



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:22 AM UTC

PDB ID : 8EZQ / pdb_00008ezq
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.dev132
MolProbity : 4-5-2 with Phenix2.0
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)
Validation Pipeline (wwPDB-VP) : 2.49

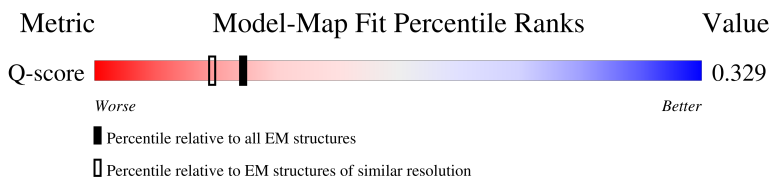
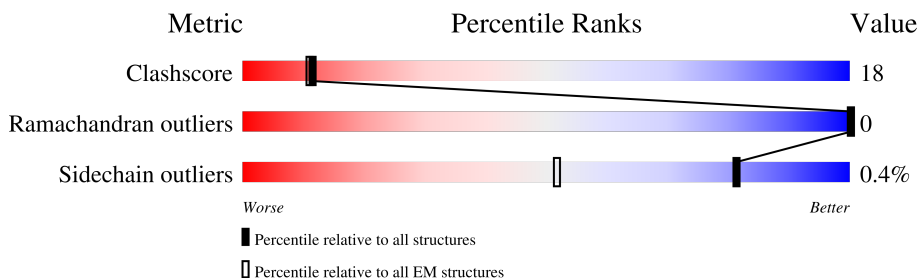
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1483	 57% 29% 14%
1	B	1483	 56% 30% 14%

2 Entry composition

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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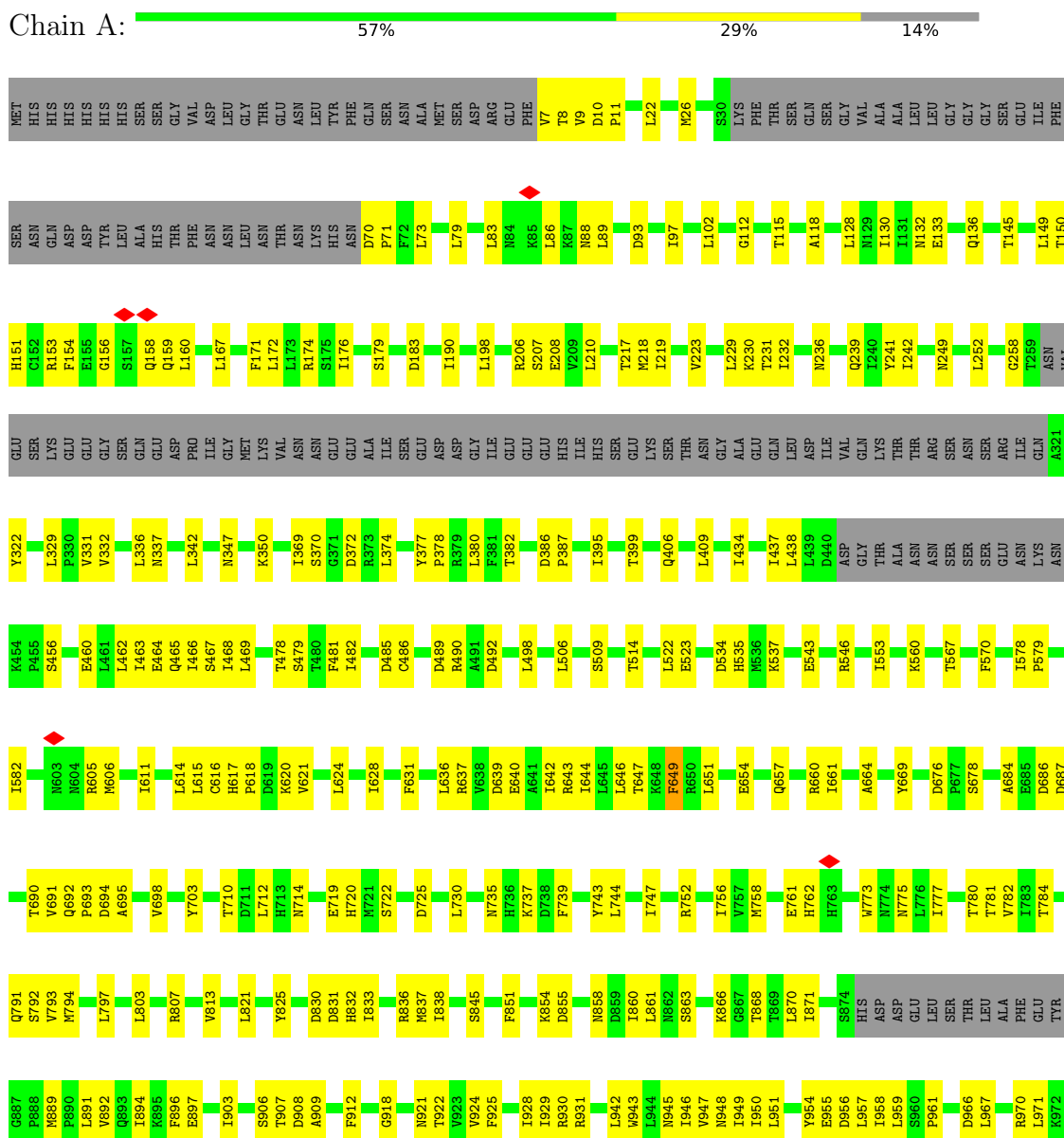
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	HIS	-	expression tag	UNP P39993
B	-20	HIS	-	expression tag	UNP P39993
B	-19	HIS	-	expression tag	UNP P39993
B	-18	HIS	-	expression tag	UNP P39993
B	-17	HIS	-	expression tag	UNP P39993
B	-16	SER	-	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

