



## Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 10:42 PM EST

PDB ID : 6VBU  
EMDB ID : EMD-21144  
Title : Structure of the bovine BBSome complex  
Authors : Singh, S.K.; Gui, M.; Koh, F.; Yip, M.C.J.; Brown, A.  
Deposited on : 2019-12-19  
Resolution : 3.10 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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

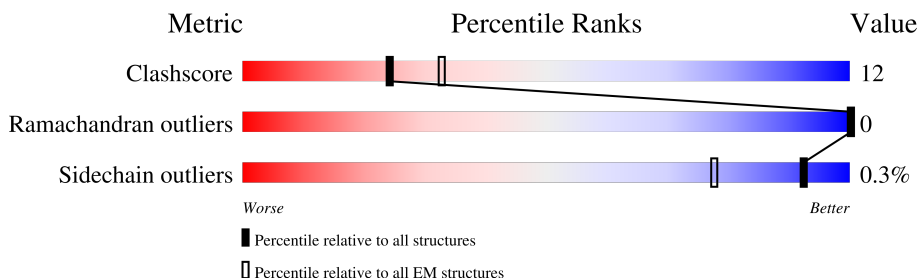
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	0	69	<div> <div>13%</div> <div>62%</div> <div>13%</div> <div>25%</div> </div>
2	1	592	<div> <div>39%</div> <div>56%</div> <div>26%</div> <div>18%</div> </div>
3	2	721	<div> <div>10%</div> <div>65%</div> <div>26%</div> <div>9%</div> </div>
4	4	519	<div> <div>10%</div> <div>57%</div> <div>18%</div> <div>26%</div> </div>
5	5	341	<div> <div>13%</div> <div>60%</div> <div>28%</div> <div>12%</div> </div>
6	7	715	<div> <div>67%</div> <div>66%</div> <div>31%</div> <div>.</div> </div>
7	8	501	<div> <div>75%</div> <div>20%</div> <div>5%</div> </div>
8	9	887	<div> <div>60%</div> <div>26%</div> <div>14%</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 30209 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 Bardet-Biedl syndrome 18 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	52	Total	C	N	O	S	0	0
			421	270	70	77	4		

- Molecule 2 is a protein called BBS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	486	Total	C	N	O	S	0	0
			3767	2418	657	673	19		

- Molecule 3 is a protein called Bardet-Biedl syndrome 2 protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	659	Total	C	N	O	S	0	0
			5145	3245	896	977	27		

- Molecule 4 is a protein called Bardet-Biedl syndrome 4 protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	386	Total	C	N	O	S	0	0
			3113	2016	513	564	20		

- Molecule 5 is a protein called Bardet-Biedl syndrome 5 protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	300	Total	C	N	O	S	0	0
			2411	1533	422	450	6		

- Molecule 6 is a protein called Bardet-Biedl syndrome 7 protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	698	Total	C	N	O	S	0	0
			5519	3498	931	1068	22		

- Molecule 7 is a protein called Bardet-Biedl syndrome 8 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	475	Total	C	N	O	S	0	0
			3797	2417	655	705	20		

- Molecule 8 is a protein called Bardet-Biedl syndrome 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	764	Total	C	N	O	S	0	0
			6034	3857	1018	1128	31		

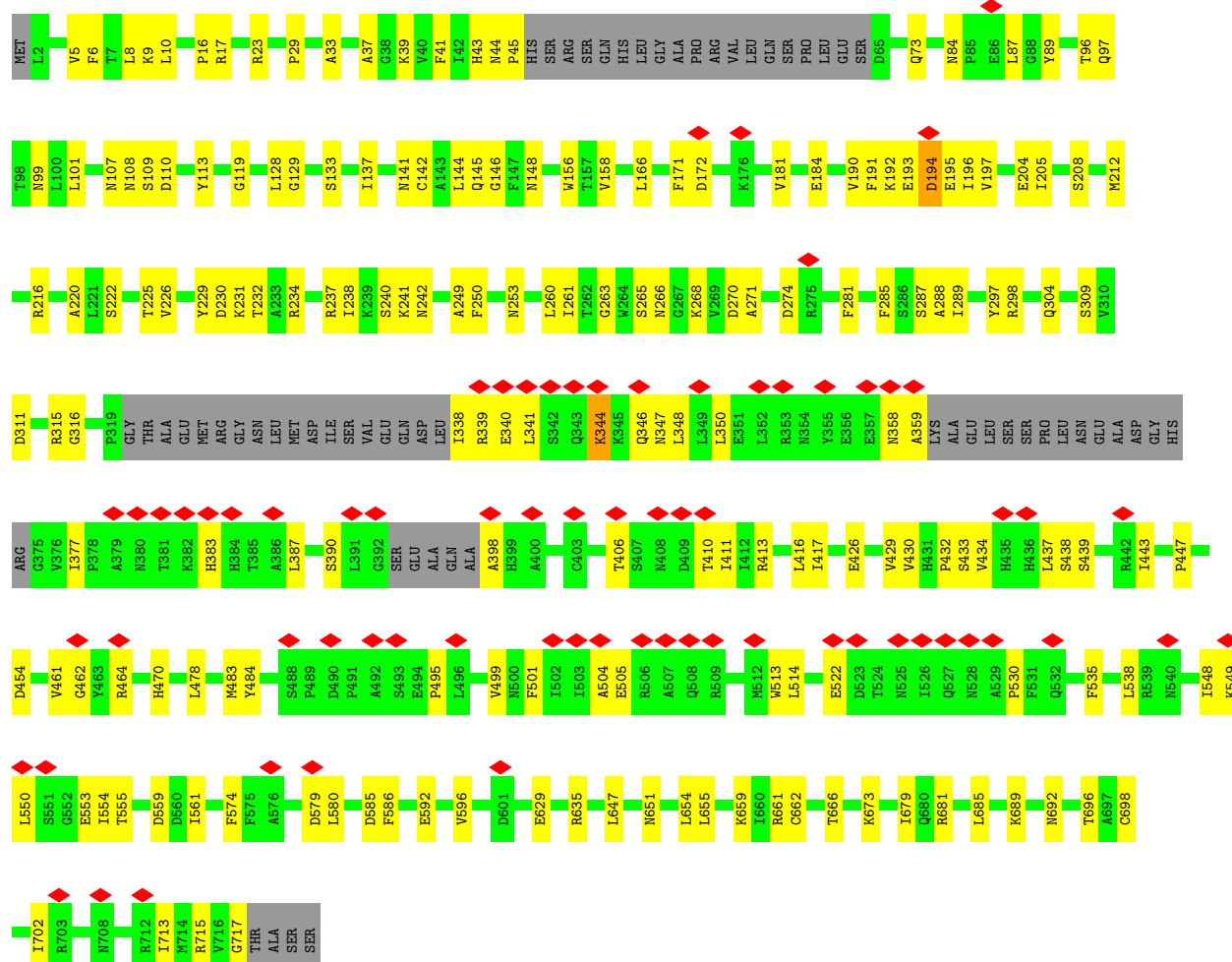
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
9	2	2	Total	Ca	0
			2	2	



