



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:22 am BST

PDB ID : 8ROR / pdb\_00008ror  
EMDB ID : EMD-19402  
Title : Single-particle cryo-EM of Mycoplasma pneumoniae adhesin P1 complexed with the anti-adhesive Fab fragment.  
Authors : Vizarraga, D.; Kawamoto, A.; Marcos-Silva, M.; Fita, I.; Miyata, M.; Pinyol, J.; Namba, K.; Kenri, T.  
Deposited on : 2024-01-12  
Resolution : 2.39 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

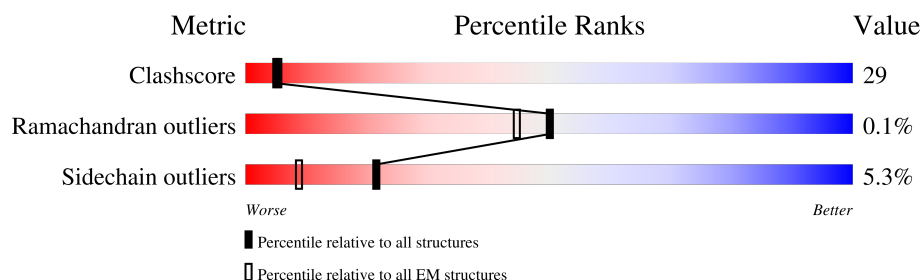
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.39 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1	1457	<div> <div>71%</div> <div>44%</div> <div>47%</div> <div>7%</div> </div>
2	L	218	<div> <div>69%</div> <div>57%</div> <div>39%</div> <div>.</div> </div>
3	H	222	<div> <div>84%</div> <div>59%</div> <div>36%</div> <div>5%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14205 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 Adhesin P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1349	Total	C	N	O	S	9	0
			10563	6659	1841	2053	10		

- Molecule 2 is a protein called Light Chain Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	218	Total	C	N	O	S	0	0
			1698	1066	288	337	7		

- Molecule 3 is a protein called Heavy Chain Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	222	Total	C	N	O	S	0	0
			1675	1057	271	337	10		

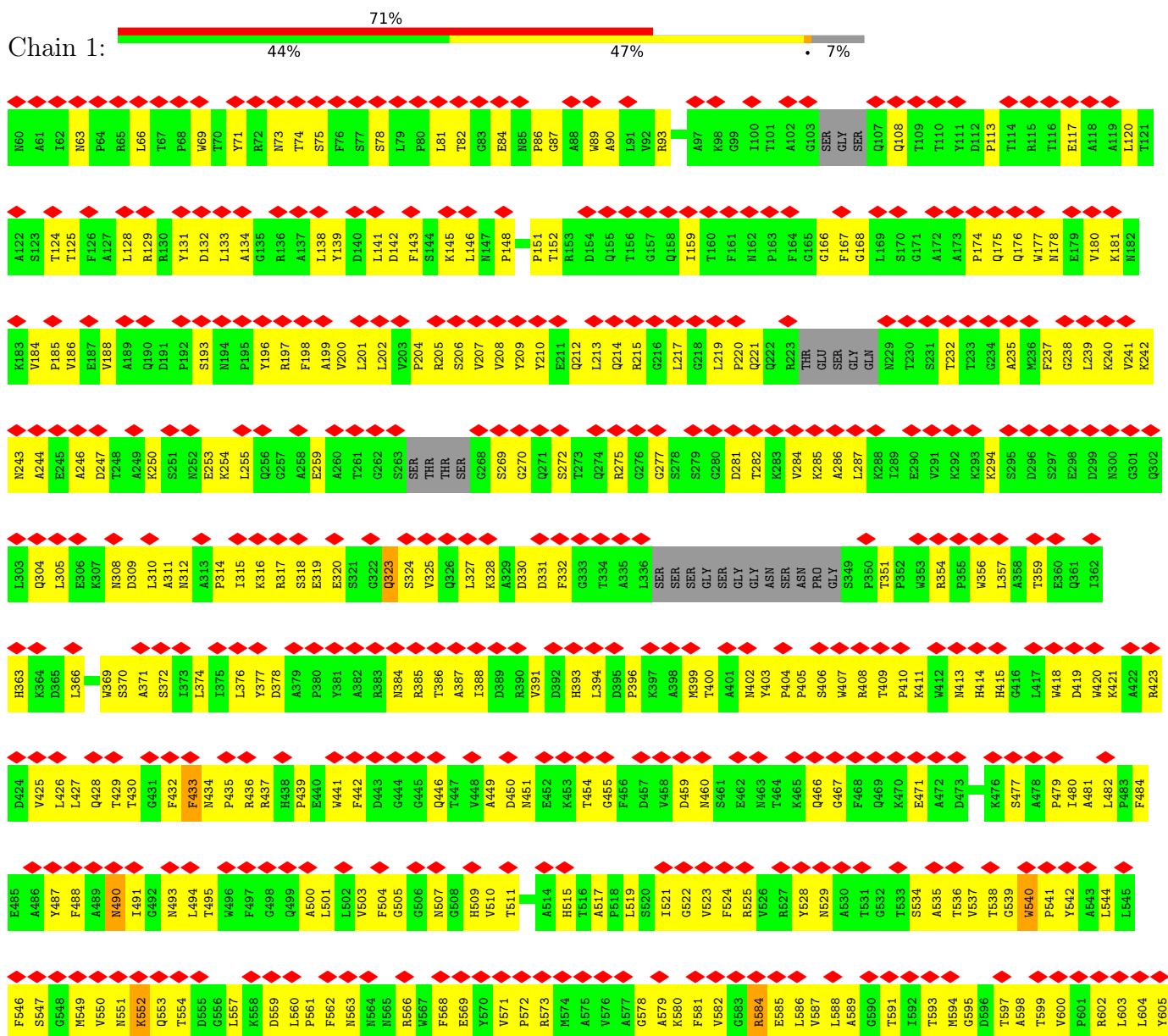
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	1	267	Total	O	0
			267	267	
4	H	2	Total	O	0
			2	2	

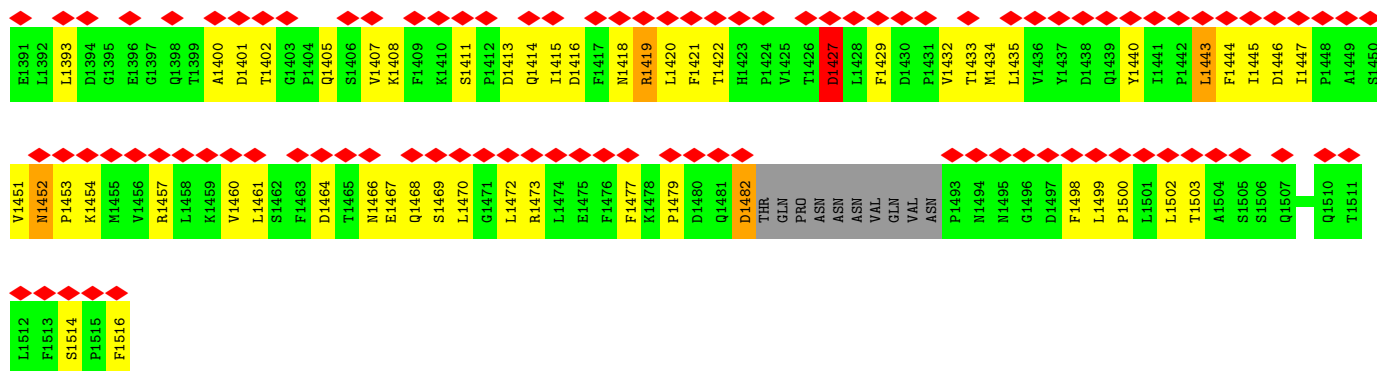
### 3 Residue-property plots

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: Adhesin P1



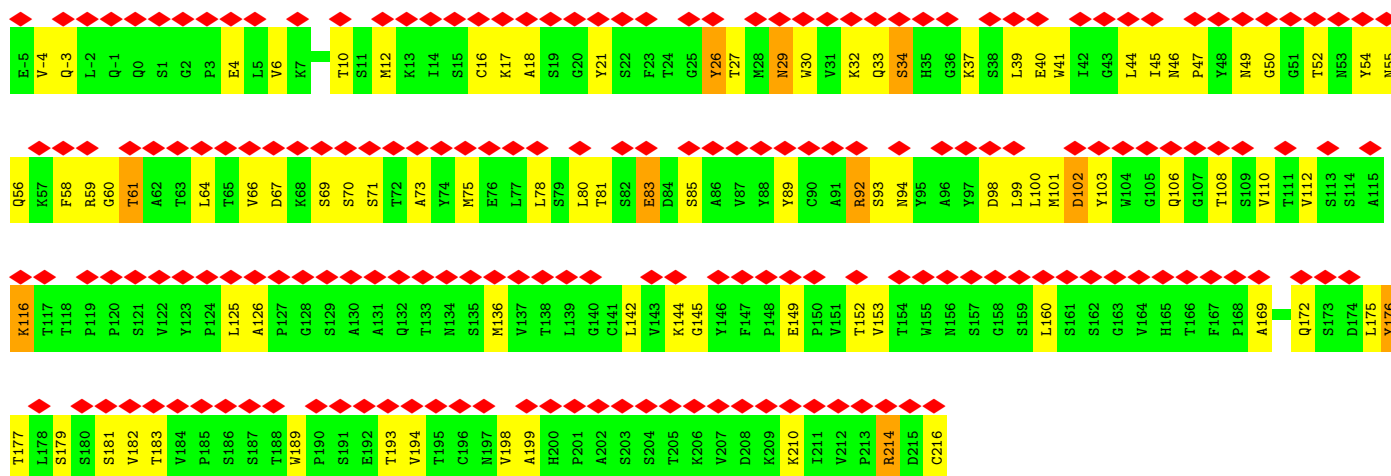
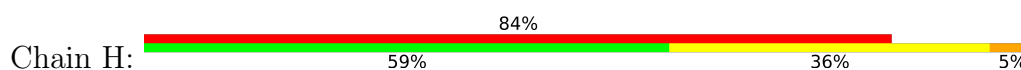
K1330	V1331	S1332	G1333	W1334	L1335	G1336	G1337	Q1338	L1339	P1340	S1341	T1342	SER	ASP	GLY	ASN	THR	SER	S1349	T1350	N1351	N1352	L1353	A1354	P1355	N1356	T1357	N1358	T1359	G1360	N1361	D1362	V1363	V1364	G1365	V1366	G1367	R1368	L1369	S1370	E1371	S1372	GLY	GLY	ALA	GLY	GLY	SER	SER	GLY	ALA	THR	ARG	ASN	A1202	L1203	P1204	H1205	H1206	P1207	N1208	A1209																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								</
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### • Molecule 2: Light Chain Fab



### • Molecule 3: Heavy Chain Fab



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4312408	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	188.0, 188.0, 188.0	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	1	0.32	0/10826	0.52	3/14749 (0.0%)
2	L	0.27	0/1739	0.51	0/2361
3	H	0.27	0/1718	0.51	0/2349
All	All	0.31	0/14283	0.52	3/19459 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1443	LEU	CA-CB-CG	5.59	128.16	115.30
1	1	1427	ASP	CB-CG-OD1	5.55	123.29	118.30
1	1	433	PHE	C-N-CA	-5.42	108.16	121.70

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	1	10563	0	10175	661	0
2	L	1698	0	1638	72	0
3	H	1675	0	1630	78	0
4	1	267	0	0	14	0
4	H	2	0	0	0	0
All	All	14205	0	13443	784	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 29.