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



VAL	K1353	L1271	K1187	T1074	S974	SER	T790	T796	T861	S874	HIS	ASP	ASP	GLU	LEU
GLU	I1354	T1272	V1188	I1075	H975	THR	Q791	L797	N862	S875	ASP	ASP	ASP	GLU	LEU
ILE	L1355		T1189	A1076	L976	LEU	ALA	T798	S863	S864	ASP	ASP	ASP	GLU	LEU
GLU	T1356	L1275	A1190	A1077		ALA	PHE		I864	A865					
ALA	S1357	L1276	M1191	F1078	P981	THR			T868						
THR	S1358	E1277	K1192		E982	ALA									
ALA	T1359	D1278	E1193	C1081		LEU									
PRO	L1360	N1279	Q1194		X989	LEU									
ILE	T1361	N1280	S1197	E1084	GLU	LEU									
ASP	T1362	D1281	I1198	E1085	SER	LEU									
ASP	T1363	L1282	T1198	E1086	LYS	LEU									
ASN					GLY	LEU									
THR	V1366	I1287	V1201	K1094		LEU									
ASP	Y1367		L1202	V1095		LEU									
ASP	L1368	T1290	N1203	F1096		LEU									
ASP	H1369	I1291	E1204			SER									
ASN	V1370	L1294	S1205	R1111		THR									
LYS	L1371	A1295	T1208	T1114		PHE									
PRO	K1372	H1296	E1216	Y1115		ALA									
LYS		Q1297	F1218	I1117		SER									
LEU	T1376	C1302	M1219	Q1126		ALA									
SER	S1377	K1303	V1220	I1134		SER									
ASP	N1378	Q1304	V1221	N1135		LEU									
VAL	E1379	S1306	L1224	D1136		LEU									
GLU	T1380	E1307	L1225	E1137		LEU									
LYS	F1381	L1313	D1226	L1138		LEU									
ASP	L1382		E1227	L1139		LEU									
	K1383	T1316	I1228	F1150		LEU									
	L1384	L1317	M1231	A1151		LEU									
	L1385	N1318	G1232	G1155		LEU									
		I1320	A1233	K1156		LEU									
	D1396	I1321	M1236	E1157		LEU									
		E1322				LEU									
	K1400	I1323	E1239	R1161		LEU									
		P1324	I1240	L1162		LEU									
	I1405	T1325	N1241	F1163		LEU									
		N1326	Y1242	T1166		LEU									
	K1409	E1327	K1243	E1167		LEU									
		M1328	L1245	S1169		LEU									
	E1412	E1329	T1246	Y1171		LEU									
GLY	K1413	G1338	I1252	F1174		LEU									
ASN		L1339	K1253	L1175		LEU									
GLY		L1340	K1254			LEU									
SER		P1341	E1255			LEU									
SER		L1342	N1256			LEU									
SER		L1343	K1257			LEU									
HIS		N1344	P1258			LEU									
GLY		S1345	Y1258			LEU									
GLU		S1346				LEU									
THR		Q1349	S1261			LEU									
PRO		E1350				LEU									
GLU		D1351	S1268			LEU									
SER		Q1352				LEU									
ASN						LEU									
ASP						LEU									

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.20	0/10392	0.36	0/14039
1	B	0.18	0/10404	0.38	0/14056
All	All	0.19	0/20796	0.37	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	371	0
1	B	10233	0	10436	374	0
All	All	20456	0	20853	735	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 18.

