



Full wwPDB EM Validation Report ⓘ

Jun 3, 2026 – 05:46 PM EDT

PDB ID : 9YEE / pdb_00009yee
EMDB ID : EMD-72849
Title : Rod-hook protein in *Vibrio cholerae* at assembled, opened state
Authors : Guo, W.; Yue, J.
Deposited on : 2025-09-24
Resolution : 3.44 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

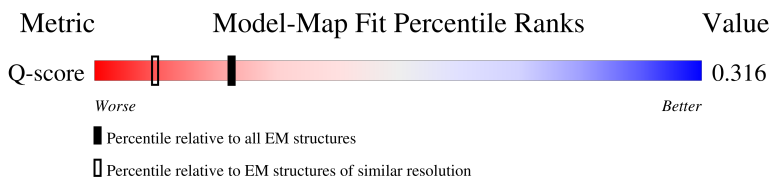
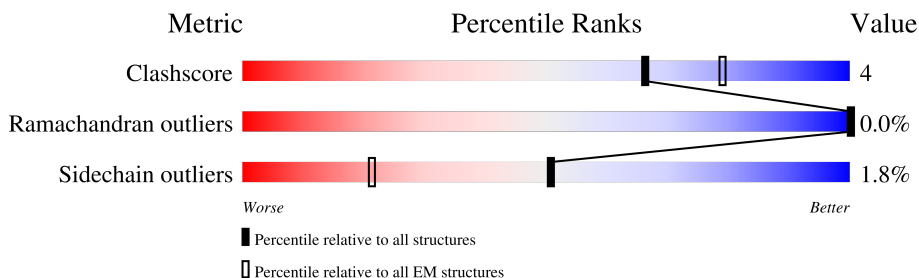
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.44 Å.

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













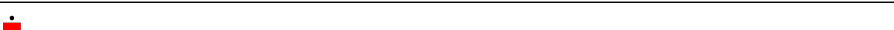

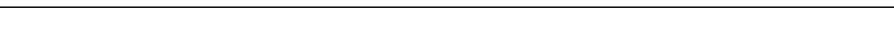
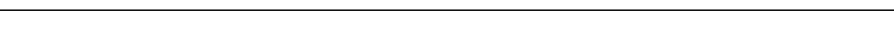











Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13877 (2.94 - 3.94)

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	Ba	262	
1	Bb	262	
1	Bc	262	
1	Bd	262	











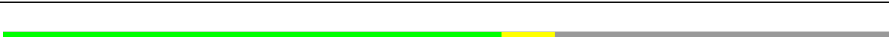


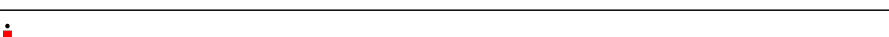
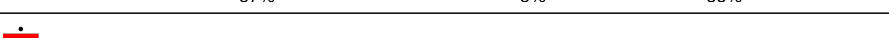
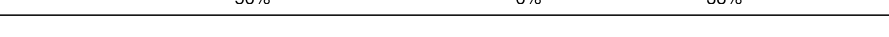

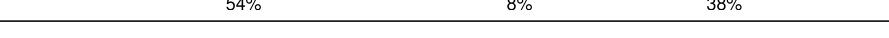

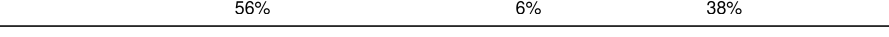
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Be	262	
1	Bf	262	
1	Bg	262	
1	Bh	262	
1	Bi	262	
1	Bj	262	
1	Bk	262	
1	Bl	262	
1	Bm	262	
1	Bn	262	
1	Bo	262	
1	Bp	262	
1	Bq	262	
1	Br	262	
1	Bs	262	
1	Bt	262	
1	Bu	262	
1	Bv	262	
1	Bw	262	
1	Bx	262	
1	By	262	
1	Bz	262	
1	Cb	262	
2	Ca	249	
2	Cc	249	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Cd	249	 87% 10%
2	Cv	249	 82% 11% 7%
2	Cw	249	 88% 12%
3	Ce	434	 55% 7% 38%
3	Cf	434	 55% 6% 38%
3	Cg	434	 58% 38%
3	Ch	434	 58% 38%
3	Ci	434	 58% 38%
3	Cj	434	 56% 6% 38%
3	Ck	434	 58% 5% 38%
3	Cl	434	 56% 6% 38%
3	Cm	434	 55% 7% 38%
3	Cn	434	 57% 5% 38%
3	Co	434	 57% 5% 38%
3	Cp	434	 56% 6% 38%
3	Cq	434	 55% 7% 38%
3	Cr	434	 54% 8% 38%
3	Cs	434	 57% 6% 38%
3	Ct	434	 56% 6% 38%
3	Cu	434	 58% 38%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 96589 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 Flagellar basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ba	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bb	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bc	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bd	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Be	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bf	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bg	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bh	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bi	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bj	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bk	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bl	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bm	262	Total 1966	C 1215	N 339	O 403	S 9	0	0
1	Bn	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bo	262	Total 1969	C 1217	N 339	O 403	S 10	0	0
1	Bp	252	Total 1893	C 1173	N 323	O 387	S 10	0	0
1	Bq	262	Total 1969	C 1217	N 339	O 403	S 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Br	247	Total	C	N	O	S	0	0
			1863	1156	317	380	10		
1	Bs	262	Total	C	N	O	S	0	0
			1969	1217	339	403	10		
1	Bt	251	Total	C	N	O	S	0	0
			1889	1171	322	386	10		
1	Bu	262	Total	C	N	O	S	0	0
			1969	1217	339	403	10		
1	Bv	247	Total	C	N	O	S	0	0
			1859	1154	316	379	10		
1	Bw	262	Total	C	N	O	S	0	0
			1969	1217	339	403	10		
1	Bx	249	Total	C	N	O	S	0	0
			1876	1163	320	383	10		
1	By	248	Total	C	N	O	S	0	0
			1864	1158	316	380	10		
1	Bz	249	Total	C	N	O	S	0	0
			1873	1161	319	383	10		
1	Cb	253	Total	C	N	O	S	0	0
			1900	1178	324	388	10		

- Molecule 2 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ca	241	Total	C	N	O	S	0	0
			1811	1112	327	361	11		
2	Cc	249	Total	C	N	O	S	0	0
			1870	1149	336	373	12		
2	Cd	244	Total	C	N	O	S	0	0
			1833	1125	331	365	12		
2	Cv	232	Total	C	N	O	S	0	0
			1737	1066	312	347	12		
2	Cw	249	Total	C	N	O	S	0	0
			1868	1147	336	373	12		

- Molecule 3 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ce	268	Total	C	N	O	S	0	0
			2045	1273	354	414	4		
3	Cf	268	Total	C	N	O	S	0	0
			2045	1273	354	414	4		

Continued on next page...

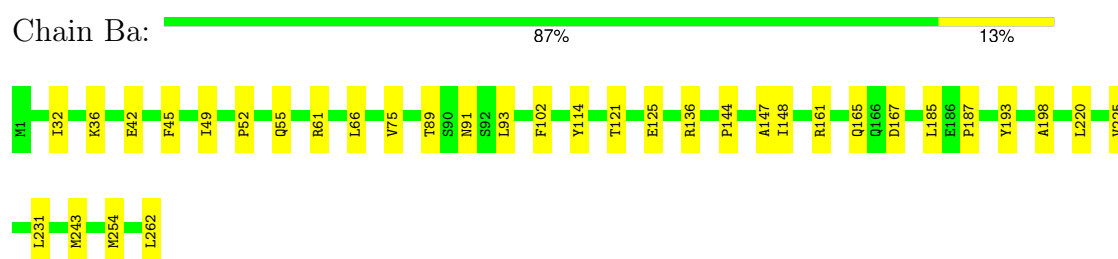
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Cg	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Ch	268	Total 2045	C 1273	N 354	O 414	S 4	0	0
3	Ci	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Cj	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Ck	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Cl	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Cm	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Cn	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Co	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Cp	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Cq	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Cr	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Cs	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Ct	270	Total 2065	C 1285	N 359	O 417	S 4	0	0
3	Cu	270	Total 2065	C 1285	N 359	O 417	S 4	0	0

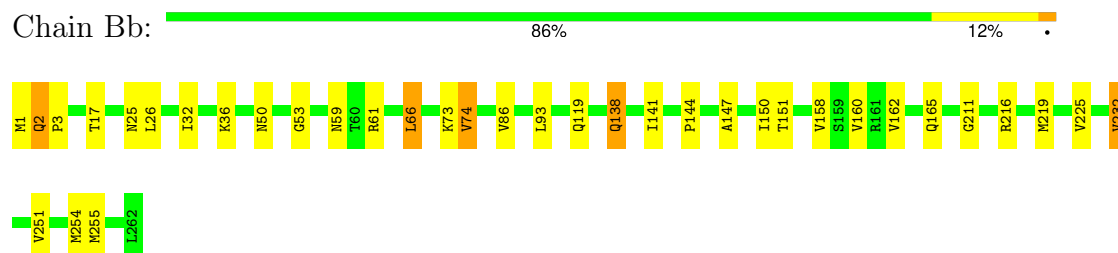
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

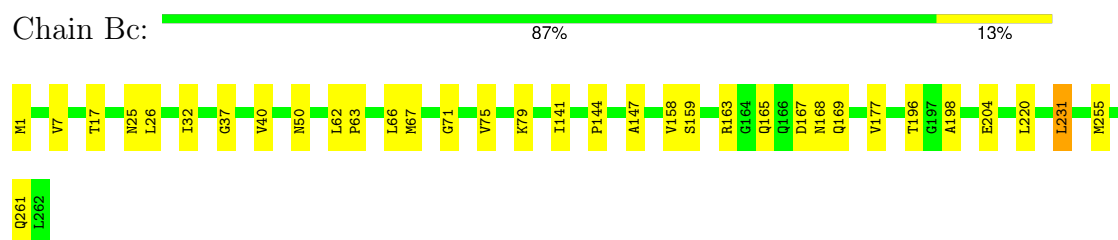
- Molecule 1: Flagellar basal-body rod protein FlgG



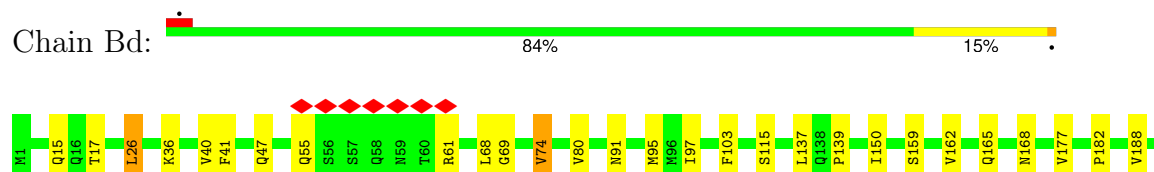
- Molecule 1: Flagellar basal-body rod protein FlgG



- Molecule 1: Flagellar basal-body rod protein FlgG



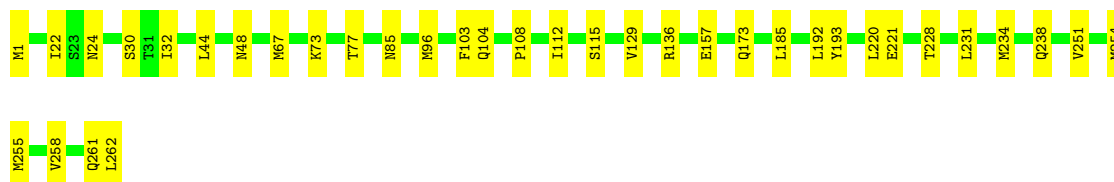
- Molecule 1: Flagellar basal-body rod protein FlgG





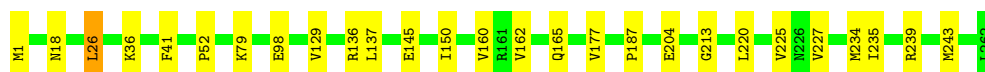
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Be: 86% 14%



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bf: 90% 10%



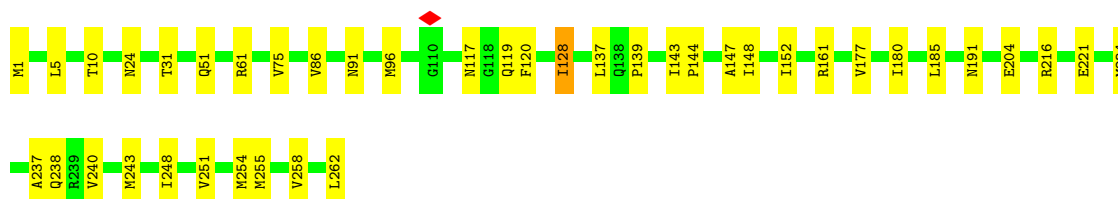
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bg: 88% 11%



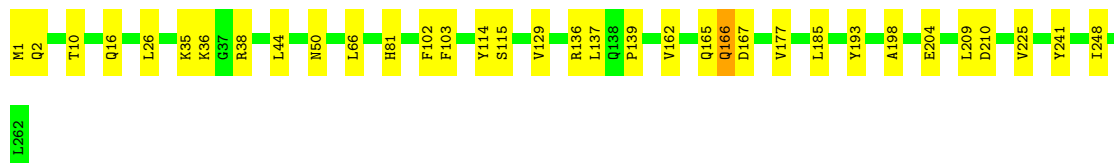
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bh: 84% 15%




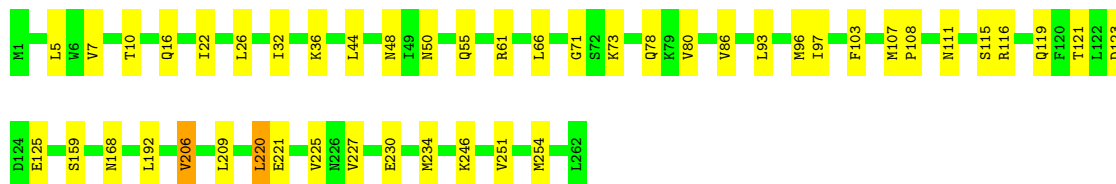
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bi: 87% 13%




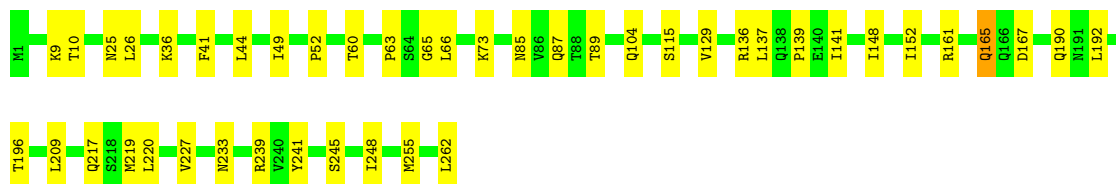
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bj:  82% 17%




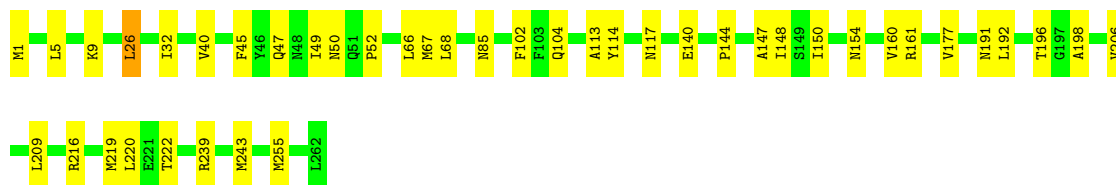
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bk:  83% 16%



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bl:  84% 16%



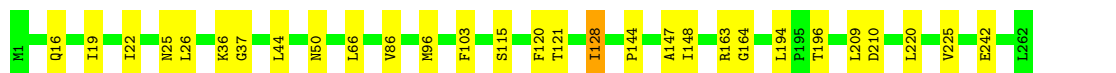
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bm:  87% 12%




- Molecule 1: Flagellar basal-body rod protein FlgG

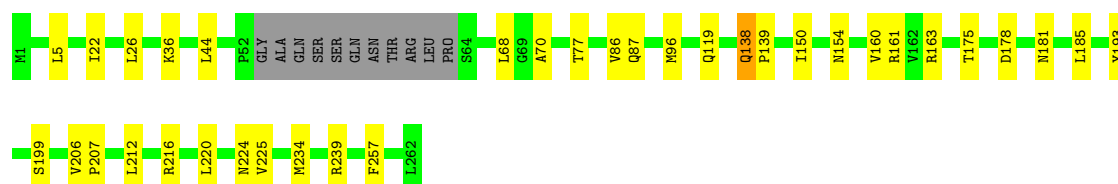
Chain Bn:  89% 11%



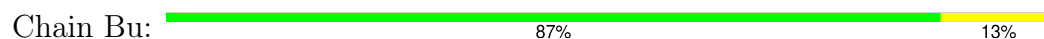
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bo:  86% 14%

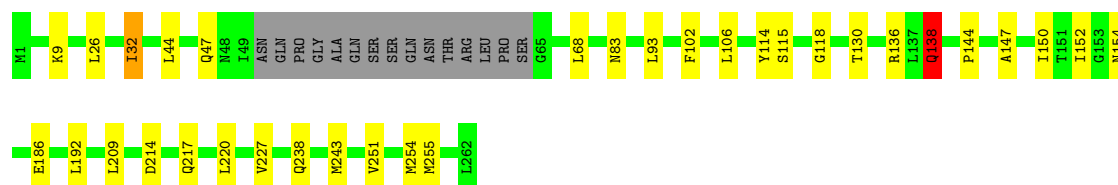
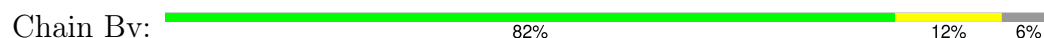




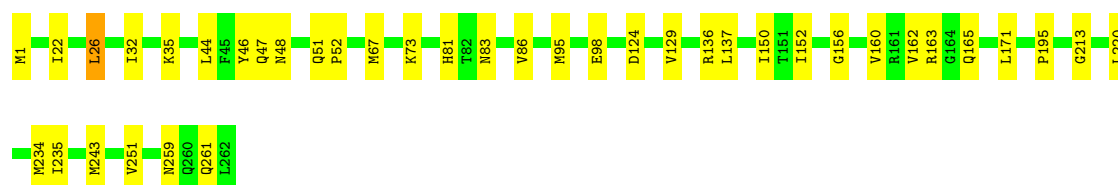
- Molecule 1: Flagellar basal-body rod protein FlgG



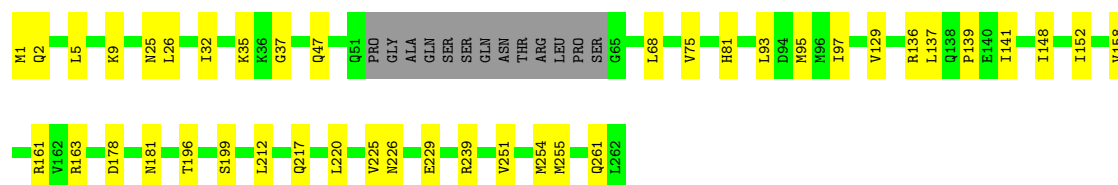
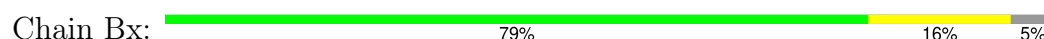
- Molecule 1: Flagellar basal-body rod protein FlgG



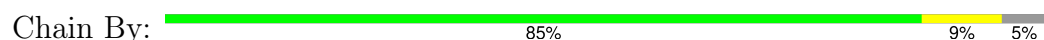
- Molecule 1: Flagellar basal-body rod protein FlgG

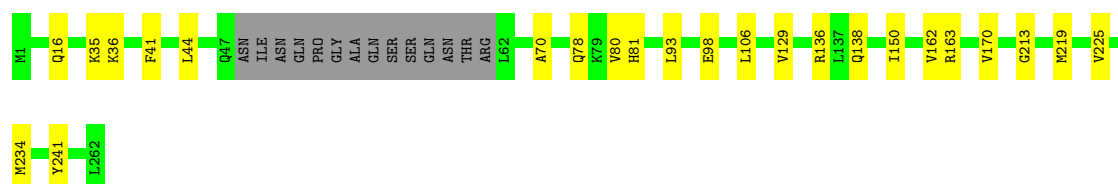


- Molecule 1: Flagellar basal-body rod protein FlgG



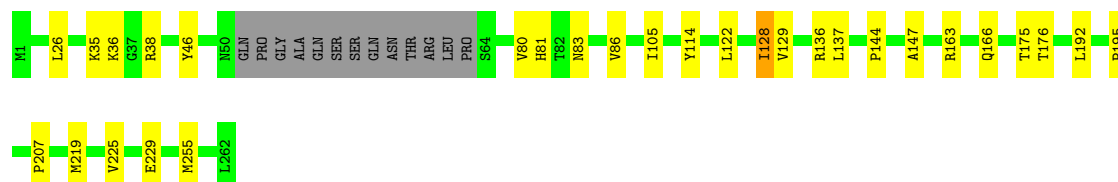
- Molecule 1: Flagellar basal-body rod protein FlgG





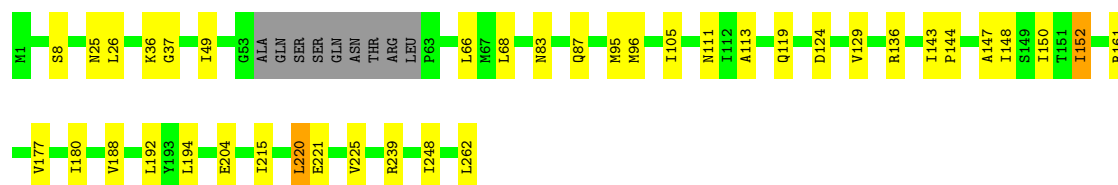
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Bz: 84% 11% 5%



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain Cb: 82% 14% ..