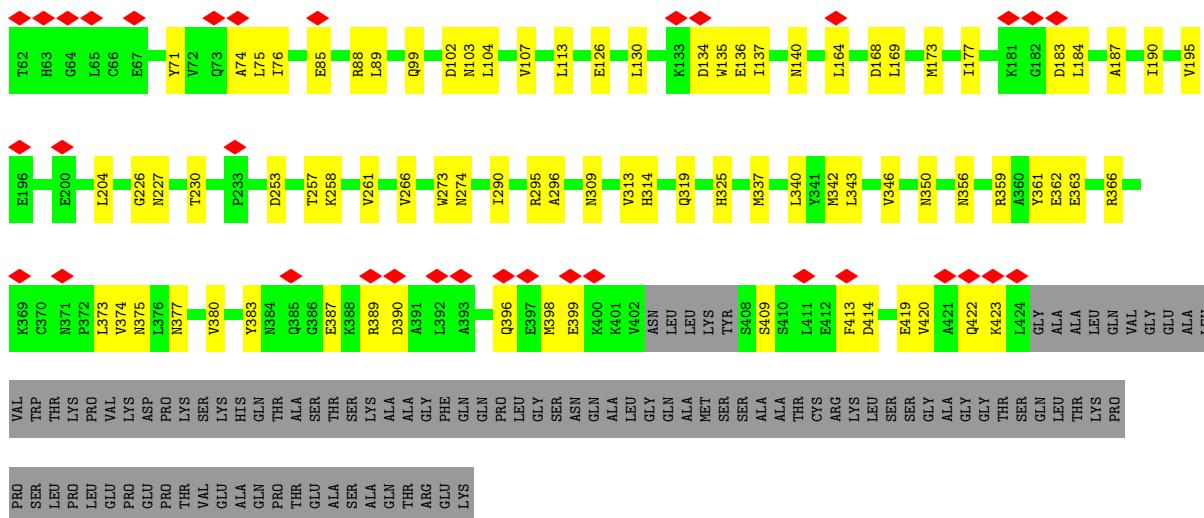


• Molecule 3: Bardet-Biedl syndrome 2 protein homolog

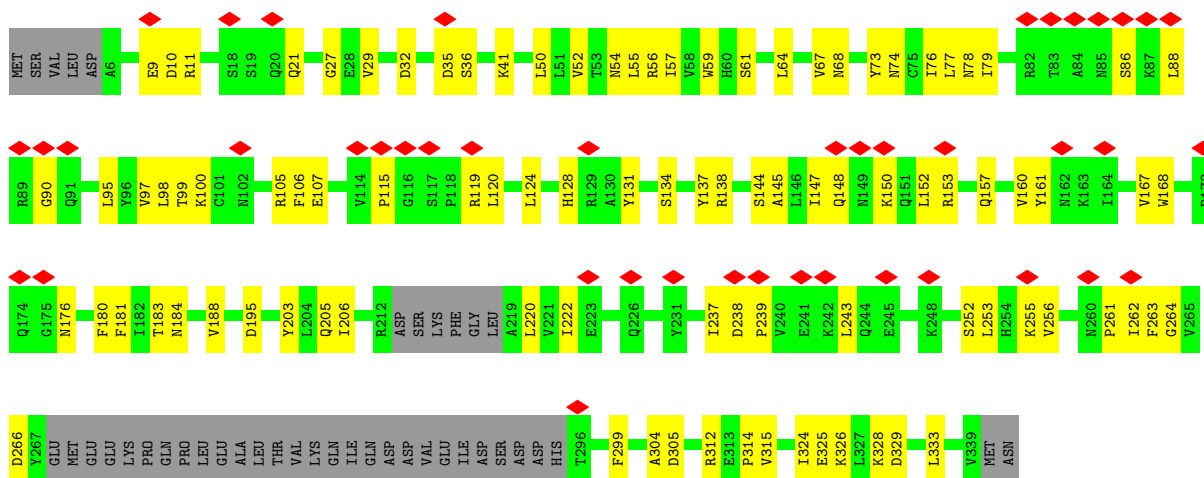


• Molecule 4: Bardet-Biedl syndrome 4 protein homolog

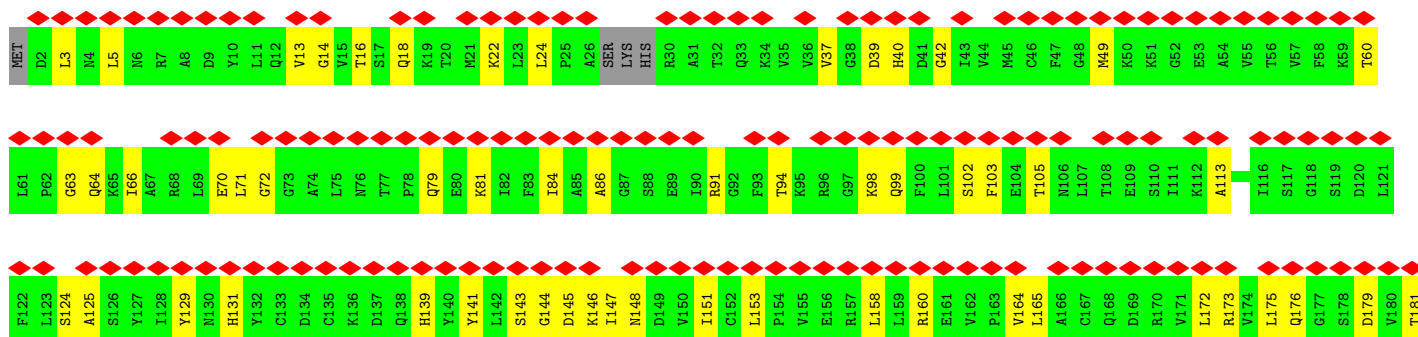


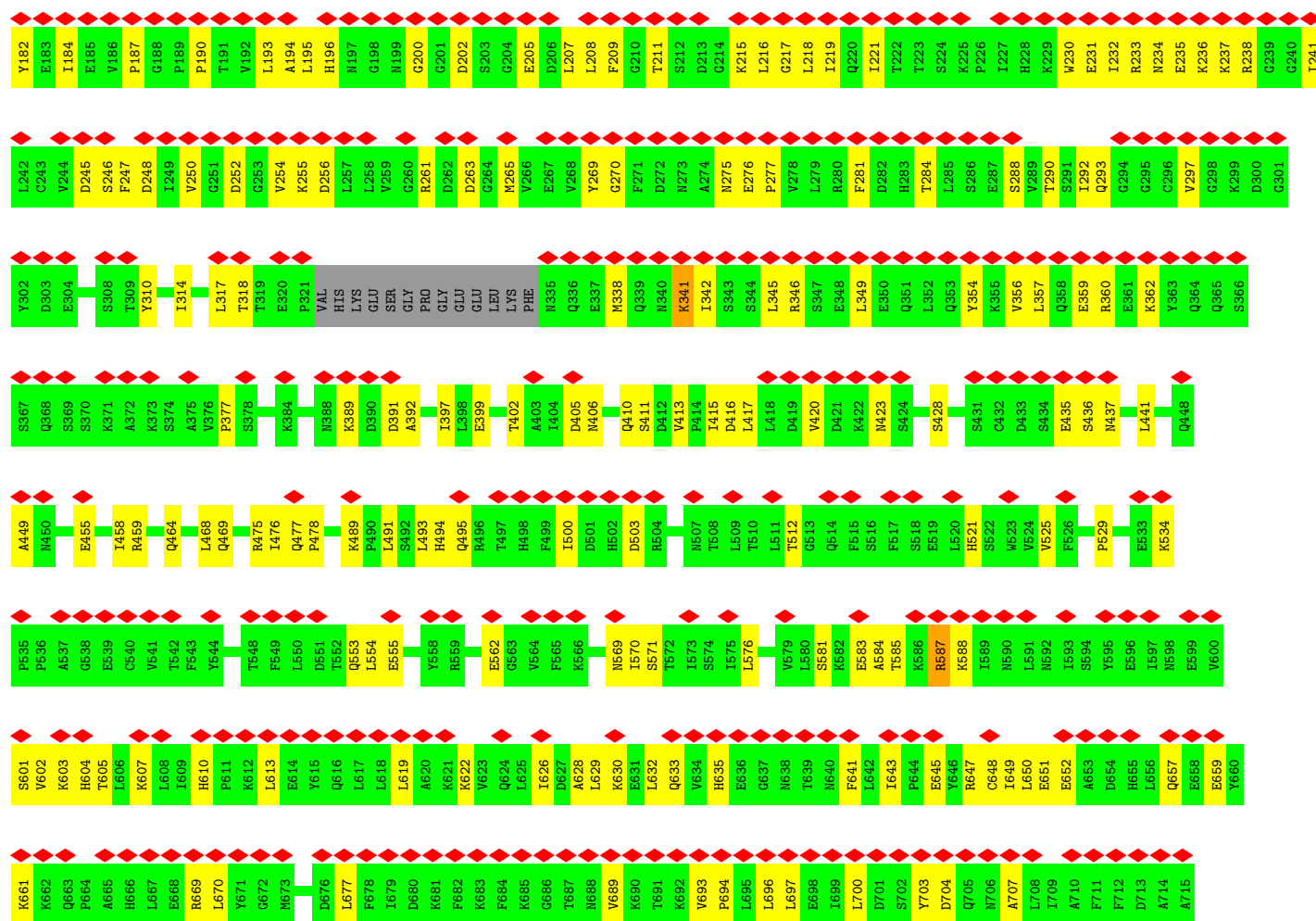


• Molecule 5: Bardet-Biedl syndrome 5 protein homolog



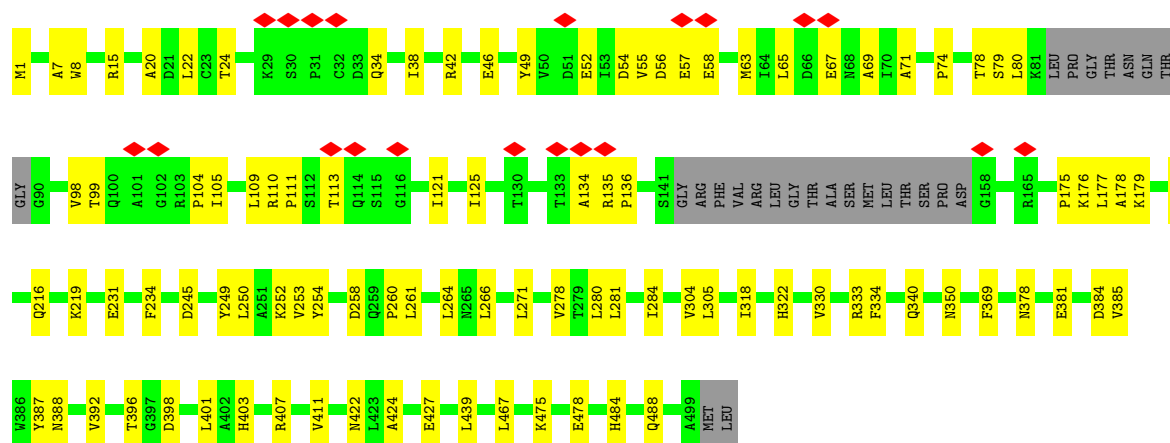
• Molecule 6: Bardet-Biedl syndrome 7 protein homolog





• Molecule 7: Bardet-Biedl syndrome 8 protein

Chain 8: 75% 20% 5%



• Molecule 8: Bardet-Biedl syndrome 9

Chain 9: 60% 26% 14%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	152942	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 ( $e^-/\text{\AA}^2$ )	56	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

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

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

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	0	0.39	0/426	0.53	0/572
2	1	0.28	0/3840	0.50	0/5205
3	2	0.30	0/5237	0.47	0/7092
4	4	0.29	0/3178	0.42	0/4295
5	5	0.29	0/2456	0.48	0/3324
6	7	0.27	0/5618	0.49	0/7596
7	8	0.33	0/3883	0.42	0/5262
8	9	0.32	0/6153	0.48	0/8325
All	All	0.30	0/30791	0.47	0/41671

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 [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	0	421	0	450	13	0
2	1	3767	0	3926	104	0
3	2	5145	0	5109	142	0
4	4	3113	0	3135	67	0
5	5	2411	0	2412	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	7	5519	0	5523	161	0
7	8	3797	0	3740	67	0
8	9	6034	0	6068	168	0
9	2	2	0	0	0	0
All	All	30209	0	30363	718	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 12.

