



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:43 AM UTC

PDB ID : 8IZL / pdb_00008izl
EMDB ID : EMD-35864
Title : Structure of the Mumps Virus L Protein Bound by Phosphoprotein Tetramer
Authors : Li, T.H.; Shen, Q.T.
Deposited on : 2023-04-07
Resolution : 2.93 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

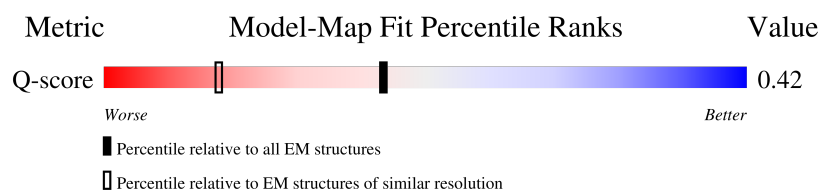
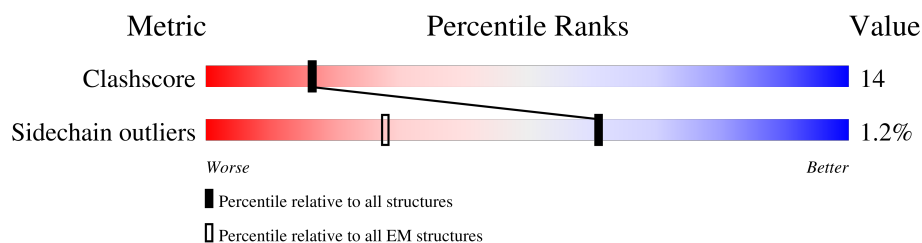
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.93 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13037 (2.43 - 3.43)

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

Mol	Chain	Length	Quality of chain
1	B	391	
1	C	391	
1	D	391	
1	E	391	
2	A	2261	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18612 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	60	Total	C	N	O	S	0	0
			459	284	79	90	6		
1	E	58	Total	C	N	O	S	0	0
			440	272	76	87	5		
1	B	69	Total	C	N	O	S	0	0
			517	321	89	101	6		
1	C	91	Total	C	N	O	S	0	0
			680	420	119	135	6		

- Molecule 2 is a protein called RNA-directed RNA polymerase L.

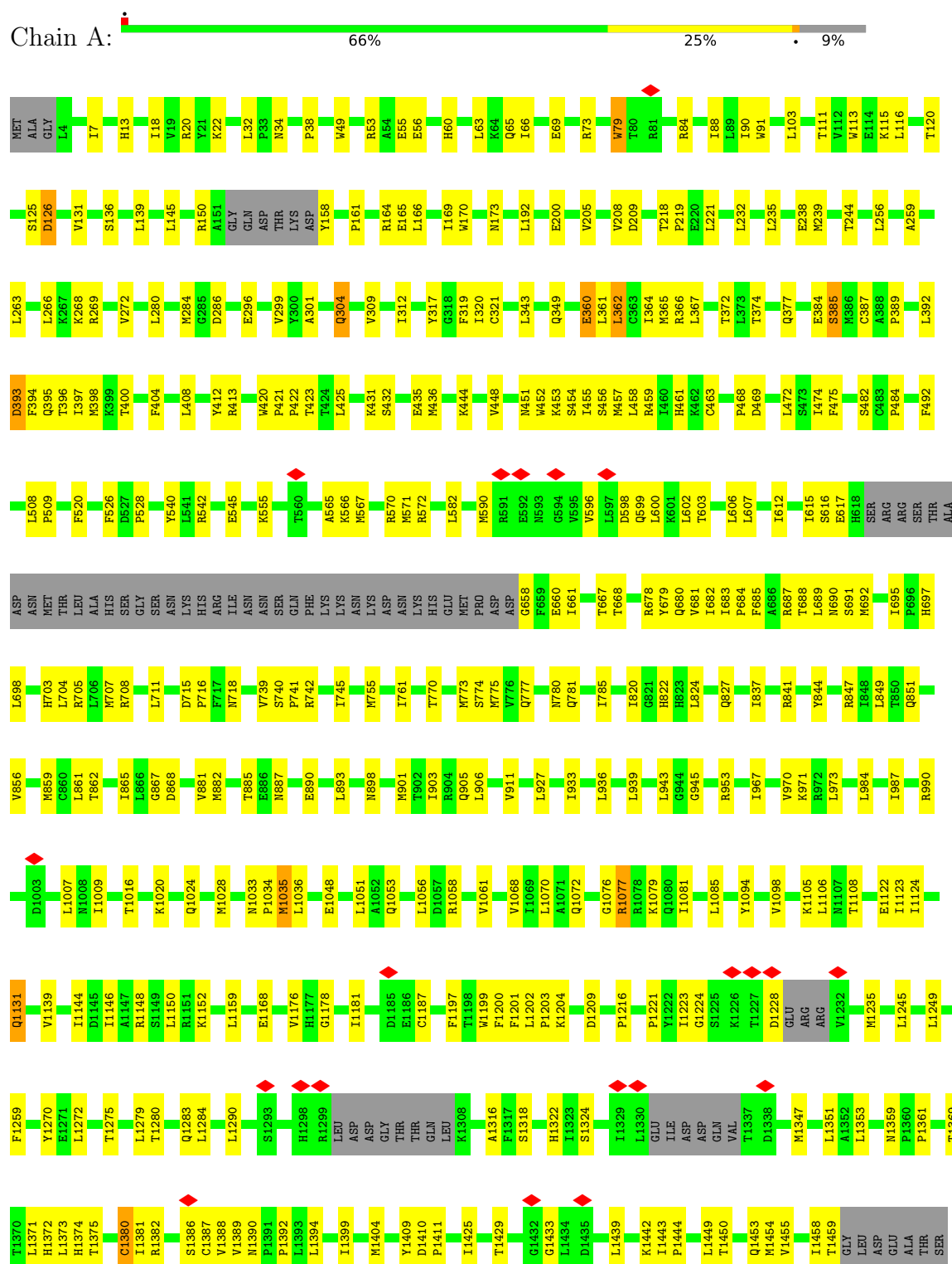
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2067	Total	C	N	O	S	0	0
			16514	10585	2805	3039	85		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	



- Molecule 2: RNA-directed RNA polymerase L





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	438014	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.500	Depositor
Minimum map value	-0.051	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	233.19998, 233.19998, 233.19998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.53, 0.53, 0.53	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: ZN

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	B	0.57	0/520	1.06	1/701 (0.1%)
1	C	0.56	0/686	0.95	2/926 (0.2%)
1	D	0.49	0/459	0.84	0/614
1	E	0.65	0/440	0.96	0/590
2	A	0.32	7/16861 (0.0%)	0.49	13/22897 (0.1%)
All	All	0.35	7/18966 (0.0%)	0.56	16/25728 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1932	ALA	C-N	-7.63	1.23	1.33
2	A	1845	PRO	C-O	-7.35	1.16	1.24
2	A	200	GLU	C-N	6.17	1.42	1.33
2	A	1933	GLN	C-N	5.50	1.40	1.34
2	A	38	PRO	C-N	-5.33	1.26	1.33
2	A	570	ARG	C-N	-5.29	1.25	1.33
2	A	658	GLY	C-N	-5.27	1.26	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	LEU	N-CA-C	-9.05	101.42	111.28
2	A	361	LEU	N-CA-C	-8.15	103.43	112.72
2	A	1388	VAL	CA-C-N	-6.09	114.76	122.43
2	A	1388	VAL	C-N-CA	-6.09	114.76	122.43
2	A	455	ILE	N-CA-C	-5.97	103.63	111.09
2	A	1636	VAL	N-CA-C	-5.89	107.55	113.20
2	A	2191	TYR	O-C-N	5.59	129.72	122.89
2	A	362	LEU	N-CA-C	-5.43	106.24	112.92
2	A	385	SER	N-CA-C	-5.31	105.39	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1932	ALA	O-C-N	-5.25	116.56	122.12
2	A	1678	LEU	CA-C-N	5.22	129.76	121.72
2	A	1678	LEU	C-N-CA	5.22	129.76	121.72
2	A	1077	ARG	CB-CA-C	-5.16	102.08	110.85
2	A	1035	MET	N-CA-C	-5.05	102.22	110.20
1	C	250	THR	CA-C-N	-5.03	113.50	120.38
1	C	250	THR	C-N-CA	-5.03	113.50	120.38

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	B	517	0	545	53	0
1	C	680	0	702	57	0
1	D	459	0	487	38	0
1	E	440	0	466	41	0
2	A	16514	0	16753	415	0
3	A	2	0	0	0	0
All	All	18612	0	18953	528	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 14.