All (784) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:214:ARG:H	3:H:214:ARG:HD3	1.39	0.86
1:1:374:LEU:HD13	1:1:388:ILE:HG12	1.61	0.82
1:1:1088:LYS:NZ	1:1:1253:LYS:O	2.12	0.82
1:1:733:LEU:HD21	1:1:1122:VAL:HG11	1.63	0.81
1:1:515:HIS:HE1	1:1:1209:ALA:HB3	1.48	0.79
1:1:217:LEU:HD11	1:1:439:PRO:HG2	1.65	0.78
1:1:202:LEU:O	1:1:371:ALA:HA	1.83	0.77
1:1:139:TYR:OH	1:1:378:ASP:OD1	2.01	0.77
1:1:399:MET:HG2	1:1:482:LEU:HD22	1.69	0.74
1:1:809:PRO:HA	1:1:816:ARG:HA	1.70	0.74
1:1:806:ASP:OD2	1:1:852:PRO:HB2	1.87	0.74
3:H:93:SER:HB3	3:H:101:MET:H	1.52	0.73
1:1:711:ASN:HB3	1:1:723:VAL:HG22	1.70	0.73
1:1:749:LYS:HA	1:1:749:LYS:HE2	1.71	0.73
1:1:851:LEU:HD12	1:1:1037:LEU:HD13	1.70	0.72
1:1:582:VAL:HG21	1:1:1128:VAL:HG21	1.70	0.72
1:1:704:TRP:HB2	1:1:983:SER:HA	1.68	0.72
1:1:640:LEU:HD12	1:1:693:ILE:HD13	1.71	0.72
3:H:102:ASP:OD1	3:H:103:TYR:N	2.21	0.72
1:1:525:ARG:NH2	1:1:748:ASP:OD1	2.22	0.72
1:1:617:GLN:O	1:1:728:TYR:OH	2.06	0.72
1:1:517:ALA:HA	1:1:1101:GLN:HE22	1.55	0.71
1:1:733:LEU:HD13	1:1:1117:LEU:HD22	1.73	0.71
1:1:1216:VAL:HG21	1:1:1252:ASP:HB3	1.72	0.71
1:1:1427:ASP:O	3:H:49:ASN:ND2	2.23	0.70
1:1:801:LEU:HD23	1:1:992:ARG:HB3	1.72	0.70
3:H:149:GLU:HG2	3:H:176:TYR:HE2	1.56	0.70
1:1:629:PHE:O	1:1:1043:GLY:N	2.21	0.69
1:1:787:LEU:HD21	1:1:790:PHE:HB3	1.73	0.69
1:1:132:ASP:HB2	1:1:1502:LEU:HD13	1.73	0.69
1:1:617:GLN:NE2	1:1:624:GLU:O	2.25	0.69
2:L:189:GLU:OE2	2:L:213:ARG:NH2	2.26	0.69
1:1:1206:HIS:HB3	1:1:1209:ALA:HB2	1.74	0.69
1:1:460:ASN:H	1:1:466:GLN:HE21	1.41	0.68
2:L:21:ARG:HG3	2:L:21:ARG:HH11	1.57	0.68
2:L:81:GLU:OE2	2:L:81:GLU:N	2.26	0.68
1:1:81:LEU:O	1:1:86:PRO:HA	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:998:ARG:HD2	1:1:1001:LEU:HD12	1.74	0.68
1:1:561:PRO:HG2	1:1:594:MET:HB2	1.76	0.68
2:L:37:TRP:HB2	2:L:50:ILE:HB	1.73	0.68
1:1:1038:ASN:HA	1:1:1080:ILE:HG12	1.75	0.68
1:1:73:ASN:ND2	1:1:491:ILE:O	2.27	0.68
1:1:415:HIS:HB2	1:1:419:ASP:HB2	1.77	0.67
1:1:602:ARG:H	1:1:638:PRO:HB3	1.59	0.67
1:1:426:LEU:HD22	1:1:608:LEU:HD21	1.76	0.67
1:1:975:THR:HA	1:1:987:LYS:HE3	1.77	0.67
1:1:146:LEU:HD21	1:1:386:THR:HG21	1.76	0.67
2:L:49:LEU:HA	2:L:60:VAL:HG21	1.76	0.67
1:1:701:MET:N	1:1:983:SER:O	2.25	0.67
2:L:56:ARG:NH1	2:L:64:PHE:O	2.28	0.67
1:1:1434:MET:O	1:1:1460:VAL:N	2.24	0.66
1:1:584:ARG:NH2	2:L:71:THR:OG1	2.26	0.66
1:1:730:PRO:HB2	1:1:1100:PRO:HB2	1.76	0.66
1:1:1356:ASN:ND2	1:1:1369:LEU:O	2.28	0.66
1:1:1164:GLY:O	1:1:1175:SER:HA	1.95	0.66
1:1:180:VAL:HG21	1:1:391:VAL:HG11	1.78	0.66
1:1:674:VAL:HG22	1:1:678:ILE:HD12	1.77	0.66
1:1:604:LEU:HD11	1:1:660:HIS:HA	1.78	0.65
1:1:1172[A]:ARG:NH2	1:1:1373:ASN:OD1	2.30	0.65
1:1:235:ALA:HB1	1:1:239:LEU:HB3	1.78	0.65
1:1:1284:GLN:O	1:1:1286:GLN:NE2	2.30	0.65
1:1:1106:LEU:HD11	1:1:1113:VAL:HB	1.79	0.65
1:1:467:GLY:HA3	1:1:762:GLU:HG2	1.78	0.65
3:H:47:PRO:HA	3:H:66:VAL:HG21	1.79	0.65
1:1:394:LEU:HD11	1:1:503:VAL:HG21	1.79	0.64
1:1:573:ARG:NH2	1:1:727:ALA:O	2.24	0.64
1:1:585:GLU:HB3	1:1:737:ILE:HG23	1.80	0.64
1:1:662:ASN:ND2	1:1:932:GLY:O	2.31	0.64
1:1:509:HIS:NE2	1:1:1102:ASP:OD1	2.30	0.64
1:1:1009:ASN:ND2	1:1:1079:LYS:O	2.20	0.64
3:H:152:THR:HB	3:H:199:ALA:HB3	1.80	0.64
1:1:1369:LEU:HD12	1:1:1373:ASN:HB3	1.79	0.63
1:1:1447:ILE:HG21	1:1:1453:PRO:HG3	1.80	0.63
1:1:418:TRP:HB2	1:1:641:PRO:HB3	1.79	0.63
1:1:1332:SER:O	1:1:1336:VAL:HG23	1.98	0.63
1:1:611:ASN:HD22	1:1:630:THR:HB	1.64	0.63
1:1:310:LEU:HD13	1:1:418:TRP:HD1	1.64	0.63
1:1:725:GLU:OE1	1:1:726:ASN:N	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:197:ARG:NH1	4:1:1644:HOH:O	2.31	0.62
1:1:594:MET:N	1:1:731:ASN:OD1	2.28	0.62
3:H:94:ASN:HB2	3:H:99:LEU:HB2	1.81	0.62
1:1:629:PHE:CG	1:1:974:PRO:HG3	2.35	0.62
1:1:796:LEU:HD13	1:1:800:VAL:HG12	1.81	0.62
1:1:244:ALA:HB3	1:1:605:TYR:HB2	1.81	0.62
1:1:394:LEU:HA	1:1:537:VAL:HG11	1.81	0.62
1:1:519:LEU:O	4:1:1601:HOH:O	2.16	0.62
1:1:536:THR:OG1	1:1:748:ASP:OD2	2.15	0.62
2:L:119:ILE:HG21	2:L:211:PHE:HB3	1.80	0.62
1:1:901:ASP:OD1	1:1:914:LYS:N	2.30	0.61
1:1:1354:ALA:O	1:1:1368:ARG:NH2	2.23	0.61
1:1:1179:LEU:HD11	1:1:1288:LEU:HB2	1.82	0.61
1:1:1126:ASP:HB2	1:1:1131:ARG:H	1.63	0.61
1:1:515:HIS:CE1	1:1:1209:ALA:HB3	2.33	0.61
1:1:602:ARG:NH2	4:1:1656:HOH:O	2.34	0.61
1:1:285:LYS:O	1:1:657:TYR:OH	2.12	0.61
1:1:436:ARG:HA	1:1:449:ALA:HB1	1.82	0.61
1:1:372:SER:HA	1:1:393:HIS:HA	1.83	0.60
1:1:811:ILE:HB	1:1:1120:TRP:HE1	1.66	0.60
1:1:1381:VAL:HG22	1:1:1393:LEU:HB3	1.82	0.60
1:1:625:ASP:OD1	1:1:728:TYR:N	2.34	0.60
1:1:731:ASN:ND2	4:1:1662:HOH:O	2.34	0.60
2:L:22:PHE:HB2	2:L:71:THR:HB	1.82	0.60
1:1:1039:LEU:HD13	1:1:1049:LEU:HD12	1.82	0.60
1:1:504:PHE:HD2	1:1:588:LEU:HD13	1.66	0.60
1:1:1005:PRO:HB2	1:1:1091:LEU:HD22	1.83	0.60
1:1:1078:PHE:HE1	1:1:1080:ILE:HD13	1.66	0.60
3:H:172:GLN:HE22	3:H:177:THR:HB	1.66	0.60
1:1:404:PRO:HD3	1:1:541:PRO:HG3	1.83	0.60
1:1:582:VAL:HB	1:1:1128:VAL:HG11	1.83	0.60
1:1:423:ARG:HB2	1:1:430:THR:HG22	1.84	0.60
1:1:809:PRO:HD2	1:1:1120:TRP:HH2	1.67	0.60
3:H:17:LYS:NZ	3:H:70:SER:O	2.32	0.60
1:1:413:ASN:ND2	1:1:419:ASP:OD2	2.26	0.60
1:1:956:ALA:O	1:1:957:ILE:HG13	2.02	0.60
1:1:1338:GLN:HG2	1:1:1364:VAL:HG23	1.84	0.60
1:1:851:LEU:HB2	1:1:1025[A]:TRP:HE3	1.66	0.60
3:H:160:LEU:HD21	3:H:182:VAL:HG21	1.84	0.59
1:1:275:ARG:NH1	1:1:667:ASP:OD2	2.35	0.59
1:1:493:ASN:ND2	1:1:505:GLY:O	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1113:VAL:HG23	1:1:1124:PHE:HB2	1.84	0.59
1:1:987:LYS:HG2	1:1:1047:GLY:HA2	1.84	0.59
2:L:194:TYR:HB2	2:L:211:PHE:CE1	2.36	0.59
1:1:200:VAL:HB	1:1:374:LEU:HG	1.85	0.59
1:1:426:LEU:HA	1:1:608:LEU:HD11	1.83	0.59
1:1:523:VAL:HG23	1:1:542:TYR:CE1	2.38	0.59
1:1:420:TRP:NE1	1:1:451:ASN:O	2.33	0.59
1:1:482:LEU:HG	1:1:487:TYR:HA	1.85	0.59
1:1:547:SER:HB3	1:1:568:PHE:HE1	1.67	0.59
1:1:566:ARG:HD2	1:1:755:GLU:HB2	1.83	0.59
1:1:603:LEU:HD11	1:1:614:LEU:HB3	1.84	0.59
1:1:184:VAL:HG12	1:1:186:VAL:HG13	1.85	0.59
1:1:862:LYS:HD2	1:1:891:GLN:HG2	1.84	0.59
1:1:1009:ASN:HB3	1:1:1089:ALA:HB2	1.84	0.59
1:1:563:ASN:HB3	1:1:720:ALA:HB2	1.85	0.58
1:1:1098:TRP:HE1	1:1:1153:ILE:HG23	1.67	0.58
2:L:91:PHE:HE1	2:L:98:TRP:HB3	1.67	0.58
2:L:110:ARG:NH1	2:L:173:SER:O	2.36	0.58
1:1:328:LYS:O	1:1:436:ARG:NH1	2.35	0.58
2:L:97:PRO:HB3	3:H:55:ASN:HB2	1.83	0.58
1:1:423:ARG:HD3	1:1:430:THR:HA	1.84	0.58
1:1:1000:LEU:HD12	1:1:1117:LEU:HD23	1.86	0.58
1:1:1025[B]:TRP:HE1	1:1:1061:THR:HG21	1.68	0.58
3:H:116:LYS:HE2	3:H:116:LYS:H	1.67	0.58
1:1:796:LEU:HD11	1:1:1135:LEU:HD22	1.86	0.58
1:1:1357:THR:HB	1:1:1359:THR:HG22	1.85	0.58
1:1:1415:ILE:HD13	1:1:1420:LEU:HD22	1.85	0.58
2:L:40:GLN:OE1	3:H:33:GLN:NE2	2.27	0.58
1:1:242:LYS:HB3	1:1:325:VAL:HG11	1.85	0.58
1:1:410:PRO:HG2	1:1:442:PHE:CE2	2.39	0.58
1:1:1007:LEU:O	1:1:1078:PHE:HB2	2.04	0.58
1:1:142:ASP:O	1:1:146:LEU:N	2.37	0.58
1:1:319:GLU:HA	1:1:324:SER:HA	1.85	0.58
1:1:540:TRP:HB3	1:1:544:LEU:HD23	1.86	0.58
1:1:602:ARG:NH1	4:1:1650:HOH:O	2.37	0.58
1:1:973:THR:O	1:1:986:ASN:ND2	2.37	0.58
1:1:1432:VAL:O	2:L:28:HIS:NE2	2.37	0.58
1:1:584:ARG:HH22	2:L:71:THR:HG1	1.50	0.57
1:1:219:LEU:HD13	1:1:237:PHE:HB3	1.84	0.57
2:L:146:ILE:HD11	2:L:198:ALA:HB1	1.86	0.57
1:1:894:THR:O	1:1:971:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:247:ASP:N	1:1:314:PRO:O	2.31	0.57
1:1:1124:PHE:HA	1:1:1137:LEU:HD12	1.86	0.57
1:1:623:ARG:NH1	4:1:1683:HOH:O	2.37	0.57
1:1:956:ALA:HB2	1:1:962:ALA:HB2	1.87	0.57
1:1:957:ILE:HD12	1:1:958:ASP:HB2	1.86	0.57
1:1:394:LEU:HD22	1:1:524:PHE:HB3	1.86	0.57
1:1:1025[A]:TRP:HE1	1:1:1061:THR:HG21	1.70	0.57
1:1:661:ASN:ND2	1:1:700:GLY:O	2.30	0.57
1:1:311:ALA:O	1:1:421:LYS:NZ	2.35	0.57
1:1:419:ASP:OD1	1:1:602:ARG:NH2	2.37	0.57
1:1:896:ALA:O	1:1:975:THR:OG1	2.20	0.57
1:1:427:LEU:O	1:1:619:GLN:HB3	2.05	0.56
1:1:308:ASN:HD21	1:1:762:GLU:HG3	1.70	0.56
1:1:544:LEU:HD21	1:1:750:VAL:HG11	1.87	0.56
1:1:1183:TRP:NE1	1:1:1285:PRO:O	2.30	0.56
2:L:38:TYR:OH	3:H:100:LEU:O	2.23	0.56
1:1:1415:ILE:HB	1:1:1420:LEU:HD13	1.87	0.56
1:1:1120:TRP:CE3	1:1:1139:LEU:HB3	2.41	0.56
1:1:714:THR:HG1	1:1:719:SER:HG	1.50	0.56
1:1:305:LEU:HD23	1:1:308:ASN:HB2	1.88	0.56
1:1:1162:PHE:HE1	1:1:1175:SER:HB3	1.70	0.56
1:1:1470:LEU:HG	1:1:1472:LEU:HD21	1.87	0.56
2:L:108:ILE:N	2:L:168:GLN:OE1	2.38	0.56
1:1:198:PHE:CE2	1:1:378:ASP:HB3	2.41	0.56
1:1:859:VAL:HB	1:1:895:GLY:HA2	1.88	0.56
1:1:977:ASP:HA	1:1:985:THR:HG23	1.87	0.56
1:1:1033:ASP:OD1	1:1:1035:THR:OG1	2.23	0.56
1:1:653:HIS:ND1	1:1:935:ASP:OD1	2.33	0.56
3:H:33:GLN:HB2	3:H:39:LEU:HD23	1.87	0.56
3:H:54:TYR:HE2	3:H:64:LEU:HD13	1.71	0.56
1:1:124:THR:O	1:1:205:ARG:NH1	2.39	0.55
1:1:269:SER:OG	1:1:270:GLY:N	2.38	0.55
1:1:405:PRO:HB3	1:1:408:ARG:HH22	1.71	0.55
3:H:27:THR:O	3:H:93:SER:OG	2.24	0.55
1:1:1126:ASP:HB3	1:1:1131:ARG:HE	1.70	0.55
1:1:410:PRO:HG2	1:1:442:PHE:HE2	1.72	0.55
1:1:517:ALA:HA	1:1:1101:GLN:NE2	2.21	0.55
1:1:856:ASN:ND2	1:1:975:THR:O	2.35	0.55
1:1:869:LEU:HD22	1:1:965:TYR:CG	2.41	0.55
1:1:897:GLY:HA3	1:1:973:THR:HG21	1.89	0.55
1:1:1096:LEU:O	1:1:1208:ASN:ND2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:781:SER:O	1:1:784:SER:OG	2.25	0.55
1:1:800:VAL:HG13	1:1:1331:VAL:HG11	1.89	0.55
1:1:1212:PHE:HB2	1:1:1262:LEU:HD21	1.88	0.55
2:L:138:LEU:HB2	2:L:177:MET:HB3	1.89	0.55
1:1:703:ALA:HA	1:1:988:ASN:HB3	1.88	0.55
2:L:90:CYS:O	2:L:101:GLY:N	2.38	0.55
1:1:557:LEU:HD11	1:1:801:LEU:HD22	1.89	0.54
2:L:194:TYR:HB2	2:L:211:PHE:HE1	1.72	0.54
1:1:237:PHE:CE2	1:1:1262:LEU:HD13	2.42	0.54
1:1:853:THR:HG22	1:1:1048:LEU:HB2	1.90	0.54
1:1:1002:GLY:HA3	1:1:1096:LEU:HD12	1.90	0.54
1:1:1464:ASP:O	1:1:1468:GLN:N	2.40	0.54
3:H:149:GLU:HG2	3:H:176:TYR:CE2	2.42	0.54
1:1:580:LYS:NZ	4:1:1701:HOH:O	2.40	0.54
3:H:64:LEU:HD12	3:H:75:MET:HG3	1.88	0.54
1:1:73:ASN:HB2	1:1:510:VAL:HB	1.88	0.54
1:1:89:TRP:CZ3	1:1:128:LEU:HB3	2.42	0.54
1:1:359:THR:HG23	1:1:396:PRO:HB2	1.89	0.54
1:1:418:TRP:CH2	1:1:639:ASP:HA	2.42	0.54
1:1:429:THR:HG21	1:1:437:ARG:HG3	1.89	0.54
1:1:519:LEU:HD21	1:1:1101:GLN:HG2	1.89	0.54
1:1:519:LEU:HD11	1:1:730:PRO:HD3	1.90	0.54
1:1:589:ALA:HA	1:1:735:ALA:HA	1.88	0.54
1:1:219:LEU:HD21	1:1:1203:LEU:HD22	1.89	0.54
1:1:221:GLN:NE2	1:1:330:ASP:O	2.41	0.54
1:1:255:LEU:HD21	1:1:309:ASP:HB3	1.89	0.54
1:1:899:ARG:CZ	1:1:972:LEU:HG	2.37	0.54
1:1:1178:ASP:OD2	1:1:1180:LYS:NZ	2.39	0.54
1:1:133:LEU:HD21	1:1:1499:LEU:HB3	1.90	0.54
1:1:1044:GLU:HA	1:1:1091:LEU:HD21	1.89	0.54
1:1:152:THR:N	1:1:168:GLY:O	2.32	0.53
1:1:184:VAL:O	1:1:202:LEU:HA	2.08	0.53
1:1:819:ASN:HB3	1:1:850[A]:PHE:HD2	1.73	0.53
1:1:1009:ASN:HA	1:1:1258:LEU:HD21	1.89	0.53
1:1:945:SER:O	1:1:948:SER:OG	2.26	0.53
2:L:89:TYR:OH	3:H:33:GLN:NE2	2.41	0.53
3:H:16:CYS:HB3	3:H:73:ALA:HB3	1.91	0.53
1:1:74:THR:HG21	1:1:493:ASN:H	1.74	0.53
1:1:829:ALA:O	1:1:831:GLN:NE2	2.38	0.53
1:1:1288:LEU:HD11	1:1:1374:ALA:HB1	1.91	0.53
1:1:1454[A]:LYS:O	3:H:56:GLN:NE2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:810:TRP:HD1	1:1:817:TYR:HH	1.56	0.53
1:1:423:ARG:NH2	1:1:724:ASN:O	2.40	0.53
1:1:488:PHE:HA	1:1:491:ILE:HB	1.91	0.53
1:1:1405:GLN:N	1:1:1405:GLN:OE1	2.42	0.53
1:1:641:PRO:HD2	1:1:693:ILE:HD11	1.90	0.52
1:1:87:GLY:HA3	1:1:131:TYR:O	2.09	0.52
1:1:237:PHE:HE2	1:1:1262:LEU:HD13	1.74	0.52
1:1:557:LEU:HB2	1:1:560:LEU:HD11	1.90	0.52
1:1:1411:SER:OG	1:1:1413:ASP:OD1	2.26	0.52
3:H:34:SER:HB2	3:H:37:LYS:HD3	1.90	0.52
1:1:174:PRO:HG2	1:1:177:TRP:HB2	1.90	0.52
1:1:286:ALA:HB2	1:1:695:PRO:HD3	1.90	0.52
1:1:510:VAL:HG13	1:1:511:THR:HG23	1.92	0.52
1:1:562:PHE:HB2	1:1:713:LEU:HG	1.91	0.52
1:1:597:THR:HG22	1:1:710:SER:HB2	1.92	0.52
1:1:459:ASP:OD1	1:1:459:ASP:N	2.43	0.52
1:1:494:LEU:HG	1:1:501:LEU:HD21	1.92	0.52
1:1:721:ASP:HA	1:1:770:LEU:HD13	1.90	0.52
1:1:1005:PRO:HD2	1:1:1045:VAL:HG21	1.92	0.52
1:1:1042:TYR:HE1	1:1:1215:SER:HB3	1.75	0.52
1:1:239:LEU:HD22	1:1:1213:GLN:HG3	1.90	0.52