All (718) 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)
3:2:387:LEU:HD11	3:2:478:LEU:HD23	1.45	0.98
2:1:41:PRO:HD3	2:1:45:GLN:HE21	1.43	0.83
1:0:12:LEU:HD21	4:4:346:VAL:HG11	1.61	0.82
7:8:52:GLU:HG2	7:8:219:LYS:HD2	1.62	0.81
1:0:8:PHE:HB2	4:4:380:VAL:HG13	1.63	0.79
2:1:503:LEU:HD21	2:1:566:VAL:HG11	1.67	0.77
8:9:183:PRO:HB2	8:9:248:ILE:HG22	1.67	0.77
3:2:406:THR:HG21	3:2:410:THR:HB	1.66	0.75
6:7:42:GLY:HA3	6:7:63:GLY:H	1.50	0.75
3:2:250:PHE:HB3	3:2:261:ILE:HD13	1.68	0.75
3:2:263:GLY:HA3	3:2:289:ILE:HG21	1.69	0.75
8:9:281:LYS:HD2	8:9:318:VAL:HG13	1.68	0.74
5:5:324:ILE:HG13	8:9:359:LEU:HB2	1.67	0.73
6:7:147:ILE:HD12	6:7:165:LEU:HD21	1.69	0.73
1:0:35:PRO:HB2	7:8:109:LEU:HG	1.71	0.73
4:4:135:TRP:HB3	4:4:164:LEU:HD22	1.69	0.73
3:2:387:LEU:HD11	3:2:478:LEU:CD2	2.19	0.73
6:7:5:LEU:HA	6:7:318:THR:O	1.89	0.73
1:0:8:PHE:HZ	4:4:423:LYS:HD2	1.54	0.72
6:7:632:LEU:HD21	8:9:676:ILE:HG12	1.71	0.72
8:9:475:GLU:CD	8:9:475:GLU:H	1.91	0.72
8:9:108:VAL:HG22	8:9:123:ILE:HG22	1.70	0.72
6:7:72:GLY:HA2	6:7:79:GLN:HB3	1.72	0.72
3:2:194:ASP:O	3:2:692:ASN:ND2	2.23	0.71
2:1:296:VAL:HG13	2:1:335:LEU:HG	1.71	0.71
7:8:1:MET:HB2	8:9:77:PRO:HG2	1.71	0.71
3:2:430:VAL:HG21	3:2:443:ILE:HG12	1.71	0.71
6:7:626:ILE:HD11	6:7:657:GLN:HE21	1.55	0.71
6:7:22:LYS:HA	6:7:293:GLN:HE21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:8:PHE:CZ	4:4:423:LYS:HD2	2.26	0.70
3:2:242:ASN:OD1	3:2:266:ASN:ND2	2.24	0.70
3:2:340:GLU:HG2	3:2:341:LEU:HD12	1.72	0.70
2:1:349:ALA:HB2	2:1:376:LEU:HD11	1.73	0.69
3:2:225:THR:HA	3:2:238:ILE:O	1.91	0.69
6:7:99:GLN:NE2	6:7:102:SER:OG	2.25	0.69
6:7:397:ILE:HG12	6:7:455:GLU:HG2	1.73	0.69
8:9:656:ARG:NH1	8:9:770:GLU:OE2	2.26	0.69
8:9:780:LEU:HD23	8:9:784:LEU:HD12	1.75	0.68
3:2:661:ARG:NH1	8:9:686:ASP:O	2.25	0.68
4:4:58:GLN:HA	4:4:61:GLU:HG2	1.74	0.68
8:9:151:LEU:HB2	8:9:165:GLU:HA	1.76	0.68
3:2:348:LEU:HD22	6:7:356:VAL:HG21	1.75	0.67
8:9:613:THR:HG21	8:9:733:LEU:HD13	1.76	0.67
5:5:168:TRP:HD1	5:5:176:ASN:HB3	1.59	0.67
8:9:274:ASN:HD21	8:9:276:GLN:HE21	1.42	0.67
7:8:80:LEU:HG	7:8:260:PRO:HG3	1.77	0.67
6:7:113:ALA:HB3	6:7:124:SER:HB3	1.76	0.66
4:4:35:GLN:NE2	4:4:58:GLN:OE1	2.29	0.66
4:4:36:ASN:OD1	4:4:58:GLN:NE2	2.28	0.66
2:1:23:LEU:HD21	2:1:32:TYR:HB3	1.78	0.66
2:1:206:LEU:O	2:1:218:CYS:N	2.27	0.66
3:2:417:ILE:HD11	3:2:443:ILE:HD13	1.77	0.66
8:9:656:ARG:HG3	8:9:720:LEU:HD11	1.77	0.66
5:5:148:GLN:HG3	5:5:153:ARG:HG2	1.78	0.66
8:9:314:ILE:HD13	8:9:322:TRP:HB3	1.78	0.65
8:9:80:GLN:NE2	8:9:82:GLU:OE2	2.29	0.65
8:9:189:ARG:HG3	8:9:258:SER:HB2	1.77	0.65
4:4:274:ASN:OD1	4:4:309:ASN:ND2	2.29	0.65
7:8:340:GLN:O	8:9:325:GLN:NE2	2.30	0.65
3:2:651:ASN:ND2	8:9:677:GLN:OE1	2.25	0.64
7:8:110:ARG:HG2	7:8:113:THR:HG23	1.79	0.64
3:2:43:HIS:ND1	3:2:297:TYR:OH	2.30	0.64
5:5:181:PHE:HB2	5:5:188:VAL:HG22	1.79	0.64
8:9:748:GLN:HE22	8:9:824:ARG:HD2	1.62	0.64
7:8:57:GLU:OE1	7:8:135:ARG:NH2	2.28	0.64
2:1:249:ALA:HB2	2:1:268:ARG:HG3	1.80	0.64
6:7:632:LEU:HD23	6:7:641:PHE:HE2	1.61	0.64
3:2:242:ASN:HB3	3:2:265:SER:HB2	1.78	0.63
2:1:471:LEU:HD22	8:9:395:VAL:HG21	1.81	0.63
2:1:529:ALA:HB2	2:1:555:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:42:GLY:HA3	6:7:63:GLY:N	2.13	0.63
6:7:629:LEU:HB3	6:7:650:LEU:HD21	1.80	0.63
2:1:230:VAL:HB	2:1:240:ALA:HB3	1.81	0.63
5:5:203:TYR:HD1	5:5:206:ILE:HD12	1.63	0.63
8:9:781:LYS:O	8:9:791:GLN:NE2	2.31	0.63
3:2:662:CYS:HB3	8:9:689:PRO:HB3	1.80	0.63
2:1:361:LYS:HG3	2:1:362:VAL:HG13	1.81	0.62
5:5:10:ASP:OD2	5:5:11:ARG:NH2	2.31	0.62
3:2:338:ILE:HG13	3:2:339:ARG:H	1.64	0.62
6:7:254:VAL:HG13	6:7:255:LYS:H	1.64	0.62
5:5:105:ARG:NH1	5:5:305:ASP:OD1	2.33	0.62
3:2:585:ASP:OD1	3:2:715:ARG:NH1	2.33	0.62
4:4:314:HIS:HD2	4:4:319:GLN:HG3	1.64	0.62
5:5:237:ILE:HG22	5:5:239:PRO:HD2	1.82	0.61
2:1:75:ALA:HB3	2:1:79:PRO:HA	1.83	0.61
2:1:207:LYS:HD3	2:1:211:ALA:HA	1.83	0.61
2:1:438:THR:OG1	4:4:319:GLN:NE2	2.34	0.61
2:1:440:ARG:HH11	8:9:367:GLN:HG2	1.66	0.61
6:7:153:LEU:HD13	6:7:205:GLU:HG3	1.83	0.61
3:2:530:PRO:HD3	3:2:550:LEU:HB2	1.82	0.60
5:5:50:LEU:HD23	5:5:120:LEU:HD21	1.83	0.60
5:5:160:VAL:HA	5:5:183:THR:HG22	1.84	0.60
7:8:245:ASP:OD1	8:9:282:LYS:NZ	2.32	0.60
6:7:410:GLN:OE1	6:7:469:GLN:NE2	2.34	0.60
3:2:635:ARG:HD3	8:9:764:GLN:HB3	1.83	0.60
5:5:167:VAL:HG21	5:5:180:PHE:HB2	1.83	0.60
6:7:22:LYS:HB3	6:7:71:LEU:HD23	1.83	0.60
6:7:236:LYS:HE2	6:7:237:LYS:HE2	1.82	0.60
7:8:38:ILE:HD13	8:9:179:LEU:HD23	1.83	0.60
3:2:172:ASP:H	3:2:231:LYS:HE2	1.66	0.60
6:7:392:ALA:HB1	6:7:493:LEU:HD11	1.83	0.60
5:5:312:ARG:HH21	5:5:326:LYS:HG2	1.66	0.60
6:7:389:LYS:HD3	6:7:495:GLN:HE22	1.67	0.60
2:1:356:ARG:NH1	2:1:357:ILE:O	2.35	0.60
2:1:72:PHE:HB3	2:1:205:THR:HG21	1.84	0.59
2:1:440:ARG:HE	8:9:367:GLN:HE21	1.50	0.59
2:1:378:PHE:HD1	2:1:388:LEU:HD12	1.66	0.59
5:5:134:SER:O	5:5:138:ARG:NH2	2.35	0.59
8:9:106:TYR:HD1	8:9:125:LEU:HA	1.66	0.59
8:9:554:LYS:O	8:9:597:GLN:NE2	2.34	0.59
8:9:559:LEU:HD13	8:9:592:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:151:LEU:HD23	8:9:151:LEU:H	1.68	0.59
6:7:449:ALA:O	6:7:475:ARG:NH2	2.34	0.59
5:5:9:GLU:HB3	5:5:56:ARG:HD3	1.83	0.59
7:8:378:ASN:HB2	7:8:381:GLU:HG3	1.84	0.59
2:1:268:ARG:HG2	4:4:40:HIS:NE2	2.17	0.59
3:2:341:LEU:O	3:2:344:LYS:HG3	2.02	0.58
3:2:411:ILE:HG13	3:2:464:ARG:HD3	1.85	0.58
3:2:107:ASN:HB3	7:8:261:LEU:HD12	1.84	0.58
6:7:153:LEU:HD11	6:7:221:ILE:HD11	1.84	0.58
4:4:342:MET:HG3	4:4:374:VAL:HA	1.84	0.58
2:1:472:GLU:HG3	8:9:514:ARG:HH21	1.68	0.58
5:5:86:SER:O	5:5:88:LEU:HD23	2.04	0.58
8:9:134:THR:HG23	8:9:157:VAL:HG12	1.83	0.58
6:7:184:ILE:HD13	6:7:219:ILE:HG21	1.85	0.58
8:9:196:VAL:HG22	8:9:202:VAL:HG22	1.84	0.58
8:9:50:ARG:HG2	8:9:71:GLU:HG3	1.86	0.58
6:7:215:LYS:HG2	6:7:233:ARG:HA	1.86	0.58
6:7:554:LEU:HD21	6:7:576:LEU:HD11	1.86	0.58
2:1:373:VAL:HA	2:1:392:THR:HA	1.85	0.57
3:2:348:LEU:HB3	6:7:356:VAL:HG11	1.85	0.57
8:9:10:TRP:NE1	8:9:67:ASP:OD2	2.38	0.57
8:9:461:VAL:HG23	8:9:462:GLN:H	1.70	0.57
4:4:134:ASP:HB3	4:4:137:ILE:HD12	1.87	0.57
8:9:70:LEU:HD13	8:9:72:VAL:HG23	1.86	0.57
5:5:57:ILE:HD12	5:5:124:LEU:HD11	1.87	0.57
3:2:358:ASN:OD1	3:2:359:ALA:N	2.38	0.57
6:7:628:ALA:HB2	8:9:694:HIS:ND1	2.20	0.57
3:2:629:GLU:OE1	8:9:674:ARG:NH2	2.38	0.56
8:9:455:ILE:HG12	8:9:508:TYR:HB3	1.86	0.56
3:2:212:MET:HG2	3:2:249:ALA:HB2	1.87	0.56
8:9:448:ASN:ND2	8:9:477:MET:HG3	2.20	0.56
5:5:32:ASP:OD2	5:5:119:ARG:NH2	2.38	0.56
7:8:34:GLN:HG3	8:9:179:LEU:HD21	1.88	0.56
8:9:490:TYR:HA	8:9:533:LEU:HD21	1.87	0.56
8:9:549:THR:HG22	8:9:600:ARG:HG3	1.87	0.56
3:2:216:ARG:HG2	3:2:230:ASP:OD1	2.06	0.56
5:5:76:ILE:HA	5:5:99:THR:HG22	1.86	0.56
8:9:392:ILE:O	8:9:395:VAL:HG12	2.06	0.56
2:1:357:ILE:HG22	2:1:365:ASN:HB2	1.87	0.56
5:5:29:VAL:H	5:5:54:ASN:HB2	1.71	0.56
6:7:694:PRO:HA	6:7:697:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:232:THR:O	3:2:232:THR:HG22	2.05	0.56
2:1:519:VAL:HG22	2:1:568:VAL:HG22	1.86	0.56
6:7:184:ILE:HG21	6:7:219:ILE:HG21	1.88	0.56
8:9:14:LEU:HD11	8:9:52:PHE:HZ	1.71	0.56
8:9:154:ILE:HD12	8:9:164:PHE:CE2	2.41	0.56
2:1:386:ASN:HB3	2:1:402:LEU:HB3	1.88	0.55
7:8:387:TYR:HE2	7:8:422:ASN:ND2	2.03	0.55
3:2:240:SER:OG	3:2:241:LYS:N	2.39	0.55
4:4:136:GLU:O	4:4:140:ASN:ND2	2.26	0.55
6:7:216:LEU:O	6:7:231:GLU:HG3	2.06	0.55
4:4:173:MET:O	4:4:177:ILE:HG13	2.05	0.55
8:9:779:LEU:O	8:9:783:CYS:HB2	2.07	0.55
2:1:26:PHE:HB2	2:1:98:LEU:HG	1.88	0.55
5:5:262:ILE:HG22	5:5:264:GLY:H	1.70	0.55
7:8:176:LYS:HG3	7:8:177:LEU:HD12	1.89	0.55
8:9:642:LEU:HD11	8:9:812:ILE:HG22	1.88	0.55
3:2:377:ILE:HD11	3:2:410:THR:HG21	1.87	0.55
6:7:66:ILE:HD12	6:7:84:ILE:HD12	1.88	0.55
3:2:513:TRP:HE3	3:2:514:LEU:HD12	1.70	0.55
3:2:679:ILE:HD11	3:2:702:ILE:HD12	1.88	0.55
6:7:377:PRO:HG3	6:7:478:PRO:HG2	1.89	0.55
7:8:56:ASP:HB2	7:8:252:LYS:HE3	1.89	0.55
7:8:8:TRP:CZ3	8:9:136:CYS:HB2	2.41	0.55
8:9:333:VAL:O	8:9:334:ARG:NH1	2.40	0.55
3:2:411:ILE:HB	3:2:462:GLY:O	2.07	0.55
3:2:434:VAL:HA	3:2:437:LEU:HD13	1.88	0.55
5:5:64:LEU:HD13	8:9:377:ASN:HD21	1.72	0.55
6:7:521:HIS:O	6:7:525:VAL:HG23	2.07	0.55
2:1:336:LEU:HB2	2:1:347:MET:HG3	1.89	0.54
8:9:187:SER:HB2	8:9:250:ILE:HD13	1.88	0.54
8:9:191:ASP:OD2	8:9:208:GLN:NE2	2.40	0.54
2:1:569:LEU:HB3	2:1:576:PRO:HA	1.88	0.54
6:7:696:LEU:O	6:7:700:LEU:HG	2.08	0.54
7:8:278:VAL:HG13	7:8:304:VAL:HG13	1.89	0.54
4:4:253:ASP:O	4:4:257:THR:HG23	2.08	0.54
6:7:181:THR:HG22	6:7:182:TYR:HD1	1.72	0.54
6:7:72:GLY:O	6:7:81:LYS:HB2	2.07	0.54
6:7:288:SER:HB2	6:7:310:TYR:HB2	1.87	0.54
1:0:7:MET:HE3	1:0:7:MET:HA	1.90	0.54
7:8:135:ARG:HG2	7:8:136:PRO:HD2	1.90	0.54
7:8:234:PHE:HB2	7:8:250:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:39:LEU:H	2:1:39:LEU:HD23	1.72	0.54
2:1:53:GLY:N	2:1:381:TYR:OH	2.41	0.54
6:7:84:ILE:HD11	6:7:91:ARG:HD3	1.90	0.54
6:7:245:ASP:OD1	6:7:246:SER:N	2.40	0.54
8:9:652:HIS:ND1	8:9:769:GLU:OE2	2.30	0.54
7:8:350:ASN:ND2	7:8:388:ASN:OD1	2.38	0.54
7:8:478:GLU:OE2	7:8:488:GLN:NE2	2.30	0.54
1:0:13:PRO:CD	4:4:343:LEU:HD21	2.38	0.53
3:2:454:ASP:OD1	3:2:454:ASP:N	2.41	0.53
6:7:124:SER:OG	6:7:125:ALA:N	2.42	0.53
7:8:219:LYS:HD3	7:8:249:TYR:CZ	2.42	0.53
3:2:184:GLU:HA	3:2:205:ILE:HG22	1.90	0.53
3:2:208:SER:HB2	3:2:220:ALA:HB3	1.89	0.53
5:5:78:ASN:HB3	5:5:98:LEU:HB3	1.90	0.53
6:7:143:SER:OG	6:7:173:ARG:NH1	2.41	0.53
2:1:32:TYR:CE2	2:1:380:ARG:HD3	2.44	0.53
4:4:113:LEU:HD22	7:8:467:LEU:HD12	1.90	0.53
2:1:97:ASN:HB3	2:1:99:LYS:HG3	1.90	0.53
8:9:610:TRP:HB2	8:9:733:LEU:HB2	1.91	0.53
2:1:534:PHE:HB3	8:9:460:TYR:CE2	2.44	0.53
5:5:35:ASP:OD1	5:5:36:SER:N	2.41	0.53
6:7:420:VAL:HG23	6:7:423:ASN:HB2	1.91	0.53
7:8:54:ASP:O	7:8:111:PRO:HG2	2.09	0.53
8:9:491:LEU:HB2	8:9:534:VAL:HG12	1.89	0.53
6:7:569:ASN:OD1	6:7:571:SER:N	2.41	0.53
5:5:144:SER:OG	5:5:145:ALA:N	2.40	0.53
6:7:619:LEU:HD11	6:7:659:GLU:HB2	1.90	0.53
2:1:13:ASN:O	2:1:49:LYS:NZ	2.42	0.52
6:7:476:ILE:HG22	6:7:478:PRO:HD2	1.91	0.52
2:1:343:LEU:HD13	2:1:364:LEU:HD13	1.90	0.52
5:5:195:ASP:OD1	5:5:195:ASP:N	2.42	0.52
5:5:220:LEU:HB2	5:5:243:LEU:HD11	1.92	0.52
6:7:435:GLU:HG2	6:7:436:SER:N	2.24	0.52
2:1:440:ARG:NH1	8:9:367:GLN:HG2	2.25	0.52
3:2:387:LEU:CD1	3:2:478:LEU:HD23	2.29	0.52
4:4:42:TYR:HB3	4:4:51:CYS:HB2	1.91	0.52
8:9:27:LEU:HD21	8:9:336:GLY:HA3	1.91	0.52
5:5:157:GLN:NE2	5:5:266:ASP:OD1	2.43	0.52
6:7:601:SER:O	6:7:605:THR:HG23	2.10	0.52
8:9:10:TRP:CD2	8:9:54:PRO:HB3	2.44	0.52
3:2:426:GLU:HG2	6:7:428:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:653:PHE:HE1	8:9:802:PRO:HD2	1.74	0.52
3:2:181:VAL:HG21	3:2:191:PHE:HD2	1.75	0.52
3:2:253:ASN:OD1	3:2:253:ASN:N	2.40	0.52
6:7:3:LEU:HD11	6:7:250:VAL:HG12	1.90	0.52
6:7:630:LYS:HA	6:7:633:GLN:HG2	1.92	0.52
2:1:508:THR:O	2:1:508:THR:OG1	2.28	0.52
3:2:87:LEU:HD22	3:2:89:TYR:HE1	1.74	0.52
6:7:342:ILE:O	6:7:346:ARG:HG2	2.10	0.52
6:7:583:GLU:HB3	6:7:587:ARG:HH21	1.75	0.52
8:9:559:LEU:HD21	8:9:590:LEU:HG	1.92	0.52
3:2:144:LEU:O	3:2:156:TRP:HA	2.10	0.51
3:2:194:ASP:OD1	3:2:194:ASP:C	2.49	0.51
3:2:499:VAL:HG11	3:2:685:LEU:HD21	1.90	0.51