All (528) 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)
2:A:1290:LEU:CD2	2:A:1691:LYS:HE3	1.65	1.26
1:D:256:LEU:HD11	1:C:256:LEU:HD23	1.14	1.11
1:D:256:LEU:CD1	1:C:256:LEU:HD23	1.85	1.07
2:A:1290:LEU:HD21	2:A:1691:LYS:CE	1.86	1.05
2:A:2090:LEU:HD13	2:A:2150:ASN:HD22	1.20	1.03
2:A:1290:LEU:HD21	2:A:1691:LYS:HE3	1.00	0.98
1:C:271:ALA:O	2:A:395:GLN:HB2	1.68	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LEU:HD11	1:C:256:LEU:CD2	1.99	0.91
1:D:253:LYS:HD3	1:C:252:ILE:HG22	1.55	0.87
1:C:303:PRO:HG2	2:A:459:ARG:HB2	1.53	0.87
2:A:1290:LEU:CD2	2:A:1691:LYS:CE	2.50	0.83
2:A:1324:SER:OG	2:A:1849:ASN:HB2	1.79	0.82
1:E:259:VAL:HG22	1:B:263:LEU:HD22	1.61	0.81
2:A:2090:LEU:HD13	2:A:2150:ASN:ND2	1.96	0.80
1:E:273:VAL:HG21	1:B:270:MET:HE3	1.65	0.79
2:A:1914:VAL:HG11	2:A:1940:THR:HG22	1.66	0.77
2:A:1529:ARG:HH11	2:A:1573:LYS:HZ1	1.32	0.77
2:A:136:SER:HB2	2:A:145:LEU:HB3	1.67	0.77
1:E:259:VAL:HG23	1:B:260:LYS:CE	2.14	0.76
1:E:259:VAL:HG23	1:B:260:LYS:HE2	1.67	0.76
1:C:280:ASN:HB3	2:A:387:CYS:HB3	1.67	0.75
2:A:777:GLN:HG2	2:A:780:ASN:O	1.87	0.74
2:A:1624:ALA:HB2	2:A:1651:HIS:NE2	2.01	0.74
2:A:1502:LEU:HB3	2:A:1622:LEU:HD11	1.69	0.74
2:A:841:ARG:HH12	2:A:887:ASN:HD21	1.36	0.73
2:A:1558:ILE:HD12	2:A:1574:LEU:HD22	1.70	0.72
2:A:2105:VAL:HG13	2:A:2132:ILE:HD12	1.70	0.72
1:B:249:VAL:O	1:B:252:ILE:HG22	1.89	0.72
1:D:263:LEU:HD21	1:C:259:VAL:HG13	1.72	0.71
2:A:1176:VAL:HG12	2:A:1375:THR:HG22	1.74	0.70
1:D:263:LEU:CD2	1:C:259:VAL:HG13	2.21	0.69
2:A:360:GLU:HG3	2:A:851:GLN:HA	1.74	0.69
1:E:256:LEU:O	1:E:259:VAL:HG12	1.93	0.69
1:D:266:ILE:HG22	1:C:266:ILE:HD13	1.76	0.68
2:A:1810:HIS:HB2	2:A:1833:ILE:HD13	1.74	0.68
1:C:239:VAL:HA	1:C:242:VAL:HG22	1.77	0.67
2:A:111:THR:O	2:A:115:LYS:HG2	1.93	0.67
2:A:615:ILE:HD11	2:A:661:ILE:HG22	1.76	0.67
2:A:703:HIS:O	2:A:707:MET:HG2	1.94	0.67
2:A:1902:ILE:O	2:A:1906:VAL:HG22	1.96	0.66
2:A:715:ASP:HB3	2:A:718:ASN:HB2	1.78	0.66
2:A:1811:LEU:HB3	2:A:1914:VAL:HG22	1.77	0.66
2:A:615:ILE:HD12	2:A:660:GLU:HG2	1.79	0.65
2:A:20:ARG:HB2	2:A:372:THR:HB	1.78	0.65
2:A:1061:VAL:HG21	2:A:1159:LEU:HD22	1.77	0.65
2:A:1200:PHE:HB2	2:A:1371:LEU:HB3	1.79	0.65
2:A:2158:THR:HA	2:A:2161:THR:HG22	1.79	0.65
1:E:269:MET:HE1	1:B:271:ALA:HA	1.77	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1123:ILE:HG13	2:A:1124:ILE:HG23	1.79	0.64
2:A:13:HIS:NE2	2:A:862:THR:O	2.26	0.64
2:A:1028:MET:HE1	2:A:1036:LEU:HD13	1.79	0.64
2:A:425:LEU:HD23	2:A:458:LEU:HD13	1.79	0.64
2:A:469:ASP:HB3	2:A:528:PRO:HG2	1.79	0.64
2:A:280:LEU:O	2:A:284:MET:HG3	1.99	0.63
1:E:259:VAL:HG22	1:B:263:LEU:CD2	2.29	0.63
2:A:2104:GLU:O	2:A:2108:ILE:HG12	1.99	0.63
2:A:1202:LEU:HB3	2:A:1369:THR:HG22	1.81	0.62
2:A:1520:ILE:HD11	2:A:1625:ILE:HG22	1.80	0.62
1:B:276:MET:O	2:A:680:GLN:HG2	1.99	0.62
2:A:881:VAL:HG11	2:A:898:ASN:HB2	1.80	0.62
2:A:1866:ILE:HD11	2:A:1878:GLN:HB2	1.81	0.62
2:A:1550:ARG:HH22	2:A:1858:ILE:HD12	1.64	0.62
2:A:1777:HIS:HD2	2:A:1781:ARG:HH21	1.48	0.62
2:A:1056:LEU:HD22	2:A:1061:VAL:HG13	1.82	0.62
1:B:249:VAL:O	1:B:250:THR:C	2.43	0.62
2:A:55:GLU:HG3	2:A:56:GLU:HG3	1.81	0.62
1:E:273:VAL:CG2	1:B:270:MET:CE	2.78	0.61
1:C:284:VAL:O	2:A:739:VAL:HG11	1.99	0.61
2:A:820:ILE:HG13	2:A:822:HIS:HD2	1.66	0.61
2:A:1785:LEU:HD23	2:A:1785:LEU:H	1.64	0.61
1:E:256:LEU:HD22	1:E:259:VAL:CG1	2.30	0.61
1:B:227:GLY:O	1:B:231:ARG:HG2	2.00	0.61
2:A:1531:ILE:HD11	2:A:1536:ILE:HD12	1.83	0.61
2:A:1790:TRP:HB2	2:A:1823:LEU:HD13	1.83	0.61
2:A:2172:ARG:HD2	2:A:2174:ARG:HH22	1.66	0.61
2:A:319:PHE:HE2	2:A:827:GLN:HG3	1.66	0.61
2:A:301:ALA:HB2	2:A:320:ILE:HD12	1.83	0.60
2:A:1813:LEU:HD23	2:A:1916:VAL:HG22	1.83	0.60
1:E:266:ILE:CD1	1:B:266:ILE:HG22	2.32	0.60
2:A:235:LEU:HA	2:A:239:MET:HE2	1.84	0.60
2:A:1858:ILE:HA	2:A:1863:TYR:HD2	1.66	0.60
2:A:1290:LEU:HD22	2:A:1691:LYS:HE3	1.75	0.60
2:A:526:PHE:H	2:A:1034:PRO:HG2	1.66	0.60
1:D:257:SER:O	1:D:261:THR:HG23	2.02	0.60
2:A:268:LYS:O	2:A:272:VAL:HG23	2.02	0.60
2:A:1359:ASN:HB3	2:A:1361:PRO:HD2	1.83	0.60
2:A:1481:TRP:H	2:A:1542:THR:HG22	1.66	0.60
2:A:520:PHE:O	2:A:1033:ASN:ND2	2.34	0.59
2:A:1203:PRO:HB2	2:A:1216:PRO:HG3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2048:ASP:HA	2:A:2163:ARG:HH12	1.67	0.59
1:E:273:VAL:HG21	1:B:270:MET:CE	2.32	0.59
1:C:284:VAL:CG1	1:C:288:GLU:HB2	2.32	0.59
2:A:2180:MET:N	2:A:2180:MET:SD	2.74	0.59
2:A:492:PHE:HA	2:A:716:PRO:HA	1.85	0.59
2:A:1235:MET:HE1	2:A:1429:THR:HG21	1.85	0.58
2:A:1318:SER:HB2	2:A:1351:LEU:HD22	1.86	0.58
2:A:715:ASP:OD2	2:A:718:ASN:ND2	2.37	0.58
2:A:1870:ILE:HD12	2:A:1870:ILE:H	1.67	0.58
2:A:139:LEU:HB3	2:A:1353:LEU:HD11	1.85	0.58
2:A:678:ARG:O	2:A:681:VAL:HG12	2.03	0.58
2:A:1558:ILE:HD11	2:A:1578:ALA:HB2	1.85	0.57
2:A:2142:ARG:HA	2:A:2145:MET:HE2	1.85	0.57
2:A:695:ILE:HG21	2:A:698:LEU:HB2	1.86	0.57
2:A:1663:GLN:HG2	2:A:1664:ILE:HG23	1.86	0.57
2:A:1790:TRP:CD1	2:A:2066:ILE:HD12	2.39	0.57
1:B:276:MET:HA	2:A:683:ILE:HG21	1.86	0.57
2:A:451:ASN:HD21	2:A:454:SER:HB2	1.70	0.57
2:A:1790:TRP:O	2:A:1794:ILE:HG12	2.03	0.57
2:A:2095:ALA:HA	2:A:2182:ILE:HD13	1.86	0.57
2:A:2160:LEU:O	2:A:2164:GLN:HG2	2.05	0.57
2:A:113:TRP:HB2	2:A:911:VAL:HG11	1.85	0.57
2:A:1425:ILE:HD12	2:A:1682:PRO:CB	2.35	0.57
2:A:1670:ARG:O	2:A:1674:ILE:HG12	2.05	0.57
2:A:847:ARG:NH2	2:A:1209:ASP:OD1	2.38	0.57
2:A:906:LEU:HD23	2:A:933:ILE:HG23	1.86	0.57
2:A:1439:LEU:HA	2:A:1442:LYS:HD2	1.86	0.57
2:A:484:PRO:HB3	2:A:545:GLU:HG3	1.85	0.56
1:C:274:LYS:NZ	2:A:393:ASP:CG	2.63	0.56
2:A:1936:ALA:O	2:A:1940:THR:HG23	2.05	0.56
2:A:1068:VAL:O	2:A:1072:GLN:HG2	2.04	0.56
2:A:150:ARG:O	2:A:158:TYR:N	2.39	0.56
2:A:2051:ILE:HG21	2:A:2163:ARG:HD2	1.88	0.56
2:A:847:ARG:HG2	2:A:1316:ALA:HA	1.87	0.56
2:A:943:LEU:HB3	2:A:987:ILE:HD13	1.88	0.56
2:A:1425:ILE:HD12	2:A:1682:PRO:HB2	1.88	0.56
2:A:1822:SER:O	2:A:1826:THR:HG23	2.06	0.56
2:A:1484:GLU:HG3	2:A:1693:LEU:HD22	1.87	0.56
1:B:276:MET:HG2	2:A:683:ILE:CG2	2.36	0.56
1:B:272:THR:O	1:B:275:ILE:HG13	2.05	0.56
2:A:2090:LEU:HD11	2:A:2094:MET:CE	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:384:GLU:HG3	2:A:385:SER:N	2.20	0.55