All (735) 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:570:PHE:CD1	1:A:606:MET:HE1	2.28	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:B:1359:ILE:C	1:B:1362:ILE:HG12	2.19	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:774:ASN:HA	1:B:777:ILE:HG22	1.77	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:1236:ASN:CG	1:A:1302:CYS:SG	2.81	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:892:VAL:HG12	1:B:893:GLN:N	2.11	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:647:THR:HG23	1:B:779:SER:OG	2.00	0.62
1:A:478:THR:HG23	1:A:794:MET:HE1	1.81	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:821:LEU:HD22	1:A:837:MET:HE1	1.82	0.61
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:B:1138:LEU:O	1:B:1187:LYS:NZ	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ARG:O	1:A:605:ARG:NH2	2.34	0.60
1:B:821:LEU:HD22	1:B:837:MET:HE1	1.83	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
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:198:LEU:HD13	1:B:218:MET:HE2	1.84	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:889:MET:HE3	1:A:889:MET:HA	1.87	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: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:1228:ILE:HA	1:B:1231:MET:HE2	1.88	0.55
1:B:1294:LEU:HD22	1:B:1313:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:1258:TYR:O	1:B:1261:SER:OG	2.21	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: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:B:1316:THR:HG22	1:B:1320:LYS:HZ3	1.72	0.54
1:A:855:ASP:OD1	1:A:855:ASP:N	2.40	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:A:1393:GLU:O	1:A:1394:ASP:CG	2.50	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:570:PHE:CG	1:A:606:MET:HE1	2.44	0.53
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: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:1326:ASN:O	1:A:1327:GLU:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:207:SER:OG	1:A:208:GLU:N	2.41	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:1362:ILE:HG13	1:B:1363:ILE:N	2.25	0.51
1:A:1326:ASN:HD22	1:A:1327:GLU:CD	2.19	0.50
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:1125:ASP:O	1:A:1171:TYR:OH	2.27	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:A:10:ASP:N	1:A:10:ASP:OD1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:26:MET:HE3	1:A:73:LEU:HD13	1.94	0.48
1:B:1349:GLN:O	1:B:1351:ASP:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:734:CYS:C	1:B:736:HIS:H	2.21	0.48
1:B:926:PHE:HD1	1:B:929:ILE:HD11	1.77	0.48
1:A:637:ARG:HG3	1:A:743:TYR:CE1	2.49	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:510:ALA:O	1:B:513:THR:OG1	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:132:ASN:CG	1:A:133:GLU:H	2.24	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:26:MET:HE1	1:B:72:PHE:HB2	1.98	0.46
1:B:1382:LEU:O	1:B:1385:LEU:HG	2.15	0.46
1:A:249:ASN:CG	1:A:337:ASN:ND2	2.74	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:B:636:LEU:HD12	1:B:636:LEU:C	2.41	0.46
1:A:83:LEU:HA	1:A:86:LEU:HD12	1.98	0.46
1:A:347:ASN:HA	1:A:350:LYS:HZ3	1.81	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:1281:ASP:C	1:A:1282:LEU:HG	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1396:ASP:O	1:B:1400:LYS:NZ	2.48	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:198:LEU:HD22	1:A:218:MET:HE2	1.99	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
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:1393:GLU:C	1:A:1395:SER:H	2.25	0.45
1:A:1412:GLU:HA	1:A:1415:ASN:HD21	1.82	0.45
1:A:793:VAL:O	1:A:793:VAL:HG12	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:958:ILE:HB	1:A:1020:MET:CE	2.48	0.44
1:B:176:ILE:O	1:B:179:SER:OG	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:176:ILE:O	1:A:179:SER:OG	2.35	0.44
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:909:ALA:HA	1:A:957:LEU:HD11	1.98	0.44
1:A:956:ASP:O	1:A:957:LEU:HB2	2.16	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:780:THR:C	1:A:782:VAL:H	2.27	0.43
1:A:1048:LEU:HD21	1:A:1074:THR:HG21	2.00	0.43
1:B:536:MET:HE3	1:B:847:ILE:HG12	2.00	0.43
1:B:908:ASP:OD1	1:B:908:ASP:N	2.50	0.43
1:A:567:THR:HG21	1:A:605:ARG:HG2	2.00	0.43
1:A:646:LEU:HD13	1:A:758:MET:HE2	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1343:LEU:C	1:B:1345:SER:H	2.26	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: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
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:472:ARG:O	1:B:473:SER:OG	2.30	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:A:79:LEU:HD11	1:A:97:ILE:HA	2.00	0.43
1:A:1176:LEU:C	1:A:1217:ASN:HD21	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1409:LYS:HZ2	1:B:1412:GLU:HB3	1.84	0.42
1:A:676:ASP:OD2	1:A:678:SER:OG	2.23	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: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: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
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:A:479:SER:HB2	1:A:794:MET:HE2	2.02	0.42
1:B:397:GLN:OE1	1:B:433:ARG:NH1	2.53	0.42
1:B:1034:GLY:C	1:B:1036:GLU:H	2.27	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:A:1123:CYS:SG	1:A:1124:ALA:N	2.92	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:B:1060:SER:C	1:B:1062:TYR:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:690:THR:O	1:A:691:VAL:C	2.63	0.41
1:B:963:ILE:HG23	1:B:964:PHE:HD1	1.86	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:A:1374:GLY:C	1:A:1375:LYS:HG2	2.45	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:734:CYS:C	1:B:736:HIS:N	2.76	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:862:ASN:CG	1:B:942:LEU:HD23	2.46	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: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:685:GLU:HA	1:B:742:TRP:CE2	2.55	0.41
1:B:1007:GLU:H	1:B:1007:GLU:CD	2.24	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:A:871:ILE:HD13	1:A:945:ASN:HA	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1113:LEU:HD13	1:A:1137:GLU:HG2	2.02	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
1:A:1328:MET:HE2	1:A:1328:MET:HB2	1.95	0.40
1:B:551:MET:C	1:B:553:ILE:H	2.29	0.40
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