1:1:259:GLU:HG2	1:1:285:LYS:HG2	1.90	0.52
1:1:495:THR:HG21	1:1:586:LEU:HD11	1.92	0.52
1:1:998:ARG:NH2	1:1:1003:SER:O	2.43	0.52
1:1:1461:LEU:HD11	1:1:1473:ARG:HB2	1.91	0.52
1:1:808:VAL:HG22	1:1:1366:VAL:HG11	1.90	0.52
1:1:1018:PHE:CZ	1:1:1023:GLN:HB2	2.44	0.52
1:1:1203:LEU:HD12	1:1:1204:PRO:HD2	1.90	0.52
1:1:1421:PHE:HB3	1:1:1468:GLN:HG2	1.90	0.52
1:1:1042:TYR:CE1	1:1:1215:SER:HB3	2.44	0.52
3:H:41:TRP:HZ2	3:H:44:LEU:HD23	1.74	0.52
3:H:136:MET:SD	3:H:183:THR:HB	2.49	0.52
1:1:175:GLN:O	1:1:176:GLN:HG2	2.10	0.52
1:1:184:VAL:HG11	1:1:208:VAL:HG21	1.92	0.52
1:1:581:PHE:HE1	1:1:740:PRO:HG3	1.75	0.52
1:1:698:TYR:HB3	1:1:704:TRP:HH2	1.75	0.52
1:1:809:PRO:HD2	1:1:1120:TRP:CH2	2.43	0.52
1:1:519:LEU:HB2	1:1:573:ARG:HB3	1.92	0.51
1:1:254:LYS:HG2	1:1:646:SER:HB3	1.92	0.51
1:1:407:TRP:CH2	1:1:571:VAL:HG13	2.44	0.51
1:1:1000:LEU:HD21	1:1:1139:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:232:THR:HG22	1:1:1250:GLN:HE22	1.75	0.51
1:1:410:PRO:HB2	1:1:433:PHE:O	2.10	0.51
1:1:1001:LEU:HD21	1:1:1117:LEU:HD11	1.93	0.51
1:1:1012:GLY:N	1:1:1016:ASN:O	2.41	0.51
3:H:153:VAL:HG22	3:H:198:VAL:HG22	1.93	0.51
1:1:1097:ALA:HB1	1:1:1207:PRO:HG2	1.92	0.51
2:L:149:LYS:O	2:L:197:GLU:N	2.39	0.51
1:1:255:LEU:HD12	1:1:644:ALA:HB2	1.92	0.51
1:1:404:PRO:HD2	1:1:407:TRP:CD2	2.46	0.51
1:1:437:ARG:HG2	1:1:620:GLY:HA2	1.92	0.51
1:1:636:ASN:ND2	4:1:1693:HOH:O	2.43	0.51
1:1:1432:VAL:HG11	3:H:100:LEU:HD11	1.93	0.51
1:1:167:PHE:HZ	1:1:196:TYR:HB3	1.75	0.51
1:1:851:LEU:HB2	1:1:1025[A]:TRP:CE3	2.44	0.51
1:1:1440:TYR:HD1	1:1:1443:LEU:HD21	1.76	0.51
2:L:93:GLY:O	2:L:98:TRP:NE1	2.43	0.51
1:1:315:ILE:HD11	1:1:646:SER:HB2	1.92	0.51
1:1:941:ASN:HB3	1:1:956:ALA:HA	1.93	0.51
1:1:1125:THR:OG1	1:1:1126:ASP:OD1	2.28	0.51
1:1:1261:LEU:HD22	1:1:1267:VAL:HG22	1.91	0.51
1:1:1479:PRO:HB2	1:1:1482:ASP:HA	1.92	0.51
1:1:89:TRP:HB3	1:1:188:VAL:HG21	1.93	0.51
1:1:856:ASN:OD1	1:1:987:LYS:NZ	2.44	0.51
1:1:1429:PHE:CG	1:1:1460:VAL:HG21	2.45	0.51
3:H:32:LYS:HD2	3:H:58:PHE:CZ	2.46	0.51
2:L:37:TRP:CH2	2:L:90:CYS:HB3	2.46	0.51
1:1:217:LEU:HB3	1:1:515:HIS:HB2	1.92	0.50
1:1:912:HIS:HA	1:1:970:PRO:HD3	1.93	0.50
1:1:1063:ALA:HB3	1:1:1073:SER:HB3	1.93	0.50
1:1:1135:LEU:N	1:1:1300:GLY:O	2.41	0.50
1:1:627:GLN:OE1	1:1:1046:ASN:ND2	2.44	0.50
1:1:729:GLN:NE2	4:1:1643:HOH:O	2.31	0.50
1:1:201:LEU:HD11	1:1:491:ILE:HG23	1.93	0.50
1:1:429:THR:OG1	1:1:437:ARG:NE	2.37	0.50
1:1:593:THR:HB	1:1:727:ALA:HB3	1.94	0.50
1:1:327:LEU:HD11	1:1:619:GLN:HB2	1.93	0.50
1:1:561:PRO:HD3	1:1:990:ALA:HB2	1.93	0.50
1:1:584:ARG:NH1	2:L:22:PHE:O	2.45	0.50
3:H:46:ASN:O	3:H:50:GLY:N	2.44	0.50
1:1:405:PRO:HB3	1:1:408:ARG:NH2	2.26	0.50
3:H:32:LYS:O	3:H:40:GLU:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:143:PHE:HE2	1:1:185:PRO:HB3	1.77	0.50
1:1:406:SER:HB2	1:1:758:PHE:CZ	2.47	0.50
1:1:108:GLN:NE2	1:1:214:GLN:O	2.45	0.50
1:1:370:SER:OG	1:1:393:HIS:HB3	2.11	0.50
1:1:620:GLY:HA2	1:1:728:TYR:HE2	1.76	0.50
1:1:610:SER:HB3	1:1:1245:PRO:HG2	1.94	0.50
1:1:627:GLN:CD	1:1:991:GLN:HB2	2.32	0.50
1:1:199:ALA:HB1	1:1:501:LEU:HD22	1.94	0.50
3:H:61:THR:O	3:H:78:LEU:N	2.44	0.50
1:1:407:TRP:CG	1:1:480:ILE:HD12	2.47	0.49
2:L:117:VAL:HG22	2:L:138:LEU:HG	1.93	0.49
1:1:1160:ALA:O	1:1:1163:ARG:NH1	2.43	0.49
1:1:1362:ASP:OD1	1:1:1362:ASP:N	2.41	0.49
1:1:275:ARG:HA	1:1:656:PRO:HG3	1.94	0.49
1:1:759:ALA:HB1	1:1:764[A]:GLU:HB3	1.94	0.49
1:1:632:TYR:CD2	1:1:1245:PRO:HD2	2.47	0.49
1:1:1123:THR:O	1:1:1137:LEU:HA	2.13	0.49
1:1:402:ASN:ND2	1:1:538:THR:OG1	2.44	0.49
1:1:413:ASN:HA	1:1:758:PHE:CZ	2.48	0.49
1:1:1012:GLY:O	1:1:1017:LYS:NZ	2.41	0.49
1:1:1302:LEU:HD22	1:1:1331:VAL:HG22	1.93	0.49
1:1:66:LEU:HD21	1:1:125:THR:HB	1.95	0.49
1:1:132:ASP:HB3	1:1:138:LEU:HD11	1.95	0.49
1:1:415:HIS:HB3	1:1:418:TRP:CE2	2.47	0.49
1:1:611:ASN:HB3	1:1:630:THR:HB	1.95	0.49
1:1:673:VAL:HG22	1:1:942:ILE:HD12	1.94	0.49
1:1:677:PHE:CZ	1:1:942:ILE:HD11	2.48	0.49
1:1:1161:ALA:O	1:1:1178:ASP:N	2.24	0.49
1:1:1249:THR:H	1:1:1252:ASP:HB2	1.77	0.49
3:H:80:LEU:HB3	3:H:112:VAL:HG11	1.94	0.49
1:1:411:LYS:HD3	1:1:450:ASP:O	2.13	0.49
1:1:669:PRO:HD2	1:1:965:TYR:OH	2.12	0.49
1:1:675:ASP:HA	1:1:679:LYS:HB2	1.94	0.49
1:1:1334:TRP:CH2	1:1:1364:VAL:HA	2.48	0.49
3:H:194:VAL:H	3:H:210:LYS:HZ2	1.60	0.49
1:1:557:LEU:HD21	1:1:801:LEU:HD22	1.94	0.49
1:1:408:ARG:HA	1:1:479:PRO:HB3	1.94	0.49
2:L:91:PHE:CE1	2:L:98:TRP:HB3	2.46	0.49
3:H:45:ILE:HD12	3:H:52:THR:HG22	1.95	0.49
1:1:204:PRO:HD2	1:1:488:PHE:CZ	2.47	0.48
1:1:584:ARG:HH11	1:1:584:ARG:HG2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:691:LYS:H	1:1:766:PHE:HZ	1.60	0.48
1:1:210:TYR:CD2	1:1:213:LEU:HD12	2.48	0.48
1:1:305:LEU:HD11	1:1:763:TYR:HB2	1.96	0.48
1:1:434:ASN:N	1:1:725:GLU:OE2	2.32	0.48
1:1:441:TRP:CH2	1:1:573:ARG:HD2	2.49	0.48
1:1:523:VAL:HG23	1:1:542:TYR:HE1	1.79	0.48
1:1:978:TRP:O	1:1:985:THR:OG1	2.32	0.48
1:1:1024:LYS:HB2	1:1:1036:LYS:HB3	1.95	0.48
1:1:1338:GLN:HG3	1:1:1360:GLY:HA2	1.95	0.48
1:1:612:LEU:HB3	1:1:1213:GLN:CB	2.43	0.48
1:1:667:ASP:HB3	1:1:673:VAL:HG11	1.95	0.48
1:1:1025[B]:TRP:NE1	1:1:1061:THR:HG21	2.28	0.48
1:1:1477:PHE:CG	3:H:56:GLN:HG2	2.49	0.48
2:L:135:VAL:HG12	2:L:180:THR:HG23	1.95	0.48
3:H:18:ALA:HB3	3:H:71:SER:HG	1.79	0.48
1:1:220:PRO:HB3	1:1:331:ASP:HB3	1.96	0.48
1:1:407:TRP:HB3	1:1:480:ILE:HB	1.94	0.48
1:1:487:TYR:O	1:1:491:ILE:HG12	2.14	0.48
1:1:821:HIS:CD2	1:1:852:PRO:HD3	2.48	0.48
1:1:133:LEU:CD2	1:1:1499:LEU:HB3	2.43	0.48
1:1:897:GLY:HA2	1:1:1239:TYR:CD2	2.48	0.48
1:1:1008:VAL:HG23	1:1:1258:LEU:HD11	1.95	0.48
1:1:1010:ARG:HB2	1:1:1018:PHE:HB2	1.95	0.48
1:1:446:GLN:HA	1:1:449:ALA:HB2	1.95	0.48
1:1:359:THR:OG1	1:1:481:ALA:HB1	2.14	0.48
1:1:490:ASN:O	1:1:490:ASN:ND2	2.44	0.48
1:1:528:TYR:CD2	1:1:535:ALA:HB2	2.49	0.48
1:1:629:PHE:CE2	1:1:631:PRO:HG3	2.49	0.48
1:1:828:THR:HA	1:1:1027:TYR:H	1.79	0.48
1:1:1432:VAL:HG11	3:H:100:LEU:HD21	1.95	0.48
1:1:560:LEU:O	1:1:713:LEU:N	2.46	0.48
2:L:93:GLY:HA3	3:H:100:LEU:CD1	2.44	0.48
1:1:87:GLY:HA2	1:1:133:LEU:HA	1.95	0.47
3:H:144:LYS:HD2	3:H:177:THR:HG21	1.95	0.47
1:1:277:GLY:HA2	1:1:281:ASP:HB3	1.96	0.47
1:1:432:PHE:O	1:1:726:ASN:ND2	2.47	0.47
1:1:433:PHE:HE2	1:1:441:TRP:HB2	1.79	0.47
3:H:126:ALA:O	3:H:214:ARG:NH2	2.48	0.47
1:1:86:PRO:HG3	1:1:1500:PRO:HG3	1.95	0.47
1:1:419:ASP:OD2	1:1:423:ARG:HD2	2.14	0.47
1:1:243:ASN:HB3	1:1:606:ASP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:428:GLN:NE2	4:1:1650:HOH:O	2.40	0.47
1:1:631:PRO:HA	1:1:634:TRP:CD2	2.49	0.47
1:1:678:ILE:O	1:1:682:GLU:N	2.48	0.47
1:1:901:ASP:OD2	1:1:1235:ASN:HB2	2.14	0.47
1:1:494:LEU:HB3	1:1:501:LEU:HD11	1.95	0.47
1:1:549:MET:HG2	1:1:787:LEU:HD22	1.95	0.47
1:1:1419:ARG:HH22	1:1:1440:TYR:HE1	1.63	0.47
2:L:119:ILE:HD11	2:L:209:LYS:HB3	1.97	0.47
3:H:125:LEU:HD11	3:H:142:LEU:HB2	1.97	0.47
1:1:402:ASN:HB2	1:1:539:GLY:O	2.14	0.47
1:1:117:GLU:HB2	1:1:369:TRP:CH2	2.49	0.47
1:1:399:MET:HA	1:1:539:GLY:O	2.15	0.47
1:1:403:TYR:OH	1:1:521:ILE:HG21	2.14	0.47
1:1:566:ARG:HH22	1:1:768:GLN:HB2	1.79	0.47
1:1:599:THR:HA	1:1:614:LEU:HD11	1.97	0.47
1:1:896:ALA:HB3	1:1:1049:LEU:HD13	1.96	0.47
1:1:1408:LYS:NZ	1:1:1503:THR:O	2.43	0.47
1:1:1452:ASN:HD22	1:1:1453:PRO:HD2	1.79	0.47
1:1:159:ILE:HG13	1:1:377:TYR:CZ	2.50	0.47
1:1:490:ASN:ND2	1:1:522:GLY:O	2.38	0.47
1:1:587:VAL:HG11	1:1:1113:VAL:HG21	1.96	0.47
1:1:1149:GLN:HG2	1:1:1288:LEU:HD21	1.96	0.47
1:1:63:ASN:O	1:1:129:ARG:NH2	2.47	0.47
1:1:84:GLU:HG3	1:1:1473:ARG:HH22	1.79	0.47
1:1:310:LEU:HD13	1:1:418:TRP:CD1	2.48	0.47
1:1:642:ILE:HG13	4:1:1698:HOH:O	2.15	0.47
2:L:212:ASN:OD1	2:L:213:ARG:N	2.48	0.47
1:1:1407:VAL:HG13	1:1:1445:ILE:HD12	1.96	0.47
2:L:117:VAL:HB	2:L:209:LYS:HG3	1.96	0.47
1:1:74:THR:HG21	1:1:493:ASN:N	2.31	0.46
1:1:113:PRO:HA	1:1:356:TRP:CH2	2.50	0.46
1:1:405:PRO:HD3	1:1:752:TYR:CG	2.50	0.46
1:1:563:ASN:ND2	1:1:719:SER:OG	2.37	0.46
1:1:566:ARG:HH11	1:1:755:GLU:HA	1.80	0.46
1:1:742:LEU:O	1:1:746:LEU:N	2.48	0.46
1:1:1098:TRP:CZ2	1:1:1153:ILE:HA	2.50	0.46
1:1:71:TYR:CG	1:1:186:VAL:HB	2.50	0.46
1:1:631:PRO:HA	1:1:634:TRP:CE2	2.50	0.46
3:H:-4:VAL:HG11	3:H:92:ARG:HD3	1.97	0.46
1:1:167:PHE:CE2	1:1:377:TYR:HB3	2.51	0.46
1:1:240[B]:LYS:O	1:1:619:GLN:NE2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:420:TRP:CD1	1:1:454:THR:HG21	2.50	0.46
1:1:1454[B]:LYS:HE2	3:H:60:GLY:HA3	1.97	0.46
2:L:39:LEU:HB2	2:L:49:LEU:HD11	1.98	0.46
2:L:151:LYS:HB2	2:L:195:THR:HG22	1.96	0.46
1:1:78:SER:HA	1:1:90:ALA:HA	1.98	0.46
1:1:504:PHE:HA	1:1:523:VAL:HG22	1.96	0.46
1:1:544:LEU:HG	1:1:783:PHE:CG	2.50	0.46
1:1:546:PHE:HB3	1:1:549:MET:SD	2.55	0.46
1:1:503:VAL:HB	1:1:524:PHE:HB2	1.97	0.46
1:1:622:LEU:HD22	1:1:1212:PHE:HA	1.96	0.46
1:1:1039:LEU:HD12	1:1:1040:PRO:HD2	1.98	0.46
2:L:57:PHE:CZ	3:H:102:ASP:HB2	2.50	0.46
1:1:239:LEU:HD11	1:1:615:VAL:HG12	1.98	0.46
1:1:287:LEU:HB2	1:1:693:ILE:HB	1.96	0.46
1:1:396:PRO:O	1:1:400:THR:HG23	2.15	0.46
1:1:563:ASN:O	1:1:711:ASN:HB2	2.16	0.46
1:1:240[A]:LYS:O	1:1:619:GLN:NE2	2.44	0.46
1:1:743:LEU:HA	1:1:746:LEU:HD12	1.96	0.46
2:L:87:VAL:HA	2:L:105:LYS:HA	1.97	0.46
1:1:131:TYR:CZ	1:1:1385:VAL:HG21	2.51	0.46
1:1:807:TYR:OH	1:1:1360:GLY:HA3	2.16	0.46
1:1:1144:ALA:O	1:1:1150:ARG:HB2	2.15	0.46
1:1:525:ARG:CZ	1:1:540:TRP:HZ2	2.28	0.46
1:1:640:LEU:HB3	1:1:644:ALA:HB3	1.97	0.46
1:1:854:PHE:CD1	1:1:995:LEU:HD13	2.51	0.46
1:1:1176:VAL:HB	1:1:1384:ILE:HD11	1.98	0.46
1:1:1185:ASP:HA	1:1:1188:GLN:HG2	1.98	0.46
1:1:113:PRO:HA	1:1:356:TRP:CZ2	2.51	0.45
1:1:525:ARG:NH1	1:1:746:LEU:O	2.44	0.45
1:1:711:ASN:OD1	1:1:711:ASN:N	2.48	0.45
1:1:810:TRP:CZ3	1:1:1057:TYR:HA	2.51	0.45
1:1:1150:ARG:HD2	1:1:1275:PHE:CD2	2.51	0.45
1:1:1174:GLU:HG2	1:1:1291:THR:HG23	1.97	0.45
1:1:134:ALA:HB2	1:1:1402:THR:HG23	1.98	0.45
1:1:317:ARG:HG2	1:1:425:VAL:HA	1.98	0.45
1:1:400:THR:HA	1:1:403:TYR:CG	2.51	0.45
1:1:862:LYS:HE3	1:1:893:TRP:NE1	2.30	0.45
1:1:1055:GLU:OE2	1:1:1062:ARG:N	2.47	0.45
1:1:1464:ASP:O	1:1:1468:GLN:CA	2.64	0.45
3:H:54:TYR:CE2	3:H:64:LEU:HD13	2.51	0.45
1:1:554:THR:HA	1:1:790:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:573:ARG:HH21	1:1:726:ASN:HB3	1.82	0.45
1:1:620:GLY:HA2	1:1:728:TYR:CE2	2.51	0.45
1:1:629:PHE:HA	1:1:702:TRP:HE1	1.82	0.45
1:1:664:ASP:CG	1:1:899:ARG:HH12	2.20	0.45
1:1:755:GLU:OE1	1:1:775:THR:OG1	2.34	0.45
2:L:26:ILE:HA	2:L:95:HIS:CE1	2.52	0.45
1:1:730:PRO:HD2	1:1:1100:PRO:HG2	1.99	0.45
1:1:1214:VAL:HG22	1:1:1216:VAL:HG22	1.98	0.45
3:H:83:GLU:H	3:H:83:GLU:CD	2.19	0.45
1:1:244:ALA:N	1:1:605:TYR:O	2.50	0.45
1:1:507:ASN:HB2	1:1:1101:GLN:O	2.16	0.45
1:1:573:ARG:NH2	1:1:726:ASN:HB3	2.31	0.45
1:1:595:GLY:HA3	1:1:711:ASN:OD1	2.17	0.45
1:1:854:PHE:HE1	1:1:995:LEU:HD22	1.82	0.45
1:1:998:ARG:HA	1:1:1001:LEU:HD12	1.98	0.45
1:1:1416:ASP:HB2	1:1:1418:ASN:ND2	2.32	0.45
2:L:171:LYS:H	2:L:171:LYS:HG2	1.57	0.45
3:H:144:LYS:HB3	3:H:144:LYS:HE2	1.64	0.45
1:1:455:GLY:N	1:1:477:SER:HB3	2.31	0.45
1:1:1141:GLY:O	1:1:1369:LEU:N	2.40	0.45
2:L:185:LYS:O	2:L:189:GLU:HG2	2.16	0.45
3:H:-4:VAL:HG22	3:H:21:TYR:CD1	2.52	0.45
3:H:169:ALA:HB1	3:H:177:THR:H	1.81	0.45
1:1:71:TYR:CE1	1:1:510:VAL:HG21	2.51	0.45
1:1:207:VAL:O	1:1:510:VAL:HG22	2.16	0.45
1:1:707:TYR:HA	1:1:712:LYS:HD3	1.99	0.45
1:1:1097:ALA:HB3	1:1:1158:PRO:HD3	1.99	0.45
1:1:1211:ALA:O	1:1:1213:GLN:NE2	2.49	0.45
2:L:157:ARG:HH22	2:L:183:LEU:HD11	1.81	0.45
1:1:794:PHE:HB3	1:1:796:LEU:HG	1.99	0.45
1:1:1152:LEU:HD21	1:1:1177:TRP:CD2	2.51	0.45
1:1:202:LEU:O	1:1:371:ALA:CA	2.61	0.45
1:1:235:ALA:HB2	1:1:241:VAL:HG12	1.99	0.45
1:1:504:PHE:CD2	1:1:588:LEU:HD13	2.50	0.45
1:1:647:SER:HB3	1:1:654:ASN:HA	1.99	0.45
1:1:1262:LEU:HD23	1:1:1262:LEU:HA	1.68	0.45
1:1:1454[B]:LYS:O	3:H:56:GLN:NE2	2.38	0.45
1:1:594:MET:HG3	1:1:731:ASN:OD1	2.17	0.44
1:1:799:SER:O	1:1:803:GLN:HG2	2.17	0.44