2:A:1571:TYR:HA	2:A:1574:LEU:HB2	1.88	0.55
2:A:374:THR:HB	2:A:377:GLN:HG3	1.88	0.55
2:A:1380:CYS:O	2:A:1382:ARG:HG2	2.06	0.55
2:A:1937:LEU:HD22	2:A:1969:LEU:HD21	1.88	0.55
2:A:1915:HIS:HA	2:A:1951:ILE:HG23	1.87	0.55
2:A:602:LEU:HD12	2:A:775:MET:HE3	1.87	0.55
1:B:266:ILE:HD11	1:C:267:GLU:CA	2.36	0.55
1:C:273:VAL:HG23	2:A:394:PHE:HB2	1.88	0.55
2:A:366:ARG:NH2	2:A:555:LYS:O	2.40	0.55
2:A:1598:ILE:HD11	2:A:1619:LYS:HD2	1.87	0.55
2:A:319:PHE:CE2	2:A:827:GLN:HG3	2.41	0.55
2:A:1404:MET:HE3	2:A:1404:MET:HA	1.87	0.55
2:A:2215:ARG:HD3	2:A:2219:LYS:HZ2	1.71	0.55
1:B:250:THR:O	1:B:251:GLN:C	2.50	0.55
1:C:266:ILE:O	1:C:269:MET:HG2	2.07	0.55
2:A:1486:CYS:SG	2:A:1547:ARG:NH2	2.79	0.55
2:A:451:ASN:ND2	2:A:454:SER:HB2	2.22	0.54
2:A:1028:MET:HE3	2:A:1085:LEU:HD21	1.89	0.54
2:A:1199:TRP:CD2	2:A:1849:ASN:OD1	2.61	0.54
2:A:2215:ARG:O	2:A:2219:LYS:HG3	2.08	0.54
1:D:219:ASN:O	1:D:222:MET:HG2	2.08	0.54
1:E:256:LEU:HD22	1:E:259:VAL:HG12	1.90	0.54
2:A:1279:LEU:HB3	2:A:1283:GLN:HG3	1.89	0.54
2:A:2083:ASP:OD1	2:A:2083:ASP:N	2.36	0.54
2:A:841:ARG:NH2	2:A:849:LEU:O	2.39	0.54
1:E:231:ARG:O	1:E:235:LEU:HG	2.07	0.54
1:E:247:SER:O	1:E:250:THR:HG22	2.08	0.54
2:A:1775:PRO:HB2	2:A:1778:HIS:HD2	1.72	0.54
2:A:1664:ILE:HG13	2:A:1665:GLU:HG3	1.90	0.53
2:A:205:VAL:HG22	2:A:218:THR:HG22	1.89	0.53
2:A:1826:THR:HG21	2:A:2069:ALA:HA	1.89	0.53
1:D:253:LYS:HE3	1:C:255:GLU:OE1	2.08	0.53
2:A:1685:LEU:O	2:A:1690:ARG:NH1	2.42	0.53
2:A:1070:LEU:O	2:A:1076:GLY:HA3	2.09	0.53
1:B:275:ILE:HG22	1:C:299:ILE:HD11	1.90	0.53
2:A:423:THR:HB	2:A:458:LEU:HD11	1.91	0.53
2:A:1516:GLY:O	2:A:1520:ILE:HD12	2.08	0.53
2:A:1854:PRO:HG2	2:A:1857:PHE:HB3	1.91	0.53
2:A:400:THR:HG23	2:A:685:PHE:HZ	1.74	0.53
2:A:1620:LEU:HD22	2:A:1644:LYS:HE2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:VAL:O	1:C:252:ILE:HG13	2.09	0.53
2:A:169:ILE:HD11	2:A:259:ALA:HB2	1.90	0.53
2:A:1259:PHE:HA	2:A:1390:ASN:OD1	2.08	0.52
2:A:1815:GLU:OE2	2:A:1820:SER:HB2	2.10	0.52
2:A:1913:LEU:HD13	2:A:1949:LEU:HD23	1.92	0.52
2:A:1796:VAL:HG11	2:A:1951:ILE:HD12	1.91	0.52
1:B:284:VAL:HG11	2:A:691:SER:HB2	1.92	0.52
2:A:1678:LEU:HD13	2:A:1679:THR:N	2.24	0.52
1:D:228:MET:HA	1:D:228:MET:HE2	1.92	0.52
2:A:761:ILE:HG21	2:A:774:SER:HB3	1.91	0.52
1:D:225:LEU:HD21	1:E:225:LEU:HD13	1.90	0.52
2:A:1053:GLN:HG2	2:A:1394:LEU:HD22	1.92	0.52
2:A:1280:THR:HG22	2:A:1283:GLN:HG2	1.92	0.52
1:D:235:LEU:O	1:D:238:LYS:HG2	2.09	0.52
1:B:251:GLN:NE2	1:C:253:LYS:HE3	2.25	0.52
2:A:1790:TRP:CE3	2:A:1819:ALA:HB1	2.45	0.52
2:A:1952:LEU:HB3	2:A:1993:ILE:HB	1.92	0.52
2:A:422:PRO:HB2	2:A:461:HIS:HB2	1.91	0.52
2:A:2090:LEU:HD11	2:A:2094:MET:HE3	1.91	0.52
2:A:432:SER:O	2:A:436:MET:HG3	2.10	0.52
2:A:603:THR:HG23	2:A:1223:ILE:HD12	1.91	0.52
2:A:2094:MET:HG2	2:A:2143:ILE:HD12	1.92	0.52
2:A:770:THR:HG21	2:A:785:ILE:HG23	1.91	0.51
1:C:235:LEU:HA	1:C:238:LYS:HD2	1.92	0.51
2:A:397:ILE:HG12	2:A:681:VAL:HG23	1.92	0.51
1:E:259:VAL:CG1	1:E:260:LYS:N	2.74	0.51
2:A:1455:VAL:HG21	2:A:1500:ALA:HB3	1.93	0.51
2:A:2141:GLU:O	2:A:2145:MET:HG3	2.10	0.51
1:E:256:LEU:HD22	1:E:259:VAL:HG11	1.93	0.51
1:B:281:PRO:HD2	1:C:293:PHE:HB2	1.91	0.51
1:D:221:ILE:O	1:D:225:LEU:HD22	2.11	0.51
2:A:2090:LEU:CD1	2:A:2094:MET:HE3	2.40	0.51
2:A:2099:THR:HG22	2:A:2192:LEU:CD1	2.41	0.51
2:A:508:LEU:HD13	2:A:509:PRO:HD2	1.93	0.51
2:A:606:LEU:HG	2:A:775:MET:HE2	1.92	0.51
1:C:296:HIS:CE1	2:A:540:TYR:CE1	2.99	0.50
1:D:253:LYS:HD3	1:C:252:ILE:CG2	2.34	0.50
2:A:309:VAL:HB	2:A:312:ILE:HG12	1.92	0.50
1:C:274:LYS:HZ2	2:A:393:ASP:CG	2.20	0.50
2:A:1823:LEU:HD11	2:A:2065:ILE:HG22	1.92	0.50
2:A:63:LEU:O	2:A:66:ILE:HG22	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1678:LEU:HD13	2:A:1679:THR:H	1.76	0.50
1:E:273:VAL:CG2	1:B:270:MET:HE3	2.37	0.50
1:B:250:THR:O	1:B:253:LYS:N	2.44	0.50
1:C:247:SER:O	1:C:250:THR:HG22	2.12	0.49
2:A:596:VAL:HG23	2:A:598:ASP:H	1.77	0.49
2:A:688:THR:O	2:A:692:MET:HG3	2.12	0.49
1:E:228:MET:HE1	1:B:228:MET:HB2	1.94	0.49
2:A:612:ILE:HD11	2:A:773:MET:SD	2.53	0.49
2:A:1051:LEU:HD13	2:A:1399:ILE:HD11	1.94	0.49
1:E:217:SER:O	1:E:221:ILE:HG12	2.11	0.49
1:D:235:LEU:O	1:D:239:VAL:HG12	2.13	0.49
1:E:266:ILE:HD11	1:B:270:MET:HB2	1.95	0.49
1:C:296:HIS:CE1	2:A:540:TYR:HE1	2.31	0.49
2:A:393:ASP:N	2:A:393:ASP:OD1	2.45	0.49
2:A:1742:ILE:HG22	2:A:1979:LEU:HB2	1.93	0.49
1:B:275:ILE:HD13	2:A:687:ARG:HD3	1.94	0.49
2:A:582:LEU:HD21	2:A:689:LEU:HD13	1.94	0.49
2:A:602:LEU:CD1	2:A:775:MET:HE3	2.42	0.49
2:A:53:ARG:HD3	2:A:60:HIS:HE1	1.77	0.49
2:A:1178:GLY:HA2	2:A:1373:LEU:HA	1.95	0.49
2:A:1197:PHE:HE2	2:A:1199:TRP:HB2	1.78	0.49
2:A:1809:ALA:HB3	2:A:1911:CYS:HB3	1.93	0.49
1:C:275:ILE:N	2:A:392:LEU:O	2.46	0.49
1:C:280:ASN:H	2:A:387:CYS:HA	1.78	0.49
1:E:266:ILE:HD13	1:B:266:ILE:HG22	1.94	0.49
1:B:249:VAL:O	1:B:252:ILE:N	2.46	0.49
1:D:228:MET:HG2	1:E:229:ASP:OD1	2.13	0.48
1:D:245:GLN:HA	1:D:248:MET:HB3	1.95	0.48
1:D:266:ILE:CG2	1:C:266:ILE:HD13	2.43	0.48
1:E:266:ILE:HD12	1:B:267:GLU:HA	1.94	0.48
2:A:2213:LEU:HD13	2:A:2221:ILE:HD12	1.95	0.48
1:E:235:LEU:HD22	1:B:235:LEU:HD12	1.95	0.48
2:A:1410:ASP:OD1	2:A:1410:ASP:N	2.44	0.48
2:A:1609:SER:OG	2:A:1610:ASP:N	2.42	0.48
1:B:278:PRO:HG3	2:A:679:TYR:CD2	2.47	0.48
2:A:103:LEU:HD22	2:A:208:VAL:HG11	1.94	0.48
2:A:540:TYR:HD2	2:A:571:MET:HE1	1.77	0.48
2:A:1199:TRP:CE2	2:A:1849:ASN:OD1	2.66	0.48
2:A:1563:SER:OG	2:A:1565:HIS:O	2.31	0.48
2:A:1144:ILE:O	2:A:1148:ARG:HG3	2.13	0.48
1:E:263:LEU:O	1:E:267:GLU:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:88:ILE:HD12	2:A:232:LEU:HD23	1.95	0.48
2:A:740:SER:OG	2:A:742:ARG:NH1	2.46	0.48
1:C:258:THR:O	1:C:262:THR:HG22	2.13	0.48
1:C:260:LYS:HE3	1:C:260:LYS:HB3	1.43	0.48
2:A:126:ASP:OD1	2:A:126:ASP:N	2.45	0.48
2:A:412:TYR:CG	2:A:421:PRO:HG3	2.48	0.48
2:A:990:ARG:NH1	2:A:1009:ILE:HD13	2.28	0.48
2:A:166:LEU:HD21	2:A:893:LEU:HD11	1.95	0.48
2:A:299:VAL:HG11	2:A:362:LEU:HG	1.95	0.48
2:A:321:CYS:HB3	2:A:343:LEU:HD21	1.95	0.48
2:A:1007:LEU:HD11	2:A:1150:LEU:HD21	1.95	0.48