- Molecule 2: Flagellar basal-body rod protein FlgF

Chain Ca: 86% 11% .



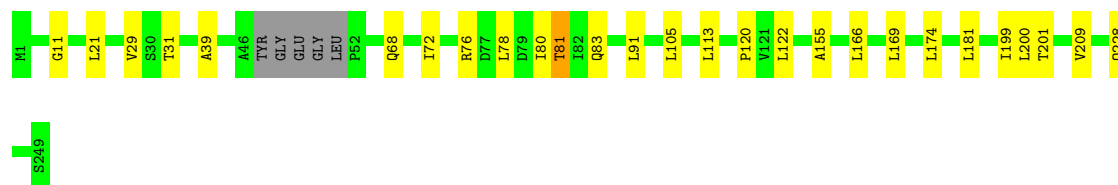
- Molecule 2: Flagellar basal-body rod protein FlgF

Chain Cc: 91% 9%

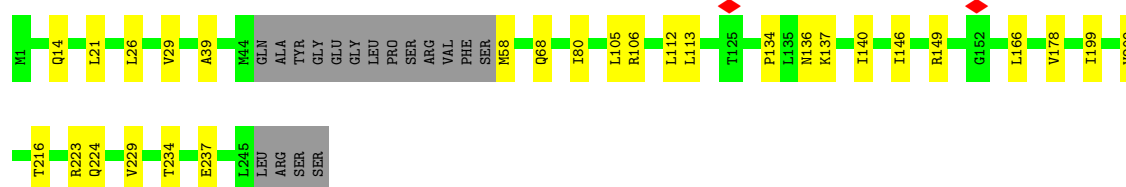
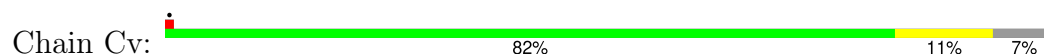


- Molecule 2: Flagellar basal-body rod protein FlgF

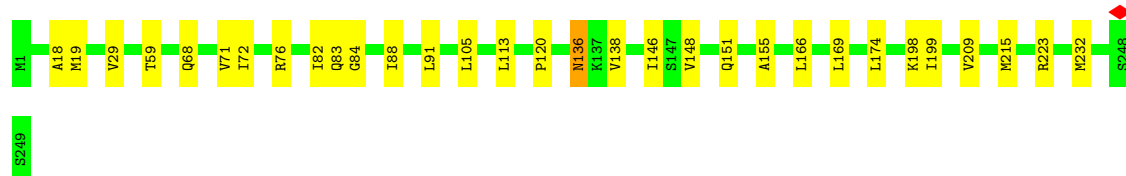
Chain Cd: 87% 10% .



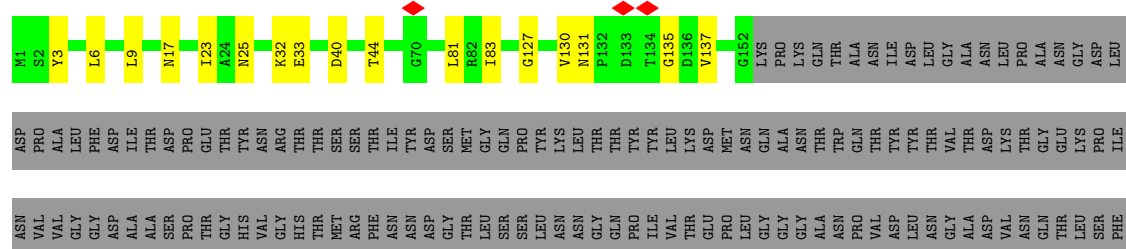
- Molecule 2: Flagellar basal-body rod protein FlgF



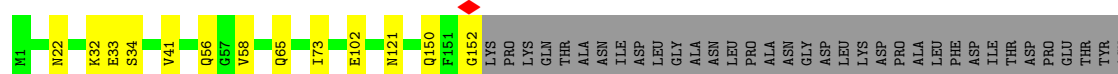
- Molecule 2: Flagellar basal-body rod protein FlgF

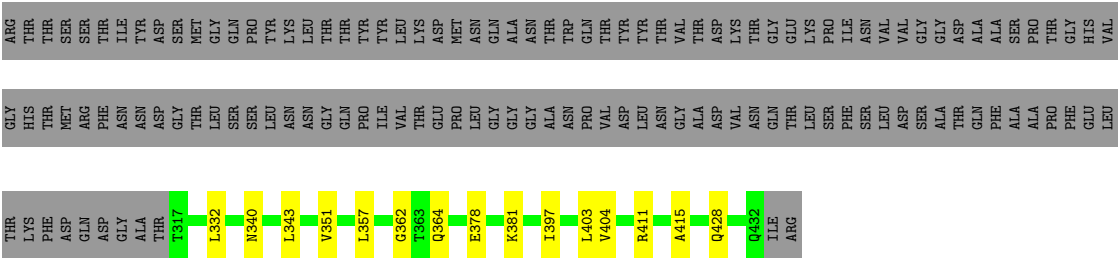


- Molecule 3: Flagellar hook protein FlgE

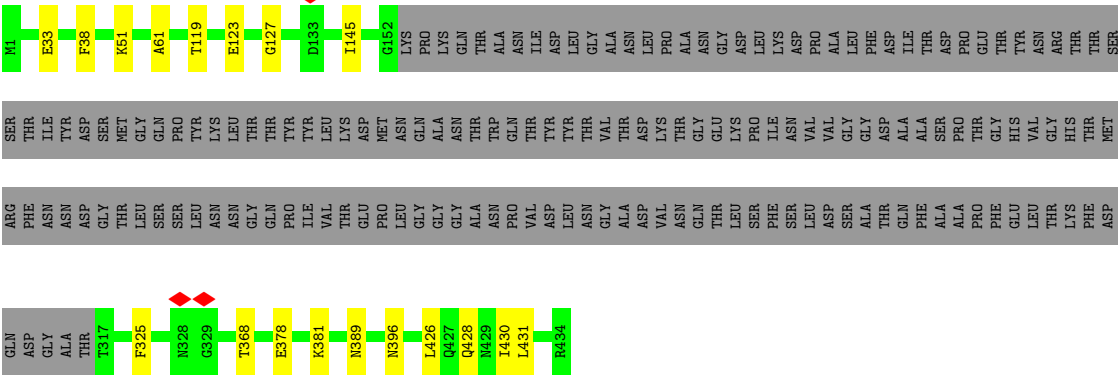


- Molecule 3: Flagellar hook protein FlgE

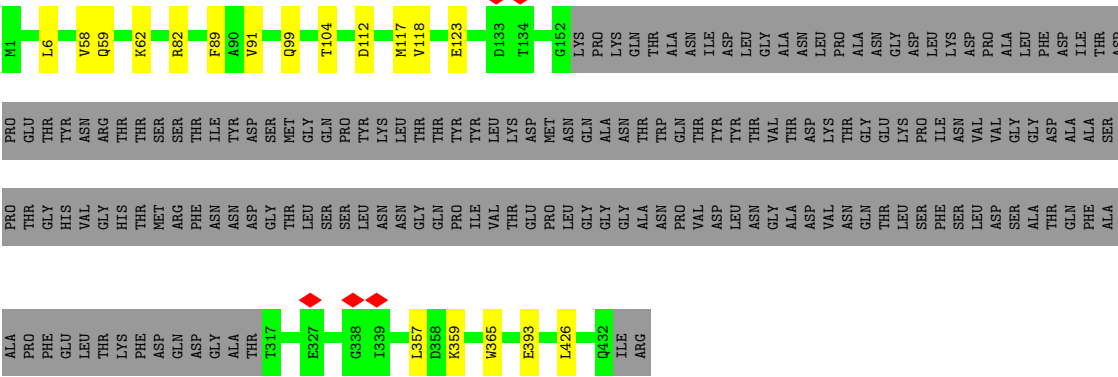




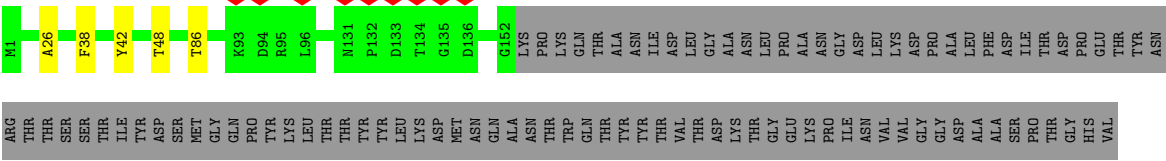
• Molecule 3: Flagellar hook protein FlgE



• Molecule 3: Flagellar hook protein FlgE



• Molecule 3: Flagellar hook protein FlgE



Response	Percentage
Used	57%
Not used	6%
Don't know	38%



Response	Percentage
Yes, the U.S. is a democracy	56%
No, the U.S. is not a democracy	6%
Don't know	38%



Response	Percentage
Yes	58%
No	38%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77446	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	13.576	Depositor
Minimum map value	-0.306	Depositor
Average map value	0.030	Depositor
Map value standard deviation	0.398	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	640.0, 640.0, 640.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ba	0.15	0/1995	0.33	0/2704
1	Bb	0.14	0/1995	0.36	0/2704
1	Bc	0.13	0/1995	0.31	0/2704
1	Bd	0.14	0/1995	0.35	1/2704 (0.0%)
1	Be	0.15	0/1995	0.37	0/2704
1	Bf	0.13	0/1995	0.34	0/2704
1	Bg	0.13	0/1995	0.34	0/2704
1	Bh	0.14	0/1995	0.36	0/2704
1	Bi	0.14	0/1995	0.35	0/2704
1	Bj	0.14	0/1995	0.33	0/2704
1	Bk	0.14	0/1995	0.35	0/2704
1	Bl	0.15	0/1995	0.35	0/2704
1	Bm	0.14	0/1992	0.37	0/2701
1	Bn	0.15	0/1995	0.35	0/2704
1	Bo	0.14	0/1995	0.33	0/2704
1	Bp	0.15	0/1917	0.34	0/2596
1	Bq	0.15	0/1995	0.36	0/2704
1	Br	0.14	0/1886	0.38	0/2554
1	Bs	0.17	0/1995	0.39	0/2704
1	Bt	0.14	0/1913	0.33	0/2591
1	Bu	0.14	0/1995	0.38	0/2704
1	Bv	0.14	0/1882	0.36	0/2548
1	Bw	0.15	0/1995	0.35	0/2704
1	Bx	0.16	0/1899	0.36	0/2571
1	By	0.13	0/1888	0.33	0/2557
1	Bz	0.14	0/1896	0.34	0/2567
1	Cb	0.14	0/1925	0.36	1/2607 (0.0%)
2	Ca	0.12	0/1830	0.33	0/2466
2	Cc	0.11	0/1891	0.28	0/2550
2	Cd	0.13	0/1852	0.34	0/2495
2	Cv	0.11	0/1753	0.31	0/2363
2	Cw	0.12	0/1888	0.32	0/2545
3	Ce	0.12	0/2080	0.33	0/2817
3	Cf	0.13	0/2080	0.33	0/2817

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Cg	0.10	0/2100	0.29	0/2842
3	Ch	0.12	0/2080	0.34	0/2817
3	Ci	0.11	0/2100	0.30	0/2842
3	Cj	0.12	0/2100	0.31	0/2842
3	Ck	0.11	0/2100	0.27	0/2842
3	Cl	0.11	0/2100	0.28	0/2842
3	Cm	0.12	0/2100	0.29	0/2842
3	Cn	0.12	0/2100	0.31	0/2842
3	Co	0.12	0/2100	0.30	0/2842
3	Cp	0.11	0/2100	0.30	0/2842
3	Cq	0.12	0/2100	0.32	0/2842
3	Cr	0.12	0/2100	0.31	0/2842
3	Cs	0.12	0/2100	0.31	0/2842
3	Ct	0.12	0/2100	0.32	0/2842
3	Cu	0.10	0/2100	0.29	0/2842
All	All	0.13	0/97962	0.33	2/132622 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Cb	188	VAL	N-CA-C	-5.50	107.44	113.43
1	Bd	188	VAL	N-CA-C	-5.33	108.09	113.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ba	1969	0	1936	21	0
1	Bb	1969	0	1936	23	0
1	Bc	1969	0	1936	20	0
1	Bd	1969	0	1936	26	0
1	Be	1969	0	1936	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Bf	1969	0	1936	17	0
1	Bg	1969	0	1936	20	0
1	Bh	1969	0	1936	26	0
1	Bi	1969	0	1936	22	0
1	Bj	1969	0	1936	31	0
1	Bk	1969	0	1936	30	0
1	Bl	1969	0	1936	25	0
1	Bm	1966	0	1929	18	0
1	Bn	1969	0	1936	15	0
1	Bo	1969	0	1936	24	0
1	Bp	1893	0	1860	17	0
1	Bq	1969	0	1936	18	0
1	Br	1863	0	1834	26	0
1	Bs	1969	0	1936	24	0
1	Bt	1889	0	1857	20	0
1	Bu	1969	0	1936	19	0
1	Bv	1859	0	1831	18	0
1	Bw	1969	0	1936	26	0
1	Bx	1876	0	1845	23	0
1	By	1864	0	1837	14	0
1	Bz	1873	0	1842	18	0
1	Cb	1900	0	1868	20	0
2	Ca	1811	0	1818	16	0
2	Cc	1870	0	1872	11	0
2	Cd	1833	0	1840	19	0
2	Cv	1737	0	1738	15	0
2	Cw	1868	0	1866	18	0
3	Ce	2045	0	1967	22	0
3	Cf	2045	0	1967	15	0
3	Cg	2065	0	1991	10	0
3	Ch	2045	0	1967	9	0
3	Ci	2065	0	1991	9	0
3	Cj	2065	0	1991	17	0
3	Ck	2065	0	1991	11	0
3	Cl	2065	0	1991	15	0
3	Cm	2065	0	1991	17	0
3	Cn	2065	0	1991	13	0
3	Co	2065	0	1991	14	0
3	Cp	2065	0	1991	13	0
3	Cq	2065	0	1991	19	0
3	Cr	2065	0	1991	20	0
3	Cs	2065	0	1991	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Ct	2065	0	1991	14	0
3	Cu	2065	0	1991	12	0
All	All	96589	0	94460	746	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 4.