2:1:200:ILE:HG21	2:1:221:LEU:HD23	1.93	0.51
3:2:204:GLU:HG3	3:2:205:ILE:H	1.75	0.51
6:7:129:TYR:HD2	6:7:141:TYR:HB3	1.75	0.51
7:8:58:GLU:HG2	7:8:63:MET:HG3	1.93	0.51
8:9:80:GLN:OE1	8:9:138:MET:N	2.43	0.51
8:9:197:SER:OG	8:9:198:SER:N	2.43	0.51
2:1:12:ALA:O	2:1:396:GLY:N	2.40	0.51
6:7:359:GLU:HA	6:7:362:LYS:HB3	1.92	0.51
7:8:20:ALA:O	7:8:24:THR:HG23	2.10	0.51
8:9:297:SER:OG	8:9:298:GLU:N	2.43	0.51
2:1:15:HIS:O	2:1:38:ASP:HB2	2.10	0.51
6:7:584:ALA:O	6:7:588:LYS:N	2.44	0.51
8:9:157:VAL:HG23	8:9:181:PRO:HG3	1.92	0.51
2:1:326:MET:HG3	2:1:330:ILE:HD11	1.93	0.51
3:2:344:LYS:O	3:2:348:LEU:HG	2.11	0.51
4:4:396:GLN:HA	4:4:399:GLU:HG2	1.92	0.51
5:5:41:LYS:HG2	5:5:107:GLU:O	2.11	0.51
6:7:265:MET:HG2	6:7:284:THR:HG22	1.92	0.51
6:7:230:TRP:NE1	6:7:275:ASN:O	2.43	0.51
6:7:643:ILE:HG23	6:7:645:GLU:HG2	1.93	0.51
7:8:398:ASP:OD1	7:8:398:ASP:N	2.44	0.51
3:2:137:ILE:HA	3:2:146:GLY:HA2	1.92	0.51
5:5:50:LEU:HD21	5:5:57:ILE:HD11	1.92	0.51
5:5:55:LEU:HD11	5:5:263:PHE:CE2	2.46	0.51
3:2:549:LYS:NZ	3:2:555:THR:OG1	2.44	0.50
3:2:655:LEU:O	3:2:659:LYS:HG2	2.11	0.50
6:7:64:GLN:HB2	6:7:86:ALA:HB1	1.93	0.50
2:1:328:ALA:HB3	2:1:350:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:287:SER:OG	3:2:288:ALA:N	2.43	0.50
2:1:260:GLU:OE2	2:1:262:ARG:NH2	2.38	0.50
8:9:272:LYS:HD2	8:9:276:GLN:HG3	1.93	0.50
8:9:652:HIS:NE2	8:9:762:ASP:OD2	2.45	0.50
3:2:181:VAL:HG21	3:2:191:PHE:CD2	2.46	0.50
3:2:713:ILE:HD12	3:2:717:GLY:HA3	1.92	0.50
6:7:230:TRP:HZ3	6:7:232:ILE:HG13	1.76	0.50
7:8:403:HIS:NE2	7:8:427:GLU:OE2	2.40	0.50
8:9:106:TYR:HE1	8:9:125:LEU:HD12	1.75	0.50
8:9:620:LEU:HD13	8:9:632:PHE:HZ	1.77	0.50
2:1:355:VAL:HB	2:1:367:ILE:HG22	1.94	0.50
2:1:564:ILE:HD12	2:1:584:MET:HE3	1.92	0.50
6:7:416:ASP:HB2	6:7:459:ARG:HB3	1.92	0.50
8:9:149:ARG:HG2	8:9:166:GLN:NE2	2.27	0.50
8:9:590:LEU:HD13	8:9:601:ILE:HG13	1.93	0.50
2:1:5:ASP:OD1	2:1:5:ASP:N	2.44	0.50
6:7:458:ILE:HD13	6:7:468:LEU:HD11	1.93	0.50
3:2:411:ILE:HG21	3:2:437:LEU:HD23	1.94	0.50
5:5:105:ARG:HB3	5:5:304:ALA:HB3	1.93	0.50
2:1:4:LEU:HD13	3:2:298:ARG:HH12	1.76	0.50
3:2:338:ILE:HG22	6:7:341:LYS:HZ3	1.76	0.50
6:7:500:ILE:HD13	6:7:555:GLU:HB2	1.94	0.50
7:8:79:SER:OG	7:8:258:ASP:OD2	2.28	0.50
1:0:8:PHE:CE2	4:4:420:VAL:HG22	2.47	0.49
7:8:250:LEU:HB3	7:8:266:LEU:HD21	1.93	0.49
2:1:488:LEU:HD13	2:1:505:LEU:HD13	1.93	0.49
3:2:347:ASN:ND2	6:7:402:THR:HG22	2.27	0.49
6:7:405:ASP:OD2	6:7:406:ASN:ND2	2.45	0.49
2:1:16:THR:HB	2:1:38:ASP:HB3	1.94	0.49
3:2:192:LYS:HG3	3:2:197:VAL:HG21	1.94	0.49
3:2:285:PHE:HZ	3:2:315:ARG:HG2	1.78	0.49
5:5:253:LEU:HA	5:5:256:VAL:HG12	1.94	0.49
2:1:435:VAL:HA	2:1:438:THR:HG22	1.94	0.49
7:8:38:ILE:O	7:8:42:ARG:HG2	2.13	0.49
6:7:583:GLU:HB3	6:7:587:ARG:NH2	2.27	0.49
3:2:44:ASN:HB3	3:2:45:PRO:HD3	1.95	0.49
3:2:195:GLU:HG2	3:2:196:ILE:N	2.27	0.49
3:2:383:HIS:CE1	3:2:461:VAL:CG1	2.96	0.49
4:4:363:GLU:O	4:4:366:ARG:HG2	2.13	0.49
6:7:49:MET:HB2	6:7:297:VAL:O	2.11	0.49
6:7:148:ASN:ND2	6:7:190:PRO:O	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:610:TRP:HA	8:9:613:THR:HG22	1.95	0.49
2:1:66:PRO:HA	2:1:87:ALA:O	2.13	0.49
3:2:268:LYS:HG2	3:2:270:ASP:OD2	2.13	0.49
3:2:495:PRO:HB3	3:2:559:ASP:HB3	1.95	0.49
8:9:204:SER:O	8:9:236:ASP:HB3	2.13	0.49
3:2:592:GLU:O	3:2:596:VAL:HG23	2.12	0.49
5:5:90:GLY:HA3	5:5:115:PRO:HB2	1.94	0.49
4:4:74:ALA:HB2	4:4:89:LEU:HB2	1.94	0.49
8:9:20:PHE:CE2	8:9:352:GLY:HA2	2.48	0.48
6:7:648:CYS:SG	6:7:649:ILE:N	2.85	0.48
3:2:548:ILE:HD12	3:2:554:ILE:HG12	1.94	0.48
4:4:419:GLU:O	4:4:422:GLN:NE2	2.39	0.48
4:4:373:LEU:HD13	4:4:413:PHE:HD1	1.78	0.48
8:9:328:HIS:ND1	8:9:349:SER:HB2	2.28	0.48
5:5:328:LYS:HG3	5:5:329:ASP:H	1.77	0.48
6:7:234:ASN:HD22	6:7:238:ARG:HA	1.78	0.48
8:9:312:LEU:HG	8:9:326:LEU:HD11	1.95	0.48
8:9:739:GLY:HA3	8:9:749:ILE:HD11	1.95	0.48
5:5:77:LEU:HD11	5:5:100:LYS:HB2	1.96	0.48
8:9:349:SER:OG	8:9:350:ASP:N	2.46	0.48
4:4:168:ASP:OD1	4:4:169:LEU:N	2.46	0.48
7:8:280:LEU:O	7:8:284:ILE:HG13	2.14	0.48
4:4:387:GLU:CD	4:4:390:ASP:H	2.17	0.48
6:7:603:LYS:HD2	6:7:607:LYS:HZ2	1.78	0.48
5:5:79:ILE:HD11	5:5:95:LEU:HD11	1.96	0.48
5:5:152:LEU:HD13	5:5:188:VAL:HG21	1.96	0.48
6:7:346:ARG:HD3	6:7:349:LEU:HD21	1.95	0.48
6:7:622:LYS:O	6:7:626:ILE:HG23	2.14	0.48
8:9:26:CYS:SG	8:9:27:LEU:N	2.87	0.48
2:1:338:GLN:HG2	2:1:341:ARG:HB3	1.96	0.47
4:4:389:ARG:N	4:4:389:ARG:HD2	2.29	0.47
6:7:158:LEU:HD21	6:7:160:ARG:HG2	1.95	0.47
7:8:121:ILE:O	7:8:125:ILE:HG12	2.14	0.47
8:9:411:LEU:HD21	8:9:446:LEU:HB2	1.95	0.47
8:9:617:ILE:O	8:9:621:GLN:HG2	2.14	0.47
2:1:333:MET:HG2	2:1:348:ALA:HA	1.95	0.47
3:2:141:ASN:HD22	3:2:673:LYS:HB2	1.79	0.47
3:2:341:LEU:HB3	6:7:345:LEU:HD21	1.96	0.47
5:5:27:GLY:CA	5:5:261:PRO:HD2	2.44	0.47
7:8:250:LEU:HG	7:8:254:TYR:CE2	2.49	0.47
2:1:26:PHE:CE1	2:1:84:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:266:ALA:HB1	2:1:292:PRO:HG2	1.96	0.47
4:4:43:TYR:OH	4:4:75:LEU:HB3	2.14	0.47
7:8:369:PHE:CE2	7:8:392:VAL:HG21	2.48	0.47
3:2:133:SER:OG	3:2:148:ASN:OD1	2.27	0.47
6:7:18:GLN:HA	6:7:290:THR:OG1	2.14	0.47
6:7:360:ARG:HE	6:7:477:GLN:HG2	1.79	0.47
6:7:648:CYS:O	6:7:652:GLU:HG3	2.14	0.47
7:8:175:PRO:HA	7:8:178:ALA:HB3	1.95	0.47
3:2:9:LYS:NZ	3:2:10:LEU:O	2.47	0.47
6:7:175:LEU:HA	6:7:181:THR:H	1.79	0.47
8:9:464:PRO:HG3	8:9:495:TYR:CE2	2.49	0.47
2:1:472:GLU:OE2	8:9:512:THR:HG21	2.15	0.47
3:2:145:GLN:HG2	3:2:156:TRP:CD1	2.49	0.47
6:7:392:ALA:HB3	6:7:669:ARG:HH12	1.79	0.47
6:7:581:SER:O	6:7:585:THR:HG23	2.15	0.47
8:9:290:PHE:HB2	8:9:305:ILE:HG12	1.97	0.47
2:1:362:VAL:HG23	2:1:364:LEU:HD22	1.97	0.47
2:1:467:TYR:HE2	7:8:407:ARG:HD2	1.80	0.47
2:1:515:LEU:HD11	8:9:827:LEU:HD21	1.96	0.47
3:2:37:ALA:HB1	6:7:635:HIS:CE1	2.48	0.47
4:4:383:TYR:CZ	4:4:423:LYS:HD3	2.50	0.47
5:5:314:PRO:HA	5:5:325:GLU:HA	1.96	0.47
6:7:195:LEU:HB3	6:7:200:GLY:HA2	1.95	0.47
6:7:248:ASP:HB2	6:7:255:LYS:HA	1.97	0.47
6:7:500:ILE:HB	6:7:553:GLN:HG2	1.97	0.47
6:7:632:LEU:HD23	6:7:641:PHE:CE2	2.47	0.47
7:8:484:HIS:O	7:8:488:GLN:HG2	2.14	0.47
8:9:68:LEU:HD11	8:9:71:GLU:HB2	1.96	0.47
6:7:338:MET:O	6:7:341:LYS:HG3	2.15	0.47
8:9:758:PRO:HG2	8:9:759:LEU:HD23	1.96	0.47
3:2:23:ARG:HA	3:2:29:PRO:HA	1.97	0.47
3:2:549:LYS:HD2	3:2:553:GLU:HB2	1.97	0.47
4:4:356:ASN:HA	4:4:359:ARG:HG2	1.95	0.47
5:5:106:PHE:HZ	5:5:299:PHE:HD2	1.63	0.47
6:7:208:LEU:HA	6:7:217:GLY:O	2.15	0.47
6:7:704:ASP:HB3	6:7:707:ALA:HB3	1.97	0.47
8:9:724:PHE:HE1	8:9:768:TRP:HB2	1.80	0.47
2:1:296:VAL:HG11	2:1:346:VAL:HG22	1.97	0.47
5:5:238:ASP:HB3	5:5:239:PRO:HD3	1.97	0.47
6:7:269:TYR:HD1	6:7:277:PRO:HB2	1.79	0.47
3:2:97:GLN:O	3:2:119:GLY:HA2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:315:VAL:HG11	5:5:326:LYS:HE2	1.95	0.46
6:7:700:LEU:O	6:7:703:TYR:HB2	2.15	0.46
5:5:79:ILE:HD13	5:5:97:VAL:HG22	1.97	0.46
6:7:602:VAL:HG13	6:7:677:LEU:HD21	1.96	0.46
8:9:589:THR:HB	8:9:602:GLN:HG2	1.96	0.46
3:2:309:SER:OG	3:2:311:ASP:OD2	2.28	0.46
4:4:136:GLU:OE1	4:4:140:ASN:ND2	2.33	0.46
5:5:76:ILE:HD11	5:5:128:HIS:CD2	2.51	0.46
8:9:88:SER:HA	8:9:166:GLN:NE2	2.30	0.46
8:9:318:VAL:O	8:9:318:VAL:CG1	2.64	0.46
8:9:672:GLN:O	8:9:676:ILE:HG13	2.16	0.46
3:2:108:ASN:H	7:8:78:THR:HB	1.79	0.46
3:2:390:SER:O	3:2:398:ALA:N	2.48	0.46
3:2:483:MET:HB3	3:2:538:LEU:HB2	1.98	0.46
6:7:176:GLN:NE2	6:7:179:ASP:OD2	2.48	0.46
8:9:16:ASP:OD1	8:9:16:ASP:N	2.46	0.46
3:2:171:PHE:CE2	3:2:190:VAL:HG21	2.51	0.46
4:4:51:CYS:SG	4:4:76:ILE:HD11	2.56	0.46
5:5:203:TYR:CD1	5:5:206:ILE:HD12	2.48	0.46
6:7:13:VAL:HG22	6:7:14:GLY:H	1.81	0.46
8:9:453:GLN:HB3	8:9:476:PHE:CE1	2.51	0.46
1:0:8:PHE:HE1	4:4:419:GLU:HB3	1.81	0.46
2:1:473:SER:HB3	2:1:475:LEU:HG	1.97	0.46
4:4:273:TRP:HB2	4:4:296:ALA:HB2	1.98	0.46
4:4:314:HIS:CD2	4:4:319:GLN:HG3	2.48	0.46
8:9:333:VAL:HG12	8:9:347:THR:HG22	1.97	0.46
2:1:522:LEU:HD11	2:1:567:LEU:HD11	1.96	0.46
2:1:458:LEU:HD21	8:9:376:LEU:HD11	1.98	0.46
3:2:172:ASP:N	3:2:231:LYS:HE2	2.30	0.46
4:4:362:GLU:HG2	4:4:366:ARG:HH21	1.80	0.46
5:5:206:ILE:HG23	5:5:222:ILE:HG23	1.98	0.46
6:7:194:ALA:O	6:7:208:LEU:HB3	2.16	0.46
6:7:647:ARG:O	6:7:651:GLU:HG2	2.14	0.46
8:9:15:GLY:HA3	8:9:18:GLU:HG3	1.97	0.46
3:2:6:PHE:CZ	3:2:316:GLY:HA3	2.50	0.46
8:9:41:ILE:HG23	8:9:51:ILE:HG12	1.98	0.46
3:2:504:ALA:O	3:2:505:GLU:HG2	2.16	0.45
5:5:76:ILE:HG22	5:5:99:THR:HG22	1.97	0.45
6:7:193:LEU:HD12	6:7:207:LEU:HD21	1.97	0.45
6:7:247:PHE:O	6:7:256:ASP:HB2	2.15	0.45
2:1:331:LEU:HD23	4:4:45:GLN:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:318:VAL:O	8:9:318:VAL:HG12	2.15	0.45
8:9:475:GLU:OE1	8:9:475:GLU:N	2.42	0.45
2:1:59:GLN:O	2:1:59:GLN:HG2	2.16	0.45
3:2:461:VAL:HG23	3:2:470:HIS:HB2	1.98	0.45
3:2:559:ASP:N	3:2:559:ASP:OD1	2.47	0.45
4:4:85:GLU:O	4:4:88:ARG:HG2	2.16	0.45
3:2:285:PHE:CD2	3:2:289:ILE:HD11	2.51	0.45
3:2:692:ASN:O	3:2:696:THR:HG23	2.17	0.45
4:4:266:VAL:HG23	4:4:266:VAL:O	2.16	0.45
6:7:413:VAL:HG13	6:7:464:GLN:HB3	1.98	0.45
7:8:212:TRP:O	7:8:216:GLN:HG2	2.16	0.45
3:2:484:TYR:HB3	3:2:535:PHE:HB3	1.98	0.45
6:7:494:HIS:O	6:7:529:PRO:HG2	2.16	0.45
7:8:231:GLU:HB2	7:8:253:VAL:HG11	1.99	0.45
8:9:673:PHE:HE1	8:9:703:TYR:HB2	1.80	0.45
8:9:823:GLY:O	8:9:824:ARG:NH1	2.48	0.45
2:1:16:THR:OG1	2:1:20:CYS:SG	2.68	0.45
6:7:196:HIS:O	6:7:196:HIS:ND1	2.50	0.45
6:7:263:ASP:OD1	6:7:263:ASP:N	2.49	0.45
3:2:344:LYS:HA	3:2:347:ASN:OD1	2.16	0.45
4:4:409:SER:HB2	4:4:414:ASP:OD2	2.15	0.45
8:9:304:LEU:HD11	8:9:312:LEU:HD13	1.97	0.45
8:9:535:CYS:SG	8:9:580:PHE:HB3	2.56	0.45
3:2:192:LYS:HB2	3:2:195:GLU:HB3	1.98	0.45
3:2:513:TRP:HB2	3:2:574:PHE:CE1	2.51	0.45
6:7:37:VAL:HG11	6:7:314:ILE:HD13	1.99	0.45
6:7:288:SER:OG	6:7:399:GLU:OE2	2.31	0.45
7:8:179:LYS:HD2	8:9:200:HIS:CD2	2.52	0.45
8:9:263:LEU:HB2	8:9:290:PHE:CD1	2.52	0.45
2:1:218:CYS:SG	2:1:233:PRO:HG3	2.56	0.45
3:2:579:ASP:OD1	3:2:580:LEU:N	2.50	0.45
4:4:325:HIS:HE2	7:8:396:THR:HA	1.81	0.45
7:8:271:LEU:HD21	7:8:281:LEU:HG	1.99	0.45
8:9:307:ASN:OD1	8:9:311:MET:HB3	2.17	0.45
2:1:434:TYR:OH	4:4:290:ILE:HD11	2.17	0.45
3:2:96:THR:HB	3:2:99:ASN:HB2	1.99	0.45
6:7:415:ILE:HG23	6:7:458:ILE:HG23	1.98	0.45
8:9:250:ILE:HG12	8:9:260:VAL:HG13	1.99	0.45
8:9:695:LEU:HD23	8:9:695:LEU:HA	1.74	0.45
2:1:234:GLU:HB2	2:1:236:PHE:CE2	2.51	0.44
3:2:212:MET:HE2	3:2:260:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:250:VAL:HG23	6:7:252:ASP:OD2	2.17	0.44
6:7:693:VAL:O	6:7:696:LEU:HG	2.17	0.44
8:9:103:LEU:HD21	8:9:152:ILE:HD11	1.99	0.44
2:1:245:PRO:HD3	2:1:282:PRO:HG3	1.98	0.44
2:1:356:ARG:HA	2:1:365:ASN:O	2.16	0.44
2:1:428:PRO:HG3	4:4:295:ARG:NH2	2.32	0.44
3:2:447:PRO:HD2	3:2:483:MET:SD	2.57	0.44
6:7:196:HIS:O	6:7:196:HIS:CG	2.70	0.44
6:7:503:ASP:OD1	6:7:503:ASP:N	2.46	0.44
8:9:245:ALA:HA	8:9:264:GLY:HA2	1.99	0.44
2:1:220:VAL:HG22	2:1:230:VAL:HG22	1.99	0.44
8:9:556:PRO:HD3	8:9:597:GLN:HA	2.00	0.44
1:0:41:LEU:HD11	7:8:134:ALA:HB1	1.99	0.44
3:2:204:GLU:HG2	3:2:222:SER:HB2	1.99	0.44
3:2:522:GLU:H	3:2:522:GLU:CD	2.21	0.44
4:4:183:ASP:OD1	4:4:184:LEU:N	2.50	0.44
4:4:195:VAL:HG22	4:4:204:LEU:HB3	2.00	0.44
3:2:226:VAL:O	3:2:237:ARG:HA	2.17	0.44