1:D:260:LYS:NZ	1:D:264:ALA:HB2	2.28	0.48
2:A:69:GLU:O	2:A:73:ARG:HG2	2.14	0.48
2:A:1181:ILE:HD11	2:A:1187:CYS:HB2	1.96	0.48
2:A:413:ARG:HD2	2:A:420:TRP:CD1	2.49	0.47
1:D:248:MET:HE1	1:E:250:THR:HA	1.96	0.47
2:A:599:GLN:O	2:A:603:THR:HG22	2.14	0.47
2:A:1805:ILE:HD11	2:A:1828:LEU:HB3	1.97	0.47
2:A:394:PHE:O	2:A:398:MET:HG2	2.14	0.47
2:A:218:THR:OG1	2:A:221:LEU:O	2.28	0.47
2:A:1272:LEU:O	2:A:1275:THR:OG1	2.22	0.47
1:C:275:ILE:HG21	2:A:680:GLN:HB3	1.97	0.47
1:C:286:VAL:HG22	1:C:290:ARG:HG3	1.95	0.47
2:A:689:LEU:HD11	2:A:755:MET:HE1	1.96	0.47
2:A:936:LEU:HB2	2:A:1124:ILE:HD13	1.97	0.47
2:A:1449:LEU:HD12	2:A:1685:LEU:HB3	1.96	0.47
2:A:1800:ILE:HA	2:A:1803:MET:HE3	1.96	0.47
2:A:683:ILE:CG2	2:A:684:PRO:HD3	2.45	0.47
1:B:246:GLY:O	1:B:247:SER:C	2.58	0.47
1:C:233:GLN:O	1:C:236:GLU:HG3	2.14	0.47
2:A:1024:GLN:HG2	2:A:1085:LEU:HB2	1.96	0.47
1:B:243:LEU:HA	1:B:243:LEU:HD23	1.82	0.47
2:A:1228:ASP:N	2:A:1228:ASP:OD1	2.48	0.47
2:A:1601:PRO:O	2:A:1611:ARG:NH2	2.48	0.47
2:A:1834:TRP:CG	2:A:1906:VAL:HG12	2.50	0.47
1:B:247:SER:O	1:B:248:MET:C	2.58	0.46
1:C:273:VAL:HG23	2:A:394:PHE:CB	2.44	0.46
2:A:865:ILE:HD13	2:A:868:ASP:H	1.80	0.46
2:A:2192:LEU:H	2:A:2197:ASN:ND2	2.12	0.46
2:A:967:ILE:HG21	2:A:1146:ILE:HB	1.97	0.46
1:C:286:VAL:O	1:C:287:ASP:C	2.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:882:MET:HE2	2:A:953:ARG:HG2	1.97	0.46
2:A:1538:GLY:O	2:A:1542:THR:HG23	2.15	0.46
1:B:258:THR:HA	1:B:261:THR:HG22	1.97	0.46
2:A:1200:PHE:HZ	2:A:1347:MET:HA	1.81	0.46
2:A:125:SER:OG	2:A:164:ARG:N	2.49	0.46
2:A:165:GLU:O	2:A:169:ILE:HG23	2.15	0.46
1:D:249:VAL:O	1:D:252:ILE:HG22	2.16	0.46
1:B:278:PRO:HG3	2:A:679:TYR:HD2	1.81	0.46
2:A:1692:LEU:O	2:A:1696:ILE:HG13	2.16	0.46
2:A:1899:VAL:HG21	2:A:1935:HIS:CD2	2.51	0.46
1:D:249:VAL:HA	1:D:252:ILE:HG22	1.98	0.46
2:A:668:THR:HB	2:A:781:GLN:HG2	1.96	0.46
1:E:220:GLU:O	1:E:224:LEU:HG	2.15	0.46
2:A:116:LEU:HD22	2:A:927:LEU:HD23	1.97	0.46
2:A:2151:TRP:CD2	2:A:2225:ILE:HD12	2.51	0.46
1:E:249:VAL:O	1:E:252:ILE:HG22	2.17	0.46
1:B:238:LYS:HB3	1:C:239:VAL:HG21	1.97	0.46
1:B:266:ILE:HD11	1:C:267:GLU:HA	1.97	0.46
2:A:1245:LEU:O	2:A:1249:LEU:HG	2.16	0.46
2:A:1536:ILE:HG21	2:A:1572:THR:HG23	1.97	0.46
2:A:404:PHE:CE1	2:A:755:MET:HE3	2.52	0.45
2:A:1779:VAL:HG21	2:A:2051:ILE:HD11	1.98	0.45
1:D:229:ASP:HA	1:D:232:LEU:HB3	1.98	0.45
1:B:242:VAL:HA	1:B:245:GLN:CD	2.41	0.45
2:A:600:LEU:HD11	2:A:1224:GLY:HA3	1.98	0.45
2:A:1122:GLU:HG2	2:A:1123:ILE:HG23	1.97	0.45
1:C:280:ASN:H	2:A:387:CYS:C	2.24	0.45
1:C:303:PRO:HG2	2:A:459:ARG:CB	2.37	0.45
1:E:264:ALA:HA	1:E:267:GLU:OE1	2.15	0.45
2:A:567:MET:HE3	2:A:567:MET:HB2	1.79	0.45
2:A:1152:LYS:HE2	2:A:1152:LYS:HB2	1.78	0.45
2:A:1386:SER:OG	2:A:1387:CYS:N	2.48	0.45
2:A:1744:ASN:OD1	2:A:1744:ASN:N	2.49	0.45
2:A:2174:ARG:HD3	2:A:2206:GLY:HA2	1.97	0.45
2:A:1513:ARG:HH21	2:A:1633:PRO:HG2	1.82	0.45
2:A:1647:ALA:HA	2:A:1650:THR:HG22	1.98	0.45
2:A:2033:TRP:O	2:A:2037:VAL:HG22	2.17	0.45
2:A:2055:VAL:HB	2:A:2058:GLN:HE21	1.81	0.45
1:B:250:THR:OG1	1:B:251:GLN:N	2.50	0.45
2:A:705:ARG:NH1	2:A:708:ARG:HB2	2.32	0.45
2:A:1544:SER:HB2	2:A:1848:ARG:HH11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1847:GLN:O	2:A:1848:ARG:NE	2.49	0.45
2:A:1962:PHE:HZ	2:A:1991:VAL:HG11	1.81	0.45
2:A:2172:ARG:HB2	2:A:2175:ASP:OD2	2.17	0.45
2:A:1409:TYR:HD2	2:A:1411:PRO:HD3	1.82	0.45
2:A:2192:LEU:H	2:A:2197:ASN:HD22	1.64	0.45
1:B:248:MET:HE2	1:B:248:MET:HB3	1.68	0.45
2:A:704:LEU:HD22	2:A:708:ARG:HH21	1.82	0.45
2:A:705:ARG:HD2	2:A:705:ARG:HA	1.70	0.45
2:A:1058:ARG:HD3	2:A:1392:PRO:HA	1.99	0.45
2:A:2097:LEU:HD12	2:A:2143:ILE:HD11	1.98	0.45
1:E:222:MET:O	1:E:226:ARG:HG2	2.17	0.45
2:A:53:ARG:HD3	2:A:60:HIS:CE1	2.52	0.45
2:A:1449:LEU:O	2:A:1453:GLN:HG3	2.17	0.45
1:D:266:ILE:HG23	1:E:270:MET:HE3	1.98	0.44
1:C:280:ASN:H	2:A:387:CYS:CA	2.30	0.44
2:A:366:ARG:HG3	2:A:366:ARG:HH11	1.81	0.44
2:A:1937:LEU:O	2:A:1941:VAL:HG23	2.17	0.44
1:C:296:HIS:NE2	2:A:540:TYR:HE1	2.14	0.44
2:A:616:SER:OG	2:A:617:GLU:N	2.51	0.44
2:A:690:ASN:HB3	2:A:695:ILE:O	2.18	0.44
2:A:1797:LEU:HD13	2:A:1800:ILE:HD11	1.98	0.44
2:A:1856:GLN:O	2:A:1860:SER:OG	2.34	0.44
2:A:2095:ALA:O	2:A:2099:THR:OG1	2.33	0.44
1:B:234:HIS:O	1:B:238:LYS:HG2	2.17	0.44
1:C:295:ASP:HA	2:A:542:ARG:HH21	1.82	0.44
2:A:79:TRP:N	2:A:79:TRP:HE3	2.15	0.44
2:A:1148:ARG:HG2	2:A:1168:GLU:CD	2.43	0.44
2:A:2189:ARG:HG3	2:A:2191:TYR:O	2.17	0.44
2:A:131:VAL:HG21	2:A:973:LEU:HD23	1.99	0.44
2:A:1199:TRP:CZ2	2:A:1201:PHE:HB2	2.53	0.44
2:A:1558:ILE:HG23	2:A:1574:LEU:HD22	2.00	0.44
2:A:1690:ARG:H	2:A:1690:ARG:HD3	1.82	0.44
1:D:236:GLU:HA	1:D:239:VAL:HG12	1.99	0.44
2:A:395:GLN:HG3	2:A:452:TRP:CH2	2.53	0.44
1:C:245:GLN:O	1:C:249:VAL:HG23	2.17	0.44
2:A:1935:HIS:HA	2:A:1938:LEU:CD2	2.47	0.44
2:A:2182:ILE:HG21	2:A:2201:PHE:HZ	1.83	0.44
1:C:277:ASP:O	2:A:389:PRO:HA	2.17	0.44
2:A:431:LYS:O	2:A:435:GLU:HG3	2.18	0.44
2:A:2191:TYR:O	2:A:2192:LEU:HB2	2.17	0.44
2:A:269:ARG:HA	2:A:349:GLN:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:890:GLU:HG3	2:A:1359:ASN:ND2	2.32	0.44
2:A:1774:PRO:HA	2:A:1775:PRO:HD3	1.88	0.44
1:B:233:GLN:HA	1:B:236:GLU:CD	2.43	0.43
2:A:32:LEU:HD11	2:A:66:ILE:HG23	1.99	0.43
1:D:243:LEU:HD21	1:C:238:LYS:HB3	1.98	0.43
2:A:412:TYR:CE2	2:A:463:CYS:HB3	2.53	0.43
2:A:2182:ILE:HG21	2:A:2201:PHE:CZ	2.53	0.43
1:D:270:MET:HG2	1:C:269:MET:HG3	2.00	0.43
2:A:1077:ARG:O	2:A:1081:ILE:HG13	2.18	0.43
2:A:1964:PHE:O	2:A:1968:VAL:HG12	2.18	0.43
2:A:2062:ASP:O	2:A:2066:ILE:HG12	2.18	0.43
1:D:258:THR:O	1:D:262:THR:HG22	2.18	0.43
2:A:301:ALA:HB1	2:A:317:TYR:HA	2.00	0.43
2:A:366:ARG:HG3	2:A:366:ARG:NH1	2.32	0.43
1:C:240:ASP:O	1:C:243:LEU:HG	2.19	0.43
2:A:7:ILE:HD11	2:A:1106:LEU:HD12	1.99	0.43
2:A:1204:LYS:HE2	2:A:1889:ASP:OD1	2.18	0.43
2:A:1443:ILE:HG23	2:A:1488:THR:HA	2.01	0.43
2:A:1960:ASN:OD1	2:A:1960:ASN:N	2.51	0.43
2:A:1614:ASN:O	2:A:1618:ARG:HG3	2.19	0.43
2:A:2028:LEU:HD23	2:A:2028:LEU:HA	1.92	0.43
2:A:22:LYS:NZ	2:A:238:GLU:OE1	2.40	0.43
2:A:192:LEU:HB3	2:A:219:PRO:HG3	2.00	0.43