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	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

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%)	1177 (100%)	5 (0%)	84	81
1	B	1183/1367 (86%)	1178 (100%)	5 (0%)	84	81
All	All	2365/2734 (86%)	2355 (100%)	10 (0%)	81	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	PHE
1	A	322	TYR
1	A	649	PHE
1	A	703	TYR
1	A	1096	PHE
1	B	72	PHE
1	B	810	PHE
1	B	916	PHE

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Mol	Chain	Res	Type
1	B	1096	PHE
1	B	1218	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	249	ASN
1	A	337	ASN
1	A	422	ASN
1	A	602	ASN
1	A	617	HIS
1	A	673	GLN
1	A	692	GLN
1	A	823	ASN
1	A	945	ASN
1	A	948	ASN
1	A	1319	ASN
1	B	91	ASN
1	B	99	GLN
1	B	151	HIS
1	B	238	ASN
1	B	657	GLN
1	B	862	ASN
1	B	948	ASN
1	B	1178	ASN
1	B	1304	GLN
1	B	1349	GLN
1	B	1352	GLN
1	B	1389	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

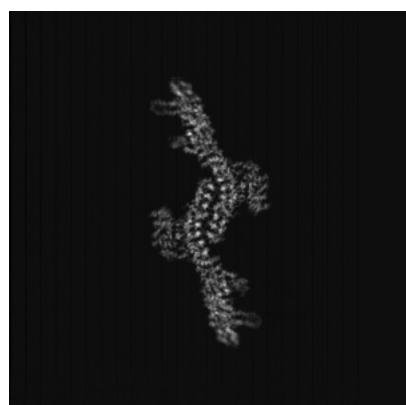
6 Map visualisation [i](#)

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.

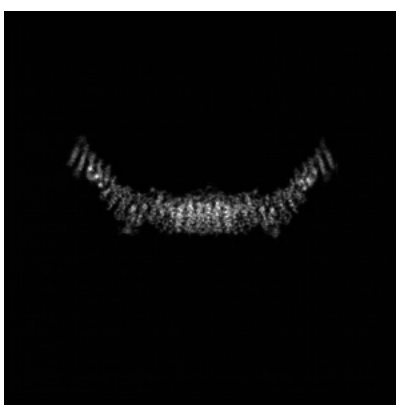
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

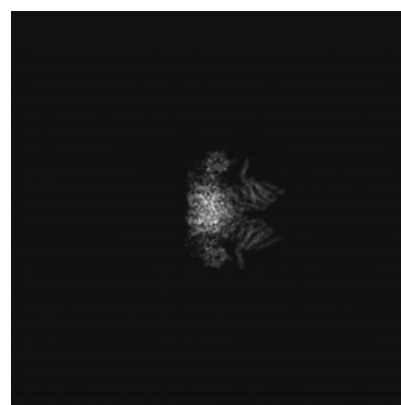
6.1.1 Primary map



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: 256



Y Index: 256



Z Index: 256

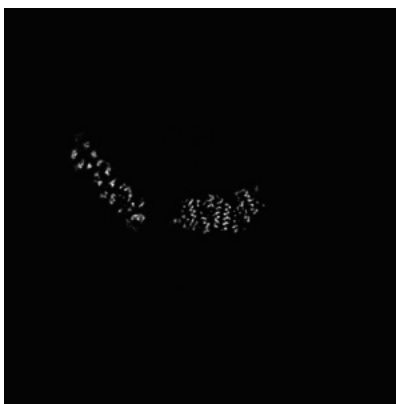
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

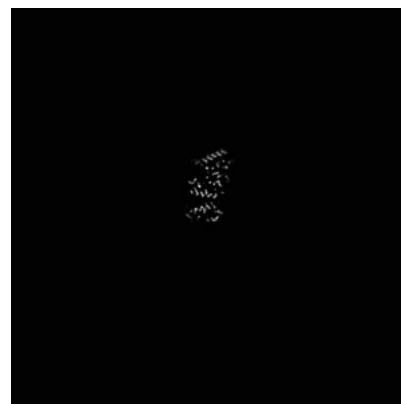
6.3.1 Primary map



X Index: 256



Y Index: 274

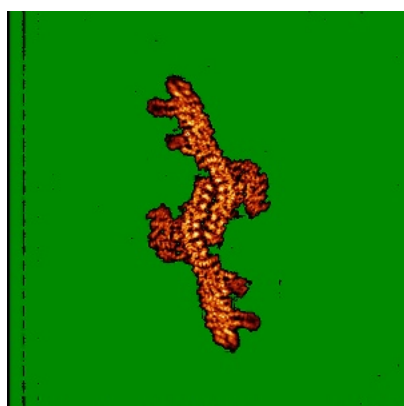


Z Index: 273

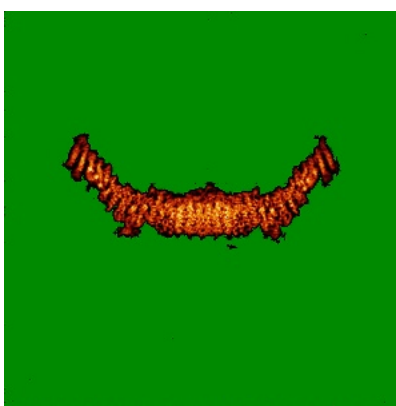
The images above show the largest variance slices of the map in three orthogonal directions.