4:4:54:VAL:O	4:4:57:GLU:HG2	2.18	0.44
6:7:292:ILE:O	6:7:293:GLN:HG2	2.18	0.44
6:7:354:TYR:O	6:7:357:LEU:HG	2.17	0.44
7:8:67:GLU:OE2	7:8:69:ALA:N	2.51	0.44
5:5:74:ASN:HB2	5:5:131:TYR:OH	2.18	0.44
5:5:131:TYR:O	5:5:138:ARG:NH1	2.37	0.44
6:7:22:LYS:HD3	6:7:293:GLN:NE2	2.32	0.44
6:7:202:ASP:OD1	6:7:202:ASP:N	2.50	0.44
8:9:135:ALA:HA	8:9:156:SER:HA	2.00	0.44
8:9:817:ASP:OD1	8:9:818:ARG:N	2.50	0.44
1:0:19:TYR:HD2	4:4:274:ASN:HD22	1.66	0.44
2:1:106:LEU:HD23	2:1:107:PRO:HD2	1.98	0.44
3:2:234:ARG:HD2	3:2:237:ARG:HD3	2.00	0.44
8:9:40:ILE:HG21	8:9:354:LEU:HD21	1.99	0.44
8:9:387:GLU:O	8:9:391:VAL:HG23	2.18	0.44
3:2:416:LEU:HD23	3:2:429:VAL:HG22	2.00	0.44
3:2:561:ILE:HD11	3:2:681:ARG:HD3	2.00	0.44
7:8:46:GLU:HA	7:8:49:TYR:HB2	2.00	0.44
8:9:292:PRO:HA	8:9:303:THR:HA	2.00	0.44
4:4:337:MET:HB3	4:4:340:LEU:HD12	1.99	0.44
6:7:42:GLY:HA2	6:7:64:GLN:O	2.18	0.44
6:7:172:LEU:HB2	6:7:184:ILE:HB	1.98	0.44
2:1:349:ALA:HB1	2:1:373:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:226:GLY:O	4:4:230:THR:HG23	2.18	0.43
6:7:217:GLY:C	6:7:218:LEU:HD12	2.38	0.43
7:8:71:ALA:HB3	7:8:74:PRO:HG3	1.99	0.43
2:1:5:ASP:HA	2:1:400:LYS:HD3	1.99	0.43
5:5:50:LEU:HD12	5:5:59:TRP:HB2	2.00	0.43
6:7:235:GLU:O	6:7:238:ARG:NH2	2.51	0.43
2:1:23:LEU:HD12	2:1:34:LEU:HD13	2.01	0.43
2:1:252:GLU:OE2	2:1:297:GLY:N	2.50	0.43
3:2:383:HIS:CE1	3:2:461:VAL:HG13	2.53	0.43
3:2:513:TRP:CE3	3:2:514:LEU:HD12	2.51	0.43
6:7:275:ASN:OD1	6:7:276:GLU:N	2.51	0.43
6:7:281:PHE:HE2	6:7:317:LEU:HD13	1.83	0.43
8:9:14:LEU:HD12	8:9:14:LEU:HA	1.77	0.43
2:1:64:ASP:HB2	2:1:88:SER:OG	2.17	0.43
4:4:169:LEU:HD23	4:4:169:LEU:HA	1.89	0.43
4:4:375:ASN:HB2	4:4:398:MET:HB2	2.00	0.43
6:7:491:LEU:HB3	6:7:494:HIS:ND1	2.33	0.43
8:9:610:TRP:O	8:9:613:THR:HG22	2.18	0.43
2:1:47:ARG:HG2	2:1:61:PRO:HA	2.00	0.43
3:2:438:SER:OG	3:2:439:SER:N	2.50	0.43
5:5:325:GLU:HG2	8:9:361:THR:H	1.84	0.43
6:7:131:HIS:HB3	6:7:139:HIS:HB2	2.00	0.43
6:7:270:GLY:O	6:7:277:PRO:HA	2.19	0.43
6:7:346:ARG:O	6:7:349:LEU:HG	2.18	0.43
6:7:493:LEU:HD12	6:7:493:LEU:HA	1.86	0.43
3:2:16:PRO:HB2	3:2:17:ARG:HD2	2.01	0.43
3:2:271:ALA:HB3	3:2:281:PHE:HB3	2.00	0.43
6:7:144:GLY:HA2	6:7:534:LYS:NZ	2.33	0.43
6:7:193:LEU:HA	6:7:209:PHE:HA	2.01	0.43
7:8:99:THR:HG23	7:8:105:ILE:HG22	1.99	0.43
7:8:475:LYS:HD3	7:8:475:LYS:HA	1.77	0.43
8:9:747:ASP:OD1	8:9:747:ASP:N	2.51	0.43
1:0:13:PRO:HD2	4:4:343:LEU:HD21	1.99	0.43
2:1:33:LYS:HG2	2:1:52:LYS:HE2	2.01	0.43
2:1:381:TYR:HB3	2:1:387:THR:HG21	2.01	0.43
4:4:258:LYS:O	4:4:261:VAL:HB	2.18	0.43
5:5:9:GLU:HG2	5:5:56:ARG:NH2	2.34	0.43
6:7:39:ASP:OD1	6:7:40:HIS:N	2.51	0.43
6:7:143:SER:HB3	6:7:147:ILE:HD11	2.00	0.43
4:4:99:GLN:HA	4:4:130:LEU:HD11	2.01	0.43
4:4:103:ASN:O	4:4:107:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:60:THR:HG21	6:7:91:ARG:HH22	1.84	0.43
6:7:103:PHE:CE2	6:7:105:THR:HB	2.54	0.43
6:7:151:ILE:HD12	6:7:194:ALA:HA	2.01	0.43
8:9:19:GLU:HB3	8:9:45:PHE:HB2	2.00	0.43
8:9:41:ILE:HG21	8:9:95:LEU:HD11	2.01	0.43
6:7:5:LEU:CA	6:7:318:THR:O	2.64	0.43
6:7:24:LEU:HD23	6:7:71:LEU:HD22	2.01	0.43
7:8:424:ALA:HB2	7:8:439:LEU:HB2	2.00	0.43
6:7:613:LEU:HG	6:7:670:LEU:HD13	2.01	0.43
8:9:752:LEU:HD21	8:9:815:PHE:CE1	2.54	0.43
3:2:107:ASN:HA	7:8:78:THR:HG21	2.01	0.42
3:2:166:LEU:HD23	3:2:181:VAL:HA	2.01	0.42
3:2:192:LYS:HG3	3:2:197:VAL:CG2	2.48	0.42
3:2:413:ARG:O	3:2:432:PRO:HD2	2.19	0.42
3:2:432:PRO:HA	6:7:437:ASN:ND2	2.33	0.42
4:4:71:TYR:OH	4:4:102:ASP:OD1	2.21	0.42
4:4:104:LEU:HD13	4:4:126:GLU:HG3	2.01	0.42
6:7:411:SER:HB3	6:7:441:LEU:HB3	2.00	0.42
6:7:604:HIS:HA	6:7:607:LYS:HZ3	1.84	0.42
7:8:65:LEU:HD22	8:9:678:ARG:HD2	2.01	0.42
7:8:305:LEU:HA	7:8:305:LEU:HD23	1.75	0.42
3:2:101:LEU:HD13	3:2:113:TYR:HD1	1.84	0.42
3:2:344:LYS:HZ1	6:7:349:LEU:HB2	1.85	0.42
8:9:686:ASP:OD1	8:9:688:THR:N	2.52	0.42
8:9:741:TRP:CH2	8:9:820:ALA:HB2	2.54	0.42
2:1:293:VAL:HG12	4:4:44:ILE:HG12	2.01	0.42
3:2:413:ARG:HD3	3:2:437:LEU:HD21	2.01	0.42
6:7:145:ASP:OD2	6:7:146:LYS:N	2.52	0.42
7:8:7:ALA:HB2	7:8:22:LEU:HD22	2.00	0.42
8:9:193:PHE:CE2	8:9:207:TYR:HD1	2.37	0.42
8:9:735:ILE:HD11	8:9:756:PHE:HB2	2.01	0.42
5:5:59:TRP:O	5:5:68:ASN:HB2	2.19	0.42
8:9:140:TYR:CB	8:9:152:ILE:HG22	2.50	0.42
2:1:430:LYS:HA	2:1:430:LYS:HD3	1.86	0.42
6:7:16:THR:OG1	6:7:290:THR:HG21	2.20	0.42
6:7:151:ILE:HG22	6:7:164:VAL:HB	2.01	0.42
6:7:196:HIS:HB3	6:7:208:LEU:HB2	2.02	0.42
6:7:415:ILE:HG22	6:7:417:LEU:HD12	2.01	0.42
8:9:20:PHE:HE2	8:9:352:GLY:HA2	1.84	0.42
8:9:551:ASP:OD1	8:9:636:PHE:N	2.48	0.42
1:0:34:LEU:HD21	7:8:384:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:460:ARG:HG2	7:8:401:LEU:HD22	2.00	0.42
3:2:37:ALA:O	3:2:39:LYS:NZ	2.46	0.42
3:2:698:CYS:O	3:2:702:ILE:HG13	2.19	0.42
4:4:309:ASN:O	4:4:313:VAL:HG23	2.19	0.42
8:9:510:ARG:O	8:9:518:GLY:HA2	2.18	0.42
8:9:512:THR:HG23	8:9:515:ASN:H	1.83	0.42
3:2:33:ALA:HB3	3:2:41:PHE:CZ	2.54	0.42
6:7:254:VAL:HG13	6:7:255:LYS:N	2.32	0.42
6:7:512:THR:HG22	6:7:562:GLU:HB3	2.01	0.42
8:9:558:SER:HB2	8:9:576:ASN:HD21	1.85	0.42
2:1:567:LEU:HD23	2:1:579:SER:HB2	2.02	0.42
3:2:298:ARG:HD3	3:2:304:GLN:HE22	1.85	0.42
3:2:433:SER:H	6:7:437:ASN:HD22	1.68	0.42
5:5:137:TYR:CD1	5:5:264:GLY:HA3	2.54	0.42
6:7:391:ASP:OD2	6:7:392:ALA:N	2.51	0.42
7:8:318:ILE:HG22	7:8:322:HIS:CD2	2.55	0.42
8:9:328:HIS:CE1	8:9:347:THR:HG1	2.37	0.42
8:9:510:ARG:O	8:9:518:GLY:CA	2.68	0.42
8:9:606:PHE:CD2	8:9:644:GLU:HG3	2.54	0.42
3:2:142:CYS:O	3:2:158:VAL:HG23	2.20	0.42
8:9:103:LEU:HD13	8:9:154:ILE:HD11	2.02	0.42
5:5:333:LEU:HD23	5:5:333:LEU:HA	1.75	0.42
8:9:531:LEU:HB2	8:9:615:GLU:OE2	2.20	0.42
2:1:8:SER:HB2	3:2:8:LEU:HD22	2.02	0.41
3:2:346:GLN:O	3:2:350:LEU:HG	2.21	0.41
4:4:342:MET:O	4:4:346:VAL:HG23	2.20	0.41
6:7:689:VAL:O	6:7:693:VAL:HG23	2.20	0.41
8:9:456:LYS:NZ	8:9:458:SER:HB3	2.35	0.41
2:1:73:LEU:HD22	2:1:216:VAL:HA	2.02	0.41
2:1:272:ILE:HD11	2:1:286:ILE:HD12	2.01	0.41
3:2:647:LEU:HD23	3:2:647:LEU:HA	1.86	0.41
6:7:70:GLU:HG3	6:7:71:LEU:H	1.85	0.41
6:7:207:LEU:HD12	6:7:207:LEU:HA	1.89	0.41
8:9:693:GLN:O	8:9:697:THR:HG23	2.19	0.41
2:1:52:LYS:HE3	2:1:57:VAL:HG21	2.01	0.41
3:2:5:VAL:N	3:2:316:GLY:O	2.53	0.41
3:2:110:ASP:OD1	3:2:110:ASP:N	2.54	0.41
3:2:662:CYS:O	3:2:666:THR:HG23	2.20	0.41
4:4:187:ALA:HA	4:4:190:ILE:HG22	2.02	0.41
8:9:295:SER:HB3	8:9:301:ILE:HA	2.02	0.41
2:1:32:TYR:HE2	2:1:380:ARG:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:476:SER:HA	7:8:411:VAL:HG22	2.01	0.41
2:1:495:LEU:HD13	2:1:588:GLU:OE1	2.20	0.41
5:5:21:GLN:O	5:5:56:ARG:NH1	2.53	0.41
6:7:402:THR:HG21	6:7:476:ILE:HD11	2.02	0.41
6:7:241:ILE:HD13	6:7:261:ARG:HD3	2.03	0.41
8:9:382:ASP:O	8:9:386:LYS:HG2	2.21	0.41
8:9:470:ASP:OD1	8:9:470:ASP:N	2.52	0.41
3:2:501:PHE:CD2	3:2:580:LEU:HD21	2.55	0.41
4:4:346:VAL:O	4:4:350:ASN:ND2	2.51	0.41
5:5:147:ILE:HD11	5:5:150:LYS:HA	2.02	0.41
5:5:181:PHE:HB2	5:5:188:VAL:CG2	2.49	0.41
8:9:483:ARG:HD3	8:9:483:ARG:HA	1.86	0.41
2:1:291:GLN:O	2:1:307:ASN:HB2	2.21	0.41
2:1:433:LEU:HD11	7:8:333:ARG:HD2	2.03	0.41
3:2:561:ILE:HG22	3:2:586:PHE:CD1	2.55	0.41
6:7:489:LYS:HG3	6:7:529:PRO:HA	2.01	0.41
6:7:569:ASN:OD1	6:7:570:ILE:N	2.53	0.41
7:8:403:HIS:HE1	7:8:407:ARG:NH2	2.18	0.41
8:9:41:ILE:HD13	8:9:95:LEU:HD13	2.02	0.41
8:9:153:CYS:SG	8:9:161:LEU:HB3	2.61	0.41
8:9:175:LEU:HD23	8:9:175:LEU:HA	1.95	0.41
8:9:185:ALA:HB2	8:9:248:ILE:HG23	2.02	0.41
3:2:274:ASP:OD1	3:2:274:ASP:N	2.50	0.41
5:5:41:LYS:HA	5:5:41:LYS:HD2	1.87	0.41
5:5:161:TYR:CE2	5:5:184:ASN:HB3	2.55	0.41
7:8:15:ARG:NH2	8:9:350:ASP:OD2	2.54	0.41
8:9:14:LEU:HD11	8:9:50:ARG:HD2	2.03	0.41
2:1:86:ILE:HG12	2:1:93:TYR:HB2	2.03	0.41
2:1:225:ASN:O	2:1:227:GLU:N	2.54	0.41
2:1:234:GLU:HB2	2:1:236:PHE:HE2	1.86	0.41
2:1:390:MET:HB2	2:1:398:ILE:HB	2.03	0.41
3:2:128:LEU:HG	3:2:129:GLY:H	1.86	0.41
3:2:387:LEU:HD21	3:2:478:LEU:CD2	2.51	0.41
4:4:361:TYR:OH	4:4:377:ASN:HB3	2.21	0.41
5:5:262:ILE:O	5:5:263:PHE:HB2	2.19	0.41
7:8:381:GLU:O	7:8:385:VAL:HG23	2.21	0.41
8:9:43:GLY:HA3	8:9:78:ILE:HG21	2.01	0.41
8:9:123:ILE:HG13	8:9:123:ILE:O	2.20	0.41
8:9:552:THR:HB	8:9:632:PHE:HE1	1.85	0.41
8:9:747:ASP:O	8:9:751:ILE:HG13	2.20	0.41
2:1:231:LEU:HD22	2:1:238:ILE:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:247:VAL:HG23	2:1:268:ARG:HD2	2.02	0.41
3:2:654:LEU:HD23	3:2:654:LEU:HA	1.78	0.41
4:4:227:ASN:O	4:4:230:THR:OG1	2.24	0.41
5:5:61:SER:HB2	5:5:67:VAL:HG23	2.03	0.41
6:7:94:THR:HG22	6:7:98:LYS:O	2.21	0.41
6:7:661:LYS:HA	6:7:661:LYS:HD3	1.84	0.41
7:8:264:LEU:HD22	7:8:284:ILE:HG23	2.02	0.41
7:8:330:VAL:O	7:8:334:PHE:HD2	2.03	0.41
2:1:298:VAL:HG12	2:1:299:HIS:N	2.36	0.40
5:5:252:SER:HA	5:5:255:LYS:HE3	2.03	0.40
8:9:342:LYS:HB3	8:9:342:LYS:HE2	1.76	0.40
2:1:487:LYS:HB3	2:1:487:LYS:HE3	1.70	0.40
3:2:84:ASN:OD1	3:2:84:ASN:N	2.54	0.40
3:2:107:ASN:O	3:2:109:SER:N	2.50	0.40
3:2:689:LYS:HE2	3:2:689:LYS:HB3	1.85	0.40
5:5:137:TYR:OH	5:5:157:GLN:N	2.36	0.40
6:7:190:PRO:HA	6:7:211:THR:HA	2.04	0.40
6:7:610:HIS:HD1	6:7:703:TYR:HH	1.61	0.40
8:9:19:GLU:HG2	8:9:45:PHE:HD2	1.87	0.40
8:9:620:LEU:HD23	8:9:620:LEU:HA	1.97	0.40
3:2:73:GLN:HG2	8:9:686:ASP:OD2	2.21	0.40
3:2:289:ILE:HD13	3:2:289:ILE:HA	1.85	0.40
6:7:187:PRO:HB2	6:7:215:LYS:NZ	2.36	0.40
7:8:52:GLU:O	7:8:55:VAL:HG12	2.22	0.40
7:8:98:VAL:HA	7:8:104:PRO:HA	2.03	0.40
2:1:268:ARG:HG2	4:4:40:HIS:CD2	2.55	0.40
3:2:285:PHE:CZ	3:2:315:ARG:HG2	2.56	0.40
5:5:52:VAL:HG13	5:5:73:TYR:OH	2.21	0.40
8:9:739:GLY:HA2	8:9:744:LEU:HB2	2.02	0.40
8:9:801:ILE:HA	8:9:802:PRO:HD3	1.93	0.40
3:2:192:LYS:O	3:2:193:GLU:C	2.59	0.40
8:9:412:LYS:O	8:9:446:LEU:HA	2.22	0.40
8:9:646:PHE:CG	8:9:809:LYS:HG2	2.56	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	0	50/69 (72%)	50 (100%)	0	0	100	100
2	1	478/592 (81%)	435 (91%)	43 (9%)	0	100	100
3	2	649/721 (90%)	620 (96%)	29 (4%)	0	100	100
4	4	382/519 (74%)	362 (95%)	20 (5%)	0	100	100
5	5	294/341 (86%)	267 (91%)	27 (9%)	0	100	100
6	7	692/715 (97%)	629 (91%)	63 (9%)	0	100	100
7	8	469/501 (94%)	452 (96%)	17 (4%)	0	100	100
8	9	752/887 (85%)	705 (94%)	47 (6%)	0	100	100
All	All	3766/4345 (87%)	3520 (94%)	246 (6%)	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	0	49/65 (75%)	48 (98%)	1 (2%)	55	80
2	1	413/499 (83%)	411 (100%)	2 (0%)	88	94
3	2	567/618 (92%)	564 (100%)	3 (0%)	88	94
4	4	331/438 (76%)	331 (100%)	0	100	100
5	5	268/307 (87%)	267 (100%)	1 (0%)	91	96
6	7	623/638 (98%)	621 (100%)	2 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	8	402/423 (95%)	402 (100%)	0	100	100
8	9	680/787 (86%)	678 (100%)	2 (0%)	92	96
All	All	3333/3775 (88%)	3322 (100%)	11 (0%)	92	96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	15	GLN
2	1	195	ARG
2	1	232	ASP
3	2	194	ASP
3	2	229	TYR
3	2	344	LYS
5	5	205	GLN
6	7	341	LYS
6	7	587	ARG
8	9	9	TRP
8	9	581	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	15	GLN
2	1	325	GLN
2	1	359	HIS
2	1	386	ASN
3	2	44	ASN
3	2	383	HIS
3	2	557	ASN
3	2	651	ASN
3	2	705	ASN
4	4	224	HIS
4	4	384	ASN
5	5	20	GLN
5	5	151	GLN
5	5	159	ASN
5	5	205	GLN
6	7	99	GLN
6	7	273	ASN
6	7	293	GLN