2:A:1562:ASN:HD21	2:A:2220:ARG:HG2	1.83	0.43
2:A:286:ASP:OD2	2:A:372:THR:OG1	2.36	0.43
2:A:304:GLN:O	2:A:304:GLN:HG3	2.19	0.43
2:A:697:HIS:CD2	2:A:697:HIS:C	2.97	0.43
2:A:1016:THR:O	2:A:1020:LYS:HG3	2.19	0.43
2:A:1144:ILE:HB	2:A:1382:ARG:NH2	2.34	0.43
2:A:1529:ARG:NH1	2:A:1573:LYS:HZ1	2.07	0.43
2:A:1945:LYS:HB2	2:A:1945:LYS:HE2	1.68	0.43
2:A:169:ILE:O	2:A:173:ASN:HB2	2.18	0.43
2:A:1094:TYR:CZ	2:A:1098:VAL:HG11	2.54	0.43
2:A:2103:LYS:HB2	2:A:2103:LYS:HE3	1.81	0.43
1:D:249:VAL:HB	1:C:248:MET:CE	2.48	0.42
2:A:73:ARG:HH12	2:A:209:ASP:HB2	1.84	0.42
2:A:590:MET:SD	2:A:755:MET:HG2	2.59	0.42
2:A:1372:HIS:HB3	2:A:1374:HIS:CD2	2.54	0.42
2:A:1669:ILE:O	2:A:1672:MET:HG2	2.19	0.42
2:A:1931:ARG:HD3	2:A:1935:HIS:HE1	1.84	0.42
2:A:2064:ASN:O	2:A:2068:GLN:HG3	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ASP:O	1:D:232:LEU:HB3	2.20	0.42
2:A:161:PRO:HG2	2:A:893:LEU:HD13	2.01	0.42
2:A:268:LYS:HE3	2:A:268:LYS:HB2	1.84	0.42
2:A:2221:ILE:O	2:A:2225:ILE:HG12	2.18	0.42
2:A:393:ASP:O	2:A:397:ILE:HG13	2.19	0.42
2:A:456:SER:O	2:A:457:MET:C	2.61	0.42
2:A:565:ALA:HB3	2:A:745:ILE:HG21	2.01	0.42
1:D:232:LEU:HB2	1:E:232:LEU:HD11	2.01	0.42
2:A:120:THR:HG22	2:A:903:ILE:HD13	2.00	0.42
2:A:939:LEU:HB3	2:A:945:GLY:HA3	2.02	0.42
2:A:1598:ILE:HB	2:A:1678:LEU:HD22	2.02	0.42
2:A:1641:PRO:O	2:A:1644:LYS:HG2	2.19	0.42
2:A:1669:ILE:HD13	2:A:1669:ILE:HA	1.86	0.42
2:A:1857:PHE:HE1	2:A:1862:PRO:HB2	1.84	0.42
2:A:1972:PHE:HD1	2:A:1973:PHE:CD1	2.37	0.42
1:E:246:GLY:HA2	1:E:249:VAL:HG12	2.00	0.42
2:A:2090:LEU:O	2:A:2091:GLN:C	2.61	0.42
1:B:266:ILE:CD1	1:C:267:GLU:HA	2.49	0.42
2:A:34:ASN:HA	2:A:88:ILE:HG21	2.00	0.42
2:A:482:SER:N	2:A:567:MET:O	2.36	0.42
2:A:1485:CYS:HA	2:A:1488:THR:HG22	2.02	0.42
2:A:1939:ILE:O	2:A:1943:VAL:HG22	2.19	0.42
2:A:53:ARG:HG2	2:A:60:HIS:ND1	2.34	0.42
2:A:90:ILE:HG22	2:A:91:TRP:H	1.85	0.42
2:A:1105:LYS:HA	2:A:1108:THR:HG22	2.02	0.42
2:A:1796:VAL:O	2:A:1800:ILE:HG12	2.20	0.42
1:B:246:GLY:O	1:B:249:VAL:N	2.52	0.42
1:B:281:PRO:HB2	1:C:296:HIS:HA	2.00	0.42
2:A:844:TYR:HD2	2:A:847:ARG:HH21	1.68	0.42
1:E:235:LEU:HD13	1:B:235:LEU:HD12	2.02	0.42
1:B:221:ILE:HD12	1:B:221:ILE:H	1.85	0.42
2:A:861:LEU:O	2:A:905:GLN:NE2	2.52	0.42
2:A:1079:LYS:HB3	2:A:1079:LYS:HE2	1.77	0.42
2:A:1458:ILE:HG13	2:A:1459:THR:N	2.34	0.42
2:A:1502:LEU:HD23	2:A:1502:LEU:HA	1.87	0.42
2:A:1670:ARG:HA	2:A:1673:ILE:HD12	2.01	0.42
2:A:1931:ARG:O	2:A:1935:HIS:ND1	2.53	0.42
2:A:2081:LEU:HB2	2:A:2149:ARG:HG2	2.02	0.42
1:D:225:LEU:HD21	1:E:225:LEU:HB3	2.01	0.42
2:A:596:VAL:HG23	2:A:598:ASP:N	2.35	0.42
2:A:667:THR:HG21	2:A:837:ILE:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:867:GLY:H	2:A:1016:THR:HG22	1.83	0.42
2:A:2131:LYS:HA	2:A:2134:THR:HG22	2.02	0.42
1:C:284:VAL:HB	1:C:289:LEU:HD21	2.01	0.41
2:A:1443:ILE:HB	2:A:1444:PRO:HD3	2.02	0.41
2:A:1450:THR:O	2:A:1454:MET:HG3	2.20	0.41
2:A:1558:ILE:HD13	2:A:1558:ILE:HA	1.93	0.41
2:A:1933:GLN:O	2:A:1937:LEU:HG	2.19	0.41
2:A:2106:ILE:HG13	2:A:2191:TYR:CE1	2.55	0.41
1:E:246:GLY:O	1:E:249:VAL:HG12	2.19	0.41
2:A:65:GLN:OE1	2:A:65:GLN:HA	2.19	0.41
2:A:436:MET:HE2	2:A:436:MET:HB3	1.95	0.41
2:A:572:ARG:HA	2:A:572:ARG:HD3	1.86	0.41
2:A:1131:GLN:H	2:A:1131:GLN:HG2	1.44	0.41
2:A:1933:GLN:HE21	2:A:1965:LEU:HD11	1.84	0.41
2:A:1934:VAL:HG23	2:A:2006:PHE:HE2	1.84	0.41
1:B:276:MET:HG2	2:A:683:ILE:HG21	2.02	0.41
1:C:275:ILE:O	2:A:392:LEU:N	2.53	0.41
2:A:1197:PHE:HB3	2:A:1374:HIS:ND1	2.35	0.41
2:A:256:LEU:HD22	2:A:856:VAL:HG21	2.02	0.41
2:A:1201:PHE:HB3	2:A:1322:HIS:HB2	2.02	0.41
2:A:2190:LYS:HA	2:A:2190:LYS:HD2	1.82	0.41
2:A:824:LEU:HD23	2:A:824:LEU:HA	1.86	0.41
2:A:859:MET:SD	2:A:901:MET:HE2	2.59	0.41
2:A:1443:ILE:HG12	2:A:1696:ILE:HD13	2.01	0.41
1:D:218:ALA:O	1:D:221:ILE:HG22	2.20	0.41
1:B:246:GLY:O	1:B:249:VAL:HB	2.21	0.41
2:A:970:VAL:HG11	2:A:984:LEU:HD13	2.02	0.41
2:A:1033:ASN:HB3	2:A:1035:MET:O	2.21	0.41
1:E:259:VAL:HG12	1:E:260:LYS:N	2.36	0.41
2:A:18:ILE:HG22	2:A:372:THR:HA	2.03	0.41
2:A:79:TRP:HE3	2:A:79:TRP:H	1.68	0.41
2:A:468:PRO:HB2	2:A:528:PRO:HB2	2.03	0.41
2:A:679:TYR:HA	2:A:682:ILE:HG13	2.03	0.41
2:A:1429:THR:O	2:A:1433:GLY:HA2	2.21	0.41
1:D:269:MET:HE3	1:D:269:MET:HB2	1.92	0.41
1:E:259:VAL:CG2	1:B:263:LEU:CD2	2.98	0.41
2:A:472:LEU:HD13	2:A:1035:MET:HE2	2.02	0.41
2:A:711:LEU:HG	2:A:741:PRO:HG3	2.03	0.41
2:A:1527:THR:O	2:A:1531:ILE:HG23	2.20	0.41
2:A:1944:LEU:HB2	2:A:1997:LEU:HD22	2.03	0.41
2:A:79:TRP:HB2	2:A:84:ARG:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:263:LEU:HD12	2:A:266:LEU:HD12	2.03	0.41
2:A:364:ILE:HA	2:A:367:LEU:HG	2.02	0.41
2:A:474:ILE:HG13	2:A:475:PHE:N	2.36	0.41
2:A:540:TYR:HD1	2:A:540:TYR:H	1.68	0.41
2:A:1270:TYR:HA	2:A:1284:LEU:CD2	2.51	0.41
2:A:1986:PRO:C	2:A:2036:ARG:HH22	2.29	0.41
1:C:225:LEU:O	1:C:226:ARG:C	2.64	0.40
2:A:1813:LEU:HD12	2:A:1893:LEU:HD21	2.03	0.40
2:A:1971:GLN:OE1	2:A:2012:ARG:HD3	2.21	0.40
2:A:2077:LYS:HE3	2:A:2077:LYS:HB3	1.79	0.40
1:D:267:GLU:HB3	1:C:266:ILE:HD11	2.03	0.40
1:B:265:THR:HG21	2:A:453:LYS:HD3	2.03	0.40
2:A:396:THR:O	2:A:400:THR:HG22	2.21	0.40
2:A:444:LYS:O	2:A:448:VAL:HG23	2.21	0.40
2:A:683:ILE:HG23	2:A:684:PRO:HD3	2.03	0.40
2:A:1907:GLY:O	2:A:1910:THR:OG1	2.38	0.40
2:A:296:GLU:HA	2:A:365:MET:HE3	2.03	0.40
2:A:482:SER:HB2	2:A:566:LYS:HG3	2.04	0.40
2:A:881:VAL:O	2:A:885:THR:HG23	2.21	0.40
2:A:971:LYS:HD2	2:A:1139:VAL:O	2.21	0.40
2:A:1989:HIS:H	2:A:2036:ARG:HH21	1.69	0.40
2:A:2090:LEU:HG	2:A:2094:MET:HE3	2.04	0.40
1:D:225:LEU:CD2	1:E:225:LEU:HD13	2.51	0.40
1:D:228:MET:SD	1:E:232:LEU:HD13	2.61	0.40
2:A:49:TRP:HB2	2:A:53:ARG:NH2	2.37	0.40
2:A:607:LEU:HD13	2:A:1221:PRO:HD2	2.03	0.40
2:A:408:LEU:HD12	2:A:692:MET:HE1	2.03	0.40
2:A:1529:ARG:HD3	2:A:1573:LYS:NZ	2.37	0.40
2:A:1883:LEU:HD13	2:A:1902:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	B	59/324 (18%)	57 (97%)	2 (3%)	32	58
1	C	78/324 (24%)	72 (92%)	6 (8%)	12	28
1	D	52/324 (16%)	52 (100%)	0	100	100
1	E	50/324 (15%)	47 (94%)	3 (6%)	17	38
2	A	1858/2037 (91%)	1844 (99%)	14 (1%)	73	84
All	All	2097/3333 (63%)	2072 (99%)	25 (1%)	61	78