All (746) 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:Cp:350:ARG:O	3:Cp:375:ILE:HB	1.90	0.71
1:Bd:103:PHE:HB2	1:Bd:115:SER:O	1.92	0.70
3:Cm:411:ARG:HH12	3:Co:424:ASN:HA	1.58	0.69
1:Be:77:THR:HG21	3:Cq:54:PRO:HG3	1.74	0.69
1:Bg:50:ASN:HB3	1:Bg:66:LEU:H	1.58	0.68
1:Bs:33:GLY:HA2	1:Bs:116:ARG:HE	1.58	0.68
1:Bi:50:ASN:HB2	1:Bi:66:LEU:H	1.58	0.68
1:Bm:1:MET:HG2	1:Bn:16:GLN:HE22	1.59	0.67
1:Bm:141:ILE:HD11	1:Bm:174:ILE:HD11	1.75	0.67
1:Bc:144:PRO:HG2	1:Bc:147:ALA:HB2	1.76	0.67
3:Cg:33:GLU:H	3:Cg:396:ASN:HD21	1.42	0.67
1:Bz:38:ARG:HD3	2:Ca:76:ARG:HH22	1.58	0.67
3:Ct:22:ASN:HD21	3:Ct:34:SER:H	1.43	0.66
1:Bc:261:GLN:HE22	1:Bj:246:LYS:HD3	1.60	0.66
1:Bc:165:GLN:HG2	1:Bc:169:GLN:HE22	1.60	0.66
3:Cq:418:ARG:HG2	3:Cs:431:LEU:HD22	1.78	0.66
1:Bl:104:GLN:HE21	1:Bl:177:VAL:HG13	1.59	0.66
3:Cl:131:ASN:HB3	3:Cl:135:GLY:H	1.61	0.66
1:Bl:216:ARG:HB3	1:Bl:219:MET:HE3	1.77	0.65
2:Cw:29:VAL:HG23	2:Cw:209:VAL:HB	1.79	0.65
3:Ce:23:ILE:HD11	3:Cu:419:ALA:HB1	1.78	0.65
1:Bd:97:ILE:HG12	1:Bd:215:ILE:HG12	1.79	0.65
3:Cm:33:GLU:HB3	3:Cm:397:ILE:HG22	1.79	0.64
2:Cw:83:GLN:HB2	2:Cw:198:LYS:HG3	1.80	0.64
1:Bc:25:ASN:HD21	1:Bc:37:GLY:H	1.46	0.64
1:Bv:209:LEU:HA	1:Bz:163:ARG:HH12	1.64	0.63
2:Cc:80:ILE:HD11	2:Cc:199:ILE:HD12	1.78	0.63
3:Cl:4:VAL:HG13	3:Cl:57:GLY:HA2	1.79	0.63
1:Bx:1:MET:HB3	1:Bx:251:VAL:HG13	1.79	0.63
1:Bd:80:VAL:HG13	1:Bh:91:ASN:HD21	1.64	0.63
1:Ba:165:GLN:HG2	1:Ba:167:ASP:H	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bh:5:LEU:HD12	1:Bh:248:ILE:HD11	1.80	0.62
1:Bl:117:ASN:HB2	1:Bl:191:ASN:HD22	1.64	0.62
1:Bs:48:ASN:HD21	1:Bs:51:GLN:HG3	1.63	0.62
2:Cv:80:ILE:HD11	2:Cv:199:ILE:HD12	1.80	0.62
1:Bc:50:ASN:HB3	1:Bc:66:LEU:H	1.64	0.62
1:Bj:36:LYS:HB3	1:Bj:225:VAL:HG22	1.82	0.62
1:Br:106:LEU:HB3	1:Br:136:ARG:HB3	1.82	0.61
3:Cj:33:GLU:HB3	3:Cj:397:ILE:HG22	1.81	0.61
1:Bi:162:VAL:HB	1:Bi:165:GLN:HE22	1.64	0.61
3:Cn:38:PHE:HB2	3:Co:28:THR:HG22	1.83	0.61
1:Bl:50:ASN:HB2	1:Bl:66:LEU:H	1.66	0.61
2:Cd:29:VAL:HG23	2:Cd:209:VAL:HB	1.82	0.61
1:Bx:148:ILE:HD11	1:Bx:163:ARG:HB2	1.82	0.61
3:Cu:348:LEU:HD21	3:Cu:387:ILE:HD11	1.83	0.61
1:Bg:103:PHE:HB2	1:Bg:115:SER:O	2.01	0.60
3:Cj:411:ARG:HH21	3:Ck:424:ASN:HB3	1.66	0.60
1:Bi:35:LYS:HD3	1:Bi:81:HIS:HA	1.83	0.60
3:Cj:348:LEU:HD12	3:Cj:384:PHE:HB3	1.83	0.60
1:Be:157:GLU:HG3	1:Be:173:GLN:HE22	1.66	0.60
3:Cj:328:ASN:HB2	3:Cj:345:ARG:HH21	1.66	0.60
1:Bh:96:MET:HB2	1:Bh:221:GLU:HG3	1.84	0.60
3:Co:32:LYS:HB2	3:Co:65:GLN:HE21	1.66	0.60
3:Co:68:HIS:HB3	3:Co:396:ASN:HD22	1.65	0.60
2:Cw:18:ALA:HB2	2:Cw:59:THR:HG21	1.84	0.60
3:Cf:22:ASN:HD21	3:Cf:34:SER:H	1.51	0.59
3:Cf:33:GLU:HB3	3:Cf:397:ILE:HG22	1.84	0.59
1:Bn:36:LYS:HD3	1:Bn:225:VAL:HA	1.84	0.59
1:Bn:148:ILE:HD11	1:Bn:163:ARG:HB2	1.84	0.59
1:Bq:144:PRO:HG2	1:Bq:147:ALA:HB2	1.84	0.59
1:Br:259:ASN:HD21	2:Cw:223:ARG:HH21	1.49	0.59
3:Ct:318:GLY:HA3	3:Ct:335:TYR:HB3	1.84	0.59
1:Bb:211:GLY:H	1:Bc:163:ARG:HH11	1.48	0.58
1:Bc:40:VAL:HG22	1:Bj:119:GLN:HE21	1.68	0.58
1:Bq:35:LYS:HD3	1:Bq:81:HIS:HA	1.85	0.58
1:Bv:152:ILE:HB	1:Bv:217:GLN:HE21	1.68	0.58
1:Bo:185:LEU:HB3	1:Bo:193:TYR:HB3	1.86	0.58
1:Bb:251:VAL:HG23	1:Bb:254:MET:HE2	1.85	0.58
1:Bu:97:ILE:HG12	1:Bu:101:GLY:HA3	1.85	0.58
1:Bw:22:ILE:HG21	1:Bw:234:MET:HB2	1.85	0.58
1:Bj:159:SER:HB2	1:Bj:168:ASN:HB3	1.86	0.58
1:Br:258:VAL:HG22	2:Cv:229:VAL:HG21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bs:36:LYS:HB3	1:Bs:225:VAL:HG22	1.86	0.58
3:Cr:128:TYR:HB2	3:Cr:345:ARG:HB3	1.86	0.58
1:Bf:36:LYS:HB3	1:Bf:225:VAL:HG22	1.85	0.58
1:Bw:51:GLN:H	2:Ca:139:GLU:HG2	1.68	0.58
1:By:78:GLN:HB3	2:Cd:76:ARG:HH22	1.69	0.58
3:Cf:332:LEU:HD21	3:Cf:340:ASN:HD21	1.67	0.57
3:Cr:408:SER:HB3	3:Cr:411:ARG:HH21	1.69	0.57
1:Bd:236:GLU:HB2	1:Bd:239:ARG:HH21	1.70	0.57
1:Bj:50:ASN:HB3	1:Bj:66:LEU:H	1.69	0.57
1:Be:258:VAL:HA	1:Be:261:GLN:HE21	1.69	0.57
1:Bt:150:ILE:HG22	1:Bt:160:VAL:HG12	1.85	0.57
3:Ck:426:LEU:HD21	3:Cn:410:GLN:HG2	1.85	0.57
1:Be:115:SER:HB2	1:Be:192:LEU:HD23	1.85	0.57
1:Br:141:ILE:HG21	1:Br:171:LEU:HB3	1.86	0.57
3:Cr:33:GLU:HB3	3:Cr:397:ILE:HG22	1.85	0.57
1:Bu:148:ILE:HB	1:Bu:161:ARG:HB2	1.86	0.57
1:Bv:144:PRO:HG2	1:Bv:147:ALA:HB2	1.85	0.57
1:Bx:152:ILE:H	1:Bx:217:GLN:HG3	1.69	0.57
3:Cn:129:GLU:H	3:Cn:143:LYS:HE2	1.69	0.57
1:Bb:1:MET:H1	1:Bb:255:MET:HG3	1.69	0.57
2:Cc:29:VAL:HG23	2:Cc:209:VAL:HB	1.87	0.57
1:Bd:168:ASN:H	3:Cj:369:GLN:HE22	1.53	0.57
1:Bt:181:ASN:HB3	1:Bt:199:SER:HA	1.87	0.57
1:Bz:46:TYR:HB2	2:Ca:178:VAL:HA	1.87	0.57
1:Bb:162:VAL:HB	1:Bb:165:GLN:HB2	1.87	0.56
1:Bl:45:PHE:HE2	1:Bv:83:ASN:HD22	1.53	0.56
1:Bl:150:ILE:HG22	1:Bl:160:VAL:HG12	1.86	0.56
1:Bt:44:LEU:HB2	1:Bt:70:ALA:HB3	1.87	0.56
3:Cs:33:GLU:HB3	3:Cs:397:ILE:HG22	1.86	0.56
1:Bi:44:LEU:HD13	1:Bt:86:VAL:HG21	1.87	0.56
1:Br:46:TYR:HB2	2:Cv:178:VAL:HA	1.88	0.56
1:Bu:53:GLY:HA2	1:Bu:61:ARG:HB3	1.87	0.56
3:Cq:4:VAL:HG13	3:Cq:57:GLY:HA2	1.86	0.56
1:Bu:36:LYS:HD2	1:Bu:225:VAL:HA	1.87	0.56
1:Bh:120:PHE:HB3	1:Bh:128:ILE:HD11	1.87	0.56
3:Cn:33:GLU:HB3	3:Cn:397:ILE:HG22	1.88	0.56
3:Cu:329:GLY:HA3	3:Cu:345:ARG:HH21	1.70	0.56
1:Bd:41:PHE:HB3	1:Bh:31:THR:HG22	1.87	0.56
1:Bw:48:ASN:HD21	1:Bw:51:GLN:HG2	1.70	0.56
1:Bx:226:ASN:HB2	1:Bx:229:GLU:HB2	1.86	0.56
3:Cq:351:VAL:HG21	3:Cq:357:LEU:HD21	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ca:9:MET:HE3	2:Ca:232:MET:HE3	1.86	0.56
2:Cd:166:LEU:HD21	2:Cd:199:ILE:HD11	1.88	0.56
1:Bw:98:GLU:O	1:Bw:213:GLY:HA3	2.05	0.56
1:Cb:177:VAL:HG22	1:Cb:204:GLU:HA	1.88	0.56
1:Br:25:ASN:HD21	1:Br:37:GLY:H	1.52	0.56
1:Bt:5:LEU:HD12	2:Cv:216:THR:HG23	1.88	0.56
3:Cm:359:LYS:HD2	3:Cm:363:THR:HA	1.88	0.55
1:Bm:35:LYS:HD3	1:Bm:81:HIS:HA	1.88	0.55
1:Bp:80:VAL:HG22	2:Cw:76:ARG:HH21	1.72	0.55
1:Bu:47:GLN:HA	1:Cb:83:ASN:HD21	1.70	0.55
1:Bz:35:LYS:HD3	1:Bz:81:HIS:HA	1.88	0.55
3:Cq:80:ASP:HB3	3:Cq:390:GLY:H	1.72	0.55
1:Bx:9:LYS:HE2	1:Bz:229:GLU:HG2	1.89	0.55
1:By:36:LYS:HB3	1:By:225:VAL:HG22	1.88	0.55
2:Cd:91:LEU:HB2	2:Cd:120:PRO:HG2	1.87	0.55
2:Cv:140:ILE:HG12	2:Cv:146:ILE:HG13	1.87	0.55
2:Ca:105:LEU:HD13	2:Ca:113:LEU:HD21	1.88	0.55
3:Co:104:THR:HB	3:Co:364:GLN:HG2	1.88	0.55
1:Bj:7:VAL:HG13	1:Bj:71:GLY:HA2	1.88	0.55
1:Be:231:LEU:HD13	3:Cs:431:LEU:HD21	1.88	0.55
3:Cl:33:GLU:HB3	3:Cl:397:ILE:HG22	1.88	0.55
1:Br:17:THR:HG21	1:Br:74:VAL:HG21	1.89	0.54
1:By:35:LYS:HD3	1:By:81:HIS:HA	1.89	0.54
3:Cf:121:ASN:HD21	3:Cf:362:GLY:HA3	1.72	0.54
1:Bf:79:LYS:HE2	1:Bf:187:PRO:HD3	1.89	0.54
1:Bl:198:ALA:HA	1:Bw:124:ASP:HB3	1.88	0.54
3:Ce:17:ASN:HD21	3:Cu:54:PRO:HG3	1.72	0.54
2:Cw:68:GLN:HE22	2:Cw:84:GLY:H	1.55	0.54
1:Bm:50:ASN:HB2	1:Bm:66:LEU:H	1.72	0.54
3:Cn:426:LEU:HD23	3:Cn:427:GLN:HG3	1.89	0.54
1:Bj:55:GLN:HA	1:Bj:61:ARG:HA	1.90	0.54
2:Ca:82:ILE:HD12	2:Ca:101:ARG:HD3	1.88	0.54
3:Cg:325:PHE:HB2	3:Cg:389:ASN:HB3	1.88	0.54
3:Cp:62:LYS:HE3	3:Cp:63:VAL:H	1.72	0.54
1:Bd:137:LEU:HG	1:Bd:139:PRO:HD2	1.89	0.54
1:Cb:96:MET:HE3	1:Cb:221:GLU:HB3	1.89	0.54
1:Ba:93:LEU:HD13	1:Ba:121:THR:HA	1.89	0.54
2:Cv:21:LEU:HD23	2:Cv:39:ALA:HB2	1.90	0.54
1:Bi:167:ASP:HA	3:Cm:369:GLN:HB3	1.90	0.54
1:Bk:209:LEU:HA	1:Bq:163:ARG:HH22	1.73	0.54
1:Bb:25:ASN:HB3	1:Bb:225:VAL:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bx:181:ASN:HB3	1:Bx:199:SER:HA	1.90	0.53
1:Cb:143:ILE:HD12	1:Cb:150:ILE:HD12	1.90	0.53
3:Cn:95:ARG:HH12	3:Cn:144:PRO:HG2	1.73	0.53
3:Co:378:GLU:HB2	3:Co:381:LYS:HE3	1.90	0.53
1:Bd:177:VAL:HG22	1:Bd:204:GLU:HG2	1.90	0.53
1:Be:108:PRO:HG2	1:Bl:154:ASN:HD21	1.74	0.53
1:Be:185:LEU:HB3	1:Be:193:TYR:HB3	1.90	0.53
1:Bk:115:SER:HB2	1:Bk:192:LEU:HD23	1.89	0.53
1:Bl:144:PRO:HG2	1:Bl:147:ALA:HB2	1.89	0.53
1:Bu:67:MET:HE1	1:Bv:186:GLU:HG3	1.91	0.53
1:Bz:114:TYR:HE2	1:Bz:195:PRO:HG3	1.73	0.53
1:Bw:35:LYS:HD3	1:Bw:81:HIS:HA	1.90	0.53
3:Cf:41:VAL:HG12	3:Cf:56:GLN:HE21	1.73	0.53
1:Bk:152:ILE:HB	1:Bk:217:GLN:HE21	1.74	0.53
3:Ct:350:ARG:O	3:Ct:375:ILE:HB	2.09	0.53
3:Cg:119:THR:HG22	3:Cg:123:GLU:H	1.73	0.53
1:Bh:1:MET:HG2	1:Bh:255:MET:HE2	1.90	0.53
3:Ct:4:VAL:HG13	3:Ct:57:GLY:HA2	1.90	0.53
1:Bu:185:LEU:HB3	1:Bu:193:TYR:HB3	1.90	0.53
1:Bb:50:ASN:HB2	1:Bb:66:LEU:H	1.74	0.53
1:Bg:1:MET:HB2	1:Bg:251:VAL:HG13	1.91	0.53
1:Bd:95:MET:HE3	1:Bd:217:GLN:HE22	1.74	0.52
1:Bw:73:LYS:HG3	1:Bz:219:MET:HE1	1.91	0.52
1:Bw:195:PRO:HB2	1:Bz:166:GLN:HG3	1.90	0.52
1:By:98:GLU:O	1:By:213:GLY:HA3	2.10	0.52
1:Ba:36:LYS:HB3	1:Ba:225:VAL:HG22	1.92	0.52
1:Ba:49:ILE:HB	1:Ba:66:LEU:HB3	1.90	0.52
1:Bi:129:VAL:HG12	1:Bi:136:ARG:HA	1.90	0.52
1:Bw:95:MET:HE1	1:Bw:152:ILE:HG21	1.90	0.52
3:Cp:29:PHE:HE2	3:Cp:107:GLY:H	1.55	0.52
1:Bj:80:VAL:HA	1:Bs:91:ASN:HD21	1.73	0.52
1:Cb:111:ASN:HD21	1:Cb:194:LEU:HD22	1.74	0.52
1:Bq:50:ASN:HB3	1:Bq:66:LEU:H	1.74	0.52
3:Cm:126:LEU:HD13	3:Cm:142:PRO:HB2	1.90	0.52
1:Be:85:ASN:HA	3:Cs:56:GLN:HB3	1.90	0.52
1:Be:129:VAL:HG12	1:Be:136:ARG:HA	1.90	0.52
1:Bm:103:PHE:HB2	1:Bm:115:SER:O	2.08	0.52
2:Cc:167:VAL:HG21	2:Cc:191:PHE:HB3	1.91	0.52
1:Bl:209:LEU:HA	1:Bw:163:ARG:HH12	1.75	0.52
1:Br:85:ASN:HD22	1:Br:86:VAL:H	1.57	0.52
1:Bw:44:LEU:HD11	1:Bw:73:LYS:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Co:353:ASN:HB3	3:Co:371:SER:HA	1.91	0.52
1:Ba:52:PRO:HB2	1:Bk:196:THR:HG21	1.91	0.52
1:Cb:144:PRO:HG2	1:Cb:147:ALA:HB2	1.92	0.52
3:Cu:81:LEU:HB2	3:Cu:107:GLY:HA3	1.92	0.52
1:Ba:231:LEU:HG	1:Bg:243:MET:HE2	1.92	0.52
1:Bc:32:ILE:HG23	1:Bc:220:LEU:HD13	1.90	0.52
1:Bn:103:PHE:HB2	1:Bn:115:SER:O	2.09	0.52
1:Bq:115:SER:HB2	1:Bq:192:LEU:HD23	1.91	0.52
1:Bs:40:VAL:HG22	1:Bt:119:GLN:HE21	1.75	0.52
1:Bz:175:THR:HA	1:Bz:207:PRO:HD3	1.92	0.52
2:Ca:21:LEU:HD22	2:Ca:39:ALA:HB2	1.92	0.52
3:Cp:348:LEU:HD21	3:Cp:387:ILE:HD11	1.91	0.52
1:Be:228:THR:HG21	3:Ct:413:PHE:HZ	1.74	0.52
1:Bk:262:LEU:HB2	1:Bo:246:LYS:HZ1	1.75	0.52
1:Bw:129:VAL:HG12	1:Bw:136:ARG:HG2	1.92	0.52
1:Bd:47:GLN:HB3	1:Bd:68:LEU:HB2	1.91	0.52
1:Bg:111:ASN:HD21	1:Bn:164:GLY:HA2	1.74	0.52
1:Cb:66:LEU:HA	2:Cc:61:ARG:HH12	1.75	0.52
1:Bv:243:MET:HG3	1:Bw:259:ASN:HD22	1.75	0.51
1:Bw:98:GLU:O	1:Bw:213:GLY:CA	2.57	0.51
2:Cd:21:LEU:HD23	2:Cd:39:ALA:HB2	1.91	0.51
1:Bd:91:ASN:HA	3:Ci:48:THR:HG22	1.91	0.51
1:Bs:261:GLN:HG3	1:Bs:262:LEU:HG	1.92	0.51
3:Ce:406:LEU:HD13	3:Cu:422:VAL:HG13	1.92	0.51
3:Cf:351:VAL:HG11	3:Cf:357:LEU:HD21	1.92	0.51
1:Bc:255:MET:HE3	1:Bk:239:ARG:HG3	1.93	0.51
1:Bj:44:LEU:HD21	1:Bj:73:LYS:HD3	1.92	0.51
1:Ba:89:THR:HG22	1:Ba:91:ASN:H	1.75	0.51
1:Bb:144:PRO:HG2	1:Bb:147:ALA:HB2	1.92	0.51
1:Bw:1:MET:HB2	1:Bw:251:VAL:HG13	1.91	0.51
1:Bx:25:ASN:HD21	1:Bx:37:GLY:H	1.59	0.51
3:Cg:51:LYS:HZ1	3:Ch:62:LYS:HA	1.75	0.51
2:Cw:105:LEU:HD13	2:Cw:113:LEU:HD21	1.91	0.51
1:Bn:120:PHE:HB3	1:Bn:128:ILE:HD11	1.92	0.51
1:Bx:1:MET:HE3	1:Bx:254:MET:HG3	1.93	0.51
3:Ci:324:ASP:HB3	3:Ci:332:LEU:HB2	1.92	0.51
1:Bj:78:GLN:HE22	1:Bs:121:THR:HB	1.75	0.51
1:Bm:105:ILE:HB	1:Bm:113:ALA:HB3	1.91	0.51
3:Ct:319:PHE:H	3:Ct:336:SER:H	1.59	0.51
2:Cv:14:GLN:HG3	2:Cv:58:MET:HA	1.92	0.51
1:Ba:187:PRO:HD2	1:Bg:67:MET:HE3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ci:357:LEU:HB3	3:Ci:365:TRP:HB3	1.93	0.51
1:Bo:36:LYS:HB3	1:Bo:225:VAL:HG22	1.92	0.51
1:Bu:188:VAL:HG11	1:Bu:194:LEU:HD12	1.93	0.51
1:Bx:47:GLN:HB3	1:Bx:68:LEU:HB2	1.92	0.51
1:Bk:129:VAL:HG12	1:Bk:136:ARG:HA	1.93	0.51
3:Cu:318:GLY:HA3	3:Cu:335:TYR:HB3	1.93	0.51
1:Ba:185:LEU:HB3	1:Ba:193:TYR:HB3	1.93	0.51
1:Bi:102:PHE:HB3	1:Bi:114:TYR:HB3	1.93	0.51
1:Bj:103:PHE:HB2	1:Bj:115:SER:O	2.10	0.51
1:Bt:22:ILE:HG21	1:Bt:234:MET:HB2	1.92	0.51
1:Be:22:ILE:HG21	1:Be:234:MET:HB2	1.93	0.50
2:Cc:106:ARG:HH21	2:Cc:118:GLY:HA2	1.76	0.50
3:Cj:328:ASN:HD22	3:Cj:345:ARG:HE	1.58	0.50
3:Ct:33:GLU:HB3	3:Ct:397:ILE:HG22	1.93	0.50
1:Bs:32:ILE:HG21	1:Bs:119:GLN:HE22	1.76	0.50
1:By:80:VAL:HG22	2:Cd:76:ARG:HH21	1.76	0.50
1:Bz:36:LYS:HE3	1:Bz:225:VAL:HA	1.94	0.50
3:Cu:92:ALA:HB2	3:Cu:126:LEU:HD11	1.94	0.50
1:Bj:97:ILE:HG23	1:Bj:116:ARG:HH21	1.76	0.50
3:Ce:9:LEU:HD11	3:Ct:404:VAL:HG13	1.94	0.50
3:Cp:33:GLU:H	3:Cp:396:ASN:HD21	1.59	0.50
3:Cq:64:ALA:HA	3:Cq:355:GLN:HE21	1.75	0.50
2:Cw:136:ASN:HB2	2:Cw:151:GLN:HA	1.93	0.50
1:Be:96:MET:HG3	1:Be:221:GLU:HB2	1.94	0.50
1:Bx:141:ILE:HD13	1:Bx:158:VAL:HG21	1.94	0.50
1:Bd:182:PRO:HG2	3:Cj:47:PHE:HE2	1.76	0.50
1:Bj:115:SER:HB2	1:Bj:192:LEU:HD23	1.94	0.50
1:Bn:144:PRO:HG2	1:Bn:147:ALA:HB2	1.94	0.50
2:Ca:112:LEU:HD11	2:Ca:128:PRO:HB2	1.93	0.50
1:Bm:52:PRO:HB2	1:Bn:196:THR:HG21	1.94	0.50
3:Co:33:GLU:HG2	3:Co:396:ASN:HD21	1.76	0.50
1:Bg:85:ASN:HD22	3:Ce:3:TYR:HD1	1.60	0.49
1:Bx:178:ASP:HB2	1:Bx:212:LEU:HD21	1.94	0.49
2:Ca:29:VAL:HG23	2:Ca:209:VAL:HB	1.92	0.49
2:Cw:91:LEU:HB2	2:Cw:120:PRO:HG2	1.93	0.49
1:Bd:247:VAL:HG22	1:Bh:234:MET:HE2	1.94	0.49
1:Bf:243:MET:HE3	1:Bl:26:LEU:HD11	1.94	0.49
1:Bm:36:LYS:HB3	1:Bm:225:VAL:HG22	1.93	0.49
1:Bo:129:VAL:HG12	1:Bo:136:ARG:HA	1.93	0.49
2:Cw:138:VAL:HG13	2:Cw:148:VAL:HG12	1.93	0.49
1:Bg:5:LEU:HD11	1:Bg:255:MET:HE1	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Br:36:LYS:HB3	1:Br:225:VAL:HG22	1.93	0.49
1:Bv:115:SER:HB2	1:Bv:192:LEU:HD23	1.94	0.49
1:Bh:61:ARG:HB2	1:Bi:198:ALA:HB2	1.93	0.49
1:Bt:185:LEU:HB3	1:Bt:193:TYR:HB3	1.95	0.49
1:Bg:161:ARG:HH11	1:Bg:168:ASN:HD21	1.60	0.49
1:Bn:50:ASN:HB2	1:Bn:66:LEU:H	1.78	0.49
3:Cf:404:VAL:HG13	3:Ch:6:LEU:HD22	1.94	0.49
3:Cs:411:ARG:HH21	3:Cu:424:ASN:HB3	1.78	0.49
1:Bl:32:ILE:HD12	1:Bl:220:LEU:HD22	1.95	0.49
1:Bu:25:ASN:HD21	1:Bu:37:GLY:H	1.60	0.49
3:Ck:380:ASN:HD21	3:Ck:386:SER:HB3	1.77	0.49
1:Bs:93:LEU:HD13	1:Bs:121:THR:HA	1.93	0.49
3:Ce:6:LEU:HA	3:Ce:9:LEU:HB3	1.95	0.49
3:Ck:4:VAL:HG13	3:Ck:57:GLY:HA2	1.95	0.49
3:Cn:328:ASN:HB3	3:Cn:345:ARG:HH12	1.78	0.49
1:Bi:177:VAL:HG22	1:Bi:204:GLU:HG3	1.95	0.48
1:Bo:125:GLU:HB3	1:Bo:136:ARG:HH12	1.77	0.48
1:Bo:196:THR:HG22	2:Cd:155:ALA:HB1	1.95	0.48
1:Bh:96:MET:HG2	1:Bh:216:ARG:HB3	1.95	0.48
1:Bo:68:LEU:HD11	1:Bp:17:THR:HG23	1.95	0.48
1:Br:185:LEU:HB3	1:Br:193:TYR:HB3	1.93	0.48
1:Bf:162:VAL:HB	1:Bf:165:GLN:HB2	1.95	0.48
1:Bw:47:GLN:HA	1:Bz:83:ASN:HD21	1.78	0.48
1:Bx:93:LEU:HA	1:Bx:217:GLN:HE22	1.78	0.48
3:Ce:25:ASN:HB2	3:Ce:33:GLU:HG3	1.95	0.48
3:Cg:428:GLN:HA	3:Cg:431:LEU:HD12	1.95	0.48
3:Ch:426:LEU:HD11	3:Cr:410:GLN:HA	1.95	0.48
1:Bc:196:THR:HG22	1:Bq:161:ARG:HH12	1.78	0.48
1:Bf:150:ILE:HG12	1:Bf:160:VAL:HG12	1.95	0.48
1:Bk:87:GLN:HB3	1:Bk:220:LEU:HG	1.95	0.48
1:Bp:144:PRO:HG2	1:Bp:147:ALA:HB2	1.94	0.48
1:Bq:243:MET:HE3	1:Br:227:VAL:HG12	1.94	0.48
3:Ck:84:ALA:O	3:Ck:385:GLY:HA3	2.13	0.48
1:Ba:102:PHE:HB3	1:Ba:114:TYR:HB3	1.95	0.48
1:Bo:137:LEU:HG	1:Bo:139:PRO:HD2	1.95	0.48
3:Ci:86:THR:HB	3:Ci:384:PHE:HA	1.94	0.48
3:Co:33:GLU:HB3	3:Co:397:ILE:HG22	1.94	0.48
1:Bk:60:THR:HG21	1:Br:135:TYR:HD1	1.78	0.48
1:Bd:255:MET:HE1	1:Bj:227:VAL:HG21	1.95	0.48
1:Bf:26:LEU:HD11	1:Bf:227:VAL:HG13	1.96	0.48
2:Ca:82:ILE:HD11	2:Ca:88:ILE:HG13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:99:GLY:HA2	3:Ce:44:THR:H	1.79	0.48
1:Bh:144:PRO:HG2	1:Bh:147:ALA:HB2	1.95	0.48
1:Bp:115:SER:HB2	1:Bp:192:LEU:HD23	1.96	0.48
3:Cr:32:LYS:HB2	3:Cr:65:GLN:HE21	1.78	0.48
2:Cv:29:VAL:HG23	2:Cv:209:VAL:HB	1.95	0.48
1:Ba:125:GLU:HB3	1:Ba:136:ARG:HH12	1.78	0.47
1:Bt:138:GLN:HG3	1:Bt:139:PRO:HD3	1.96	0.47
3:Ce:131:ASN:HB2	3:Ce:135:GLY:H	1.78	0.47
3:Cm:357:LEU:HB3	3:Cm:365:TRP:HB3	1.96	0.47
3:Cs:131:ASN:HB2	3:Cs:138:LEU:HD21	1.95	0.47
3:Cs:332:LEU:HD13	3:Cu:113:LYS:HZ1	1.79	0.47
1:Bu:130:THR:HG23	1:Bu:134:GLY:H	1.79	0.47
1:Bw:46:TYR:HB3	1:Bw:67:MET:HB3	1.97	0.47
3:Cu:9:LEU:HD22	3:Cu:416:ASN:HB3	1.96	0.47
1:Ba:55:GLN:HA	1:Ba:61:ARG:HE	1.80	0.47
1:Bf:177:VAL:HG22	1:Bf:204:GLU:HG2	1.96	0.47
1:Bz:36:LYS:HB3	1:Bz:225:VAL:HG22	1.96	0.47
3:Ce:6:LEU:HD22	3:Ce:9:LEU:HD22	1.96	0.47
3:Cq:130:VAL:HG12	3:Cq:137:VAL:HG22	1.96	0.47
3:Cr:82:ARG:HG3	3:Cr:393:GLU:HB3	1.96	0.47
3:Cr:353:ASN:HB3	3:Cr:371:SER:HA	1.96	0.47
1:Bd:69:GLY:HA3	1:Bh:24:ASN:HB2	1.96	0.47
1:Bo:47:GLN:HG3	2:Cd:68:GLN:HB3	1.96	0.47
1:Bs:177:VAL:HG22	1:Bs:204:GLU:HG2	1.96	0.47
1:Bv:93:LEU:HD21	1:Bv:150:ILE:HD12	1.95	0.47
1:Bf:129:VAL:HG12	1:Bf:136:ARG:HA	1.97	0.47
1:Bu:254:MET:HE3	1:Bv:238:GLN:HE21	1.78	0.47
1:Bw:44:LEU:HD22	1:Bz:86:VAL:HG11	1.95	0.47
2:Cv:234:THR:HA	2:Cv:237:GLU:HG2	1.96	0.47
2:Ca:219:ILE:HB	2:Ca:223:ARG:HH21	1.79	0.47
3:Cr:4:VAL:HG13	3:Cr:57:GLY:HA2	1.95	0.47
1:Bj:86:VAL:HG12	1:Bj:96:MET:HE1	1.97	0.47
1:Bk:41:PHE:HB3	1:Bq:31:THR:HG23	1.97	0.47
1:Bn:194:LEU:HD13	1:By:163:ARG:HH22	1.79	0.47
1:By:44:LEU:HB2	1:By:70:ALA:HB3	1.97	0.47
3:Cg:127:GLY:HA3	3:Cg:145:ILE:HD11	1.96	0.47
3:Ck:33:GLU:HB3	3:Ck:397:ILE:HG22	1.96	0.47
3:Cp:358:ASP:HB3	3:Cp:366:ASP:HB3	1.96	0.47
1:Bo:102:PHE:HB3	1:Bo:114:TYR:HB3	1.95	0.47
1:Bx:137:LEU:HG	1:Bx:139:PRO:HD2	1.96	0.47
3:Co:118:VAL:HG12	3:Co:124:PHE:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bj:96:MET:HG3	1:Bj:221:GLU:HB2	1.96	0.47
3:Cs:374:LYS:HD3	3:Cs:376:TRP:HE1	1.80	0.47
1:Cb:49:ILE:HG13	1:Cb:68:LEU:HD23	1.96	0.47
1:Bg:115:SER:HB2	1:Bg:192:LEU:HD23	1.97	0.46
1:Bo:80:VAL:HG13	1:Bp:91:ASN:HB3	1.97	0.46
3:Cf:411:ARG:HD2	3:Cf:411:ARG:HA	1.70	0.46
3:Cl:62:LYS:HB3	3:Cm:120:ALA:HB1	1.96	0.46
1:Bd:26:LEU:HD11	1:Bd:227:VAL:HG13	1.98	0.46
1:Bi:185:LEU:HB3	1:Bi:193:TYR:HB3	1.97	0.46
2:Ca:105:LEU:HA	2:Ca:115:ASN:HA	1.97	0.46
3:Cr:14:MET:HE2	3:Cr:63:VAL:HG21	1.96	0.46
2:Cv:105:LEU:HD13	2:Cv:113:LEU:HD21	1.96	0.46
1:Bb:66:LEU:HD11	1:Bc:17:THR:HG21	1.98	0.46
1:Bf:239:ARG:HH21	3:Cq:427:GLN:HB2	1.80	0.46
1:Bj:22:ILE:HG21	1:Bj:234:MET:HB2	1.97	0.46
1:Bk:49:ILE:HB	1:Bk:66:LEU:HD23	1.96	0.46
1:Bx:129:VAL:HG12	1:Bx:136:ARG:HA	1.98	0.46
1:Ba:254:MET:HE2	1:Bk:241:TYR:HB3	1.97	0.46
3:Ce:351:VAL:HG11	3:Ce:357:LEU:HD21	1.96	0.46
3:Ce:427:GLN:HG2	3:Ct:418:ARG:HD2	1.97	0.46
2:Cw:166:LEU:HD21	2:Cw:199:ILE:HD11	1.97	0.46
1:Bb:73:LYS:HE3	1:Bk:219:MET:HE2	1.96	0.46
1:Bd:36:LYS:HB3	1:Bd:225:VAL:HG22	1.98	0.46
1:Bd:162:VAL:HB	1:Bd:165:GLN:HB2	1.98	0.46
1:Bh:117:ASN:HB3	1:Bh:191:ASN:HD22	1.80	0.46
1:Bj:93:LEU:HD13	1:Bj:121:THR:HA	1.96	0.46
1:Bo:40:VAL:HG13	1:Bp:119:GLN:HG3	1.97	0.46
2:Cd:105:LEU:HB3	2:Cd:113:LEU:HD11	1.97	0.46
3:Cp:322:LYS:HB2	3:Cp:334:THR:HB	1.97	0.46
3:Ct:32:LYS:HB2	3:Ct:65:GLN:HE21	1.80	0.46
1:Bd:115:SER:HB2	1:Bd:192:LEU:HD23	1.98	0.46
1:Bh:262:LEU:HD21	1:Bi:248:ILE:HG23	1.97	0.46
1:Bk:52:PRO:HG3	1:Bk:65:GLY:HA3	1.97	0.46
3:Cg:38:PHE:HA	3:Cg:61:ALA:H	1.81	0.46
1:Bs:49:ILE:HB	1:Bs:66:LEU:HB3	1.98	0.46
1:Bw:152:ILE:HD11	1:Bw:156:GLY:HA2	1.98	0.46
1:Bb:3:PRO:HA	1:Bk:85:ASN:HD22	1.80	0.46
1:Be:44:LEU:HD21	1:Be:73:LYS:HB3	1.98	0.46
1:Bf:234:MET:HG2	3:Cm:422:VAL:HG21	1.98	0.46
1:Bk:245:SER:HA	1:Bk:248:ILE:HG22	1.98	0.46
1:Bo:226:ASN:HB2	1:Bo:229:GLU:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bq:211:GLY:H	1:Br:163:ARG:HD3	1.81	0.46