1:1:817:TYR:O	1:1:853:THR:OG1	2.15	0.44
1:1:978:TRP:H	1:1:985:THR:HG23	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1058:PHE:HB3	1:1:1074:PRO:HD2	1.99	0.44
2:L:112:ASP:OD1	2:L:112:ASP:N	2.50	0.44
1:1:247:ASP:HB3	1:1:250:LYS:HB2	1.98	0.44
1:1:253:GLU:O	1:1:312:ASN:HB3	2.18	0.44
1:1:542:TYR:HB2	1:1:572:PRO:O	2.17	0.44
3:H:29:ASN:OD1	3:H:29:ASN:N	2.50	0.44
1:1:482:LEU:HD12	1:1:482:LEU:HA	1.72	0.44
1:1:1140:THR:HG21	1:1:1292:THR:HA	2.00	0.44
1:1:148:PRO:HB3	1:1:388:ILE:HD12	1.98	0.44
1:1:598:ALA:HA	1:1:627:GLN:HA	2.00	0.44
2:L:52:LYS:HB3	2:L:55:ASN:OD1	2.17	0.44
1:1:134:ALA:O	1:1:1400:ALA:N	2.51	0.44
1:1:629:PHE:CZ	1:1:631:PRO:HG3	2.52	0.44
1:1:862:LYS:HD2	1:1:891:GLN:CG	2.46	0.44
1:1:997:LEU:HD21	1:1:1100:PRO:HB3	1.98	0.44
1:1:1126:ASP:O	1:1:1130:PRO:HA	2.17	0.44
1:1:1165:SER:HA	1:1:1175:SER:HA	1.99	0.44
1:1:1214:VAL:HB	1:1:1254:LEU:HG	2.00	0.44
1:1:1432:VAL:HG21	3:H:100:LEU:HD21	1.99	0.44
1:1:151:PRO:HG3	1:1:377:TYR:CD2	2.52	0.44
1:1:284:VAL:HG12	1:1:695:PRO:HG2	1.99	0.44
1:1:410:PRO:HG3	1:1:480:ILE:HG13	2.00	0.44
1:1:594:MET:SD	1:1:732:SER:HB2	2.57	0.44
1:1:166:GLY:HA3	1:1:384:ASN:HB2	1.99	0.44
1:1:285:LYS:O	1:1:695:PRO:HG3	2.17	0.44
1:1:589:ALA:HB3	1:1:1106:LEU:HD13	1.99	0.44
1:1:656:PRO:HG2	1:1:695:PRO:HA	2.00	0.44
1:1:747:PRO:HG2	1:1:779:ASN:HB2	2.00	0.44
1:1:1418:ASN:O	1:1:1422:THR:N	2.51	0.44
2:L:32:ALA:HB1	2:L:52:LYS:HD2	2.00	0.44
3:H:136:MET:HE2	3:H:136:MET:HA	2.00	0.44
1:1:206:SER:HB3	1:1:356:TRP:CZ3	2.52	0.44
1:1:357:LEU:HD12	1:1:484:PHE:CD2	2.53	0.44
1:1:515:HIS:NE2	1:1:1204:PRO:O	2.50	0.44
1:1:517:ALA:HB2	1:1:623:ARG:HH21	1.82	0.44
1:1:560:LEU:HD13	1:1:562:PHE:HE2	1.82	0.44
1:1:1139:LEU:HB2	1:1:1366:VAL:HG13	1.99	0.44
1:1:69:TRP:CH2	1:1:186:VAL:HG12	2.53	0.44
1:1:796:LEU:HD21	1:1:1135:LEU:HA	1.98	0.44
1:1:974:PRO:HB3	1:1:1046:ASN:HA	2.00	0.44
1:1:1407:VAL:HA	1:1:1446:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1418:ASN:O	1:1:1422:THR:HG23	2.17	0.44
3:H:214:ARG:HH12	3:H:216:CYS:HB3	1.82	0.44
1:1:254:LYS:HA	1:1:314:PRO:HG3	2.00	0.43
1:1:414:HIS:ND1	1:1:569:GLU:OE2	2.51	0.43
1:1:441:TRP:HE1	1:1:521:ILE:HB	1.83	0.43
1:1:604:LEU:HD12	1:1:607:GLU:HG3	2.00	0.43
1:1:811:ILE:HD11	1:1:1142:LEU:H	1.82	0.43
2:L:39:LEU:HD13	2:L:88:TYR:CE1	2.53	0.43
1:1:120:LEU:HD13	1:1:209:TYR:HD2	1.83	0.43
1:1:611:ASN:HA	1:1:1042:TYR:OH	2.18	0.43
1:1:801:LEU:O	1:1:805:LEU:HG	2.18	0.43
1:1:915:PHE:CE1	1:1:919:THR:HG21	2.53	0.43
1:1:1137:LEU:HD23	1:1:1139:LEU:HD21	2.00	0.43
1:1:1254:LEU:HD23	1:1:1254:LEU:HA	1.79	0.43
2:L:40:GLN:NE2	3:H:89:TYR:OH	2.50	0.43
2:L:150:TRP:HB3	2:L:181:LEU:HD11	1.99	0.43
3:H:30:TRP:CD1	3:H:64:LEU:HG	2.53	0.43
1:1:1467:GLU:OE2	1:1:1469:SER:HB3	2.19	0.43
1:1:407:TRP:CD2	1:1:480:ILE:HD12	2.54	0.43
1:1:415:HIS:HB2	1:1:419:ASP:CB	2.45	0.43
1:1:604:LEU:HA	1:1:658:TYR:OH	2.18	0.43
1:1:613:ASN:ND2	1:1:1213:GLN:O	2.47	0.43
1:1:1023:GLN:HG2	1:1:1025[A]:TRP:CZ2	2.53	0.43
1:1:1102:ASP:HB3	1:1:1159:TRP:CE3	2.53	0.43
1:1:275:ARG:NH1	1:1:695:PRO:O	2.38	0.43
1:1:668:ARG:HG3	1:1:963:THR:O	2.19	0.43
1:1:750:VAL:HG22	1:1:783:PHE:CZ	2.54	0.43
1:1:861:LEU:HD12	1:1:900:ASN:CG	2.39	0.43
1:1:1008:VAL:HG11	1:1:1076:ILE:HG22	2.00	0.43
1:1:1285:PRO:HG3	1:1:1376:LYS:HB3	2.01	0.43
2:L:40:GLN:NE2	3:H:33:GLN:OE1	2.37	0.43
3:H:145:GLY:HA2	3:H:175:LEU:HG	2.01	0.43
1:1:86:PRO:HB2	1:1:133:LEU:HB2	1.99	0.43
1:1:125:THR:HA	1:1:205:ARG:HH12	1.84	0.43
1:1:141:LEU:HD23	1:1:141:LEU:HA	1.76	0.43
1:1:402:ASN:HD21	1:1:538:THR:HG1	1.67	0.43
1:1:403:TYR:CE2	1:1:480:ILE:HG22	2.54	0.43
1:1:554:THR:HB	1:1:790:PHE:CE1	2.53	0.43
1:1:560:LEU:HD13	1:1:792:THR:HG21	1.99	0.43
1:1:827:ILE:HD11	1:1:1025[B]:TRP:CZ3	2.54	0.43
1:1:894:THR:HA	1:1:978:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1514:SER:O	1:1:1516:PHE:N	2.51	0.43
2:L:137:PHE:CZ	3:H:179:SER:HB2	2.53	0.43
2:L:189:GLU:HA	2:L:213:ARG:NH1	2.34	0.43
1:1:128:LEU:HD23	1:1:128:LEU:HA	1.78	0.43
3:H:26:TYR:HB2	3:H:92:ARG:HG3	2.00	0.43
1:1:429:THR:HG22	1:1:436:ARG:HB3	2.01	0.43
1:1:493:ASN:HB3	1:1:578:GLY:HA2	2.00	0.43
1:1:603:LEU:O	4:1:1602:HOH:O	2.22	0.43
1:1:941:ASN:HA	1:1:962:ALA:HA	2.00	0.43
1:1:1112:THR:HB	1:1:1125:THR:HA	2.01	0.43
1:1:1259:LYS:HB2	1:1:1259:LYS:HE2	1.88	0.43
1:1:1464:ASP:O	1:1:1468:GLN:HA	2.19	0.43
2:L:52:LYS:HD3	3:H:98:ASP:HB2	1.99	0.43
3:H:29:ASN:HA	3:H:44:LEU:HA	2.01	0.43
3:H:32:LYS:HD2	3:H:58:PHE:CE2	2.54	0.43
1:1:108:GLN:HE22	1:1:214:GLN:HB2	1.84	0.43
1:1:193:SER:HA	2:L:25:THR:HG21	2.00	0.43
1:1:587:VAL:HG11	1:1:1113:VAL:HG11	2.01	0.43
1:1:629:PHE:HZ	1:1:972:LEU:O	2.02	0.43
1:1:634:TRP:HZ2	1:1:702:TRP:CE2	2.37	0.43
1:1:1150:ARG:HA	1:1:1153:ILE:HD12	1.99	0.43
2:L:37:TRP:HB3	2:L:75:LEU:HD22	2.00	0.43
1:1:1018:PHE:HZ	1:1:1023:GLN:HB2	1.83	0.43
1:1:1038:ASN:C	1:1:1051:PRO:HG3	2.39	0.43
2:L:126:GLN:O	2:L:129:SER:OG	2.32	0.43
1:1:210:TYR:HH	1:1:215:ARG:HH11	1.66	0.42
1:1:377:TYR:HB2	1:1:387:ALA:HB3	2.00	0.42
1:1:759:ALA:HB1	1:1:764[B]:GLU:HB3	2.01	0.42
1:1:939:GLN:O	1:1:954:GLY:N	2.52	0.42
1:1:990:ALA:O	1:1:994:GLN:HG3	2.18	0.42
2:L:48:LEU:HB2	3:H:102:ASP:HA	2.01	0.42
3:H:106:GLN:OE1	3:H:106:GLN:N	2.47	0.42
1:1:627:GLN:NE2	1:1:988:ASN:OD1	2.38	0.42
1:1:811:ILE:HB	1:1:1120:TRP:NE1	2.32	0.42
1:1:1360:GLY:O	1:1:1364:VAL:N	2.49	0.42
2:L:121:PRO:HB3	2:L:211:PHE:CE2	2.55	0.42
2:L:162:LEU:HD23	2:L:162:LEU:HA	1.85	0.42
1:1:713:LEU:HD23	1:1:713:LEU:HA	1.73	0.42
2:L:39:LEU:HB3	2:L:49:LEU:HD21	2.00	0.42
2:L:173:SER:O	2:L:173:SER:OG	2.28	0.42
3:H:-3:GLN:HA	3:H:-3:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:550:VAL:HG21	1:1:552:LYS:HE3	2.02	0.42
1:1:810:TRP:CZ2	1:1:812:GLY:HA3	2.54	0.42
1:1:968:LEU:HB3	1:1:984:PHE:CE2	2.54	0.42
2:L:148:VAL:HA	2:L:198:ALA:HA	2.01	0.42
1:1:414:HIS:N	1:1:569:GLU:OE2	2.22	0.42
1:1:579:ALA:HB1	1:1:586:LEU:HD11	2.00	0.42
1:1:997:LEU:O	1:1:1001:LEU:HG	2.20	0.42
1:1:1042:TYR:CZ	1:1:1245:PRO:HB3	2.54	0.42
1:1:1106:LEU:HD12	1:1:1114:SER:O	2.20	0.42
1:1:320:GLU:N	1:1:323:GLN:O	2.53	0.42
1:1:627:GLN:O	1:1:991:GLN:NE2	2.52	0.42
1:1:1206:HIS:CD2	1:1:1264:PRO:HB2	2.54	0.42
2:L:35:LEU:HG	2:L:73:PHE:CG	2.55	0.42
3:H:41:TRP:CZ2	3:H:44:LEU:HD23	2.55	0.42
3:H:214:ARG:NH1	3:H:216:CYS:HB3	2.34	0.42
1:1:75:SER:HB2	1:1:1105:ASN:H	1.85	0.42
1:1:415:HIS:HB3	1:1:418:TRP:NE1	2.34	0.42
1:1:429:THR:HB	1:1:434:ASN:CB	2.50	0.42
1:1:491:ILE:HD13	1:1:491:ILE:HA	1.80	0.42
2:L:12:LEU:HD13	2:L:80:VAL:O	2.18	0.42
1:1:332:PHE:HZ	1:1:436:ARG:HG3	1.83	0.42
1:1:1009:ASN:HD22	1:1:1087:SER:HB2	1.84	0.42
2:L:199:THR:HG23	2:L:206:PRO:HG3	2.00	0.42
1:1:538:THR:OG1	1:1:748:ASP:O	2.33	0.42
1:1:551:ASN:ND2	1:1:713:LEU:O	2.53	0.42
1:1:584:ARG:NH1	1:1:584:ARG:HG2	2.34	0.42
1:1:811:ILE:HG12	1:1:1153:ILE:HG12	2.01	0.42
1:1:1025[B]:TRP:CD1	1:1:1025[B]:TRP:N	2.87	0.42
1:1:1178:ASP:HB2	1:1:1381:VAL:O	2.19	0.42
2:L:77:ILE:HD12	2:L:106:LEU:HD11	2.00	0.42
2:L:149:LYS:HE3	2:L:149:LYS:HB3	1.91	0.42
1:1:246:ALA:HA	1:1:315:ILE:HD13	2.02	0.42
1:1:853:THR:O	1:1:1049:LEU:N	2.50	0.42
1:1:1074:PRO:HB3	1:1:1270:LYS:HB3	2.02	0.42
1:1:1407:VAL:HG21	1:1:1451:VAL:HG11	2.02	0.42
3:H:54:TYR:CD1	3:H:59:ARG:HD2	2.55	0.42
1:1:407:TRP:HA	1:1:432:PHE:HZ	1.86	0.41
1:1:804:VAL:O	1:1:808:VAL:HG23	2.20	0.41
1:1:810:TRP:HH2	1:1:1271:LEU:HD13	1.84	0.41
1:1:1420:LEU:HD23	1:1:1421:PHE:CE2	2.55	0.41
1:1:436:ARG:HG2	1:1:619:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:742:LEU:O	1:1:746:LEU:HG	2.19	0.41
1:1:69:TRP:CD1	1:1:93:ARG:HB3	2.56	0.41
1:1:318:SER:O	1:1:325:VAL:HG12	2.19	0.41
1:1:597:THR:HA	1:1:600:VAL:HG23	2.02	0.41
1:1:998:ARG:NH1	4:1:1737:HOH:O	2.52	0.41
1:1:1444:PHE:CZ	1:1:1470:LEU:HD23	2.55	0.41
1:1:220:PRO:O	1:1:238:GLY:HA3	2.21	0.41
1:1:407:TRP:CZ2	1:1:571:VAL:HG22	2.55	0.41
1:1:423:ARG:HB3	1:1:428:GLN:HG2	2.03	0.41
1:1:636:ASN:OD1	1:1:658:TYR:HA	2.20	0.41
1:1:767:ASN:O	1:1:769:LYS:NZ	2.53	0.41
1:1:1039:LEU:HA	1:1:1051:PRO:HD3	2.01	0.41
1:1:1098:TRP:HZ2	1:1:1153:ILE:HA	1.84	0.41
1:1:1411:SER:OG	1:1:1414:GLN:HG2	2.21	0.41
3:H:6:VAL:HG11	3:H:80:LEU:HD13	2.01	0.41
1:1:549:MET:HA	1:1:553:GLN:OE1	2.20	0.41
1:1:665:TRP:HE1	1:1:933:ASN:HB3	1.85	0.41
1:1:811:ILE:O	1:1:1153:ILE:HD13	2.20	0.41
1:1:1210:LEU:HB2	1:1:1212:PHE:CE2	2.56	0.41
2:L:189:GLU:HA	2:L:213:ARG:HH12	1.85	0.41
3:H:81:THR:O	3:H:112:VAL:HG21	2.20	0.41
1:1:1113:VAL:CG2	1:1:1124:PHE:HB2	2.48	0.41
1:1:1457:ARG:NH1	2:L:96:VAL:HB	2.36	0.41
3:H:67:ASP:OD1	3:H:69:SER:OG	2.30	0.41
1:1:141:LEU:HD12	1:1:376:LEU:HD21	2.03	0.41
1:1:210:TYR:HE2	1:1:356:TRP:HB2	1.85	0.41
1:1:327:LEU:HD21	1:1:619:GLN:HB2	2.03	0.41
1:1:591:THR:HG21	1:1:1117:LEU:HD13	2.01	0.41
1:1:915:PHE:HA	1:1:968:LEU:HD11	2.02	0.41
1:1:1255:ASP:HB2	1:1:1258:LEU:HB2	2.01	0.41
2:L:137:PHE:CE1	3:H:179:SER:HB2	2.55	0.41
3:H:193:THR:HA	3:H:210:LYS:HZ3	1.85	0.41
1:1:363:HIS:O	1:1:366:LEU:HG	2.21	0.41
1:1:385:ARG:HE	1:1:385:ARG:HB2	1.60	0.41
1:1:409:THR:HB	1:1:454:THR:O	2.20	0.41
1:1:731:ASN:HB2	1:1:994:GLN:OE1	2.20	0.41
3:H:108:THR:HG22	3:H:110:VAL:HG23	2.03	0.41
1:1:178:ASN:HA	1:1:181:LYS:NZ	2.36	0.41
1:1:198:PHE:HE2	1:1:378:ASP:HB3	1.83	0.41
1:1:310:LEU:HD22	1:1:418:TRP:HB3	2.02	0.41
1:1:372:SER:HG	1:1:393:HIS:HD1	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:471:GLU:OE2	1:1:471:GLU:HA	2.21	0.41
1:1:638:PRO:HD2	1:1:709:TRP:CE3	2.56	0.41
1:1:675:ASP:HA	1:1:679:LYS:CB	2.51	0.41
1:1:677:PHE:O	1:1:694:TYR:HB3	2.20	0.41
1:1:798:GLY:O	1:1:992:ARG:HD3	2.21	0.41
1:1:803:GLN:OE1	1:1:1332:SER:HB2	2.21	0.41
1:1:851:LEU:HD22	1:1:859:VAL:HG13	2.02	0.41
1:1:1427:ASP:OD1	1:1:1427:ASP:C	2.59	0.41
1:1:561:PRO:HG2	1:1:594:MET:CB	2.47	0.41
1:1:617:GLN:HE21	1:1:624:GLU:HB3	1.86	0.41
1:1:673:VAL:HG21	1:1:963:THR:HA	2.02	0.41
1:1:1006:VAL:HG23	1:1:1053:LEU:HB3	2.02	0.41
1:1:411:LYS:HG2	1:1:435:PRO:HD2	2.02	0.40
1:1:598:ALA:HB2	1:1:625:ASP:O	2.20	0.40
1:1:1090:THR:HB	1:1:1254:LEU:HD21	2.02	0.40
2:L:188:TYR:O	2:L:213:ARG:NH1	2.45	0.40
1:1:354:ARG:HB3	1:1:354:ARG:HH11	1.85	0.40
1:1:1042:TYR:CD1	1:1:1042:TYR:C	2.95	0.40
1:1:1168:ASN:OD1	1:1:1172[B]:ARG:N	2.50	0.40
2:L:21:ARG:HG3	2:L:21:ARG:NH1	2.29	0.40
3:H:175:LEU:HD12	3:H:175:LEU:HA	1.86	0.40
1:1:159:ILE:HG13	1:1:377:TYR:CE1	2.56	0.40
1:1:369:TRP:HA	1:1:369:TRP:CE3	2.56	0.40
1:1:504:PHE:O	1:1:542:TYR:OH	2.31	0.40
1:1:587:VAL:HG22	1:1:737:ILE:CD1	2.50	0.40
1:1:612:LEU:HB3	1:1:1213:GLN:HB3	2.04	0.40
1:1:708:ASN:HB2	1:1:709:TRP:CE3	2.57	0.40
1:1:869:LEU:HD22	1:1:965:TYR:CD2	2.56	0.40
1:1:1003:SER:HB3	4:1:1669:HOH:O	2.21	0.40
1:1:1210:LEU:HB2	1:1:1212:PHE:CZ	2.56	0.40
1:1:272:SER:HB2	1:1:951:THR:O	2.21	0.40
1:1:406:SER:HB2	1:1:758:PHE:CE2	2.57	0.40
1:1:415:HIS:CB	1:1:419:ASP:HB2	2.48	0.40
1:1:504:PHE:CE2	1:1:588:LEU:HB2	2.56	0.40
1:1:529:ASN:OD1	1:1:529:ASN:N	2.54	0.40
1:1:603:LEU:HD23	1:1:634:TRP:HD1	1.87	0.40
1:1:631:PRO:HB2	1:1:701:MET:HE1	2.03	0.40
1:1:1087:SER:O	1:1:1216:VAL:HA	2.22	0.40
1:1:1502:LEU:H	1:1:1502:LEU:HG	1.60	0.40
2:L:98:TRP:HB2	3:H:41:TRP:CD2	2.57	0.40
1:1:134:ALA:HB1	1:1:1400:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:212:GLN:O	1:1:214:GLN:NE2	2.54	0.40
1:1:500:ALA:HB1	1:1:525:ARG:HD2	2.03	0.40
1:1:547:SER:HB3	1:1:568:PHE:CE1	2.53	0.40
1:1:624:GLU:OE2	1:1:998:ARG:NH1	2.55	0.40
1:1:1082:GLU:HB2	1:1:1083:GLN:NE2	2.37	0.40
1:1:1098:TRP:CH2	1:1:1158:PRO:HB2	2.56	0.40
1:1:1166:TRP:CH2	1:1:1168:ASN:HA	2.57	0.40
1:1:1258:LEU:HD12	1:1:1258:LEU:HA	1.90	0.40
1:1:1433:THR:HB	1:1:1435:LEU:HG	2.04	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	1	1330/1457 (91%)	1252 (94%)	77 (6%)	1 (0%)	48	65
2	L	216/218 (99%)	205 (95%)	11 (5%)	0	100	100
3	H	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	25	38
All	All	1766/1897 (93%)	1665 (94%)	99 (6%)	2 (0%)	50	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	957	ILE
3	H	102	ASP