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

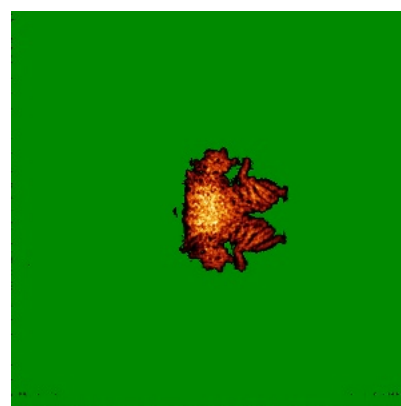
6.4.1 Primary map



X



Y

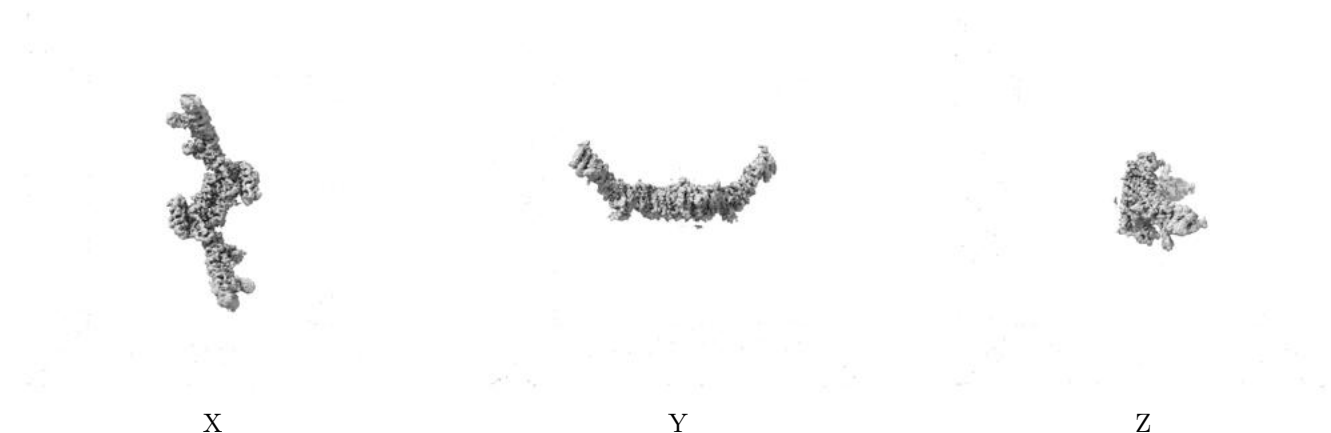


Z

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



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.

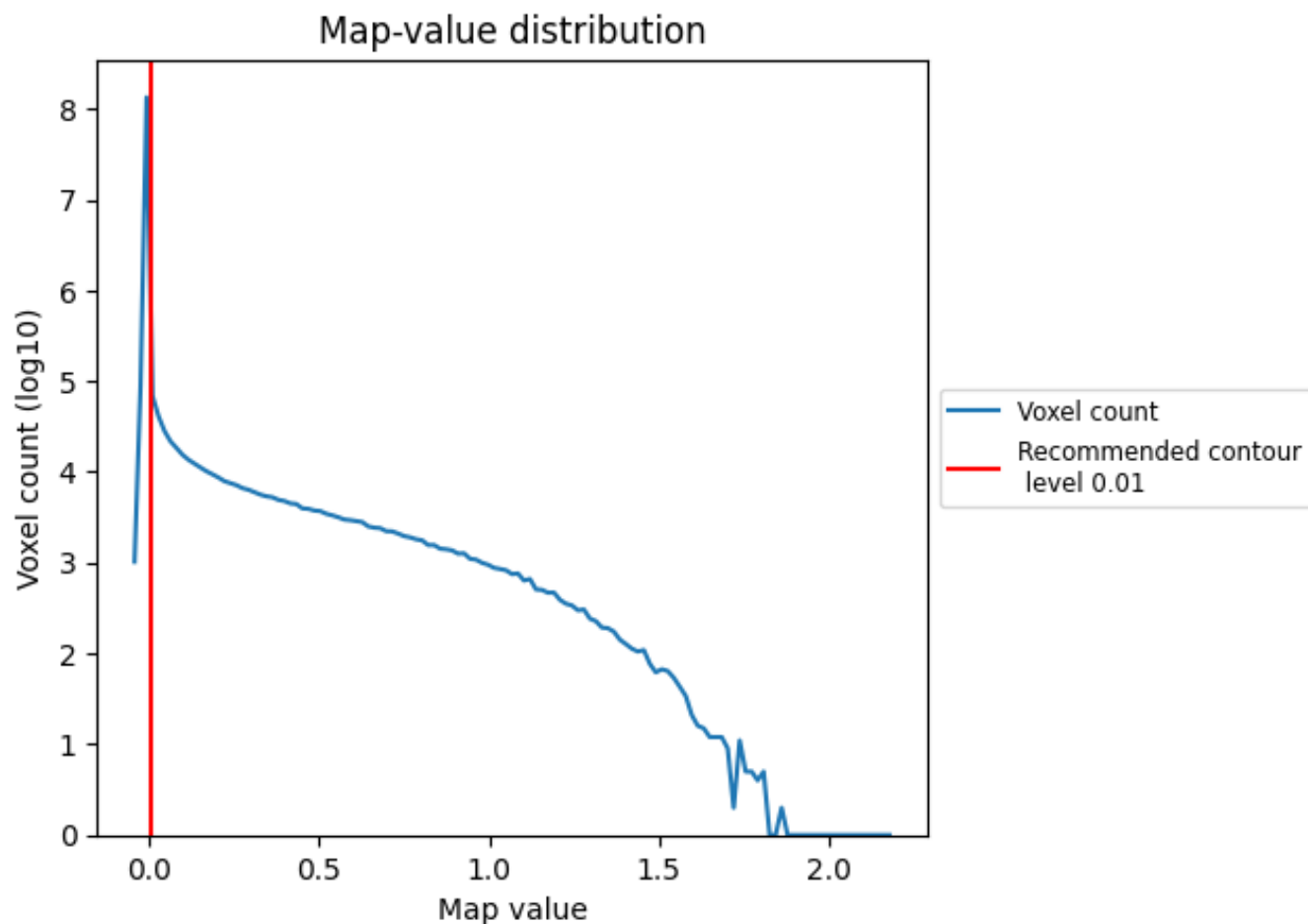
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