1:Br:22:ILE:HG21	1:Br:234:MET:HB2	1.98	0.46
1:Br:96:MET:HG3	1:Br:221:GLU:HB2	1.97	0.46
1:Bl:47:GLN:HA	1:Bv:83:ASN:HD21	1.81	0.46
1:Bo:141:ILE:HD13	1:Bo:158:VAL:HG21	1.97	0.46
1:Bp:137:LEU:HG	1:Bp:139:PRO:HD2	1.97	0.46
1:Bu:239:ARG:HA	1:Bu:239:ARG:HD3	1.69	0.46
3:Cf:150:GLN:HG3	3:Cf:152:GLY:H	1.81	0.46
3:Cj:350:ARG:HH22	3:Cj:383:SER:H	1.64	0.46
1:Bb:59:ASN:HD21	1:Bj:108:PRO:HB3	1.81	0.45
1:Bc:1:MET:HE1	1:Bj:16:GLN:HA	1.97	0.45
1:Bh:177:VAL:HG22	1:Bh:204:GLU:HA	1.98	0.45
1:Bk:10:THR:HG21	1:Bp:86:VAL:HG23	1.98	0.45
1:Bm:196:THR:HA	1:Bx:161:ARG:HH12	1.81	0.45
1:Br:86:VAL:HB	1:Br:96:MET:HE1	1.98	0.45
2:Ca:87:TRP:HB3	2:Ca:99:LEU:HB3	1.99	0.45
1:Bc:231:LEU:HD21	3:Cr:431:LEU:HD23	1.98	0.45
1:Bk:137:LEU:HG	1:Bk:139:PRO:HD2	1.98	0.45
1:Bo:45:PHE:HD1	1:Bp:189:GLY:HA3	1.81	0.45
1:Bv:47:GLN:HB3	1:Bv:68:LEU:HB2	1.98	0.45
3:Ci:426:LEU:HD21	3:Cj:410:GLN:HG3	1.98	0.45
3:Cj:415:ALA:HB2	3:Cl:399:MET:HE1	1.99	0.45
1:Ba:148:ILE:HD12	1:Ba:161:ARG:HD2	1.97	0.45
1:Bm:185:LEU:HB3	1:Bm:193:TYR:HB3	1.98	0.45
1:Ba:198:ALA:HB1	1:Bg:63:PRO:HA	1.98	0.45
1:Be:48:ASN:HB3	1:Be:67:MET:HE2	1.99	0.45
1:Be:228:THR:HG23	3:Cs:430:ILE:HG13	1.97	0.45
1:Bm:129:VAL:HG12	1:Bm:136:ARG:HA	1.98	0.45
3:Cm:15:ASP:HB2	3:Cm:38:PHE:HZ	1.82	0.45
3:Ct:81:LEU:HD21	3:Ct:387:ILE:HD11	1.97	0.45
1:Ba:262:LEU:HD21	1:Bk:248:ILE:HG23	1.98	0.45
1:Bq:129:VAL:HG12	1:Bq:136:ARG:HA	1.98	0.45
1:Bw:150:ILE:HG12	1:Bw:160:VAL:HG12	1.97	0.45
1:Cb:180:ILE:HA	2:Cc:134:PRO:HB3	1.99	0.45
3:Cl:353:ASN:HB3	3:Cl:371:SER:HA	1.98	0.45
3:Cm:32:LYS:HB2	3:Cm:65:GLN:HE21	1.81	0.45
3:Cr:378:GLU:HB2	3:Cr:381:LYS:HD2	1.97	0.45
3:Cs:83:ILE:HG13	3:Cs:387:ILE:HG12	1.99	0.45
1:Bb:36:LYS:HG3	1:Bb:225:VAL:HG23	1.99	0.45
1:Bd:55:GLN:HA	1:Bd:61:ARG:HG3	1.97	0.45
1:Bo:251:VAL:HA	1:Bo:254:MET:HE2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bx:35:LYS:HD3	1:Bx:81:HIS:HA	1.99	0.45
3:Cp:2:SER:HB2	3:Cp:423:HIS:CG	2.52	0.45
3:Cr:13:GLN:HA	3:Cr:16:LEU:HD12	1.98	0.45
1:Ba:32:ILE:HG23	1:Ba:220:LEU:HD13	1.99	0.45
1:Bb:232:VAL:HG13	3:Cr:6:LEU:HD22	1.99	0.45
1:Bd:254:MET:HE3	1:Bd:254:MET:HB3	1.75	0.45
1:Bl:52:PRO:HD3	1:Bl:67:MET:HE3	1.98	0.45
1:Bo:45:PHE:HB2	2:Cd:83:GLN:HG2	1.98	0.45
2:Cd:169:LEU:HD23	2:Cd:174:LEU:HD21	1.99	0.45
3:Ci:320:LEU:HD11	3:Ci:333:ALA:HB1	1.98	0.45
1:Bp:185:LEU:HD23	1:Bp:199:SER:HB2	1.98	0.45
1:Bt:36:LYS:HB3	1:Bt:225:VAL:HG22	1.99	0.45
1:Bu:102:PHE:HB3	1:Bu:114:TYR:HB3	1.98	0.45
1:By:41:PHE:HB2	2:Cd:31:THR:HA	1.99	0.45
3:Cj:89:PHE:HB2	3:Cj:104:THR:O	2.17	0.45
3:Cl:332:LEU:HD11	3:Cl:340:ASN:HB3	1.98	0.45
3:Cq:128:TYR:HE1	3:Cq:142:PRO:HA	1.82	0.45
1:Bj:32:ILE:HD12	1:Bj:220:LEU:HD13	1.98	0.45
1:Bt:234:MET:HE3	1:Bt:234:MET:HB3	1.88	0.45
2:Cd:80:ILE:HG22	2:Cd:201:THR:HG22	1.99	0.45
3:Ce:83:ILE:HG12	3:Ce:387:ILE:HG12	1.99	0.45
3:Co:54:PRO:HD3	3:Cq:14:MET:HE1	1.99	0.45
3:Cr:131:ASN:HB3	3:Cr:138:LEU:HD11	1.99	0.45
3:Cs:32:LYS:HG2	3:Cs:67:PHE:HA	1.98	0.45
1:Bh:10:THR:HG22	1:Bs:88:THR:HG23	1.98	0.44
1:By:234:MET:HB2	1:By:234:MET:HE2	1.80	0.44
1:Bd:40:VAL:HG13	1:Bh:119:GLN:HE21	1.82	0.44
1:Bh:237:ALA:HA	1:Bh:240:VAL:HG12	1.99	0.44
1:Bn:44:LEU:HD21	1:By:219:MET:HE2	1.99	0.44
1:Bp:239:ARG:HA	1:Bp:239:ARG:HD3	1.71	0.44
1:Bu:7:VAL:HG22	1:Bu:70:ALA:HA	1.99	0.44
3:Ck:331:VAL:HB	3:Ck:343:LEU:HB2	1.99	0.44
3:Cp:426:LEU:HD11	3:Cs:16:LEU:HD13	1.99	0.44
1:Bh:1:MET:HB3	1:Bi:16:GLN:HE22	1.82	0.44
3:Cr:148:PRO:HD2	3:Cr:343:LEU:HD13	1.99	0.44
1:Bl:49:ILE:HD12	1:Bl:68:LEU:HD23	1.98	0.44
1:Bn:19:ILE:HA	1:Bn:22:ILE:HG22	2.00	0.44
1:By:16:GLN:HG2	1:By:241:TYR:HE2	1.83	0.44
1:Bg:137:LEU:HG	1:Bg:139:PRO:HD2	1.99	0.44
3:Cm:404:VAL:HG13	3:Co:6:LEU:HD22	2.00	0.44
2:Cw:68:GLN:NE2	2:Cw:84:GLY:H	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Be:103:PHE:HB2	1:Be:115:SER:O	2.18	0.44
1:Bg:36:LYS:HB3	1:Bg:225:VAL:HG22	1.99	0.44
1:Bp:262:LEU:HD11	2:Cw:232:MET:HE3	2.00	0.44
1:Bs:166:GLN:HE21	1:Bs:166:GLN:HB3	1.57	0.44
3:Ci:38:PHE:HE2	3:Cj:27:ASN:HD22	1.66	0.44
3:Cq:91:VAL:HB	3:Cq:123:GLU:HB3	2.00	0.44
3:Ct:348:LEU:HD22	3:Ct:384:PHE:HD2	1.83	0.44
1:Bb:17:THR:HB	1:Bb:74:VAL:HG11	2.00	0.44
1:Bf:52:PRO:HB2	1:Bl:196:THR:HG21	2.00	0.44
1:Bh:251:VAL:HA	1:Bh:254:MET:HE2	1.99	0.44
3:Cm:320:LEU:HD22	3:Cm:333:ALA:HB1	2.00	0.44
1:Ba:243:MET:HE3	1:Bk:227:VAL:HB	2.00	0.44
1:Bc:7:VAL:HG13	1:Bc:71:GLY:HA2	1.99	0.44
1:Bj:10:THR:HG22	1:Br:88:THR:HG22	2.00	0.44
1:Bn:96:MET:HG3	1:Bn:220:LEU:HA	1.99	0.44
1:Br:246:LYS:HD2	1:Bs:262:LEU:HB2	2.00	0.44
3:Cr:134:THR:HG23	3:Cr:136:ASP:H	1.83	0.44
1:Bb:53:GLY:HA2	1:Bc:198:ALA:HB3	1.98	0.44
1:Bd:159:SER:HB2	1:Bd:168:ASN:HB3	2.00	0.44
1:Bw:243:MET:HB3	1:Bx:26:LEU:HD21	1.98	0.44
1:Bi:103:PHE:HB2	1:Bi:115:SER:O	2.18	0.43
1:Bj:251:VAL:HA	1:Bj:254:MET:HE3	2.00	0.43
3:Cr:348:LEU:HD11	3:Cr:387:ILE:HD11	2.00	0.43
1:Bv:138:GLN:HE21	1:Bv:138:GLN:HB3	1.64	0.43
2:Cd:91:LEU:HG	2:Cd:122:LEU:HD21	1.99	0.43
1:Be:251:VAL:HA	1:Be:254:MET:HE2	1.99	0.43
1:Bi:36:LYS:HB3	1:Bi:225:VAL:HG22	2.00	0.43
1:Bl:32:ILE:HG22	1:Bl:222:THR:HA	2.00	0.43
1:Bq:137:LEU:HG	1:Bq:139:PRO:HD2	2.00	0.43
3:Cf:32:LYS:HB2	3:Cf:65:GLN:HE21	1.83	0.43
3:Cf:102:GLU:HB3	3:Cf:364:GLN:HB3	2.01	0.43
3:Cl:35:ARG:HE	3:Cl:64:ALA:HB3	1.83	0.43
1:Bc:177:VAL:HG22	1:Bc:204:GLU:HG2	1.99	0.43
1:Bf:235:ILE:HG13	3:Co:433:ILE:HD11	2.01	0.43
1:Bp:26:LEU:HD13	1:Bp:26:LEU:HA	1.87	0.43
1:Br:94:ASP:HB3	1:Br:220:LEU:HD13	2.01	0.43
1:Bs:102:PHE:HB3	1:Bs:114:TYR:HB3	2.01	0.43
1:Cb:95:MET:HE1	1:Cb:152:ILE:HG12	2.00	0.43
1:Bg:239:ARG:HH22	3:Cf:428:GLN:HE21	1.66	0.43
1:Bn:25:ASN:HD21	1:Bn:37:GLY:H	1.66	0.43
1:Bp:180:ILE:HD11	1:Bp:203:GLN:HE22	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bw:26:LEU:HD13	1:Bw:26:LEU:HA	1.89	0.43
2:Cd:81:THR:HG23	2:Cd:200:LEU:HB3	2.00	0.43
3:Ck:42:TYR:HB2	3:Cn:361:GLY:HA2	2.00	0.43
3:Cm:65:GLN:HE22	3:Cm:365:TRP:HE1	1.67	0.43
1:Bi:209:LEU:HD23	1:Bi:210:ASP:HB2	2.00	0.43
1:Bq:36:LYS:HB3	1:Bq:225:VAL:HG22	2.00	0.43
3:Ce:127:GLY:HA2	3:Ce:347:ALA:H	1.83	0.43
3:Cj:103:LEU:HD11	3:Cj:374:LYS:HE3	2.00	0.43
3:Cl:19:THR:HG21	3:Cl:406:LEU:HB2	2.01	0.43
1:Bj:48:ASN:HD22	2:Cv:137:LYS:HD3	1.84	0.43
1:Bs:47:GLN:HG3	2:Cv:68:GLN:HG2	2.00	0.43
1:By:129:VAL:HG12	1:By:136:ARG:HA	2.01	0.43
2:Cw:82:ILE:HD11	2:Cw:88:ILE:HD11	2.00	0.43
1:Bl:243:MET:HE2	1:Bl:243:MET:HB2	1.93	0.43
1:Bm:216:ARG:HB3	1:Bm:219:MET:HG3	2.00	0.43
1:Bs:257:PHE:HA	1:Bs:260:GLN:HG2	2.00	0.43
1:Cb:8:SER:HB2	1:Cb:248:ILE:HD13	2.01	0.43
3:Ch:359:LYS:HG2	3:Ch:365:TRP:HE1	1.84	0.43
3:Cn:381:LYS:HE3	3:Cn:381:LYS:HB3	1.90	0.43
3:Cr:104:THR:HB	3:Cr:364:GLN:HG2	2.00	0.43
1:Bb:2:GLN:HE21	1:Bb:2:GLN:HB3	1.61	0.43
1:Bc:165:GLN:HG3	1:Bc:167:ASP:H	1.83	0.43
1:Bi:36:LYS:HB2	1:Bi:38:ARG:HH21	1.84	0.43
1:Bi:137:LEU:HG	1:Bi:139:PRO:HD2	2.00	0.43
1:Bv:106:LEU:HD12	1:Bv:136:ARG:HB2	2.01	0.43
1:Cb:148:ILE:HB	1:Cb:161:ARG:HB3	2.01	0.43
3:Ck:15:ASP:HB2	3:Ck:38:PHE:HZ	1.83	0.43
1:Bm:36:LYS:HG3	1:Bm:80:VAL:HB	2.00	0.43
1:Bt:96:MET:HB3	1:Bt:216:ARG:HB2	2.00	0.43
3:Cp:62:LYS:HD2	3:Cp:62:LYS:HA	1.85	0.43
3:Cq:411:ARG:CZ	3:Cs:427:GLN:HB3	2.49	0.43
1:Ba:32:ILE:HD12	1:Ba:220:LEU:HD13	2.01	0.42
1:Bg:235:ILE:HG12	3:Ce:430:ILE:HD12	2.01	0.42
1:Bk:148:ILE:HB	1:Bk:161:ARG:HB2	2.01	0.42
1:Bl:1:MET:HB3	1:Bl:255:MET:HE2	2.01	0.42
1:Bl:9:LYS:HB2	1:Bu:232:VAL:HG11	2.01	0.42
1:By:98:GLU:O	1:By:213:GLY:CA	2.67	0.42
2:Ca:14:GLN:HG3	2:Ca:58:MET:HA	2.01	0.42
3:Ce:130:VAL:HG12	3:Ce:137:VAL:HG22	2.00	0.42
3:Cj:15:ASP:HB2	3:Cj:38:PHE:HZ	1.84	0.42
1:Bc:141:ILE:HD13	1:Bc:158:VAL:HG21	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:25:ASN:HD21	1:Bk:36:LYS:HE2	1.85	0.42
1:Bp:1:MET:HE3	1:Bp:1:MET:HB3	1.93	0.42
1:Bu:50:ASN:HB2	1:Bu:66:LEU:H	1.83	0.42
1:Bw:32:ILE:HG21	1:Bw:220:LEU:HD22	2.01	0.42
1:Bz:144:PRO:HG2	1:Bz:147:ALA:HB2	2.01	0.42
2:Cc:135:LEU:HG	2:Cc:148:VAL:HB	2.00	0.42
3:Cf:403:LEU:HD13	3:Cg:430:ILE:HG21	2.00	0.42
1:Bc:159:SER:HB2	1:Bc:168:ASN:HB3	2.01	0.42
1:Bm:63:PRO:HD3	1:Bo:134:GLY:HA3	2.00	0.42
1:Br:152:ILE:HG13	1:Br:158:VAL:HA	2.01	0.42
1:Bv:251:VAL:HA	1:Bv:254:MET:HG2	2.00	0.42
3:Ce:32:LYS:HA	3:Ce:32:LYS:HD3	1.85	0.42
3:Ch:82:ARG:HG3	3:Ch:393:GLU:HB3	2.01	0.42
3:Cl:13:GLN:HA	3:Cl:16:LEU:HD12	2.01	0.42
2:Cv:223:ARG:HA	2:Cv:223:ARG:HD3	1.81	0.42
1:Bd:17:THR:HG21	1:Bd:74:VAL:HG11	2.00	0.42
1:Bi:166:GLN:HE21	1:Bi:166:GLN:HB3	1.61	0.42
1:Bq:63:PRO:HA	1:Br:198:ALA:HB1	2.01	0.42
1:Bs:61:ARG:NH2	1:Cb:124:ASP:H	2.17	0.42
1:Bv:32:ILE:HD11	1:Bv:118:GLY:H	1.83	0.42
1:Cb:119:GLN:HE22	1:Cb:220:LEU:HD22	1.85	0.42
3:Cn:330:SER:HB3	3:Cn:342:THR:HG23	2.02	0.42
3:Cq:38:PHE:HB3	3:Cq:60:ALA:HA	2.01	0.42
1:Bd:249:SER:HB2	3:Cr:433:ILE:HG12	2.01	0.42
1:Be:262:LEU:HB3	1:Bw:235:ILE:HD11	2.01	0.42
1:Bf:26:LEU:HD13	1:Bf:26:LEU:HA	1.89	0.42
1:Bg:148:ILE:HB	1:Bg:161:ARG:HB2	2.01	0.42
1:Bm:86:VAL:HG23	1:Bm:96:MET:HE1	2.01	0.42
1:Bs:38:ARG:HG3	1:Bs:78:GLN:HB3	2.01	0.42
1:Bs:52:PRO:HG3	1:Bs:65:GLY:H	1.85	0.42
1:Bt:175:THR:HA	1:Bt:207:PRO:HD3	2.02	0.42
2:Cd:181:LEU:HD13	2:Cd:181:LEU:HA	1.93	0.42
3:Cj:357:LEU:HB3	3:Cj:365:TRP:HB3	2.01	0.42
1:Bb:26:LEU:HD22	3:Cf:415:ALA:HB1	2.01	0.42
1:Bj:7:VAL:HG11	1:Bs:24:ASN:HA	2.02	0.42
1:By:106:LEU:HD13	1:By:138:GLN:HE22	1.84	0.42
3:Cf:378:GLU:HB2	3:Cf:381:LYS:HD2	2.01	0.42
1:Bj:107:MET:HB2	1:Bj:111:ASN:H	1.83	0.42
1:Bj:125:GLU:H	1:Bj:125:GLU:HG3	1.69	0.42
1:Bo:50:ASN:HB2	1:Bo:66:LEU:H	1.85	0.42
3:Ce:322:LYS:HB2	3:Ce:334:THR:HB	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ce:403:LEU:HA	3:Ce:406:LEU:HB3	2.01	0.42
1:Bb:150:ILE:HG22	1:Bb:160:VAL:HG12	2.00	0.42
1:Br:18:ASN:HB2	1:Br:41:PHE:HZ	1.85	0.42
3:Cl:42:TYR:HD1	3:Cl:42:TYR:HA	1.73	0.42
3:Cm:333:ALA:HB3	3:Cm:343:LEU:HD13	2.02	0.42
2:Cw:215:MET:HB2	2:Cw:215:MET:HE2	1.87	0.42
1:Be:67:MET:HE1	1:Bm:186:GLU:HG3	2.02	0.42
1:Bk:44:LEU:HD21	1:Bk:73:LYS:HB2	2.02	0.42
1:Bo:42:GLU:HG2	1:Bp:190:GLN:HA	2.02	0.42
1:Bo:239:ARG:HD3	1:Bo:239:ARG:HA	1.72	0.42
2:Cc:82:ILE:HD11	2:Cc:88:ILE:HD11	2.01	0.42
3:Cq:348:LEU:HD11	3:Cq:387:ILE:HD11	2.00	0.42
1:Bf:98:GLU:O	1:Bf:213:GLY:CA	2.68	0.42
1:Bw:52:PRO:HG2	1:Bx:196:THR:HG21	2.02	0.42
1:Bz:129:VAL:HG12	1:Bz:136:ARG:HA	2.01	0.42
2:Cd:11:GLY:HA3	2:Cd:228:GLN:HE22	1.85	0.42
2:Cd:76:ARG:HG2	2:Cd:78:LEU:H	1.84	0.42
3:Ci:26:ALA:HB2	3:Ci:397:ILE:HD11	2.02	0.42
3:Cn:350:ARG:HE	3:Cn:375:ILE:HD11	1.85	0.42
3:Ct:357:LEU:HB3	3:Ct:365:TRP:HB3	2.02	0.42
1:Bf:145:GLU:H	1:Bf:145:GLU:HG3	1.70	0.41
1:Bh:243:MET:HE2	1:Bi:26:LEU:HD21	2.01	0.41
1:Bk:63:PRO:HA	1:Bq:198:ALA:HB1	2.02	0.41
1:Br:180:ILE:HD12	1:Br:180:ILE:HA	1.93	0.41
1:Bv:154:ASN:HB2	1:Bv:214:ASP:HB2	2.01	0.41
1:Bx:5:LEU:HB2	1:Bx:251:VAL:HG11	2.01	0.41
1:Bx:95:MET:HE2	1:Bx:95:MET:HB2	1.96	0.41
3:Cj:322:LYS:HB3	3:Cj:334:THR:HB	2.02	0.41
3:Cj:345:ARG:HH22	3:Cj:379:SER:HB3	1.85	0.41
3:Cl:102:GLU:HG3	3:Cl:364:GLN:HG2	2.01	0.41
1:Bg:38:ARG:HE	1:Bg:78:GLN:HG2	1.85	0.41
1:Bt:154:ASN:HB3	1:Bt:216:ARG:HH21	1.85	0.41
1:Bt:178:ASP:HB2	1:Bt:212:LEU:HD21	2.01	0.41
1:Bw:162:VAL:HB	1:Bw:165:GLN:HE21	1.85	0.41
1:Bb:61:ARG:HH12	1:Bj:123:ASP:HB2	1.84	0.41
1:Bs:136:ARG:H	1:Bs:136:ARG:HG2	1.66	0.41
1:Cb:239:ARG:HA	1:Cb:239:ARG:HD3	1.73	0.41
3:Cl:91:VAL:HG12	3:Cl:125:LEU:HA	2.02	0.41
3:Co:397:ILE:HD12	3:Co:402:GLU:HG3	2.02	0.41
3:Cp:54:PRO:HB3	3:Cs:18:THR:HG22	2.02	0.41
2:Cv:26:LEU:HD23	2:Cv:26:LEU:HA	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:96:MET:HE1	1:Bg:98:GLU:HB3	2.02	0.41
1:Bk:262:LEU:HD23	1:Bq:249:SER:HB3	2.03	0.41
1:Bm:44:LEU:HB2	1:Bm:70:ALA:HB3	2.01	0.41
1:Cb:25:ASN:HD21	1:Cb:37:GLY:H	1.68	0.41
1:Cb:113:ALA:HB1	1:Cb:192:LEU:HB3	2.02	0.41
2:Cd:105:LEU:HD13	2:Cd:113:LEU:HD21	2.02	0.41
2:Cw:169:LEU:HD23	2:Cw:174:LEU:HD21	2.01	0.41
1:Bg:68:LEU:HD13	1:Bg:68:LEU:HA	1.93	0.41
1:Bh:148:ILE:HD12	1:Bh:161:ARG:HG2	2.03	0.41
1:Bm:158:VAL:HG12	1:Bm:171:LEU:HD12	2.02	0.41
1:Bt:36:LYS:HG2	1:Bt:224:ASN:HD21	1.85	0.41
1:Bx:1:MET:HE2	1:Bx:255:MET:HE2	2.03	0.41
1:Cb:36:LYS:HB3	1:Cb:225:VAL:HG22	2.02	0.41
3:Ce:414:GLN:HG3	3:Cg:431:LEU:HD23	2.02	0.41
3:Ch:357:LEU:HB3	3:Ch:365:TRP:HB3	2.01	0.41
1:Ba:144:PRO:HG2	1:Ba:147:ALA:HB2	2.03	0.41
1:Be:32:ILE:HG23	1:Be:220:LEU:HD13	2.03	0.41
1:Bi:10:THR:HG21	1:Bt:86:VAL:HG23	2.01	0.41
1:Bj:246:LYS:HB2	1:Bj:246:LYS:HE2	1.76	0.41
1:Bn:209:LEU:HD23	1:Bn:210:ASP:HB2	2.01	0.41
1:Bs:234:MET:HE2	1:Bs:234:MET:HB2	1.81	0.41
3:Cg:378:GLU:HB2	3:Cg:381:LYS:HD2	2.02	0.41
3:Cr:357:LEU:HB3	3:Cr:365:TRP:HB3	2.02	0.41
1:Bb:216:ARG:HH12	1:Bb:219:MET:HG3	1.86	0.41
1:Bf:1:MET:H1	1:Bf:1:MET:HE2	1.83	0.41
1:Bi:1:MET:HB3	1:Bi:2:GLN:H	1.55	0.41
2:Cc:36:ALA:HB2	2:Cc:209:VAL:HG22	2.03	0.41
3:Cp:403:LEU:HD23	3:Cp:406:LEU:HD21	2.03	0.41
1:Bj:206:VAL:HG13	1:Bj:209:LEU:HB2	2.02	0.41
1:Bk:165:GLN:HE22	1:Bk:167:ASP:HB3	1.86	0.41
1:Bk:190:GLN:HB2	1:Bk:192:LEU:HG	2.03	0.41
3:Ck:131:ASN:HB3	3:Ck:135:GLY:H	1.86	0.41
3:Ct:78:PRO:HA	3:Ct:390:GLY:HA2	2.03	0.41
2:Cw:19:MET:HE2	2:Cw:19:MET:HB2	1.91	0.41
1:Ba:45:PHE:CG	1:Bo:98:GLU:HG2	2.56	0.41
1:Bd:254:MET:HB2	1:Bh:238:GLN:HE22	1.85	0.41
1:Be:1:MET:HE3	1:Be:255:MET:HE3	2.02	0.41
1:Be:24:ASN:HA	3:Cq:4:VAL:HG11	2.03	0.41
1:Bh:51:GLN:HE22	1:Bt:161:ARG:HH11	1.68	0.41
1:Bh:137:LEU:HG	1:Bh:139:PRO:HD2	2.03	0.41
1:Bl:85:ASN:HB2	3:Cq:3:TYR:HD2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bl:102:PHE:HB3	1:Bl:114:TYR:HB3	2.03	0.41
1:Bl:113:ALA:HB1	1:Bl:192:LEU:HB3	2.01	0.41
1:Bq:68:LEU:HD11	1:Br:17:THR:HG23	2.03	0.41
1:Bt:87:GLN:HB2	1:Bt:220:LEU:HG	2.03	0.41
1:Bu:32:ILE:HG12	1:Bu:220:LEU:HD13	2.02	0.41
1:Bu:243:MET:HE3	1:Bu:243:MET:HB3	1.96	0.41
1:Bx:239:ARG:HA	1:Bx:239:ARG:HD3	1.86	0.41
1:Bz:176:THR:HG23	1:Bz:207:PRO:HG3	2.03	0.41
3:Ch:89:PHE:HB2	3:Ch:104:THR:O	2.21	0.41
3:Ch:91:VAL:HB	3:Ch:123:GLU:HB3	2.03	0.41
3:Cl:32:LYS:HB2	3:Cl:65:GLN:HE21	1.86	0.41
3:Cm:66:GLN:HB3	3:Cm:68:HIS:HD2	1.85	0.41
3:Cn:75:THR:HG21	3:Cn:392:LEU:HD23	2.02	0.41
1:Bl:148:ILE:HB	1:Bl:161:ARG:HB2	2.03	0.41
1:Bq:196:THR:HG22	2:Cw:155:ALA:HB1	2.03	0.41
1:Bx:32:ILE:HD12	1:Bx:220:LEU:HD13	2.03	0.41
2:Ca:5:LEU:HD22	2:Ca:232:MET:HE2	2.03	0.41
2:Cc:149:ARG:HE	2:Cc:155:ALA:HA	1.86	0.41
3:Cm:322:LYS:HE2	3:Cn:360:LYS:HE2	2.03	0.41
3:Cs:15:ASP:HB2	3:Cs:38:PHE:HZ	1.86	0.41
1:Be:104:GLN:HB3	1:Be:112:ILE:HD11	2.03	0.40
1:Bk:209:LEU:HD13	1:Bq:163:ARG:HH22	1.86	0.40
1:Br:204:GLU:H	1:Br:204:GLU:HG3	1.78	0.40
1:Bu:173:GLN:HE21	1:Bu:206:VAL:HG13	1.86	0.40
1:Bz:105:ILE:HG21	1:Bz:192:LEU:HD22	2.02	0.40
1:Cb:129:VAL:HG12	1:Cb:136:ARG:HA	2.03	0.40
3:Cc:81:LEU:HD21	3:Cc:325:PHE:CG	2.56	0.40
3:Cc:406:LEU:HD22	3:Cu:422:VAL:HG22	2.02	0.40
3:Ci:356:GLY:HA3	3:Ci:371:SER:HB3	2.02	0.40
3:Cl:411:ARG:HD3	3:Cl:411:ARG:HA	1.99	0.40
1:Bh:258:VAL:HG21	1:Bi:241:TYR:HE1	1.86	0.40
1:Bl:239:ARG:HA	1:Bl:239:ARG:HD3	1.88	0.40
1:Bo:161:ARG:HA	1:Bo:161:ARG:HD2	1.95	0.40
1:Bs:52:PRO:HB3	1:Bs:64:SER:HA	2.04	0.40
1:Bv:9:LYS:HB2	1:Bv:9:LYS:HE2	1.85	0.40
3:Cp:419:ALA:HA	3:Cs:406:LEU:HD21	2.03	0.40
3:Cq:414:GLN:HG3	3:Cs:431:LEU:HD12	2.03	0.40
1:Bb:138:GLN:HE21	1:Bb:138:GLN:HB3	1.63	0.40
1:Bc:79:LYS:HE3	1:Bc:79:LYS:HB3	1.96	0.40
1:Be:30:SER:HB2	3:Cq:412:ASN:HD21	1.85	0.40
1:Bk:9:LYS:HB3	1:Bo:232:VAL:HG11	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bt:239:ARG:HD3	1:Bt:239:ARG:HA	1.95	0.40
1:Bb:141:ILE:HD13	1:Bb:158:VAL:HG21	2.04	0.40
1:Be:238:GLN:HA	3:Cq:426:LEU:HD11	2.03	0.40
1:Bf:18:ASN:HB2	1:Bf:41:PHE:HZ	1.87	0.40
1:Bj:26:LEU:HD23	1:Bj:26:LEU:HA	1.88	0.40
1:Bv:102:PHE:HB3	1:Bv:114:TYR:HB3	2.02	0.40
1:Cb:95:MET:HE3	1:Cb:215:ILE:HG21	2.02	0.40
3:Ch:112:ASP:HB3	3:Ch:118:VAL:HG21	2.02	0.40
2:Cv:136:ASN:HB2	2:Cv:149:ARG:HB3	2.03	0.40
1:Bb:32:ILE:HG21	1:Bb:119:GLN:HE22	1.87	0.40
1:Bh:180:ILE:HD12	1:Bh:180:ILE:HA	1.93	0.40
1:Bk:255:MET:HE3	1:Bp:227:VAL:HG21	2.02	0.40
1:Br:220:LEU:HD12	1:Br:220:LEU:HA	1.93	0.40
1:Bz:128:ILE:HG12	1:Bz:137:LEU:HD23	2.04	0.40
2:Ca:13:LYS:HE2	2:Ca:13:LYS:HB3	1.92	0.40
2:Cc:133:VAL:HG21	2:Cc:150:PRO:HB3	2.02	0.40
3:Ck:330:SER:HB3	3:Ck:342:THR:HG23	2.02	0.40
3:Cm:411:ARG:HD3	3:Cm:411:ARG:HA	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	Ba	260/262 (99%)	258 (99%)	2 (1%)	0	100	100
1	Bb	260/262 (99%)	257 (99%)	3 (1%)	0	100	100
1	Bc	260/262 (99%)	257 (99%)	2 (1%)	1 (0%)	30	61
1	Bd	260/262 (99%)	257 (99%)	3 (1%)	0	100	100
1	Be	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
1	Bf	260/262 (99%)	257 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bg	260/262 (99%)	257 (99%)	3 (1%)	0	100	100
1	Bh	260/262 (99%)	258 (99%)	2 (1%)	0	100	100
1	Bi	260/262 (99%)	257 (99%)	3 (1%)	0	100	100
1	Bj	260/262 (99%)	254 (98%)	6 (2%)	0	100	100
1	Bk	260/262 (99%)	258 (99%)	2 (1%)	0	100	100
1	Bl	260/262 (99%)	258 (99%)	2 (1%)	0	100	100
1	Bm	260/262 (99%)	256 (98%)	3 (1%)	1 (0%)	30	61
1	Bn	260/262 (99%)	256 (98%)	4 (2%)	0	100	100
1	Bo	260/262 (99%)	259 (100%)	1 (0%)	0	100	100
1	Bp	248/262 (95%)	247 (100%)	1 (0%)	0	100	100
1	Bq	260/262 (99%)	255 (98%)	5 (2%)	0	100	100
1	Br	243/262 (93%)	240 (99%)	3 (1%)	0	100	100
1	Bs	260/262 (99%)	253 (97%)	6 (2%)	1 (0%)	30	61
1	Bt	247/262 (94%)	244 (99%)	3 (1%)	0	100	100
1	Bu	260/262 (99%)	256 (98%)	4 (2%)	0	100	100
1	Bv	243/262 (93%)	240 (99%)	2 (1%)	1 (0%)	30	61
1	Bw	260/262 (99%)	255 (98%)	5 (2%)	0	100	100
1	Bx	245/262 (94%)	243 (99%)	2 (1%)	0	100	100
1	By	244/262 (93%)	242 (99%)	2 (1%)	0	100	100
1	Bz	245/262 (94%)	244 (100%)	1 (0%)	0	100	100
1	Cb	249/262 (95%)	248 (100%)	1 (0%)	0	100	100
2	Ca	237/249 (95%)	234 (99%)	3 (1%)	0	100	100
2	Cc	247/249 (99%)	245 (99%)	2 (1%)	0	100	100
2	Cd	240/249 (96%)	236 (98%)	4 (2%)	0	100	100
2	Cv	228/249 (92%)	220 (96%)	7 (3%)	1 (0%)	30	61
2	Cw	247/249 (99%)	244 (99%)	3 (1%)	0	100	100
3	Ce	264/434 (61%)	260 (98%)	4 (2%)	0	100	100
3	Cf	264/434 (61%)	261 (99%)	3 (1%)	0	100	100
3	Cg	266/434 (61%)	263 (99%)	3 (1%)	0	100	100
3	Ch	264/434 (61%)	263 (100%)	1 (0%)	0	100	100
3	Ci	266/434 (61%)	263 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Cj	266/434 (61%)	265 (100%)	1 (0%)	0	100	100
3	Ck	266/434 (61%)	264 (99%)	2 (1%)	0	100	100
3	Cl	266/434 (61%)	263 (99%)	3 (1%)	0	100	100
3	Cm	266/434 (61%)	264 (99%)	2 (1%)	0	100	100
3	Cn	266/434 (61%)	265 (100%)	1 (0%)	0	100	100
3	Co	266/434 (61%)	263 (99%)	3 (1%)	0	100	100
3	Cp	266/434 (61%)	262 (98%)	4 (2%)	0	100	100
3	Cq	266/434 (61%)	263 (99%)	3 (1%)	0	100	100
3	Cr	266/434 (61%)	259 (97%)	7 (3%)	0	100	100
3	Cs	266/434 (61%)	263 (99%)	3 (1%)	0	100	100
3	Ct	266/434 (61%)	265 (100%)	1 (0%)	0	100	100
3	Cu	266/434 (61%)	264 (99%)	2 (1%)	0	100	100
All	All	12619/15697 (80%)	12468 (99%)	146 (1%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Bs	138	GLN
2	Cv	134	PRO
1	Bc	63	PRO
1	Bv	138	GLN
1	Bm	141	ILE