### 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	1	1141/1215 (94%)	1099 (96%)	42 (4%)	29	48
2	L	194/194 (100%)	170 (88%)	24 (12%)	4	5
3	H	193/193 (100%)	178 (92%)	15 (8%)	10	17
All	All	1528/1602 (95%)	1447 (95%)	81 (5%)	21	33

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	82	THR
1	1	145	LYS
1	1	282	THR
1	1	294	LYS
1	1	304	GLN
1	1	316	LYS
1	1	323	GLN
1	1	351	THR
1	1	490	ASN
1	1	534	SER
1	1	540	TRP
1	1	552	LYS
1	1	559	ASP
1	1	584	ARG
1	1	646	SER
1	1	657	TYR
1	1	688	ASP
1	1	718	LEU
1	1	725	GLU
1	1	765	ARG
1	1	768	GLN
1	1	826	ASP
1	1	891	GLN
1	1	909	ASP
1	1	940	ASP
1	1	943	SER
1	1	1084	ASN
1	1	1087	SER
1	1	1126	ASP
1	1	1169	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1	1236	SER
1	1	1253	LYS
1	1	1280	SER
1	1	1297	THR
1	1	1369	LEU
1	1	1401	ASP
1	1	1419	ARG
1	1	1427	ASP
1	1	1452	ASN
1	1	1466	ASN
1	1	1482	ASP
1	1	1498	PHE
2	L	1	MET
2	L	2	THR
2	L	6	LEU
2	L	17	SER
2	L	24	GLN
2	L	51	TYR
2	L	55	ASN
2	L	69	SER
2	L	71	THR
2	L	72	ASP
2	L	91	PHE
2	L	94	SER
2	L	105	LYS
2	L	109	LYS
2	L	112	ASP
2	L	136	CYS
2	L	147	ASN
2	L	157	ARG
2	L	159	ASN
2	L	169	ASP
2	L	174	THR
2	L	177	MET
2	L	179	SER
2	L	213	ARG
3	H	4	GLU
3	H	10	THR
3	H	12	MET
3	H	26	TYR
3	H	29	ASN
3	H	34	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	H	61	THR
3	H	83	GLU
3	H	85	SER
3	H	92	ARG
3	H	116	LYS
3	H	176	TYR
3	H	181	SER
3	H	189	TRP
3	H	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	108	GLN
1	1	415	HIS
1	1	611	ASN
1	1	1046	ASN
1	1	1101	GLN
1	1	1418	ASN
2	L	40	GLN
2	L	214	ASN
3	H	33	GLN
3	H	172	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](#)

