from the reported value 4.35 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15622 and PDB model 8ASV. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0169 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](#)

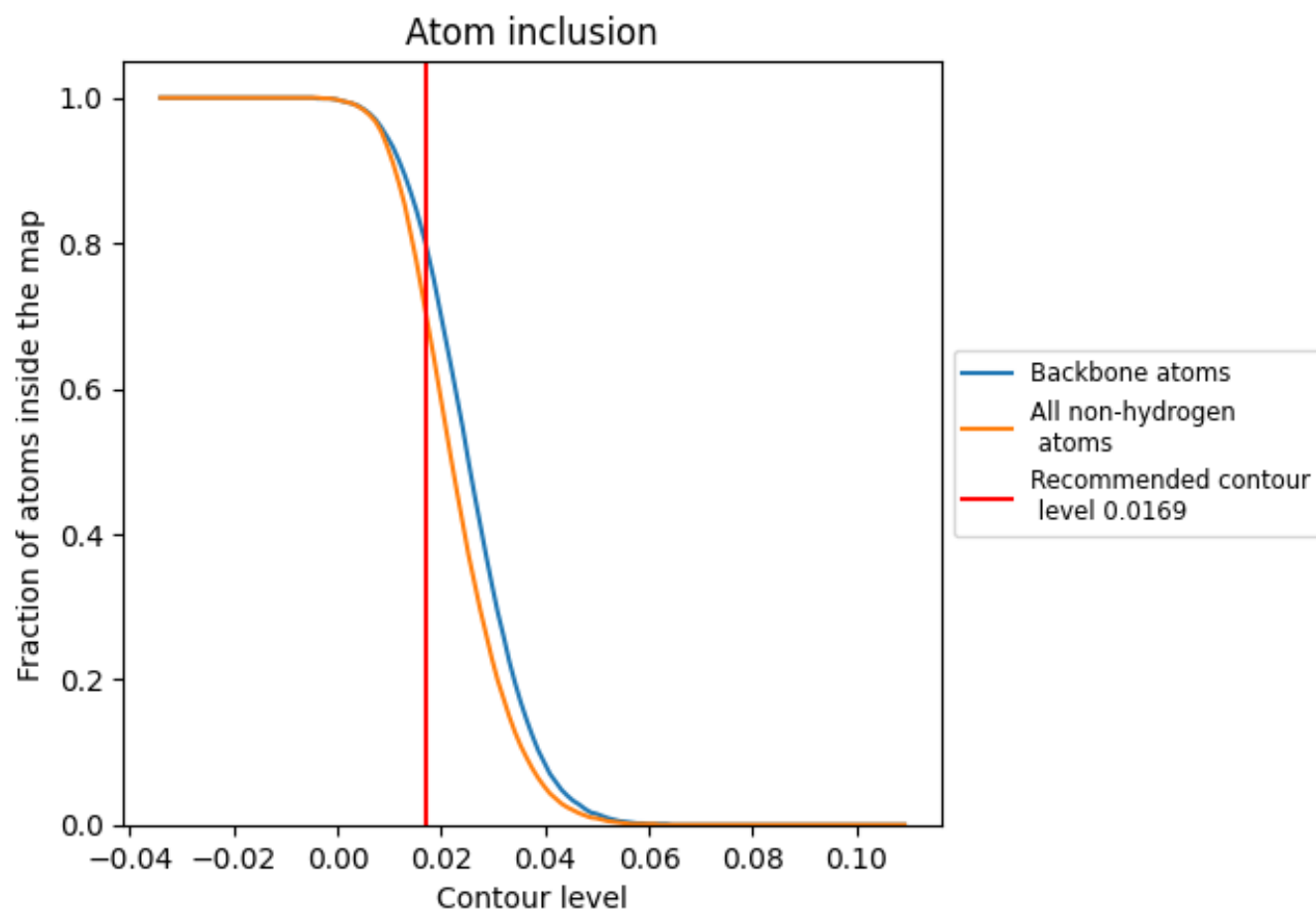


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.0169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.3720
A	0.7220	0.3690
B	0.8060	0.3970
C	0.8390	0.4550
D	0.2350	0.2490
E	0.7090	0.3850
F	0.7030	0.3510
G	0.7920	0.3900
H	0.6970	0.3580
I	0.7730	0.3900
J	0.6530	0.3280

1.0

0.0

<0.0