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	Ba	218/218 (100%)	216 (99%)	2 (1%)	70	76
1	Bb	218/218 (100%)	210 (96%)	8 (4%)	30	56
1	Bc	218/218 (100%)	213 (98%)	5 (2%)	44	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bd	218/218 (100%)	212 (97%)	6 (3%)	38	61
1	Be	218/218 (100%)	218 (100%)	0	100	100
1	Bf	218/218 (100%)	215 (99%)	3 (1%)	59	71
1	Bg	218/218 (100%)	215 (99%)	3 (1%)	59	71
1	Bh	218/218 (100%)	212 (97%)	6 (3%)	38	61
1	Bi	218/218 (100%)	217 (100%)	1 (0%)	81	81
1	Bj	218/218 (100%)	214 (98%)	4 (2%)	51	68
1	Bk	218/218 (100%)	212 (97%)	6 (3%)	38	61
1	Bl	218/218 (100%)	213 (98%)	5 (2%)	44	64
1	Bm	217/218 (100%)	214 (99%)	3 (1%)	59	71
1	Bn	218/218 (100%)	213 (98%)	5 (2%)	44	64
1	Bo	218/218 (100%)	214 (98%)	4 (2%)	51	68
1	Bp	209/218 (96%)	204 (98%)	5 (2%)	43	64
1	Bq	218/218 (100%)	213 (98%)	5 (2%)	44	64
1	Br	206/218 (94%)	202 (98%)	4 (2%)	50	67
1	Bs	218/218 (100%)	213 (98%)	5 (2%)	44	64
1	Bt	209/218 (96%)	202 (97%)	7 (3%)	33	59
1	Bu	218/218 (100%)	215 (99%)	3 (1%)	59	71
1	Bv	205/218 (94%)	197 (96%)	8 (4%)	28	55
1	Bw	218/218 (100%)	212 (97%)	6 (3%)	38	61
1	Bx	207/218 (95%)	202 (98%)	5 (2%)	43	64
1	By	206/218 (94%)	202 (98%)	4 (2%)	50	67
1	Bz	207/218 (95%)	202 (98%)	5 (2%)	43	64
1	Cb	210/218 (96%)	204 (97%)	6 (3%)	37	61
2	Ca	197/202 (98%)	194 (98%)	3 (2%)	57	71
2	Cc	202/202 (100%)	197 (98%)	5 (2%)	42	63
2	Cd	199/202 (98%)	197 (99%)	2 (1%)	68	75
2	Cv	187/202 (93%)	183 (98%)	4 (2%)	47	66
2	Cw	201/202 (100%)	197 (98%)	4 (2%)	48	66
3	Ce	221/359 (62%)	218 (99%)	3 (1%)	59	71
3	Cf	221/359 (62%)	218 (99%)	3 (1%)	59	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Cg	223/359 (62%)	221 (99%)	2 (1%)	70	76
3	Ch	221/359 (62%)	217 (98%)	4 (2%)	51	68
3	Ci	223/359 (62%)	220 (99%)	3 (1%)	61	72
3	Cj	223/359 (62%)	221 (99%)	2 (1%)	70	76
3	Ck	223/359 (62%)	222 (100%)	1 (0%)	84	82
3	Cl	223/359 (62%)	221 (99%)	2 (1%)	70	76
3	Cm	223/359 (62%)	216 (97%)	7 (3%)	35	60
3	Cn	223/359 (62%)	220 (99%)	3 (1%)	61	72
3	Co	223/359 (62%)	220 (99%)	3 (1%)	61	72
3	Cp	223/359 (62%)	219 (98%)	4 (2%)	51	68
3	Cq	223/359 (62%)	218 (98%)	5 (2%)	45	65
3	Cr	223/359 (62%)	223 (100%)	0	100	100
3	Cs	223/359 (62%)	220 (99%)	3 (1%)	61	72
3	Ct	223/359 (62%)	218 (98%)	5 (2%)	45	65
3	Cu	223/359 (62%)	221 (99%)	2 (1%)	70	76
All	All	10571/12999 (81%)	10377 (98%)	194 (2%)	51	68