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.

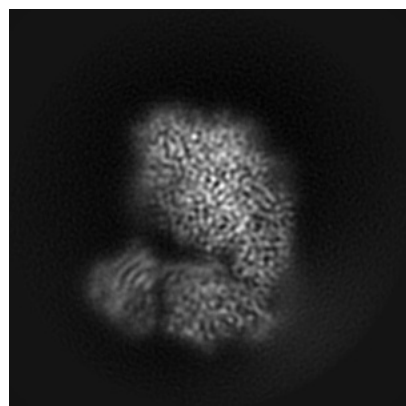
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19402. These allow visual inspection of the internal detail of the map and identification of artifacts.

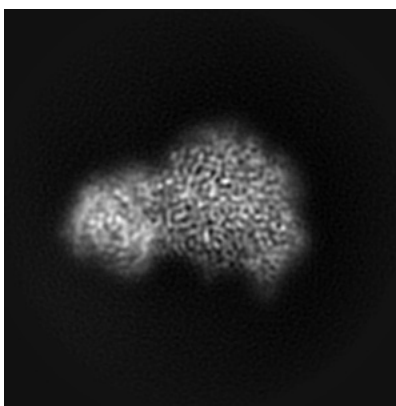
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

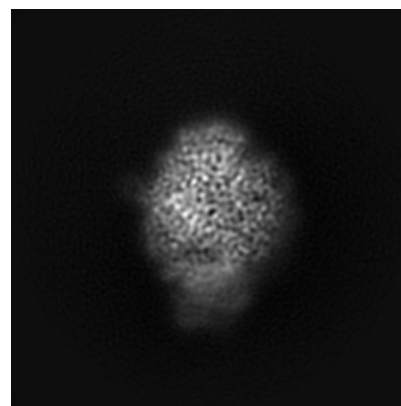
#### 6.1.1 Primary map



X

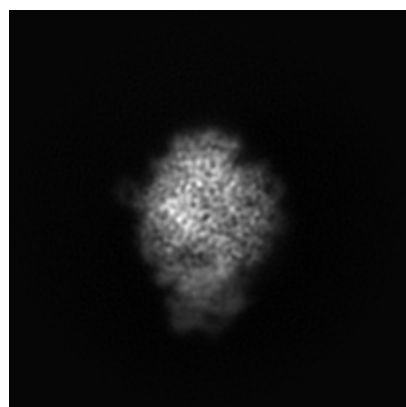


Y

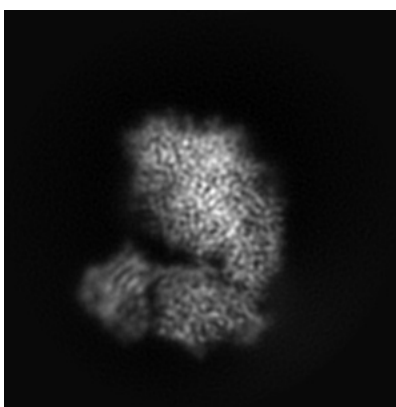


Z

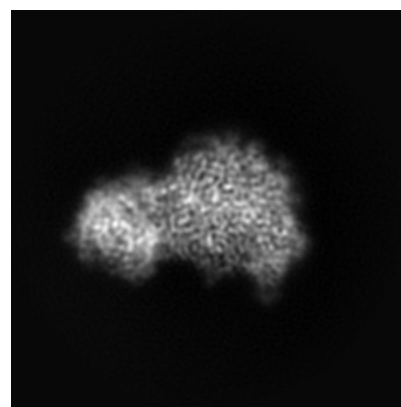
#### 6.1.2 Raw map



X



Y

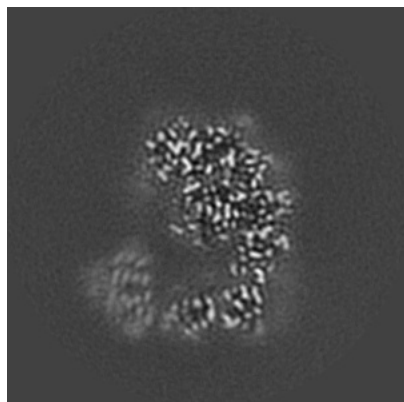


Z

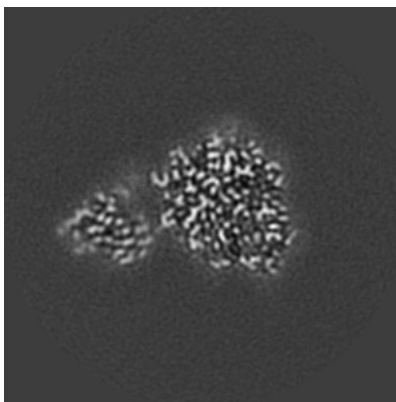
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

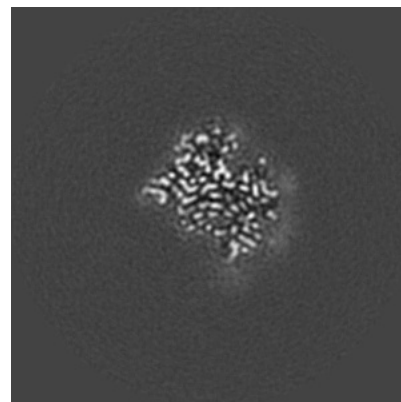
### 6.2.1 Primary map



X Index: 188

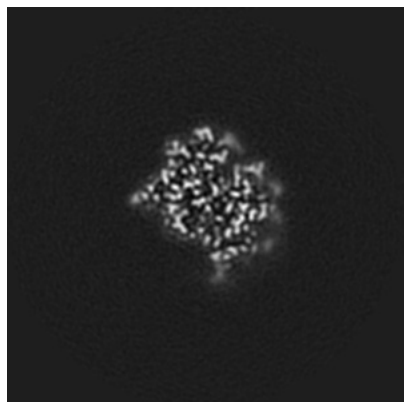


Y Index: 188

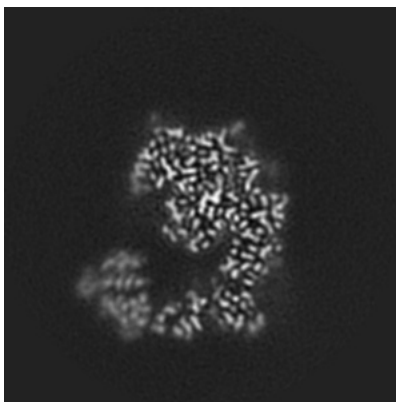


Z Index: 188

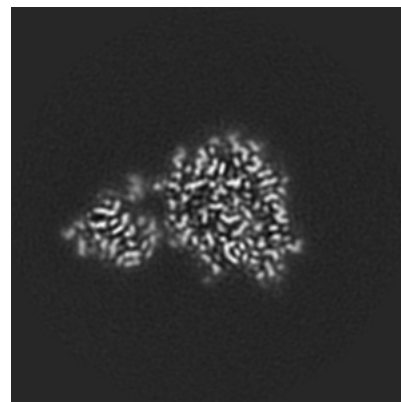
### 6.2.2 Raw map



X Index: 188



Y Index: 188

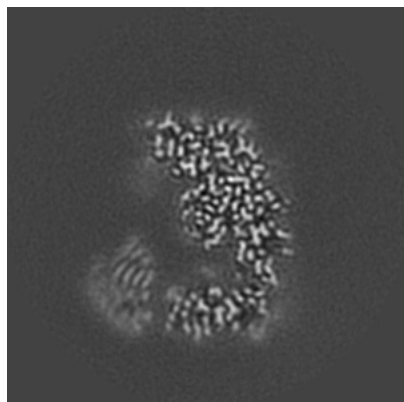


Z Index: 188

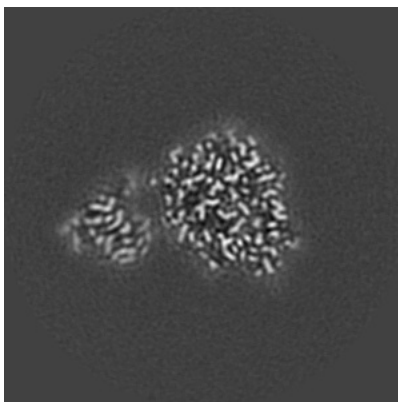
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

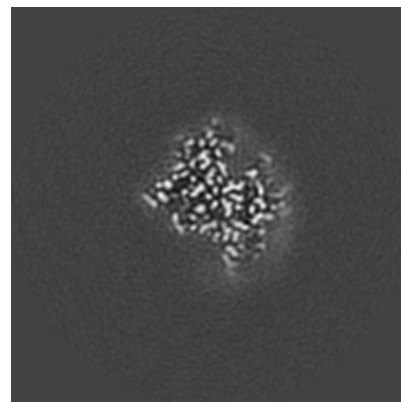
### 6.3.1 Primary map



X Index: 180

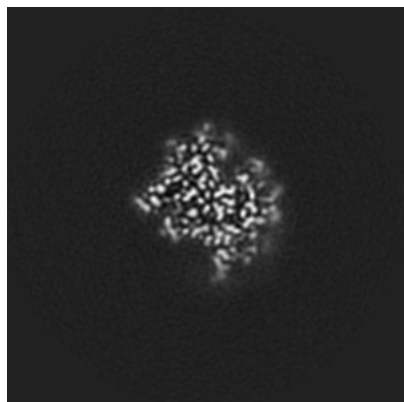


Y Index: 191

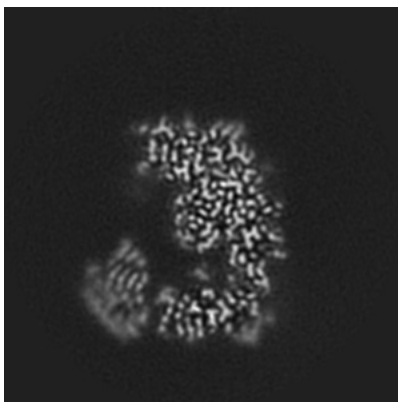


Z Index: 196

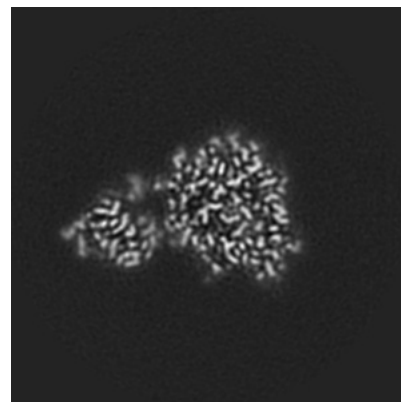
### 6.3.2 Raw map



X Index: 192



Y Index: 177

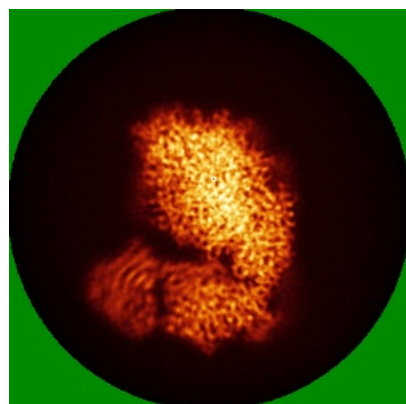


Z Index: 187

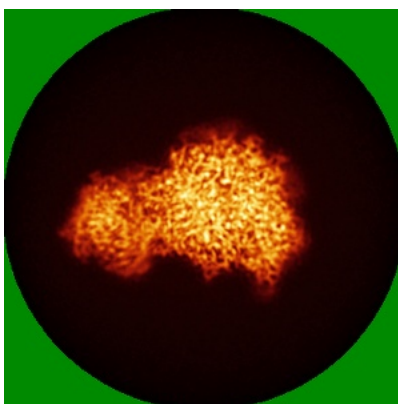
The images above show the largest variance slices of the map in three orthogonal directions.