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

Mol	Chain	Res	Type
1	E	245	GLN
1	E	259	VAL
1	E	273	VAL
1	B	232	LEU
1	B	235	LEU
1	C	250	THR
1	C	260	LYS
1	C	262	THR
1	C	263	LEU
1	C	295	ASP
1	C	297	VAL
2	A	79	TRP
2	A	126	ASP
2	A	170	TRP
2	A	244	THR
2	A	304	GLN
2	A	360	GLU
2	A	393	ASP
2	A	1048	GLU
2	A	1131	GLN
2	A	1380	CYS
2	A	1381	ILE
2	A	1389	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1678	LEU
2	A	1685	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	245	GLN
1	E	251	GLN
1	B	233	GLN
1	B	251	GLN
2	A	34	ASN
2	A	137	ASN
2	A	172	ASN
2	A	173	ASN
2	A	451	ASN
2	A	725	GLN
2	A	887	ASN
2	A	1554	ASN
2	A	1778	HIS
2	A	1933	GLN
2	A	2011	ASN
2	A	2039	GLN
2	A	2091	GLN
2	A	2150	ASN
2	A	2198	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 oligosaccharides 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.

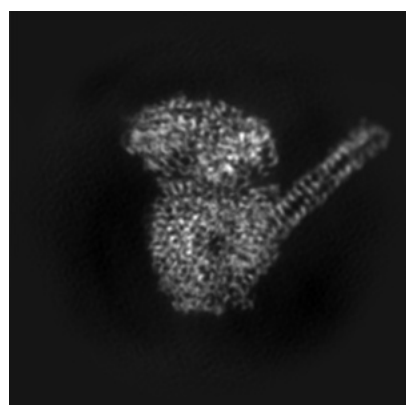
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35864. These allow visual inspection of the internal detail of the map and identification of artifacts.

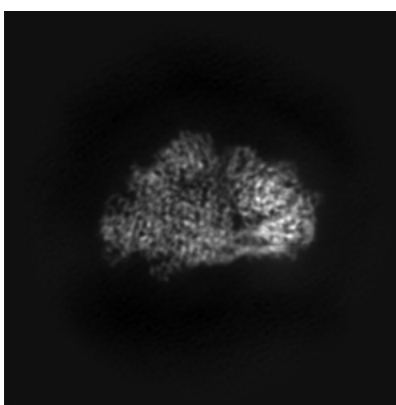
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

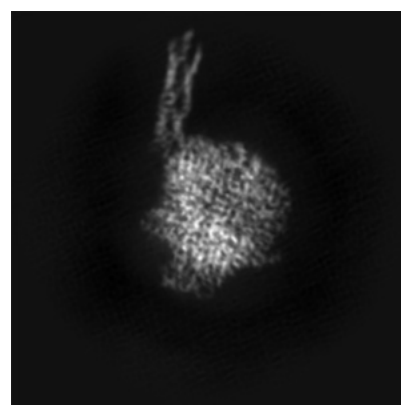
6.1.1 Primary map



X



Y



Z

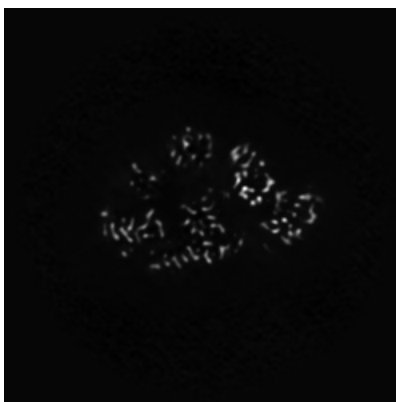
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

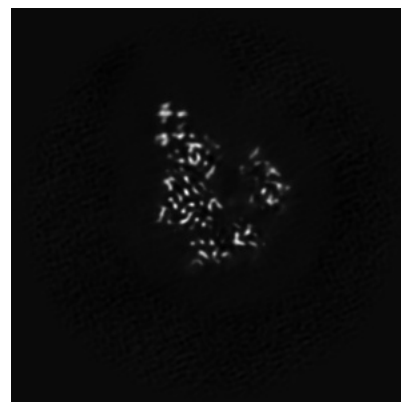
6.2.1 Primary map



X Index: 220



Y Index: 220

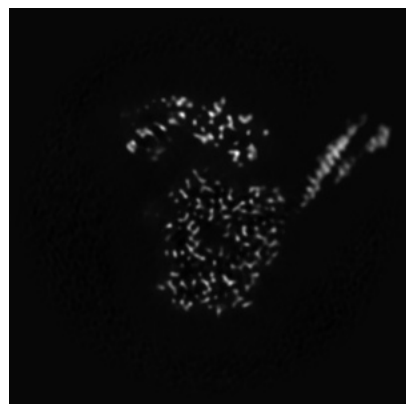


Z Index: 220

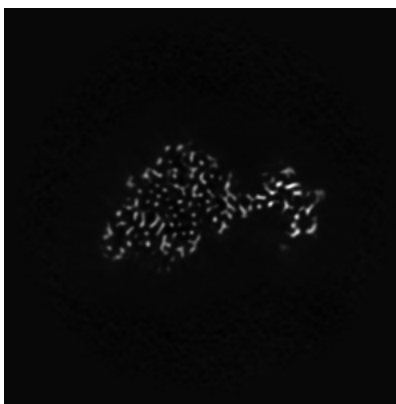
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

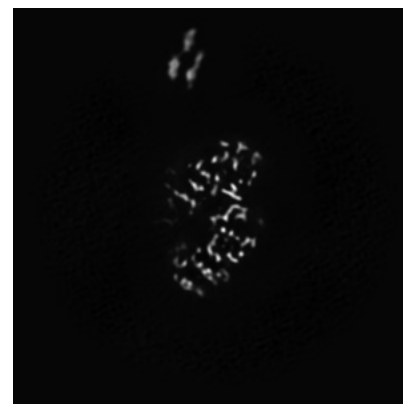
6.3.1 Primary map



X Index: 194



Y Index: 189



Z Index: 290

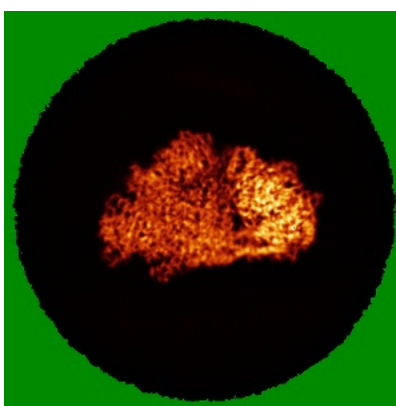
The images above show the largest variance slices of the map in three orthogonal directions.