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ba	42	GLU
1	Ba	75	VAL
1	Bb	2	GLN
1	Bb	66	LEU
1	Bb	74	VAL
1	Bb	86	VAL
1	Bb	93	LEU
1	Bb	138	GLN
1	Bb	151	THR
1	Bb	232	VAL
1	Bc	26	LEU
1	Bc	62	LEU
1	Bc	67	MET
1	Bc	75	VAL
1	Bc	231	LEU
1	Bd	15	GLN
1	Bd	26	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bd	74	VAL
1	Bd	150	ILE
1	Bd	206	VAL
1	Bd	220	LEU
1	Bf	26	LEU
1	Bf	137	LEU
1	Bf	220	LEU
1	Bg	26	LEU
1	Bg	62	LEU
1	Bg	243	MET
1	Bh	75	VAL
1	Bh	86	VAL
1	Bh	128	ILE
1	Bh	143	ILE
1	Bh	152	ILE
1	Bh	185	LEU
1	Bi	166	GLN
1	Bj	5	LEU
1	Bj	206	VAL
1	Bj	220	LEU
1	Bj	230	GLU
1	Bk	26	LEU
1	Bk	89	THR
1	Bk	104	GLN
1	Bk	141	ILE
1	Bk	165	GLN
1	Bk	233	ASN
1	Bl	5	LEU
1	Bl	26	LEU
1	Bl	40	VAL
1	Bl	140	GLU
1	Bl	206	VAL
1	Bm	93	LEU
1	Bm	258	VAL
1	Bm	262	LEU
1	Bn	26	LEU
1	Bn	86	VAL
1	Bn	121	THR
1	Bn	128	ILE
1	Bn	242	GLU
1	Bo	26	LEU
1	Bo	48	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bo	75	VAL
1	Bo	93	LEU
1	Bp	26	LEU
1	Bp	75	VAL
1	Bp	121	THR
1	Bp	150	ILE
1	Bp	170	VAL
1	Bq	5	LEU
1	Bq	26	LEU
1	Bq	74	VAL
1	Bq	86	VAL
1	Bq	209	LEU
1	Br	12	LEU
1	Br	85	ASN
1	Br	86	VAL
1	Br	128	ILE
1	Bs	85	ASN
1	Bs	116	ARG
1	Bs	166	GLN
1	Bs	206	VAL
1	Bs	227	VAL
1	Bt	26	LEU
1	Bt	68	LEU
1	Bt	77	THR
1	Bt	138	GLN
1	Bt	163	ARG
1	Bt	206	VAL
1	Bt	257	PHE
1	Bu	26	LEU
1	Bu	62	LEU
1	Bu	89	THR
1	Bv	26	LEU
1	Bv	32	ILE
1	Bv	44	LEU
1	Bv	130	THR
1	Bv	138	GLN
1	Bv	220	LEU
1	Bv	227	VAL
1	Bv	255	MET
1	Bw	26	LEU
1	Bw	83	ASN
1	Bw	86	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bw	137	LEU
1	Bw	171	LEU
1	Bw	261	GLN
1	Bx	2	GLN
1	Bx	75	VAL
1	Bx	97	ILE
1	Bx	225	VAL
1	Bx	261	GLN
1	By	93	LEU
1	By	150	ILE
1	By	162	VAL
1	By	170	VAL
1	Bz	26	LEU
1	Bz	80	VAL
1	Bz	122	LEU
1	Bz	128	ILE
1	Bz	255	MET
2	Ca	72	ILE
2	Ca	109	GLU
2	Ca	133	VAL
1	Cb	26	LEU
1	Cb	87	GLN
1	Cb	105	ILE
1	Cb	152	ILE
1	Cb	220	LEU
1	Cb	262	LEU
2	Cc	121	VAL
2	Cc	135	LEU
2	Cc	146	ILE
2	Cc	218	LEU
2	Cc	221	LEU
2	Cd	72	ILE
2	Cd	81	THR
3	Ce	40	ASP
3	Ce	363	THR
3	Ce	399	MET
3	Cf	58	VAL
3	Cf	73	ILE
3	Cf	343	LEU
3	Cg	368	THR
3	Cg	426	LEU
3	Ch	58	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Ch	59	GLN
3	Ch	99	GLN
3	Ch	117	MET
3	Ci	42	TYR
3	Ci	320	LEU
3	Ci	346	VAL
3	Cj	147	ILE
3	Cj	433	ILE
3	Ck	97	VAL
3	Cl	42	TYR
3	Cl	96	LEU
3	Cm	17	ASN
3	Cm	53	THR
3	Cm	63	VAL
3	Cm	97	VAL
3	Cm	145	ILE
3	Cm	147	ILE
3	Cm	323	ILE
3	Cn	94	ASP
3	Cn	147	ILE
3	Cn	426	LEU
3	Co	58	VAL
3	Co	97	VAL
3	Co	431	LEU
3	Cp	4	VAL
3	Cp	58	VAL
3	Cp	97	VAL
3	Cp	143	LYS
3	Cq	16	LEU
3	Cq	46	LEU
3	Cq	63	VAL
3	Cq	404	VAL
3	Cq	422	VAL
3	Cs	346	VAL
3	Cs	423	HIS
3	Cs	426	LEU
3	Ct	16	LEU
3	Ct	48	THR
3	Ct	56	GLN
3	Ct	73	ILE
3	Ct	404	VAL
3	Cu	58	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Cu	392	LEU
2	Cv	106	ARG
2	Cv	112	LEU
2	Cv	166	LEU
2	Cv	224	GLN
2	Cw	71	VAL
2	Cw	72	ILE
2	Cw	136	ASN
2	Cw	146	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (323) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ba	15	GLN
1	Ba	48	ASN
1	Ba	55	GLN
1	Ba	58	GLN
1	Ba	87	GLN
1	Ba	104	GLN
1	Ba	165	GLN
1	Ba	190	GLN
1	Ba	191	ASN
1	Ba	261	GLN
1	Bb	24	ASN
1	Bb	87	GLN
1	Bb	104	GLN
1	Bb	138	GLN
1	Bb	165	GLN
1	Bb	169	GLN
1	Bb	190	GLN
1	Bb	226	ASN
1	Bc	24	ASN
1	Bc	25	ASN
1	Bc	87	GLN
1	Bc	169	GLN
1	Bc	173	GLN
1	Bc	191	ASN
1	Bc	261	GLN
1	Bd	25	ASN
1	Bd	50	ASN
1	Bd	85	ASN
1	Bd	87	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bd	91	ASN
1	Bd	217	GLN
1	Bd	226	ASN
1	Bd	233	ASN
1	Be	2	GLN
1	Be	15	GLN
1	Be	47	GLN
1	Be	78	GLN
1	Be	85	ASN
1	Be	104	GLN
1	Be	173	GLN
1	Be	190	GLN
1	Be	217	GLN
1	Be	244	ASN
1	Be	260	GLN
1	Be	261	GLN
1	Bf	2	GLN
1	Bf	28	ASN
1	Bf	87	GLN
1	Bf	104	GLN
1	Bg	91	ASN
1	Bg	104	GLN
1	Bg	111	ASN
1	Bg	138	GLN
1	Bg	168	ASN
1	Bg	191	ASN
1	Bg	203	GLN
1	Bh	28	ASN
1	Bh	48	ASN
1	Bh	51	GLN
1	Bh	87	GLN
1	Bh	91	ASN
1	Bh	119	GLN
1	Bh	169	GLN
1	Bh	190	GLN
1	Bh	191	ASN
1	Bi	55	GLN
1	Bi	87	GLN
1	Bi	104	GLN
1	Bi	119	GLN
1	Bi	165	GLN
1	Bi	166	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bj	16	GLN
1	Bj	28	ASN
1	Bj	48	ASN
1	Bj	51	GLN
1	Bj	78	GLN
1	Bj	87	GLN
1	Bj	104	GLN
1	Bj	117	ASN
1	Bj	119	GLN
1	Bj	233	ASN
1	Bk	51	GLN
1	Bk	83	ASN
1	Bk	85	ASN
1	Bk	104	GLN
1	Bk	173	GLN
1	Bk	217	GLN
1	Bk	259	ASN
1	Bl	15	GLN
1	Bl	104	GLN
1	Bl	154	ASN
1	Bl	165	GLN
1	Bl	169	GLN
1	Bl	191	ASN
1	Bm	51	GLN
1	Bm	58	GLN
1	Bm	104	GLN
1	Bm	138	GLN
1	Bm	165	GLN
1	Bm	173	GLN
1	Bm	203	GLN
1	Bn	16	GLN
1	Bn	24	ASN
1	Bn	25	ASN
1	Bn	81	HIS
1	Bn	173	GLN
1	Bn	191	ASN
1	Bo	25	ASN
1	Bo	87	GLN
1	Bo	104	GLN
1	Bo	138	GLN
1	Bo	173	GLN
1	Bo	203	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bp	25	ASN
1	Bp	47	GLN
1	Bp	138	GLN
1	Bp	166	GLN
1	Bp	169	GLN
1	Bq	25	ASN
1	Bq	47	GLN
1	Bq	50	ASN
1	Bq	104	GLN
1	Bq	168	ASN
1	Bq	244	ASN
1	Br	24	ASN
1	Br	25	ASN
1	Br	48	ASN
1	Br	85	ASN
1	Br	117	ASN
1	Br	169	GLN
1	Br	259	ASN
1	Bs	48	ASN
1	Bs	166	GLN
1	Bs	173	GLN
1	Bs	244	ASN
1	Bs	261	GLN
1	Bt	18	ASN
1	Bt	24	ASN
1	Bt	47	GLN
1	Bt	83	ASN
1	Bt	91	ASN
1	Bt	104	GLN
1	Bt	119	GLN
1	Bt	168	ASN
1	Bt	226	ASN
1	Bt	259	ASN
1	Bu	2	GLN
1	Bu	25	ASN
1	Bu	55	GLN
1	Bu	87	GLN
1	Bu	104	GLN
1	Bu	119	GLN
1	Bu	168	ASN
1	Bu	173	GLN
1	Bu	181	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bu	217	GLN
1	Bv	2	GLN
1	Bv	16	GLN
1	Bv	18	ASN
1	Bv	78	GLN
1	Bv	83	ASN
1	Bv	138	GLN
1	Bv	203	GLN
1	Bv	217	GLN
1	Bv	238	GLN
1	Bv	261	GLN
1	Bw	2	GLN
1	Bw	48	ASN
1	Bw	51	GLN
1	Bw	58	GLN
1	Bw	78	GLN
1	Bw	85	ASN
1	Bw	87	GLN
1	Bw	104	GLN
1	Bw	111	ASN
1	Bw	117	ASN
1	Bw	181	ASN
1	Bx	2	GLN
1	Bx	16	GLN
1	Bx	47	GLN
1	Bx	104	GLN
1	Bx	138	GLN
1	Bx	169	GLN
1	Bx	173	GLN
1	Bx	260	GLN
1	By	18	ASN
1	By	25	ASN
1	By	78	GLN
1	By	104	GLN
1	By	138	GLN
1	By	260	GLN
1	By	261	GLN
1	Bz	24	ASN
1	Bz	81	HIS
1	Bz	83	ASN
1	Bz	138	GLN
1	Bz	165	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bz	260	GLN
2	Ca	17	GLN
2	Ca	83	GLN
2	Ca	170	ASN
2	Ca	224	GLN
2	Ca	228	GLN
1	Cb	15	GLN
1	Cb	25	ASN
1	Cb	28	ASN
1	Cb	111	ASN
1	Cb	119	GLN
1	Cb	238	GLN
1	Cb	261	GLN
2	Cc	65	ASN
2	Cc	151	GLN
2	Cd	170	ASN
2	Cd	228	GLN
3	Ce	13	GLN
3	Ce	17	ASN
3	Ce	25	ASN
3	Ce	100	GLN
3	Ce	110	HIS
3	Ce	340	ASN
3	Ce	380	ASN
3	Ce	423	HIS
3	Cf	13	GLN
3	Cf	22	ASN
3	Cf	25	ASN
3	Cf	121	ASN
3	Cf	340	ASN
3	Cf	424	ASN
3	Cf	428	GLN
3	Cg	65	GLN
3	Cg	77	ASN
3	Cg	380	ASN
3	Cg	396	ASN
3	Cg	428	GLN
3	Ch	21	ASN
3	Ch	49	ASN
3	Ch	65	GLN
3	Ch	114	ASN
3	Ch	380	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Ch	401	GLN
3	Ch	427	GLN
3	Ch	432	GLN
3	Ci	66	GLN
3	Ci	99	GLN
3	Ci	416	ASN
3	Ci	428	GLN
3	Cj	13	GLN
3	Cj	21	ASN
3	Cj	66	GLN
3	Cj	328	ASN
3	Cj	364	GLN
3	Cj	410	GLN
3	Cj	412	ASN
3	Ck	340	ASN
3	Ck	353	ASN
3	Ck	380	ASN
3	Ck	401	GLN
3	Ck	423	HIS
3	Ck	427	GLN
3	Ck	428	GLN
3	Cl	150	GLN
3	Cl	328	ASN
3	Cl	394	GLN
3	Cl	414	GLN
3	Cm	13	GLN
3	Cm	65	GLN
3	Cm	68	HIS
3	Cm	150	GLN
3	Cm	364	GLN
3	Cm	429	ASN
3	Cn	56	GLN
3	Cn	340	ASN
3	Co	22	ASN
3	Co	65	GLN
3	Co	100	GLN
3	Co	337	ASN
3	Co	380	ASN
3	Co	396	ASN
3	Co	414	GLN
3	Cp	22	ASN
3	Cp	65	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Cp	150	GLN
3	Cp	353	ASN
3	Cp	414	GLN
3	Cp	428	GLN
3	Cq	13	GLN
3	Cq	25	ASN
3	Cq	27	ASN
3	Cq	65	GLN
3	Cq	146	ASN
3	Cq	355	GLN
3	Cq	394	GLN
3	Cr	13	GLN
3	Cr	65	GLN
3	Cr	66	GLN
3	Cr	340	ASN
3	Cr	423	HIS
3	Cs	21	ASN
3	Cs	65	GLN
3	Cs	68	HIS
3	Cs	99	GLN
3	Cs	100	GLN
3	Cs	114	ASN
3	Cs	353	ASN
3	Cs	428	GLN
3	Cs	429	ASN
3	Cs	432	GLN
3	Ct	21	ASN
3	Ct	22	ASN
3	Ct	65	GLN
3	Ct	68	HIS
3	Ct	110	HIS
3	Ct	146	ASN
3	Ct	394	GLN
3	Cu	49	ASN
2	Cv	151	GLN
2	Cv	222	GLN
2	Cw	17	GLN
2	Cw	40	GLN
2	Cw	68	GLN
2	Cw	83	GLN
2	Cw	170	ASN
2	Cw	228	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