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

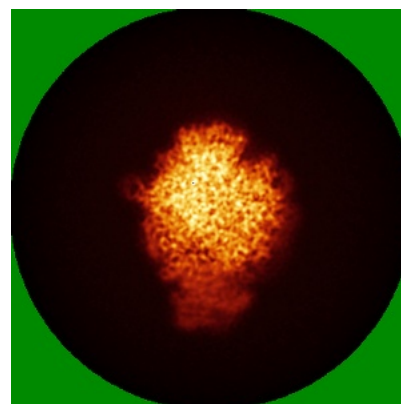
### 6.4.1 Primary map



X

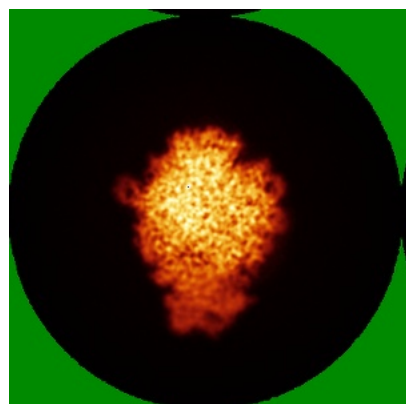


Y

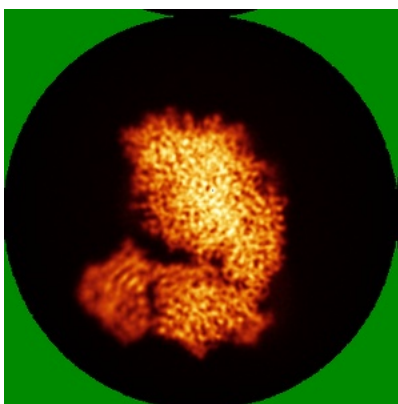


Z

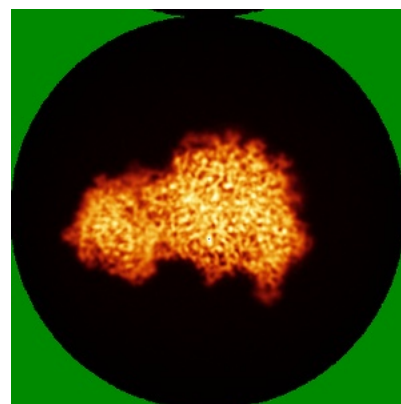
### 6.4.2 Raw map



X



Y

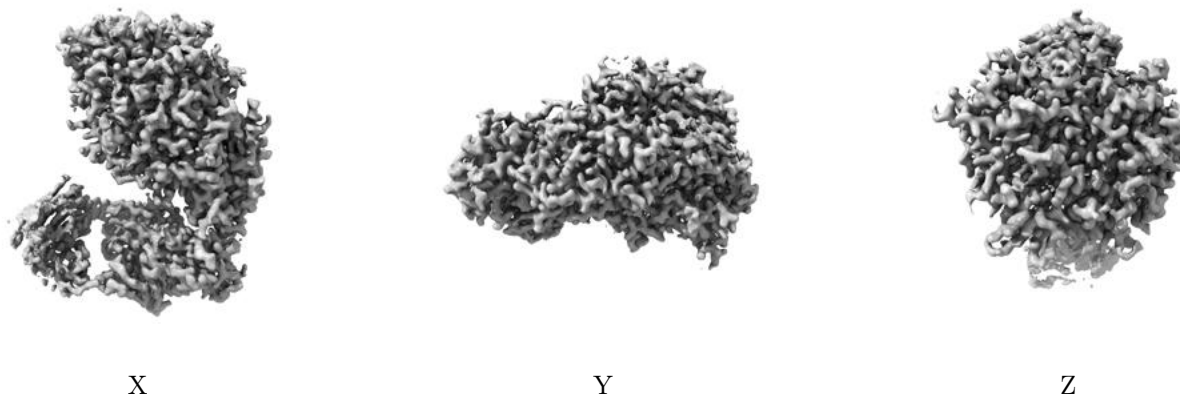


Z

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.

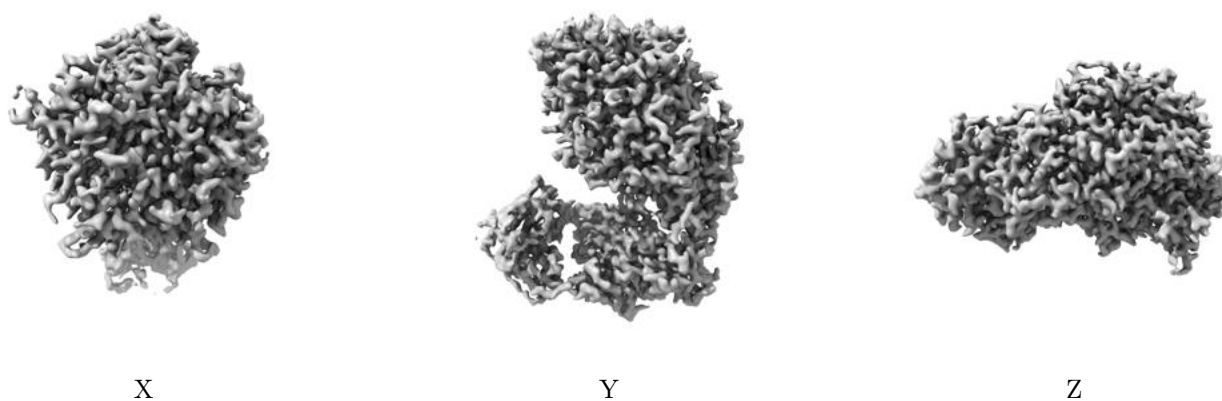
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

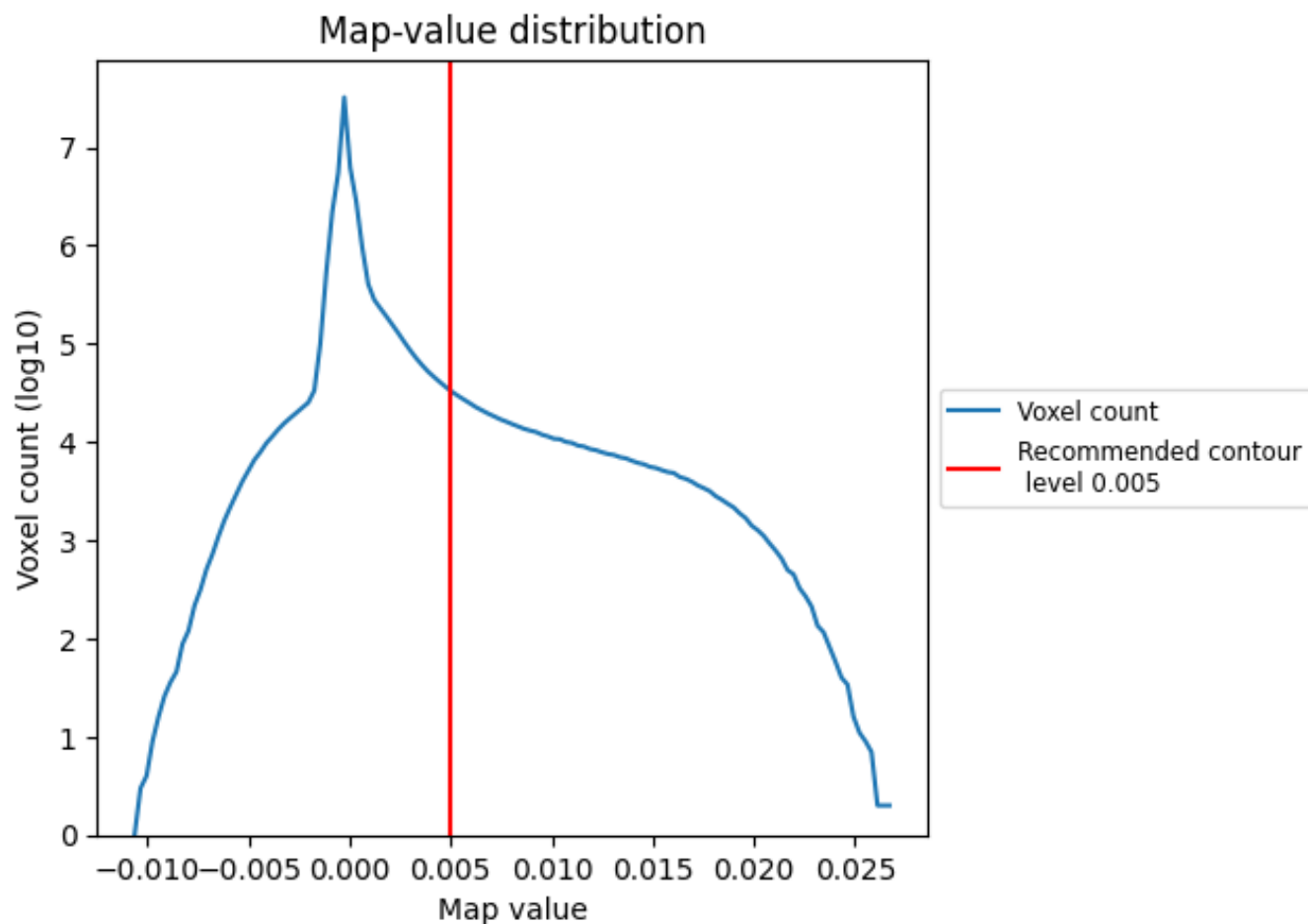
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

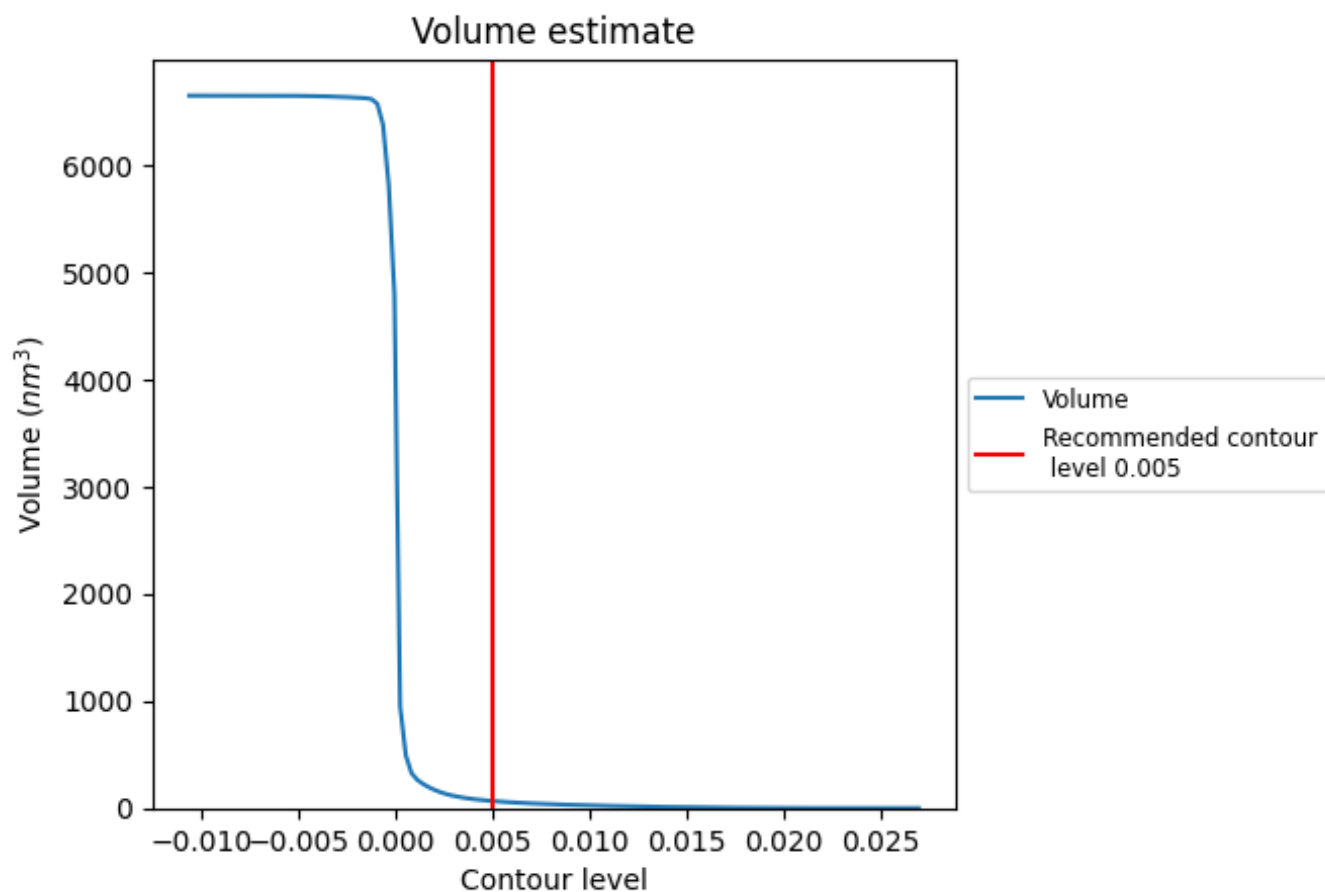
This section contains the results of statistical analysis of the map.