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

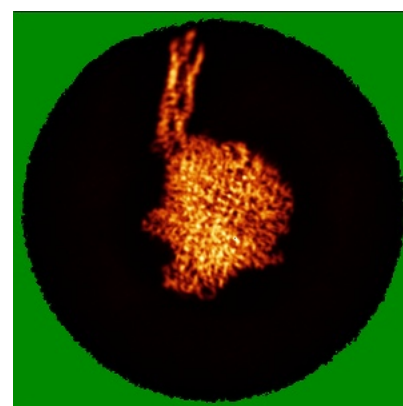
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

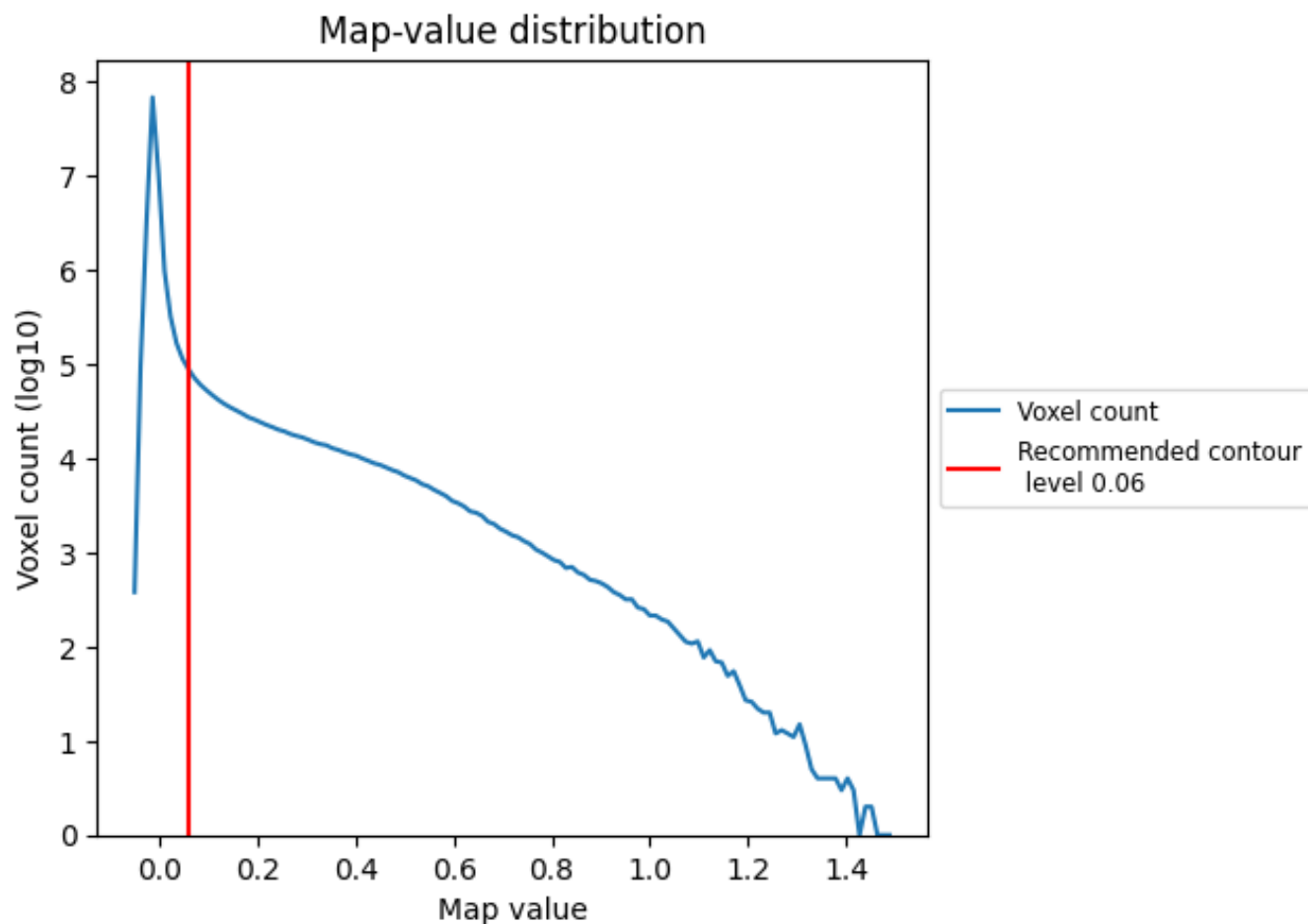
6.6 Mask visualisation

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

7 Map analysis [i](#)

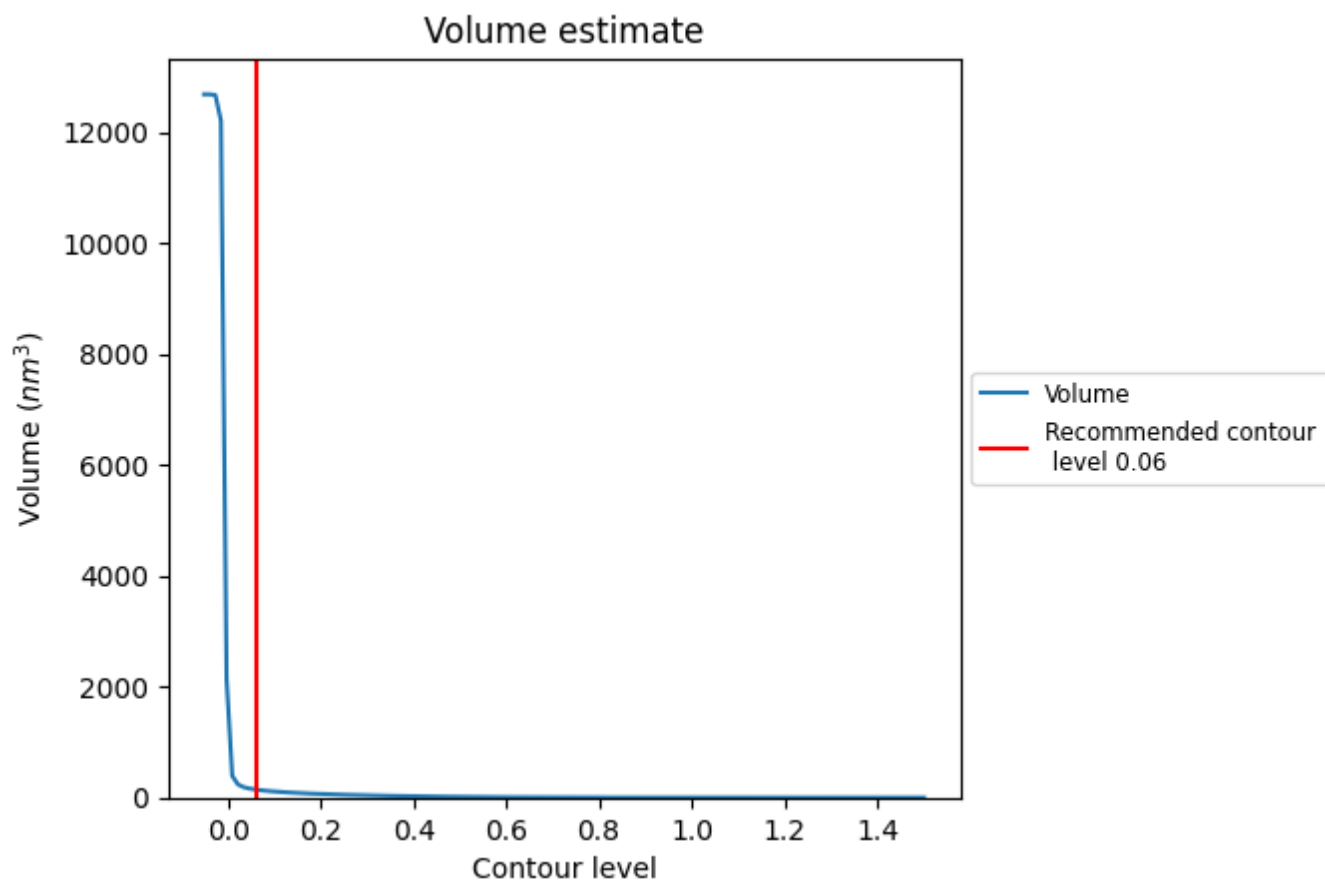
This section contains the results of statistical analysis of the map.

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.

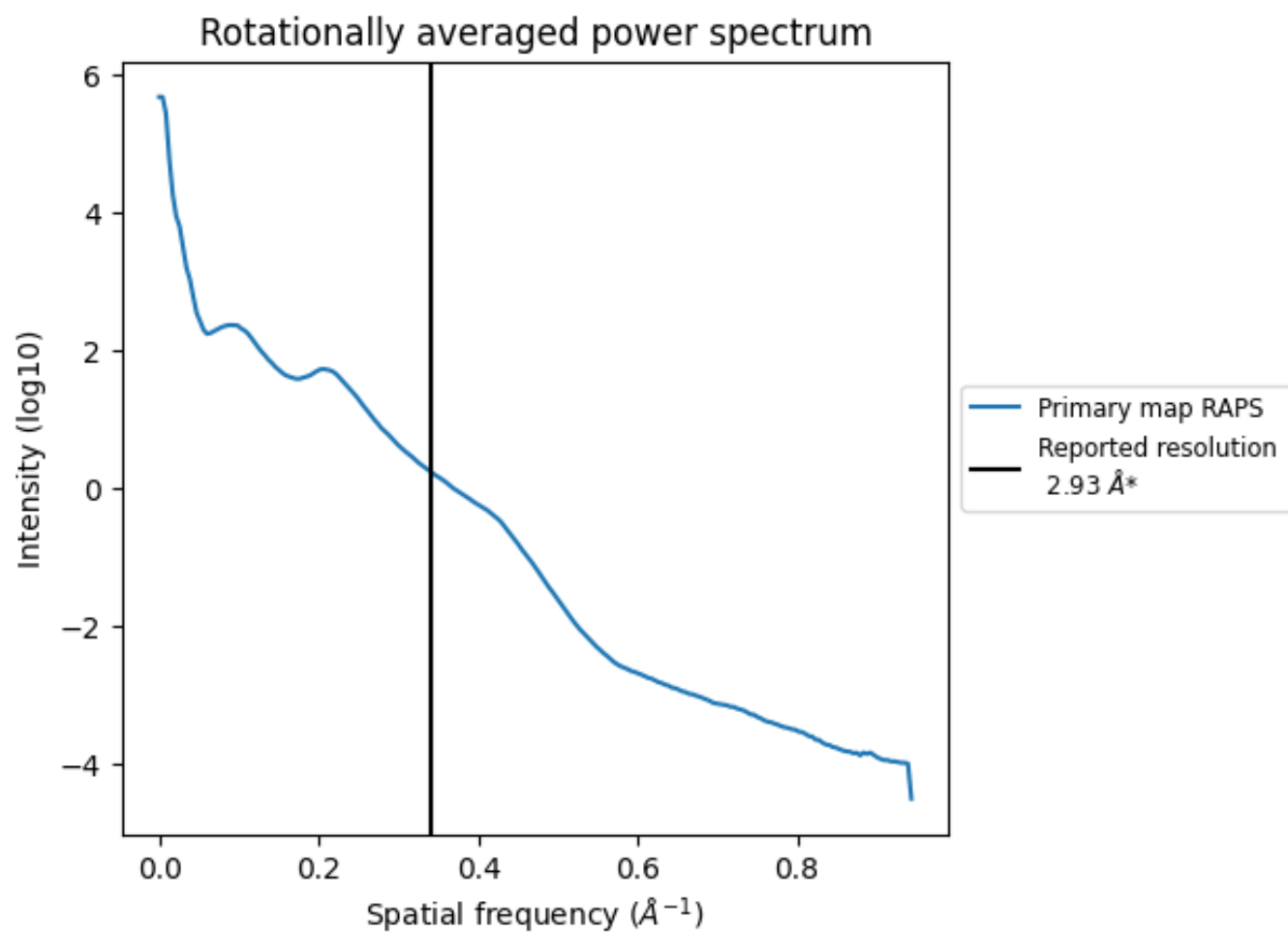
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm^3 ; this corresponds to an approximate mass of 130 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 ⓘ