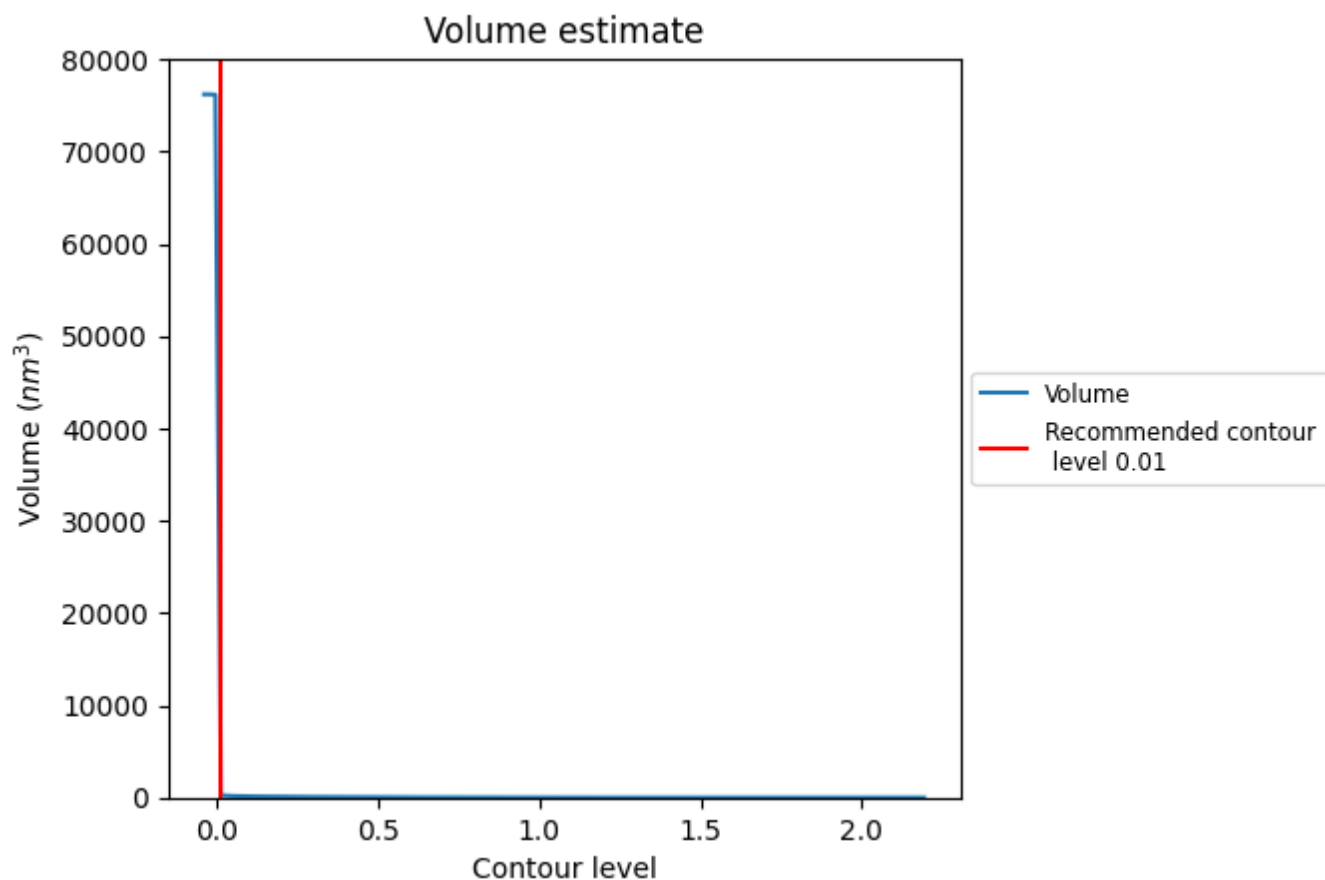
This section contains the results of statistical analysis of the map.