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Mol	Chain	Res	Type
6	7	353	GLN
6	7	388	ASN
6	7	410	GLN
6	7	437	ASN
6	7	469	GLN
6	7	477	GLN
6	7	495	GLN
6	7	598	ASN
7	8	484	HIS
7	8	496	GLN
8	9	200	HIS
8	9	276	GLN
8	9	367	GLN
8	9	377	ASN
8	9	576	ASN
8	9	677	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

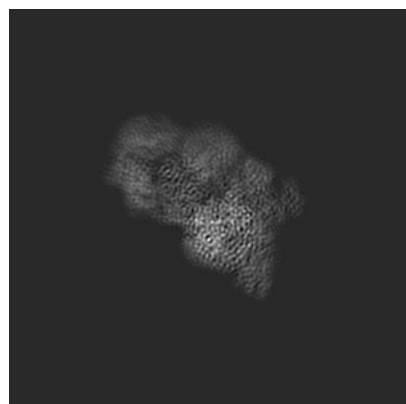
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21144. These allow visual inspection of the internal detail of the map and identification of artifacts.

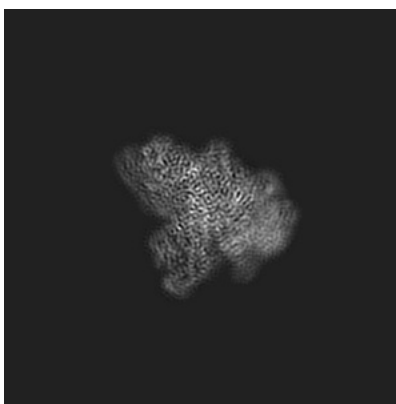
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

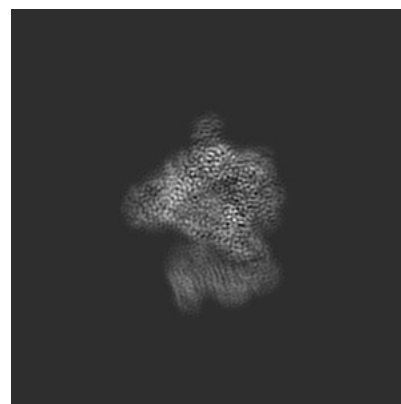
#### 6.1.1 Primary map



X

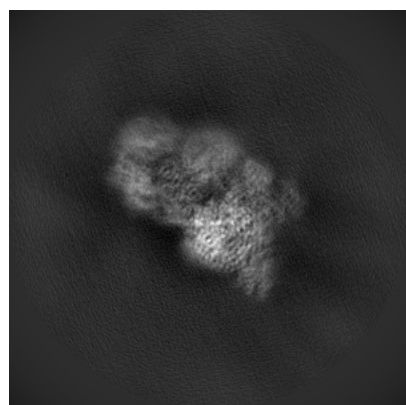


Y

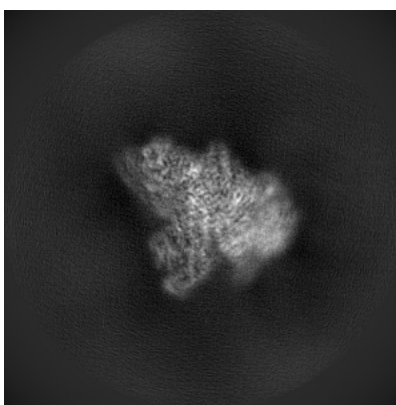


Z

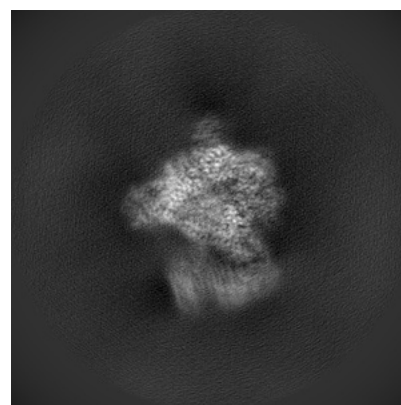
#### 6.1.2 Raw map



X



Y

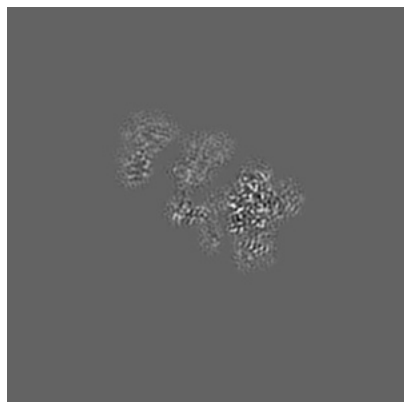


Z

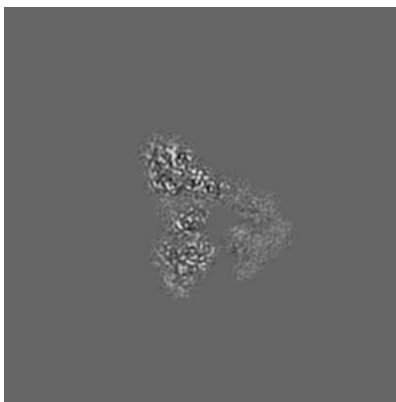
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

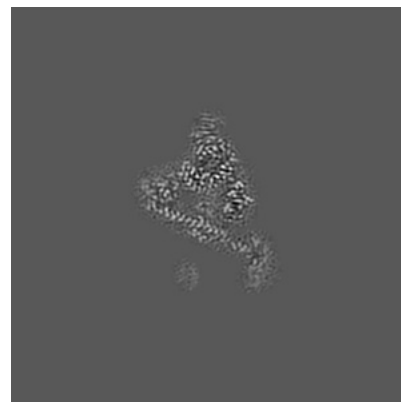
### 6.2.1 Primary map



X Index: 160

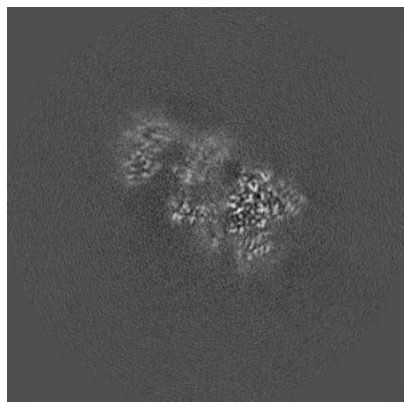


Y Index: 160

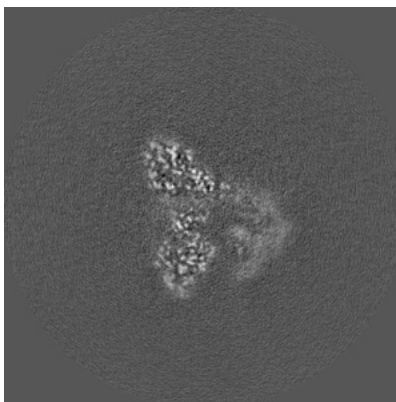


Z Index: 160

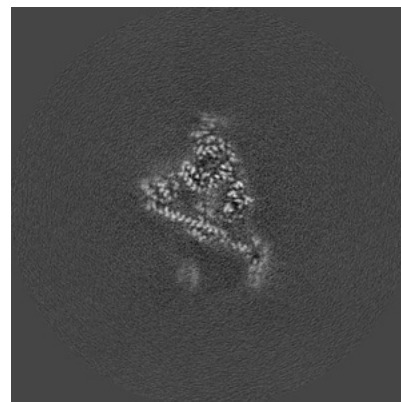
### 6.2.2 Raw map



X Index: 160



Y Index: 160

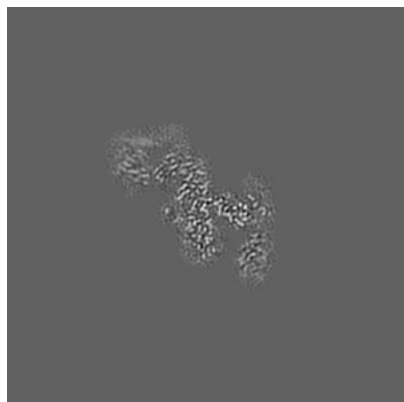


Z Index: 160

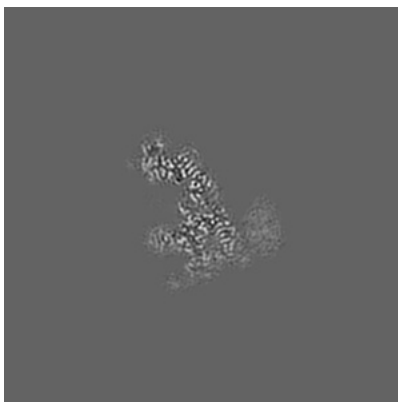
The images above show central slices of the map in three orthogonal directions.

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

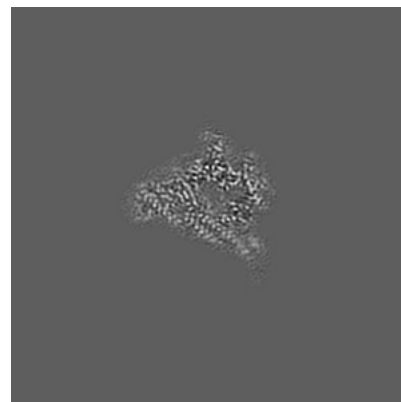
### 6.3.1 Primary map



X Index: 175

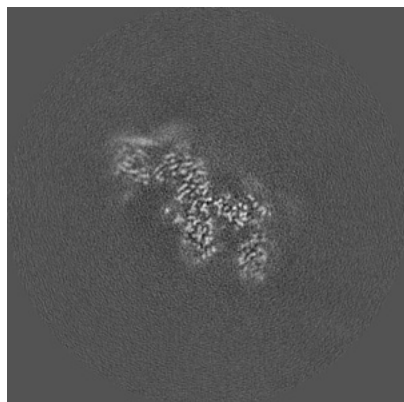


Y Index: 178

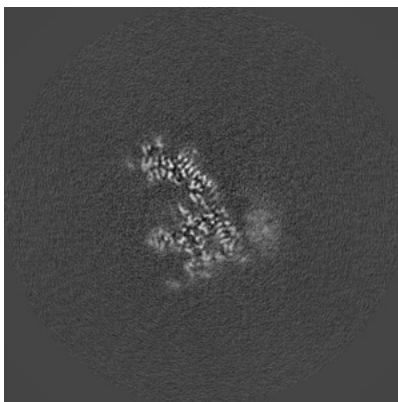


Z Index: 150

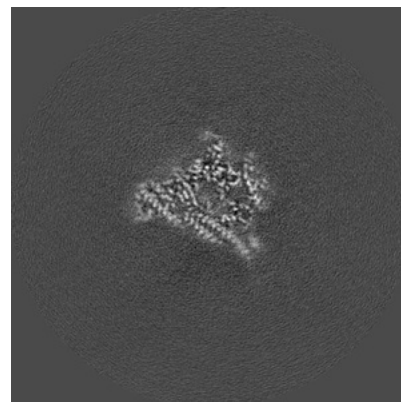
### 6.3.2 Raw map



X Index: 175



Y Index: 178

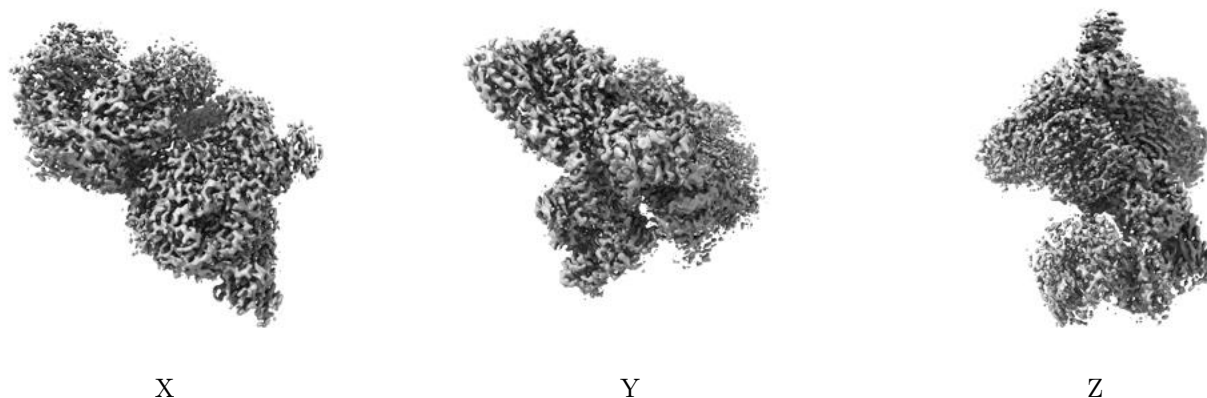


Z Index: 150

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

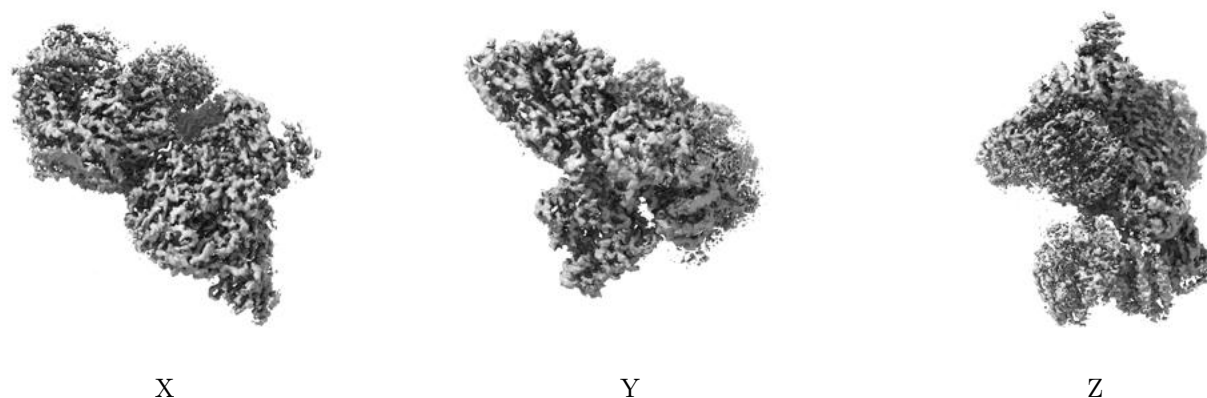
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