### 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.

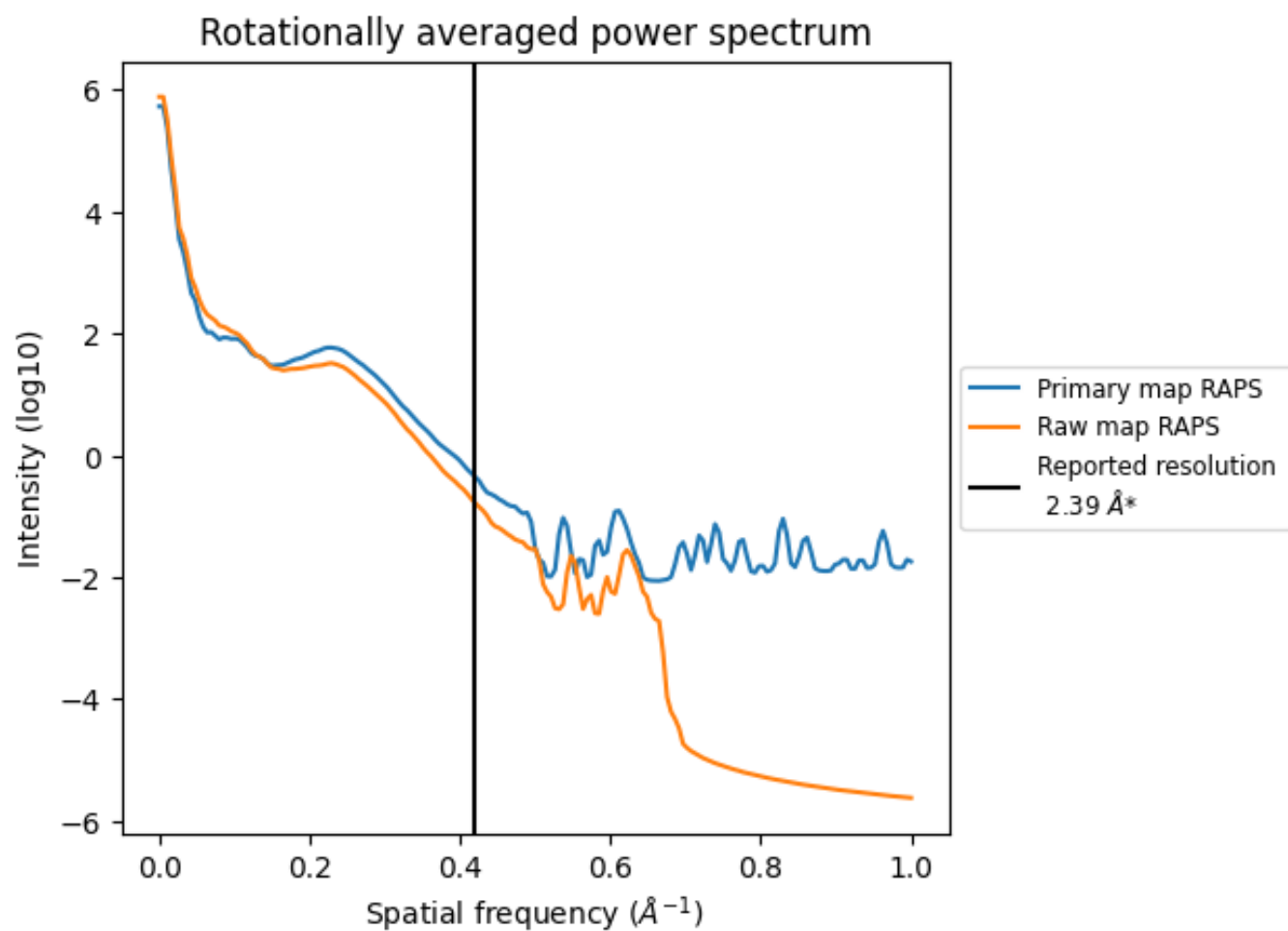
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66  $\text{nm}^3$ ; this corresponds to an approximate mass of 60 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 ⓘ

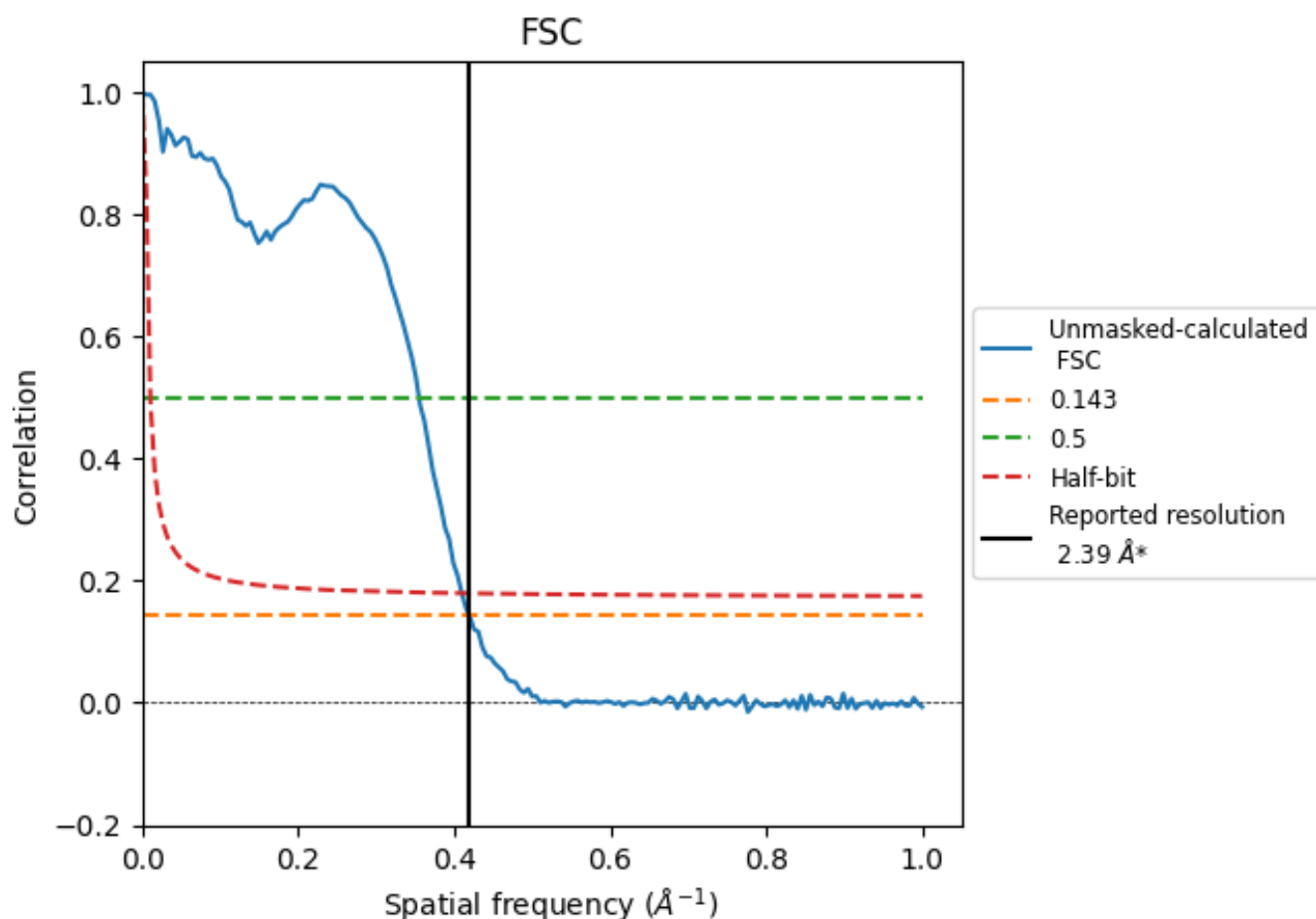


\*Reported resolution corresponds to spatial frequency of 0.418  $\text{\AA}^{-1}$

## 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 0.418  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

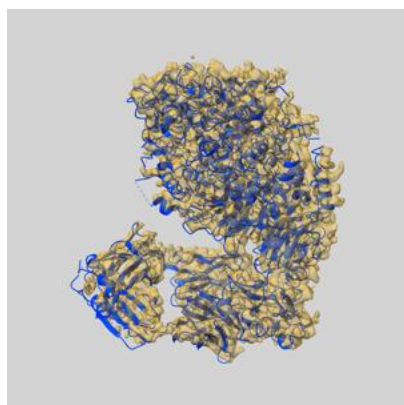
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.38	2.82	2.44

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

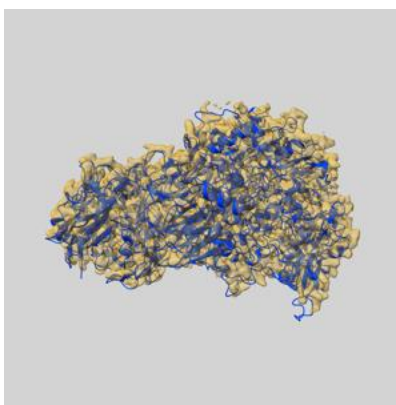
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19402 and PDB model 8ROR. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

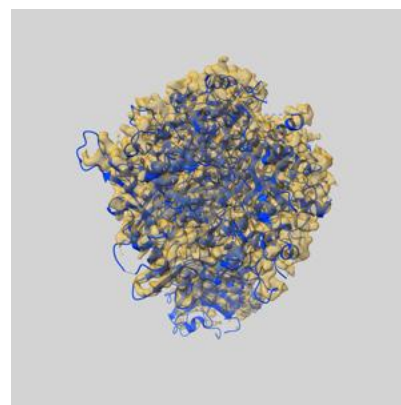
### 9.1 Map-model overlay [i](#)



X



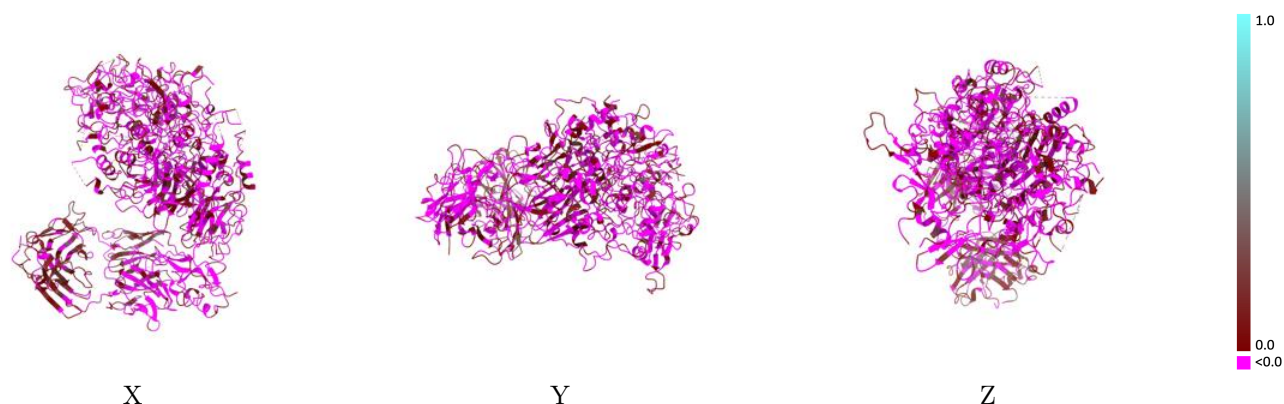
Y



Z

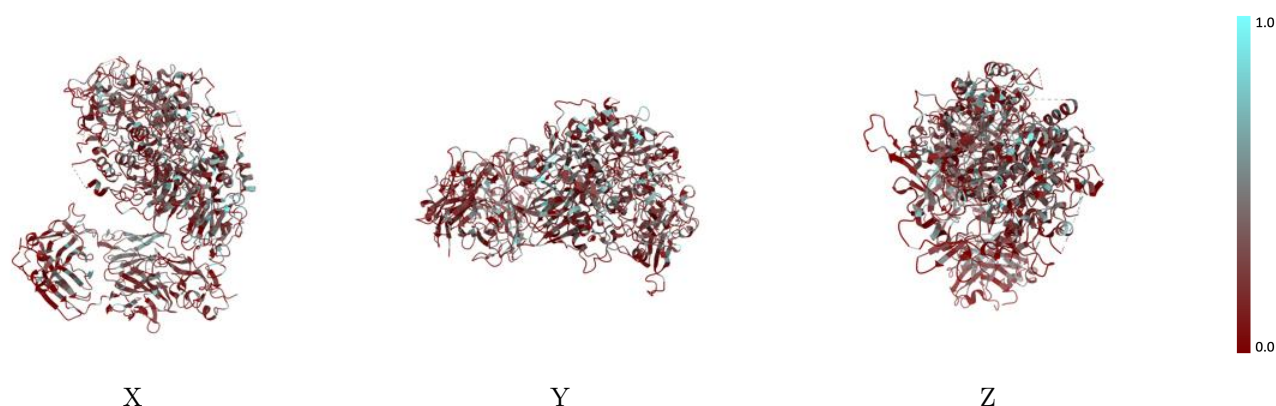
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



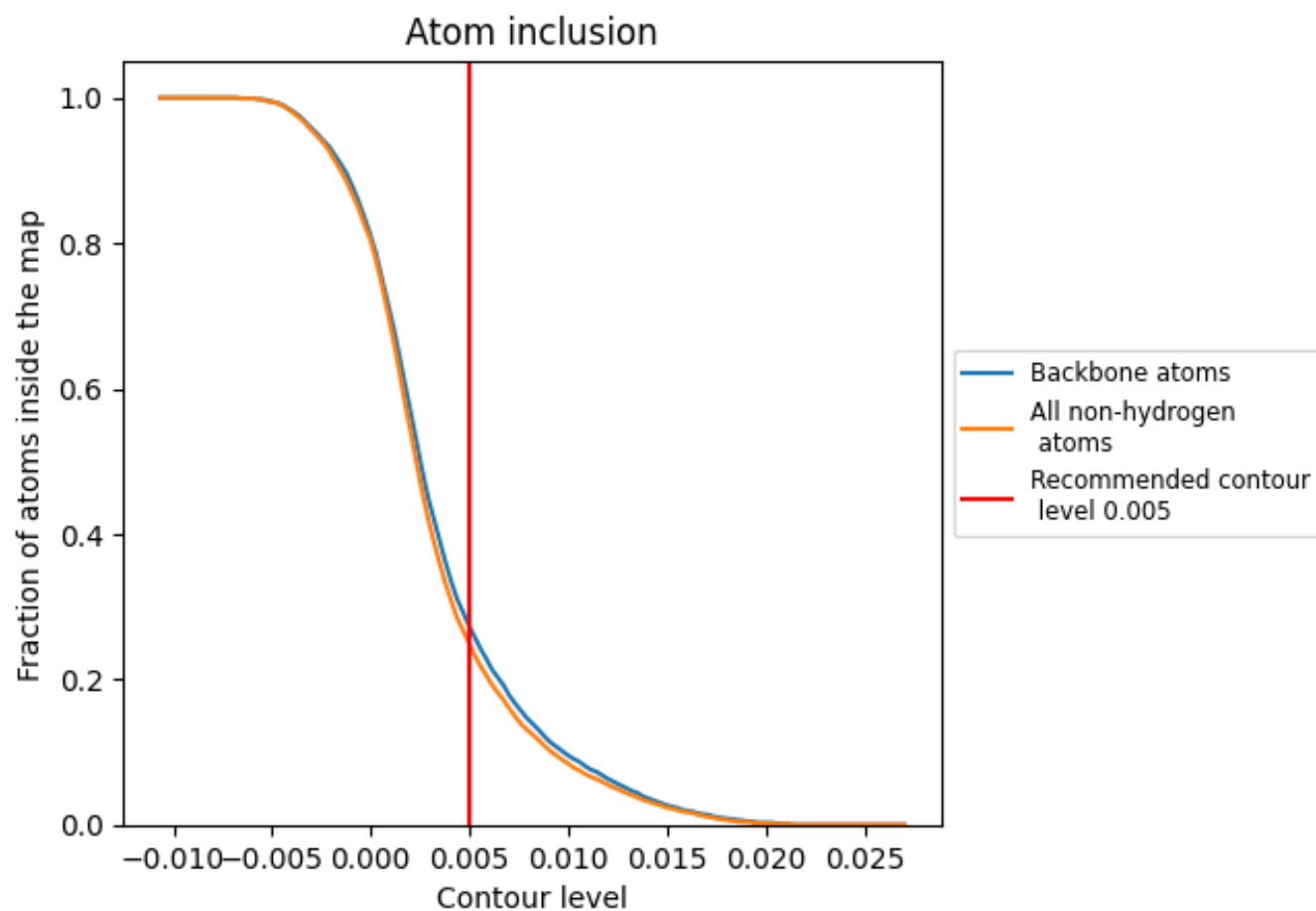
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 27% of all backbone atoms, 25% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2480	<div></div> -0.0430
1	<div></div> 0.2520	<div></div> -0.0620
H	<div></div> 0.1980	<div></div> -0.0180
L	<div></div> 0.2780	<div></div> 0.0550