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.

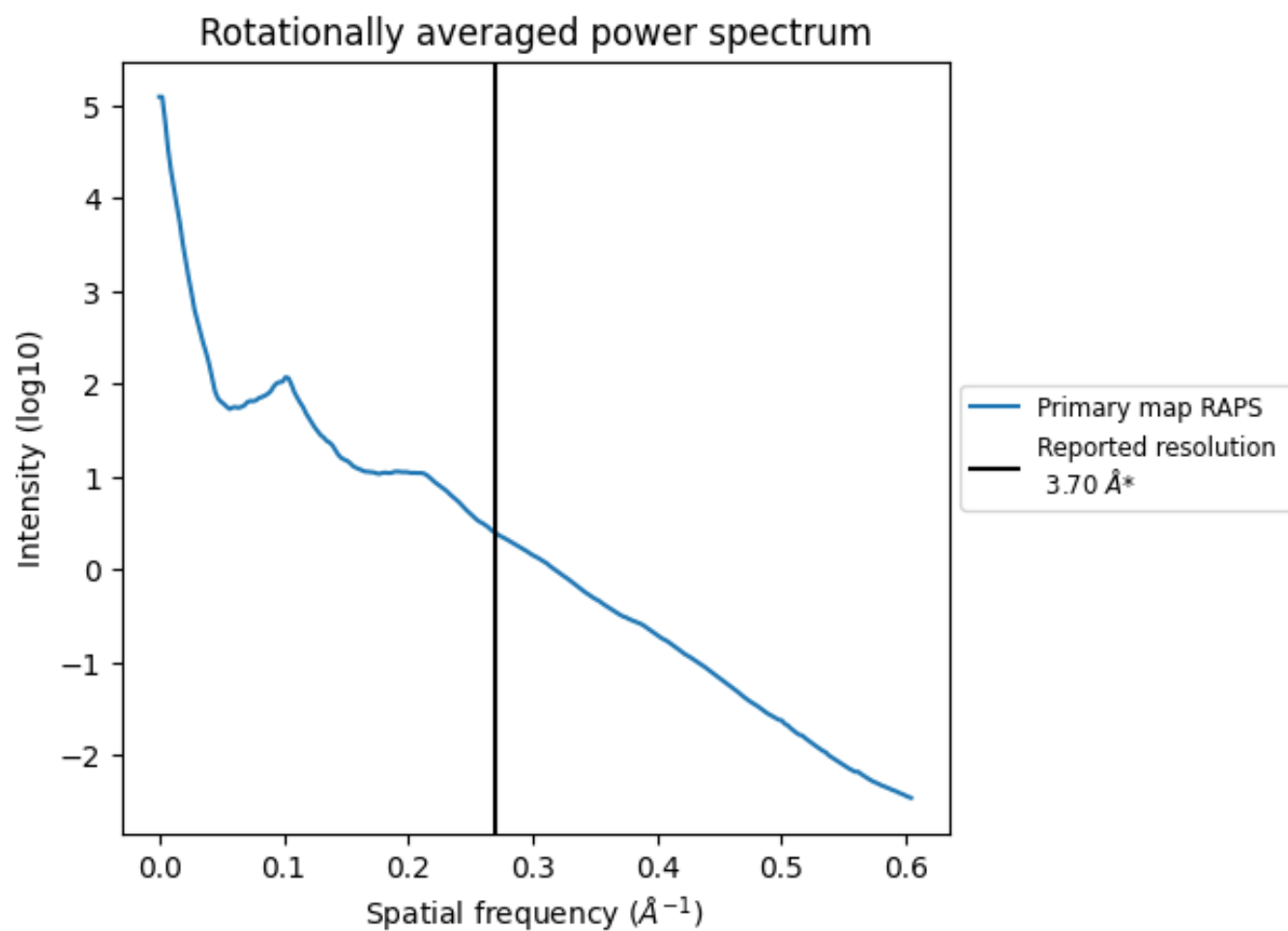
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