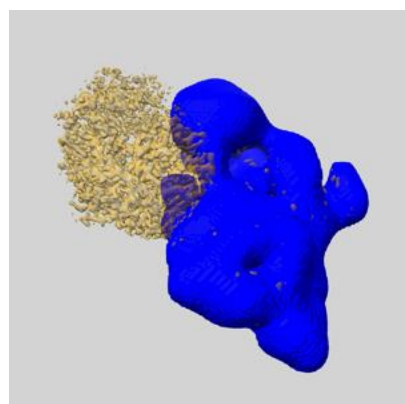
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

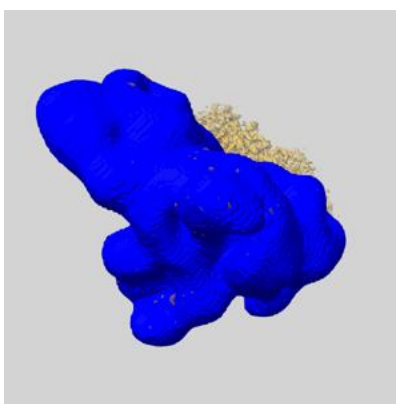
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

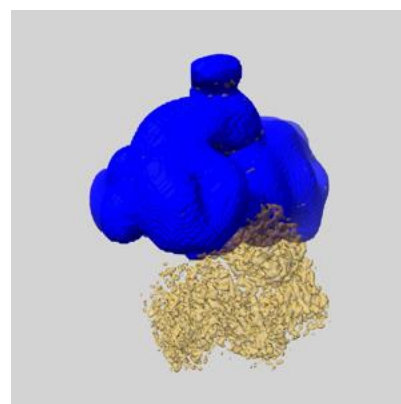
### 6.5.1 emd\_21144\_msk\_3.map [i](#)



X

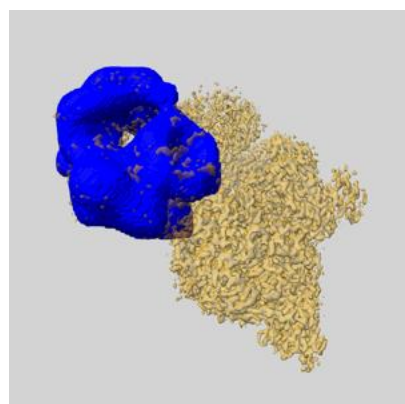


Y

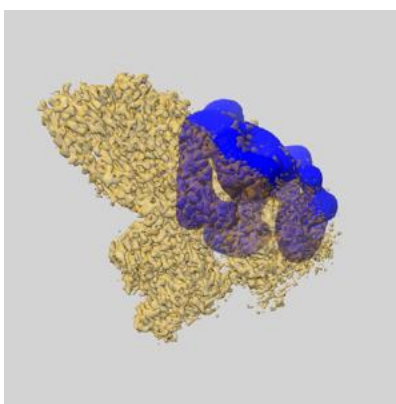


Z

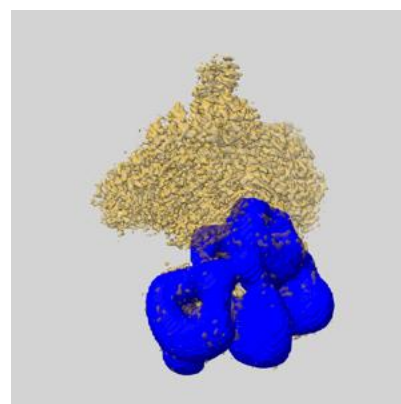
### 6.5.2 emd\_21144\_msk\_2.map [i](#)



X

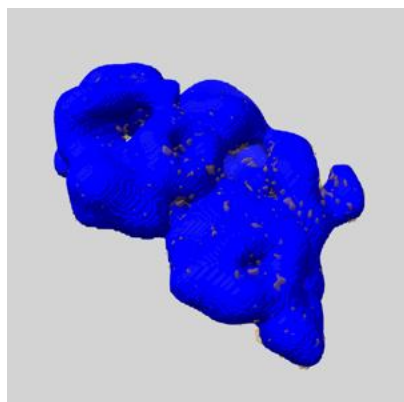


Y

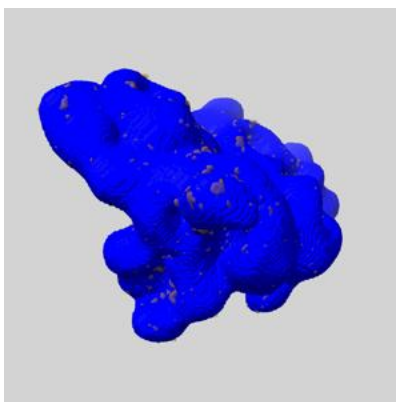


Z

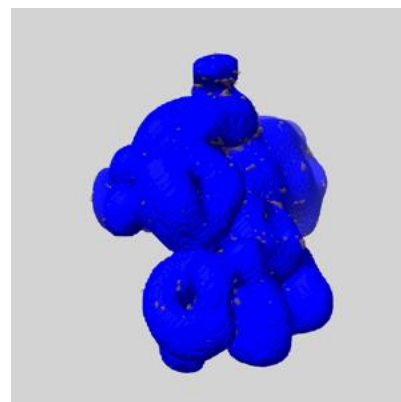
### 6.5.3 emd\_21144\_msk\_1.map [i](#)



X



Y

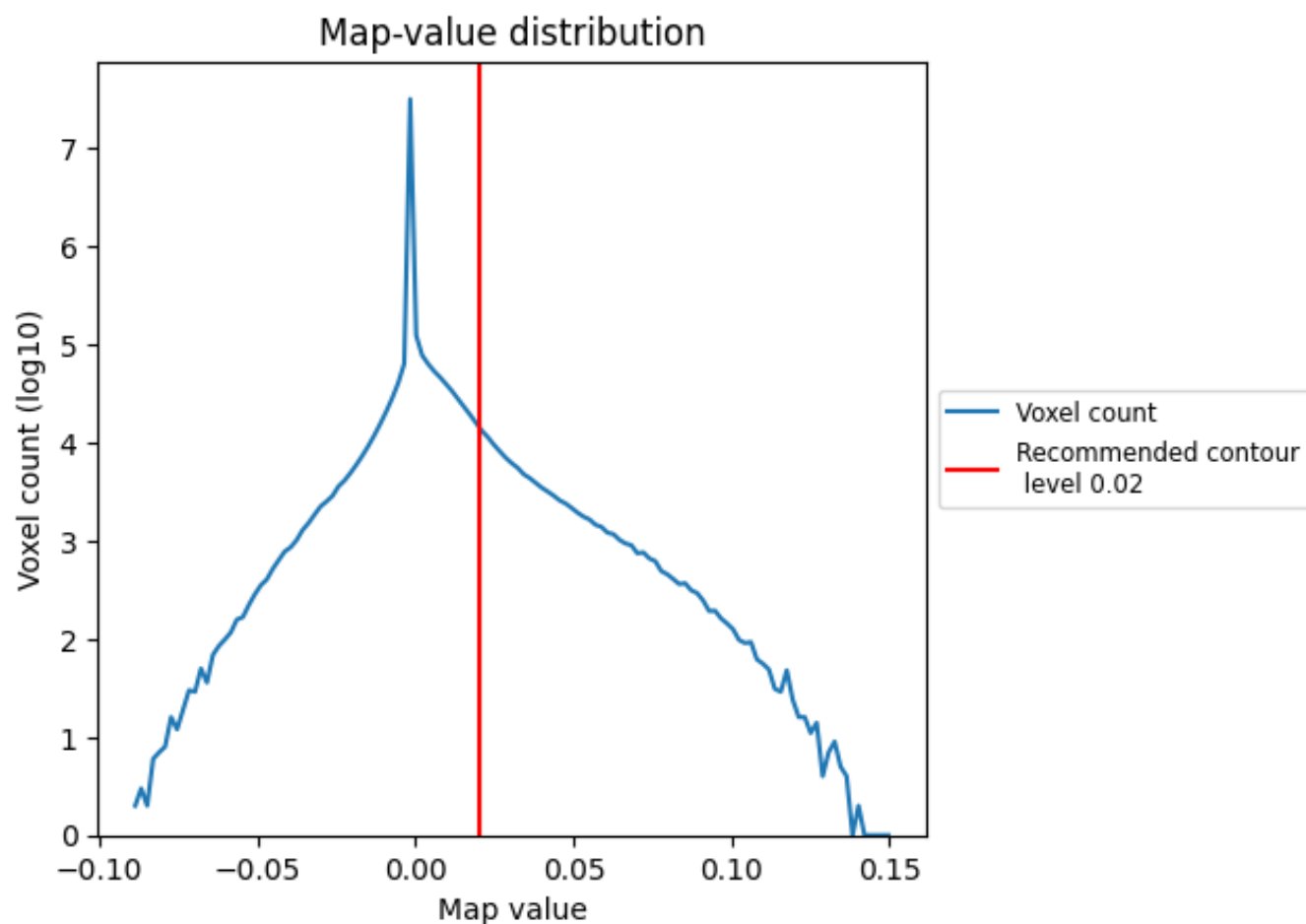


Z

## 7 Map analysis [i](#)

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

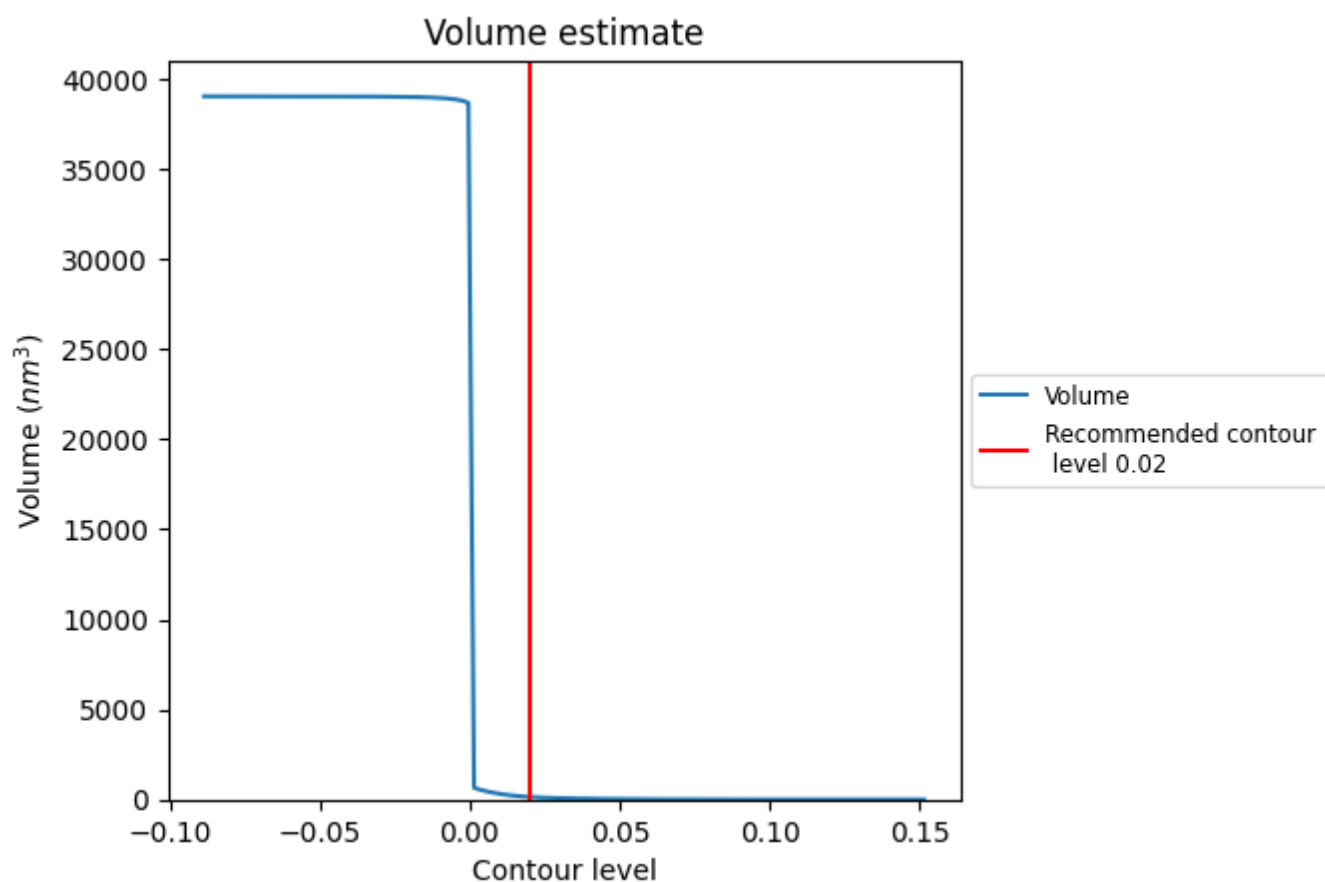
### 7.1 Map-value distribution [i](#)



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.