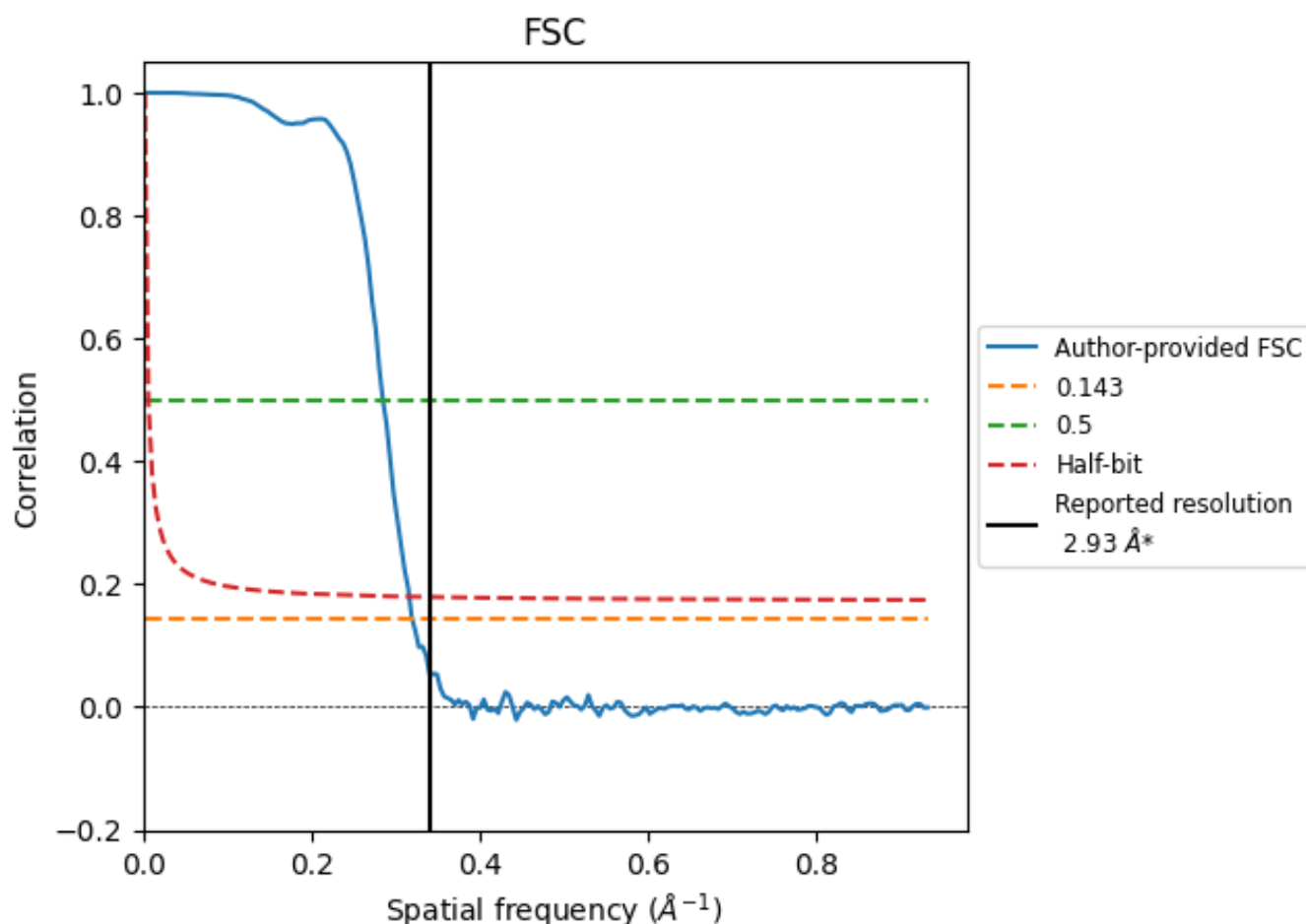


*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

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 0.341 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	3.13	3.51	3.16
Unmasked-calculated*	-	-	-

*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-35864 and PDB model 8IZL. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

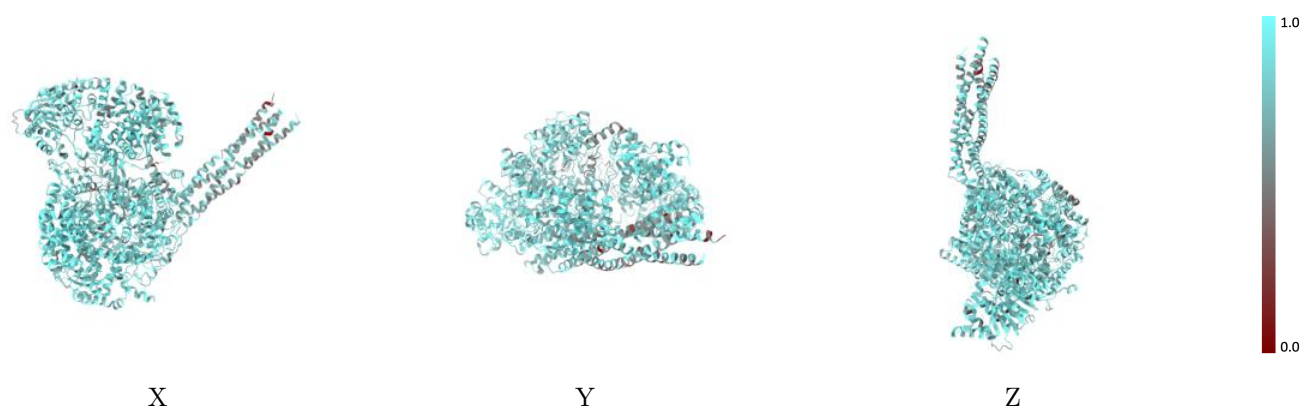
This section was not generated.

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



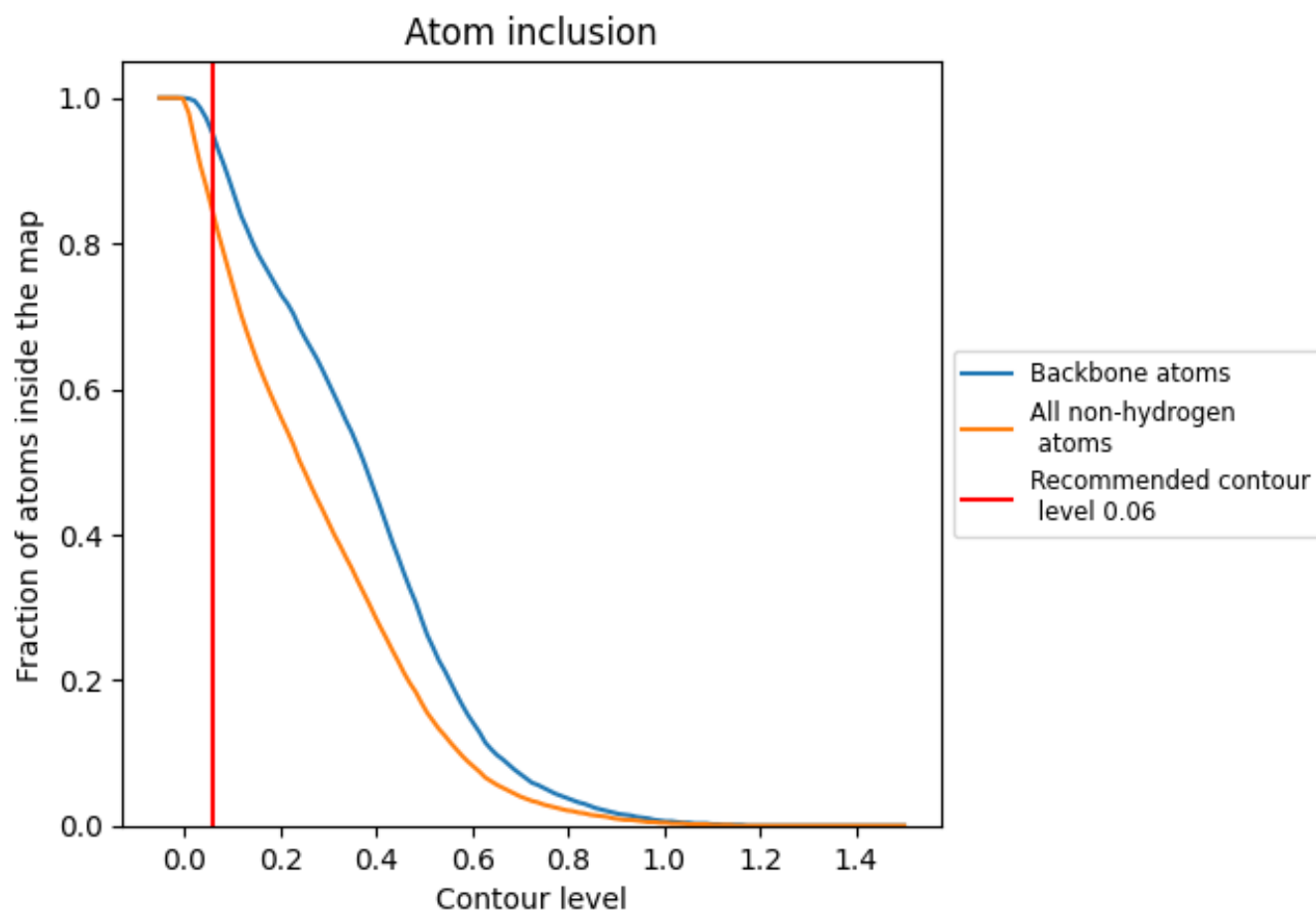
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 84% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.4200
A	0.8590	0.4450
B	0.7660	0.2650
C	0.7320	0.2430
D	0.6770	0.1700
E	0.6810	0.1670