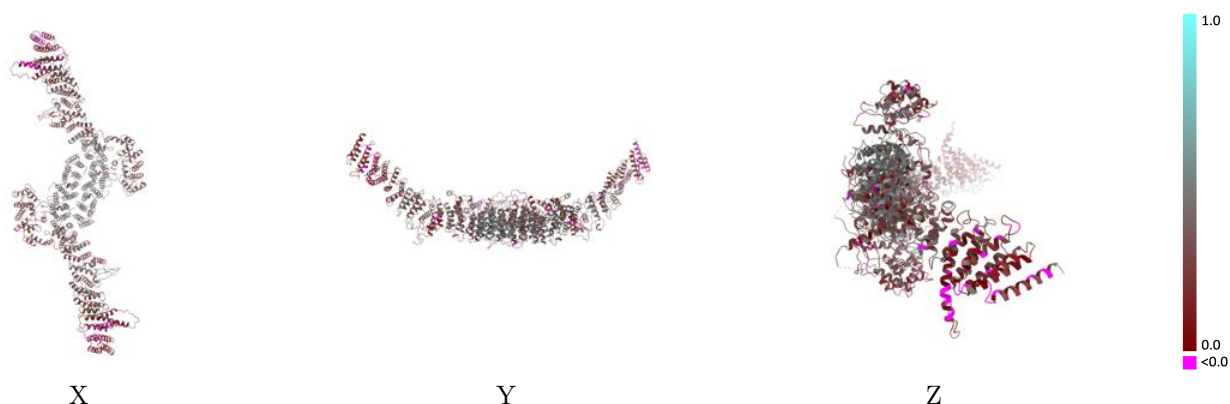
This section contains information regarding the fit between EMDB map EMD-28748 and PDB model 8EZQ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



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](#)

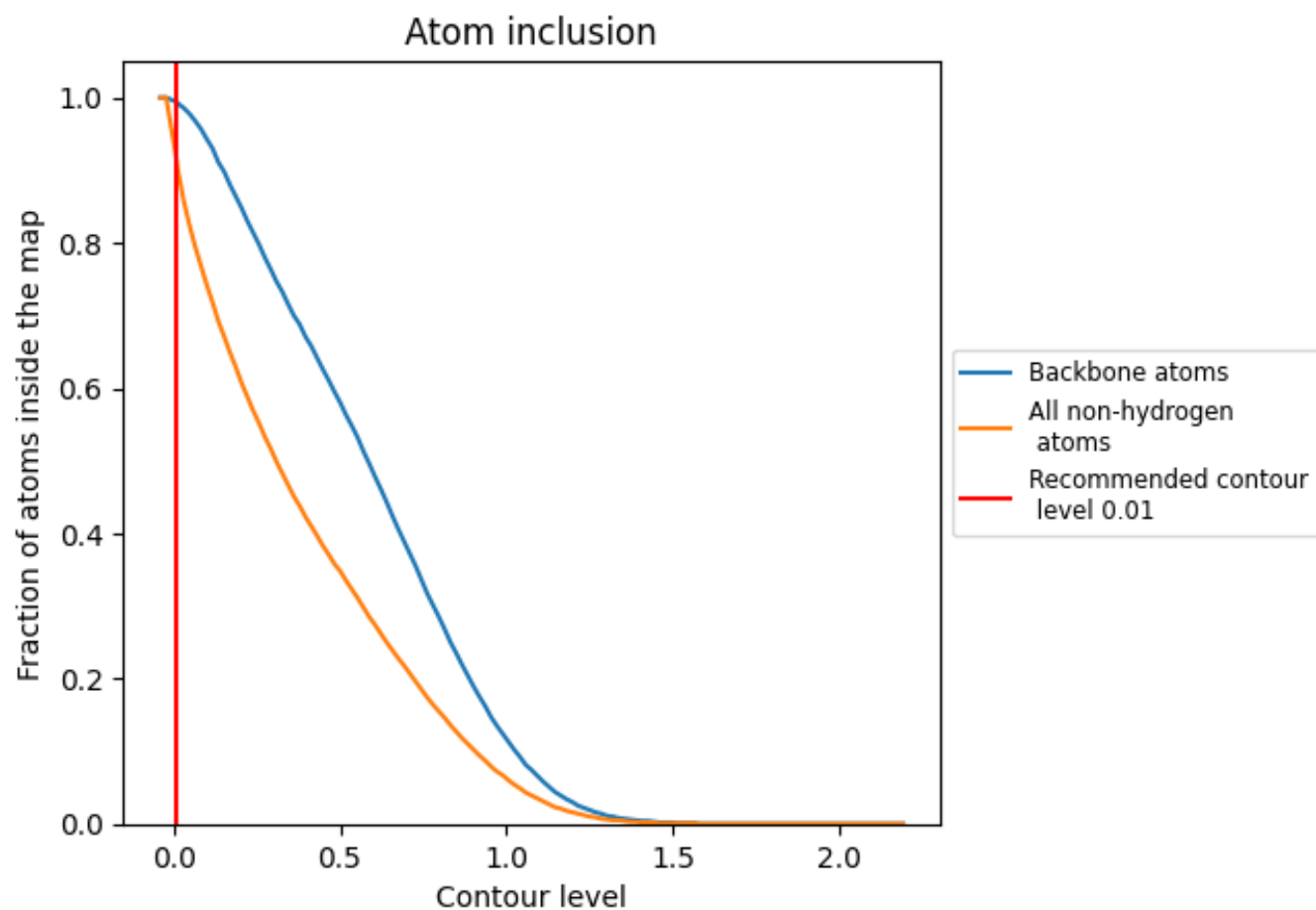


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