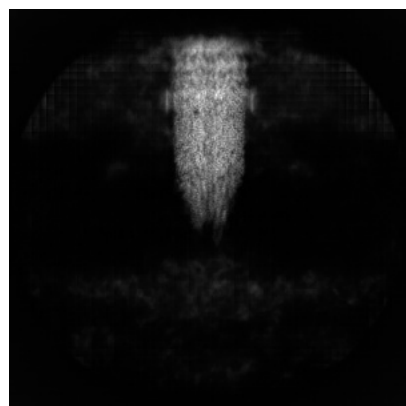
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72849. These allow visual inspection of the internal detail of the map and identification of artifacts.

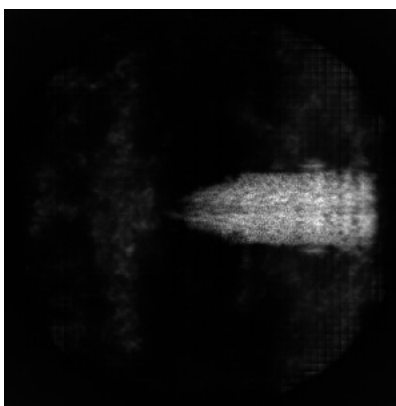
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

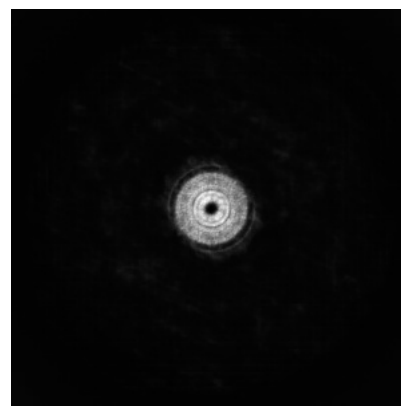
6.1.1 Primary map



X

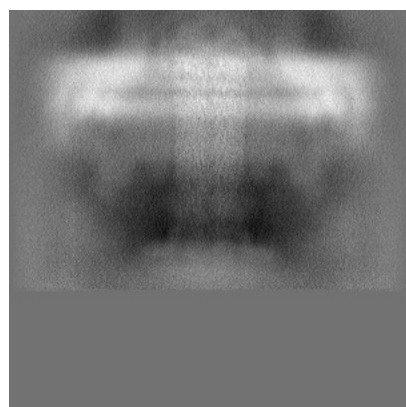


Y

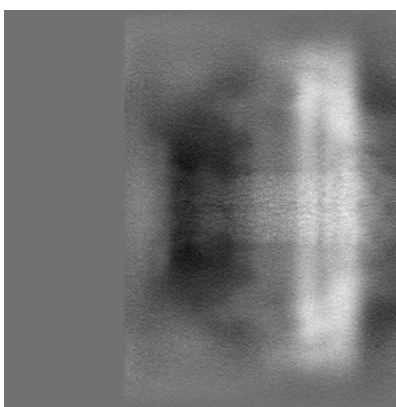


Z

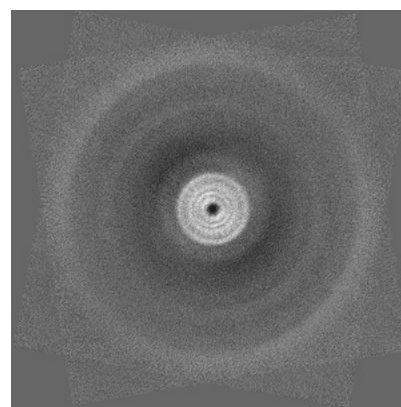
6.1.2 Raw map



X



Y

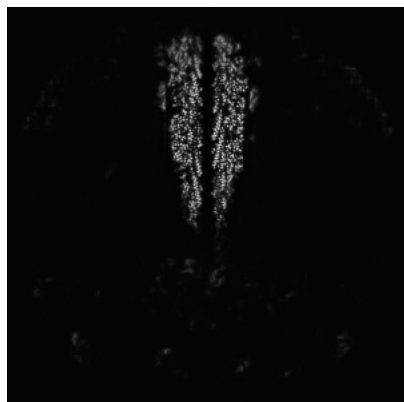


Z

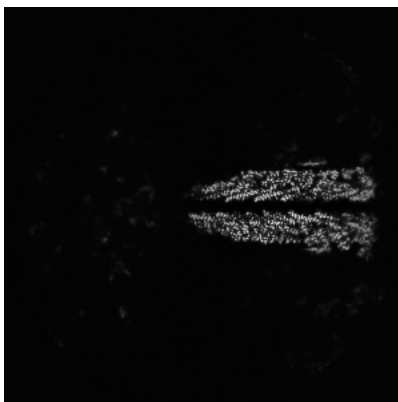
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

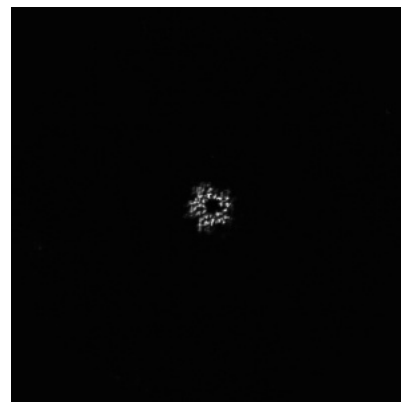
6.2.1 Primary map



X Index: 320

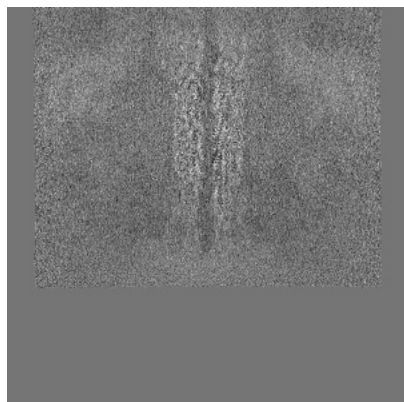


Y Index: 320

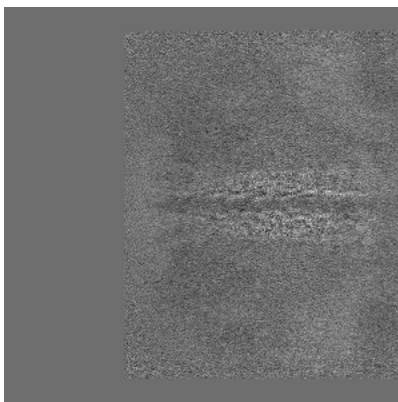


Z Index: 320

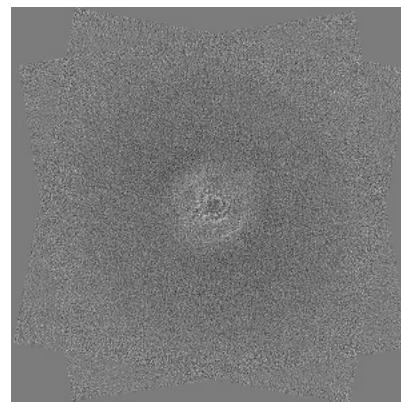
6.2.2 Raw map



X Index: 320



Y Index: 320

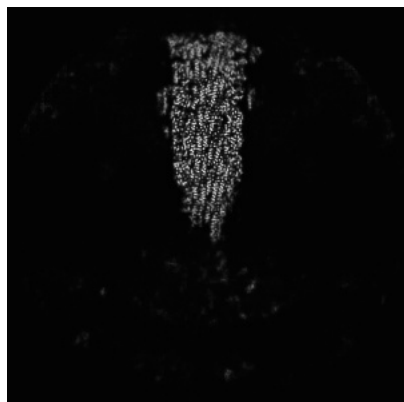


Z Index: 320

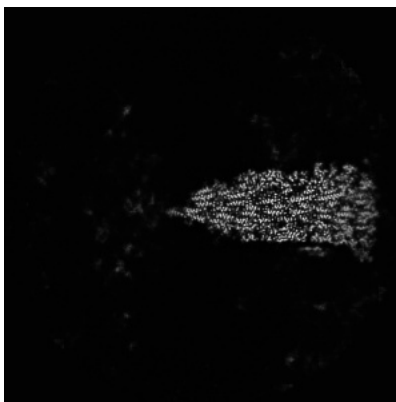
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

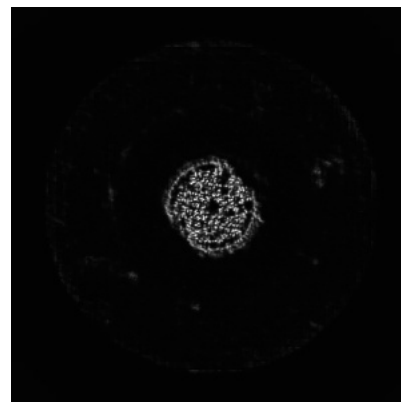
6.3.1 Primary map



X Index: 306

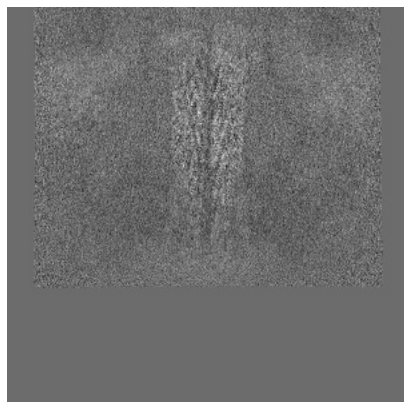


Y Index: 334

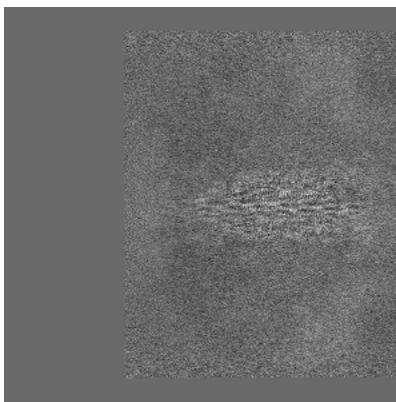


Z Index: 502

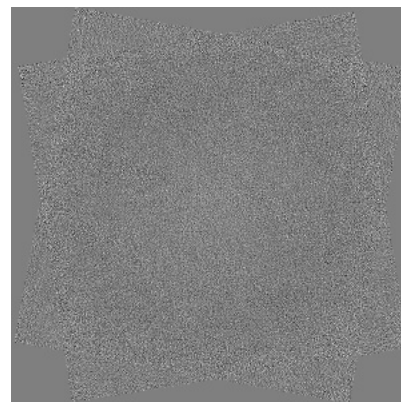
6.3.2 Raw map



X Index: 316



Y Index: 334

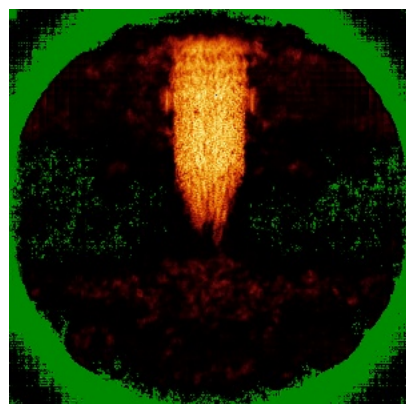


Z Index: 197

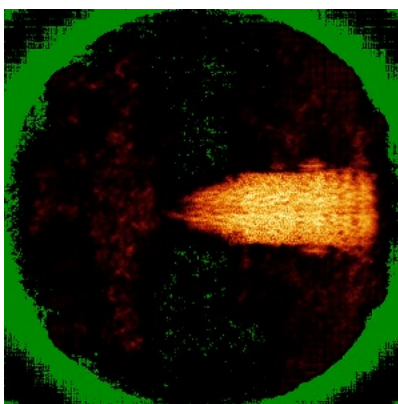
The images above show the largest variance slices of the map in three orthogonal directions.

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

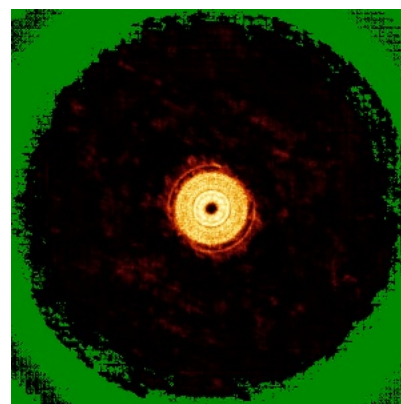
6.4.1 Primary map



X

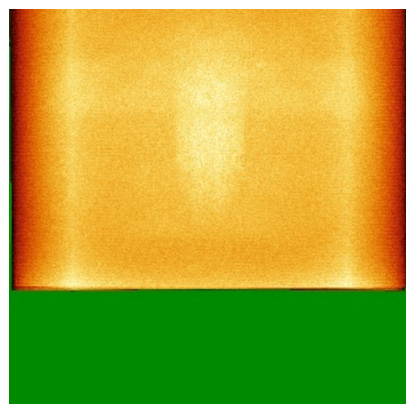


Y

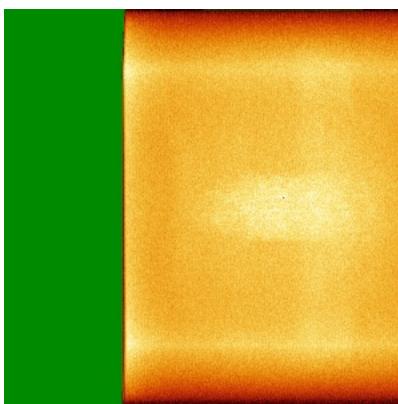


Z

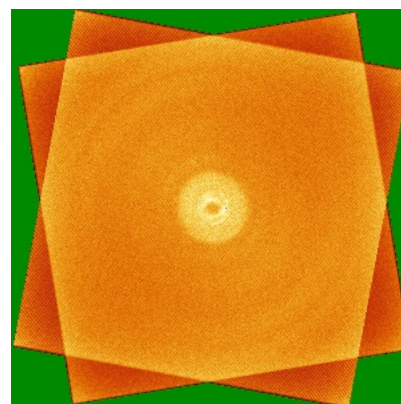
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

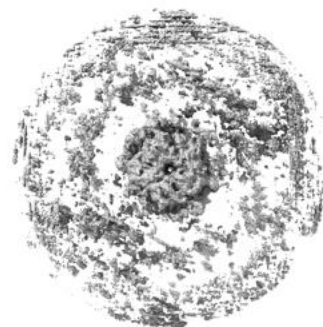
6.5.1 Primary map



X



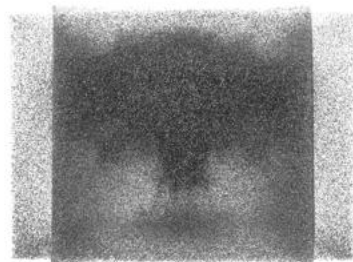
Y



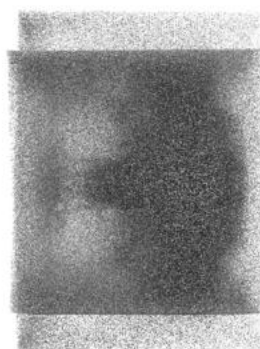
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

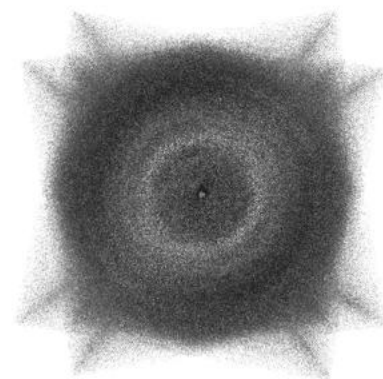
6.5.2 Raw map



X



Y



Z

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

6.6 Mask visualisation [i](#)

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

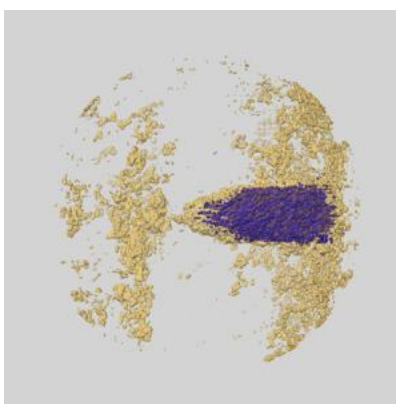
A mask typically either:

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

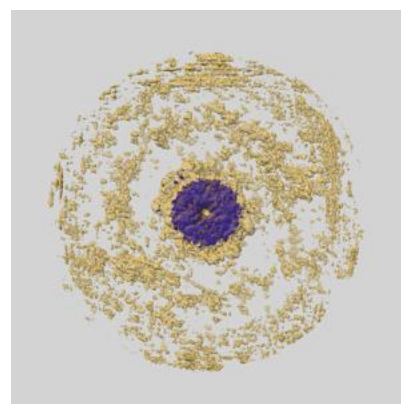
6.6.1 emd_72849_msk_1.map [i](#)



X



Y

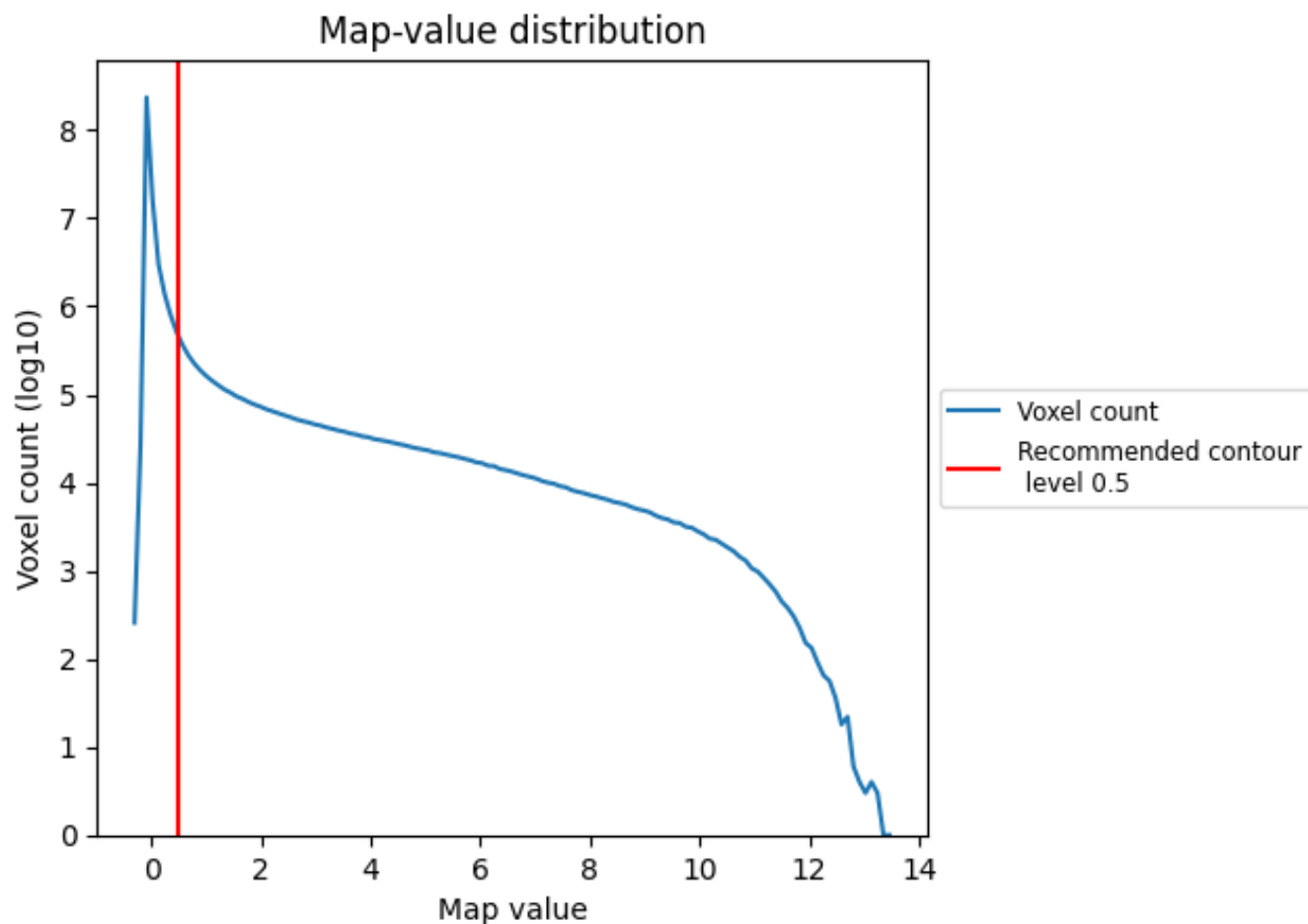


Z

7 Map analysis [i](#)

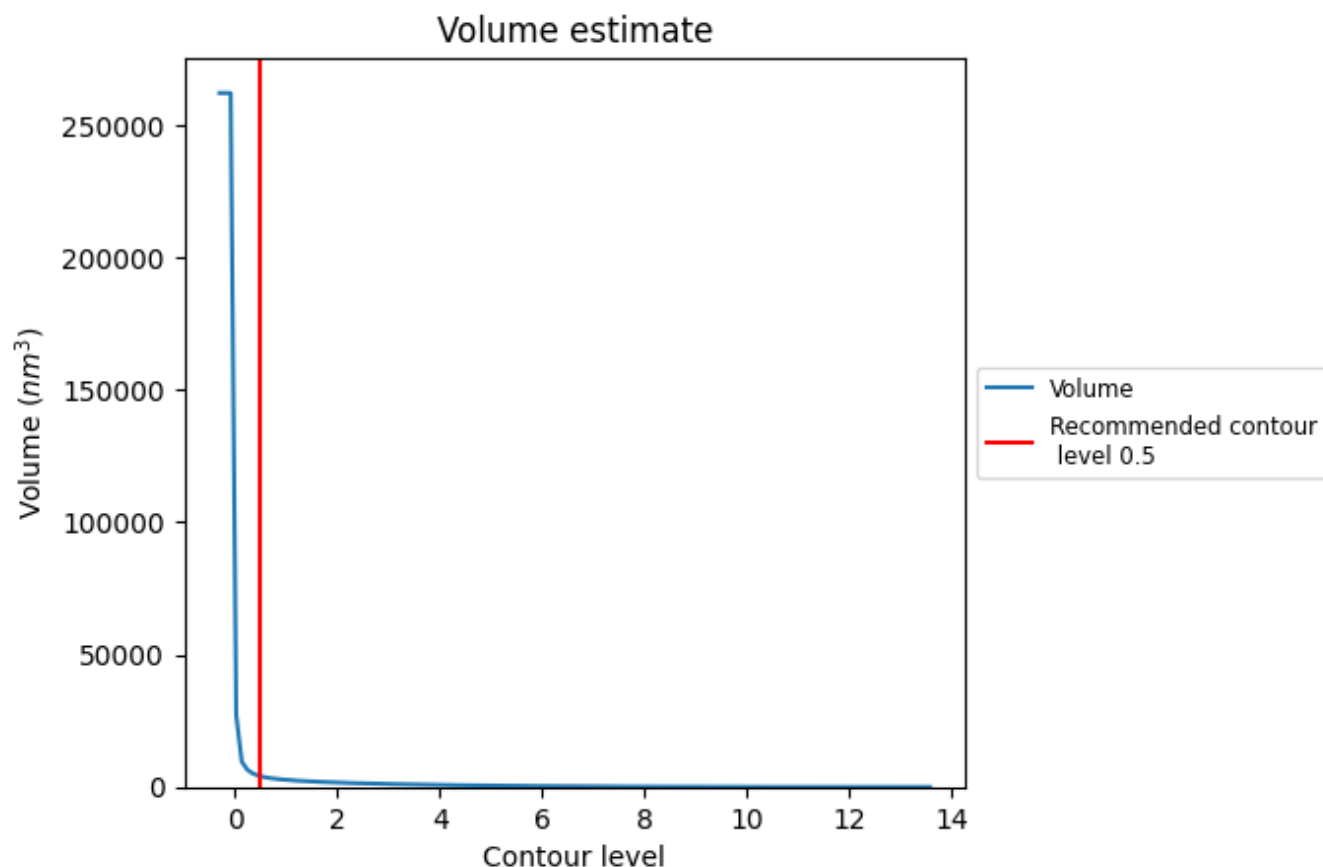
This section contains the results of statistical analysis of the map.