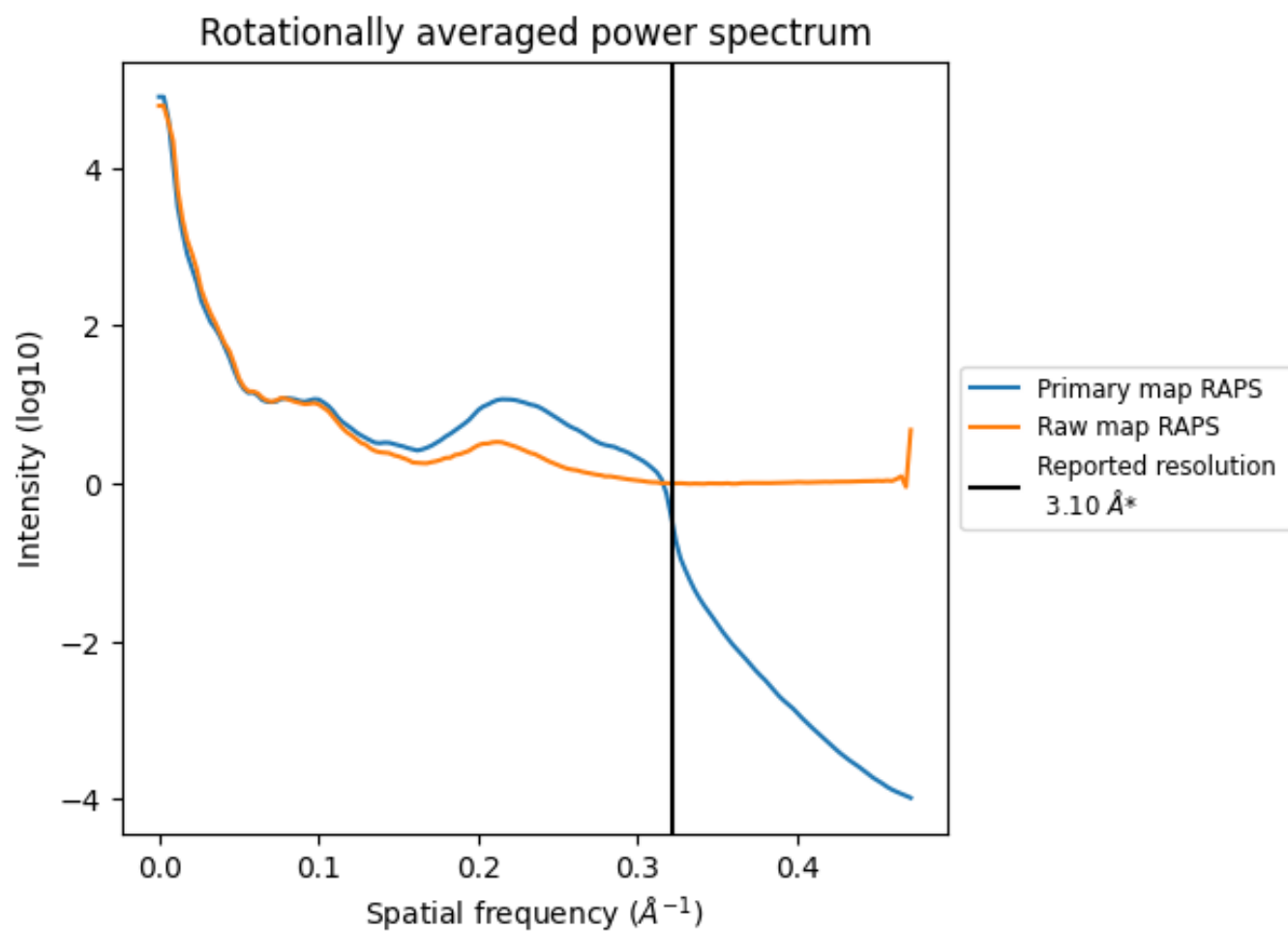
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 143  $\text{nm}^3$ ; this corresponds to an approximate mass of 129 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 ⓘ

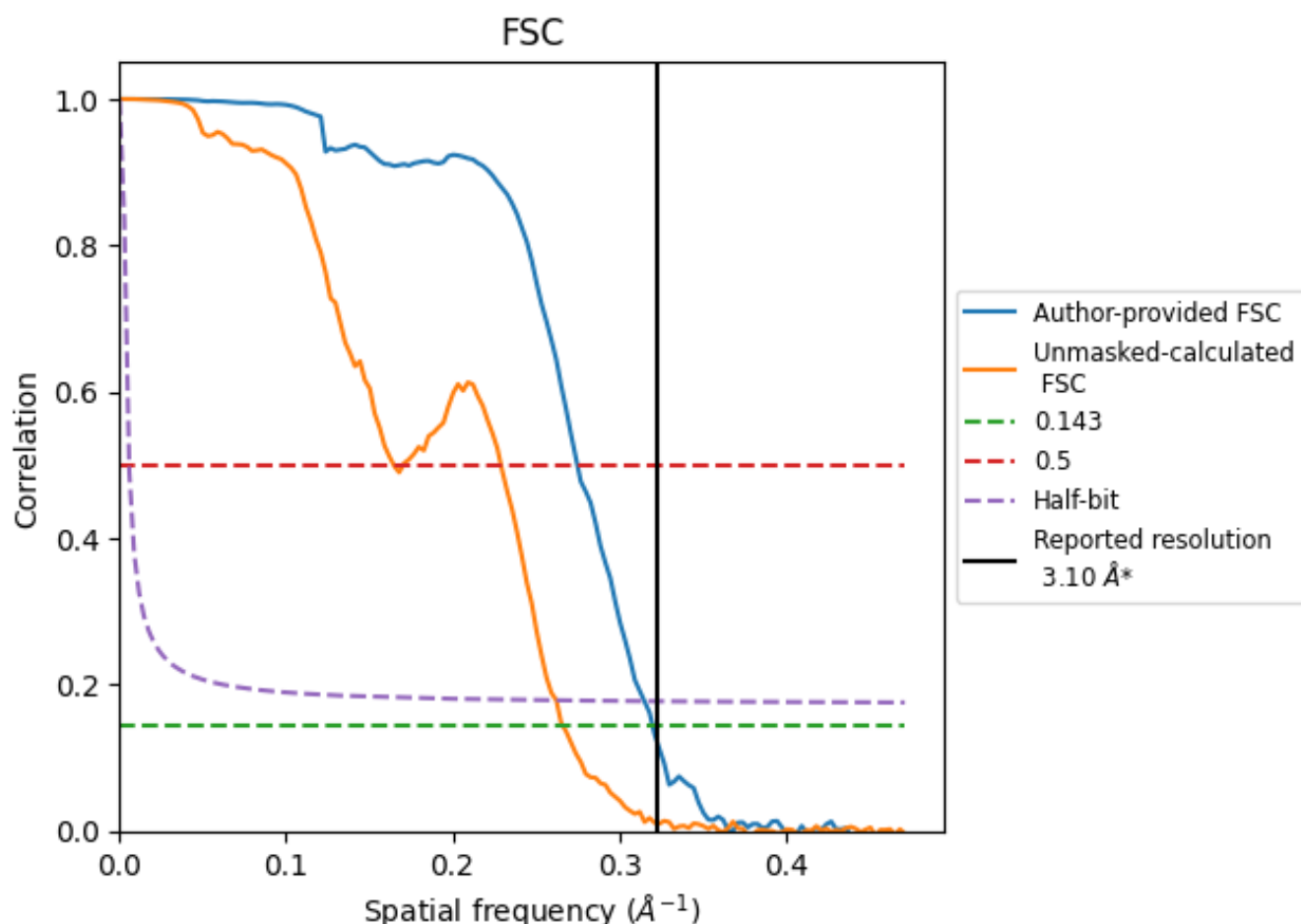


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

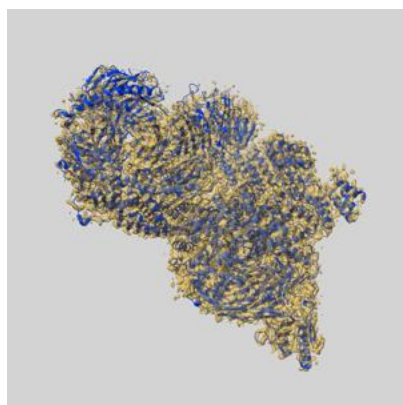
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.64	3.17
Unmasked-calculated*	3.75	6.07	3.81

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 3.1 by more than 10 %

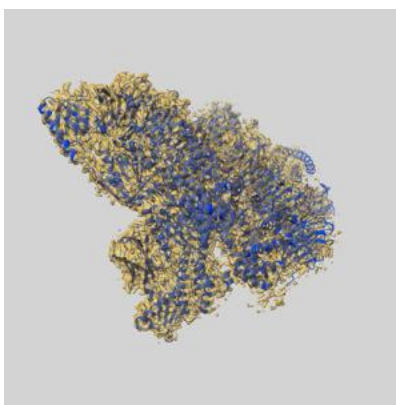
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21144 and PDB model 6VBU. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

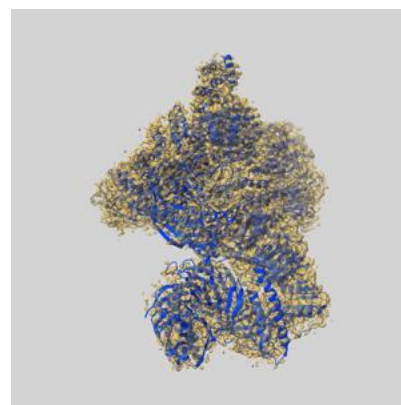
### 9.1 Map-model overlay [i](#)



X



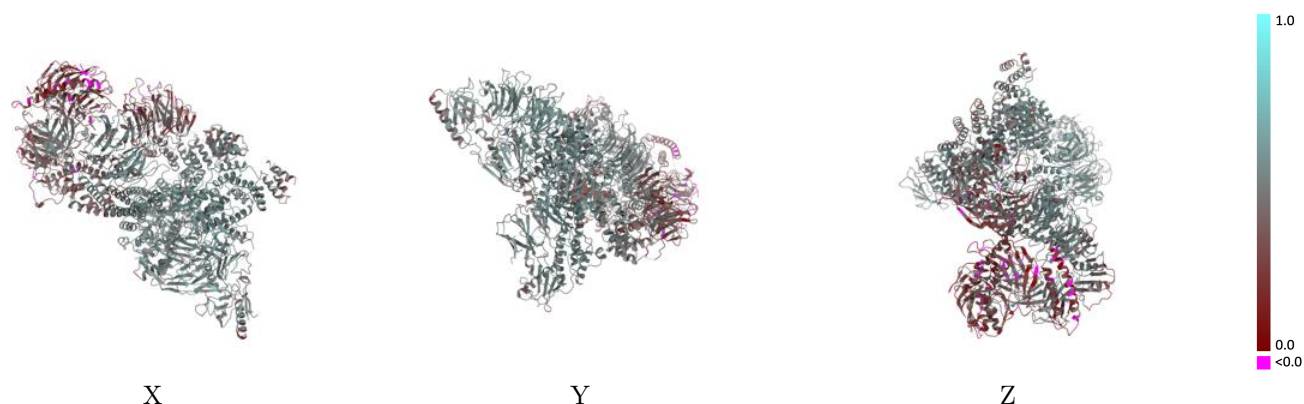
Y



Z

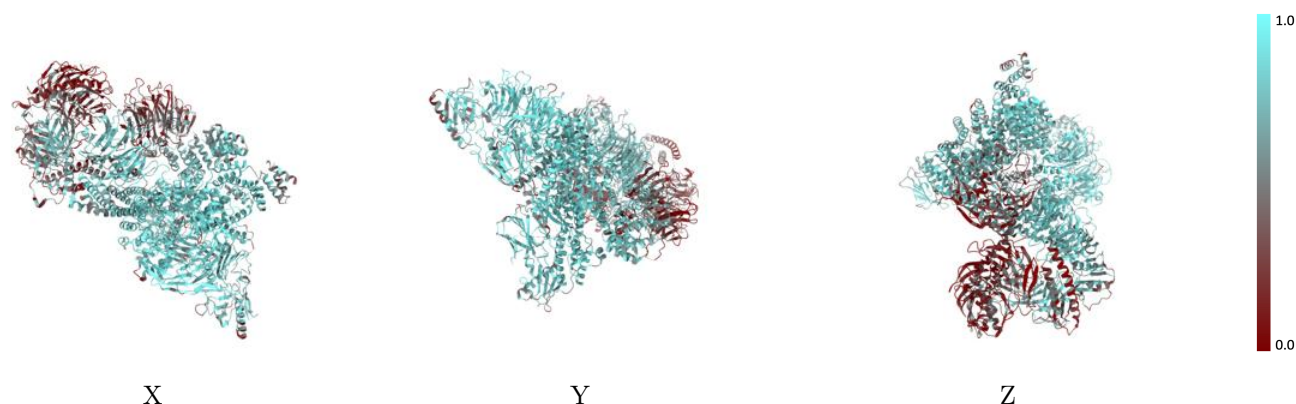
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



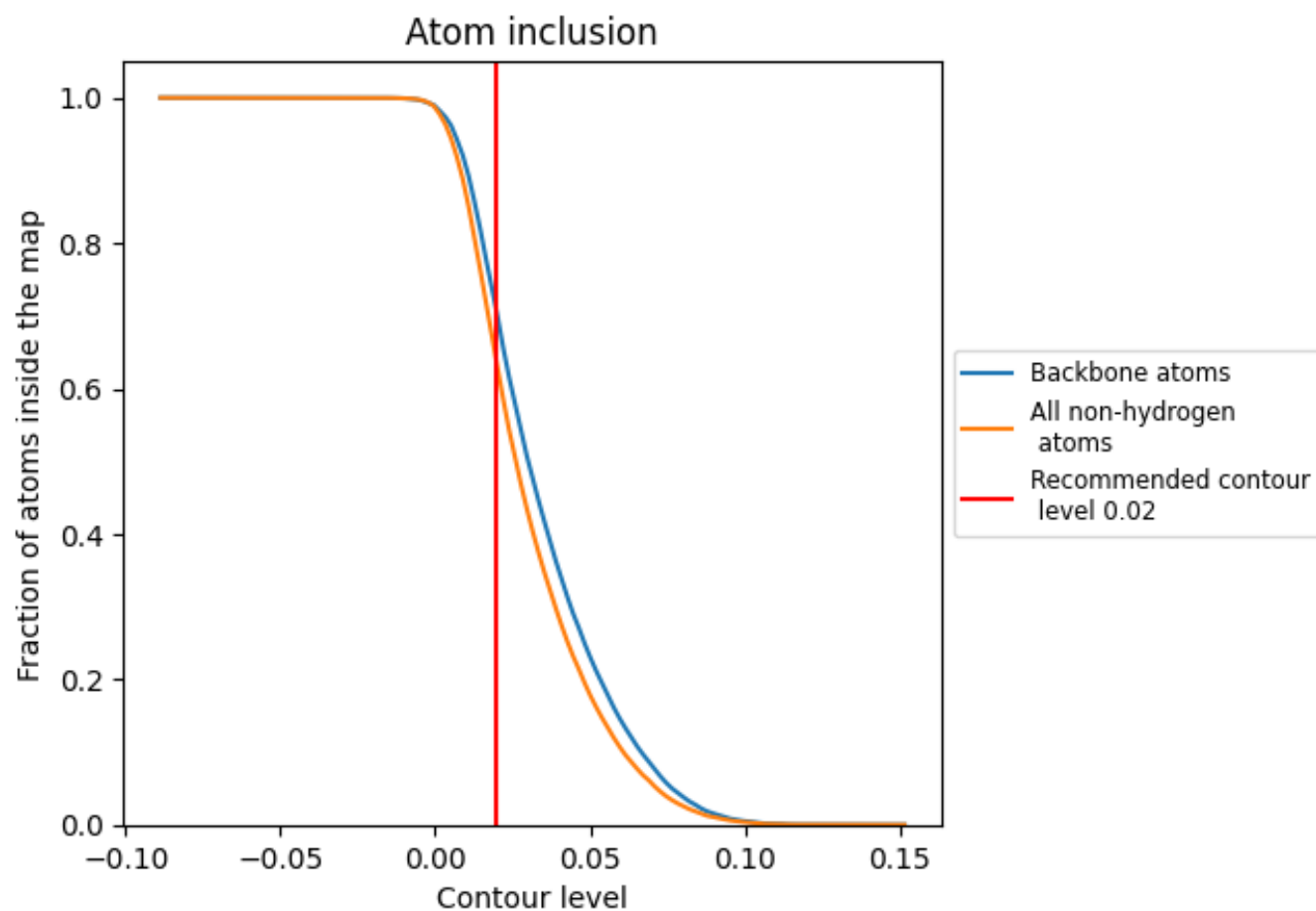
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 63% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6325	<div></div> 0.4590
0	<div></div> 0.6770	<div></div> 0.5220
1	<div></div> 0.4718	<div></div> 0.4010
2	<div></div> 0.6998	<div></div> 0.4680
4	<div></div> 0.6898	<div></div> 0.4810
5	<div></div> 0.6983	<div></div> 0.5060
7	<div></div> 0.2969	<div></div> 0.3110
8	<div></div> 0.8336	<div></div> 0.5540
9	<div></div> 0.7975	<div></div> 0.5280

1.0

0.0

<0.0