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.

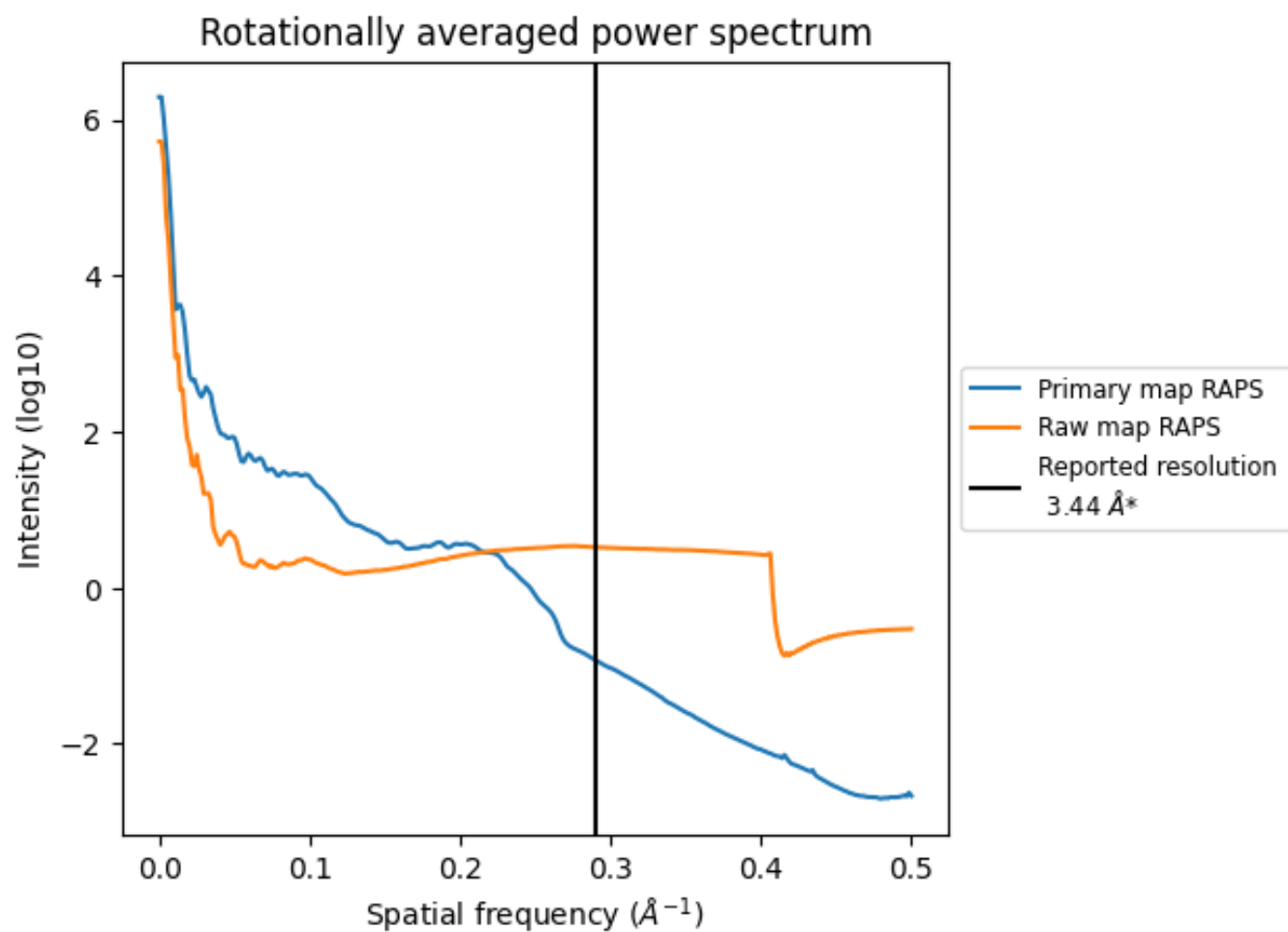
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4044 nm^3 ; this corresponds to an approximate mass of 3653 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 ⓘ

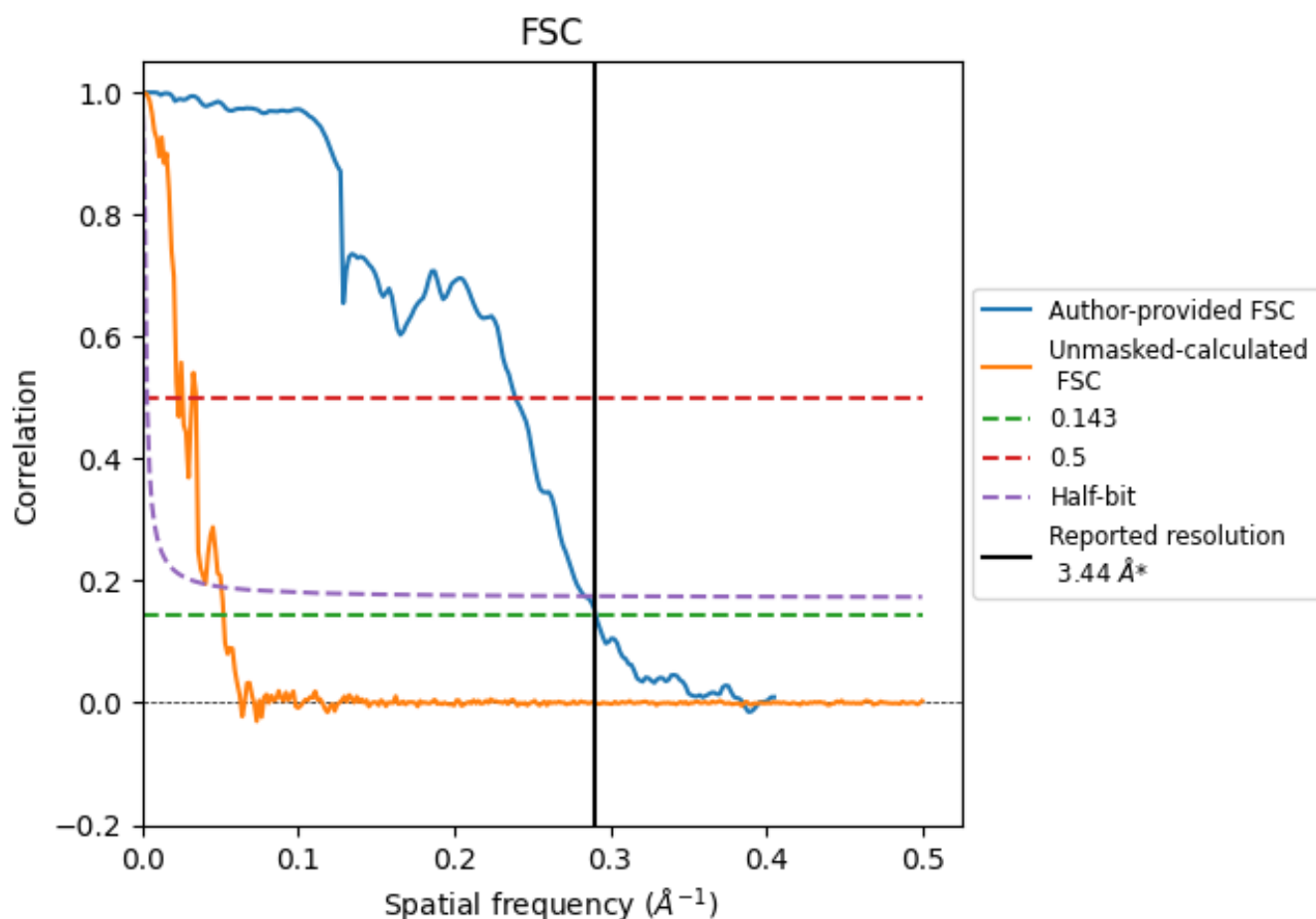


*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

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 0.291 \AA^{-1}

8.2 Resolution estimates [i](#)

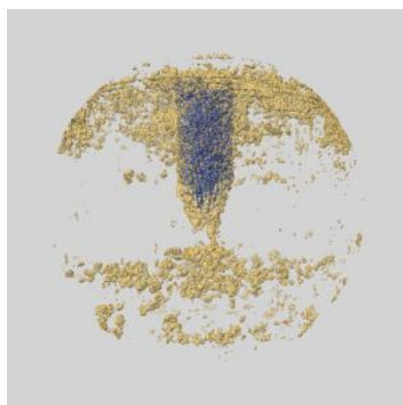
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	4.18	3.53
Unmasked-calculated*	19.19	44.25	19.72

*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 19.19 differs from the reported value 3.44 by more than 10 %

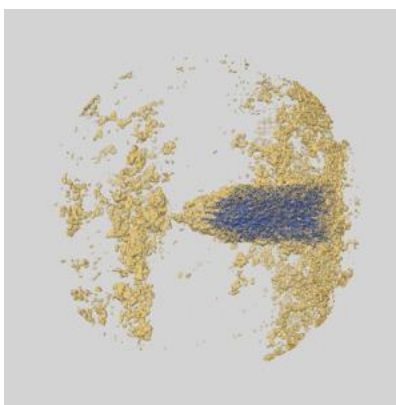
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72849 and PDB model 9YEE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

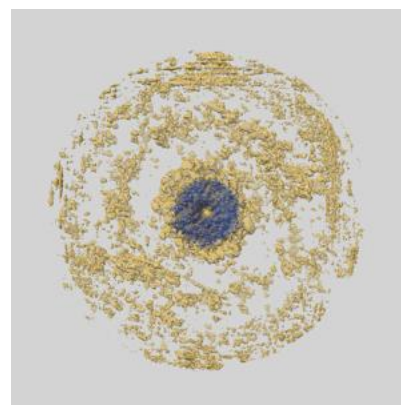
9.1 Map-model overlay [i](#)



X



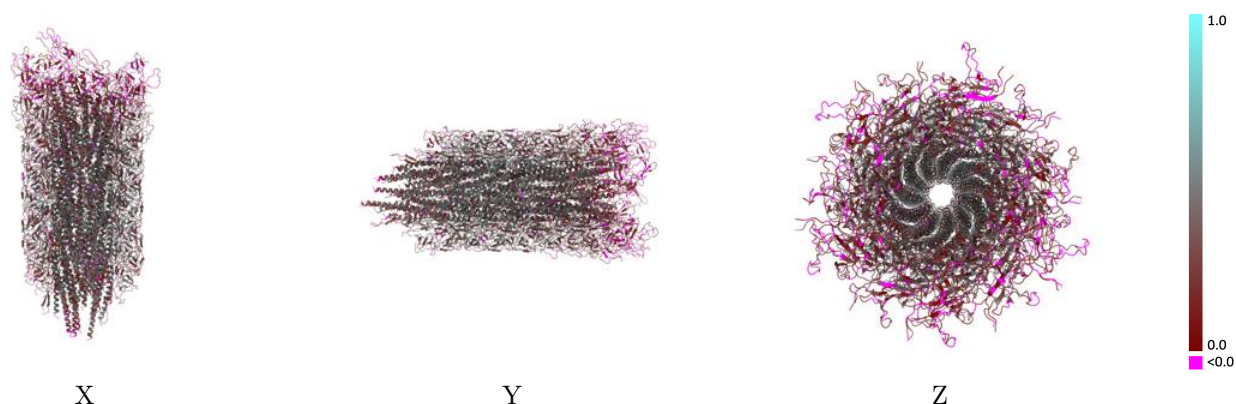
Y



Z

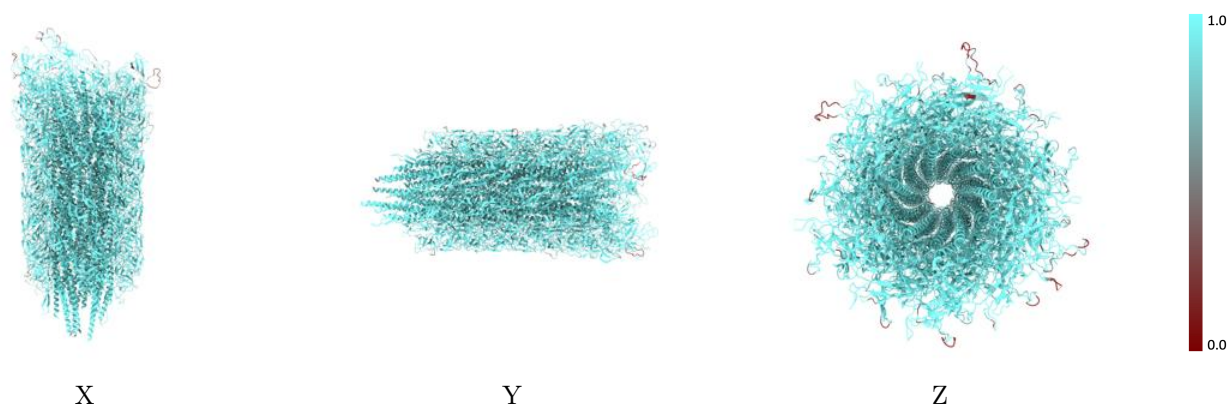
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



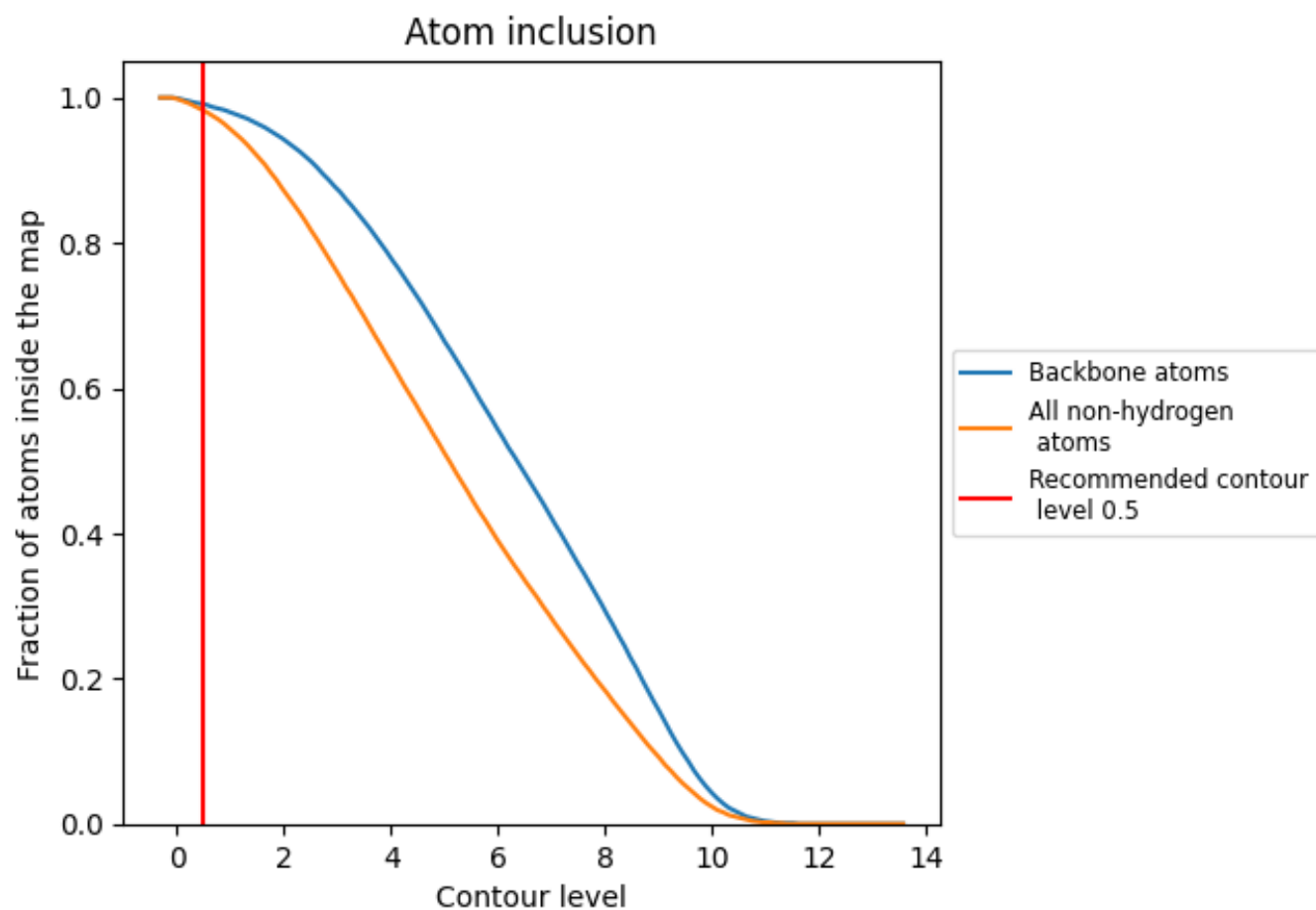
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9820	 0.3160
Ba	 0.9960	 0.3910
Bb	 0.9910	 0.3070
Bc	 0.9890	 0.3590
Bd	 0.9650	 0.3080
Be	 0.9950	 0.3660
Bf	 0.9960	 0.4030
Bg	 0.9950	 0.3430
Bh	 0.9860	 0.3430
Bi	 0.9920	 0.3920
Bj	 0.9950	 0.3740
Bk	 0.9850	 0.3610
Bl	 0.9960	 0.3920
Bm	 0.9850	 0.3800
Bn	 0.9950	 0.3760
Bo	 0.9800	 0.3750
Bp	 0.9940	 0.3600
Bq	 0.9930	 0.3590
Br	 0.9910	 0.3320
Bs	 0.9900	 0.3700
Bt	 0.9970	 0.4030
Bu	 0.9950	 0.4160
Bv	 0.9950	 0.3890
Bw	 0.9950	 0.3870
Bx	 0.9820	 0.3680
By	 0.9950	 0.3740
Bz	 0.9920	 0.3740
Ca	 0.9720	 0.3160
Cb	 0.9890	 0.3430
Cc	 0.9870	 0.3210
Cd	 0.9850	 0.3360
Ce	 0.9690	 0.1970
Cf	 0.9900	 0.3140
Cg	 0.9810	 0.1850
Ch	 0.9730	 0.2370



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ci	 0.9590	 0.1660
Cj	 0.9700	 0.2340
Ck	 0.9450	 0.1570
Cl	 0.9820	 0.2690
Cm	 0.9920	 0.3280
Cn	 0.9630	 0.2200
Co	 0.9580	 0.2640
Cp	 0.9190	 0.1730
Cq	 0.9890	 0.3230
Cr	 0.9880	 0.3020
Cs	 0.9850	 0.2710
Ct	 0.9940	 0.3270
Cu	 0.9480	 0.1750
Cv	 0.9630	 0.2550
Cw	 0.9770	 0.2600