



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 02:39 PM EDT

PDB ID : 10PL / pdb_000010pl
EMDB ID : EMD-75374
Title : Asymmetric architecture and adaptation of Treponema flagella
Authors : Wang, J.; Kurniyati, K.; Guo, W.; Botting, J.M.; Sindelar, C.V.; Li, C.; Liu, J.
Deposited on : 2026-01-30
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:

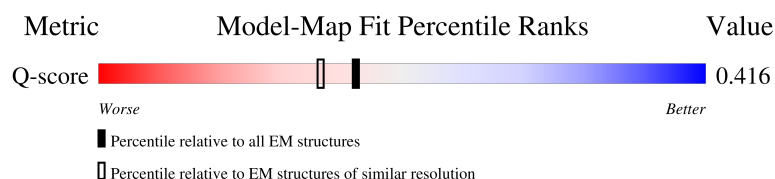
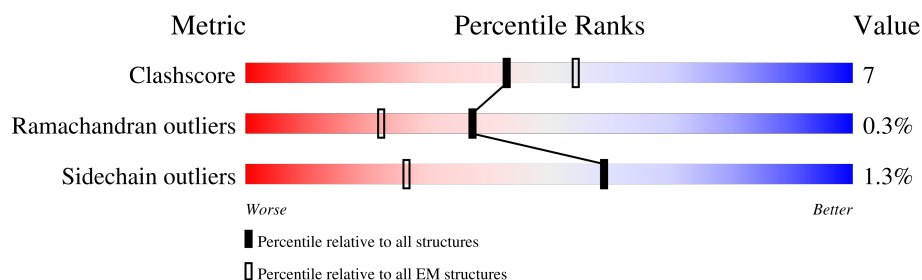
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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



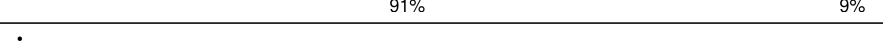

The reported resolution of this entry is 3.44 Å.

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	286	
1	Bb	286	
1	Bc	286	
1	Bd	286	

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Mol	Chain	Length	Quality of chain
1	Be	286	
1	Bf	286	
1	Bg	286	
1	Bh	286	
1	Bi	286	
1	Bj	286	
1	Bk	286	
2	F	107	
3	A	192	
4	B	201	
5	C	204	
6	D	204	
7	E	221	
8	Aa	326	
8	Ab	326	
8	Ac	326	
8	Ad	326	
8	Ae	326	
8	Af	326	
8	Ag	326	
8	Ah	326	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 53608 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 Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ba	286	Total	C	N	O	S	0	0
			2182	1328	405	431	18		
1	Bd	285	Total	C	N	O	S	0	0
			2174	1324	404	428	18		
1	Bc	286	Total	C	N	O	S	0	0
			2182	1328	405	431	18		
1	Bb	286	Total	C	N	O	S	0	0
			2182	1328	405	431	18		
1	Bk	285	Total	C	N	O	S	0	0
			2170	1322	401	429	18		
1	Bj	286	Total	C	N	O	S	0	0
			2182	1328	405	431	18		
1	Bi	286	Total	C	N	O	S	0	0
			2182	1328	405	431	18		
1	Bh	286	Total	C	N	O	S	0	0
			2182	1328	405	431	18		
1	Bg	286	Total	C	N	O	S	0	0
			2182	1328	405	431	18		
1	Bf	285	Total	C	N	O	S	0	0
			2170	1322	401	429	18		
1	Be	285	Total	C	N	O	S	0	0
			2170	1322	401	429	18		

- Molecule 2 is a protein called Flagellin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	107	Total	C	N	O	0	0
			887	583	151	153		

- Molecule 3 is a protein called HEAT repeat domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	192	Total	C	N	O	S	0	0
			1494	933	263	288	10		

- Molecule 4 is a protein called Flagellar filament outer layer protein FlaA, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	201	Total	C	N	O	S	0	0
			1622	1041	271	302	8		

- Molecule 5 is a protein called Flagellar filament outer layer protein FlaA, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	204	Total	C	N	O	S	0	0
			1680	1089	277	307	7		

- Molecule 6 is a protein called Flagellar filament outer layer protein FlaA, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	204	Total	C	N	O	S	0	0
			1676	1087	277	305	7		

- Molecule 7 is a protein called Flagellar filament outer layer protein FlaA, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	220	Total	C	N	O	S	0	0
			1760	1125	293	334	8		

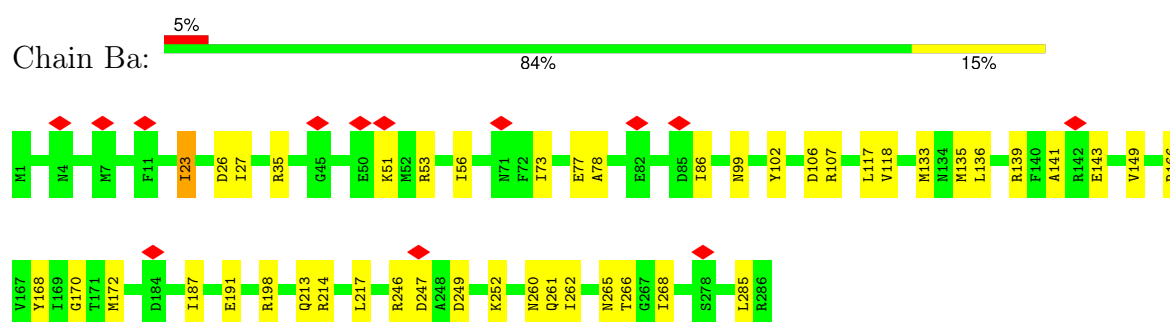
- Molecule 8 is a protein called Flagellar filament outer layer protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ab	322	Total	C	N	O	S	0	0
			2563	1628	437	491	7		
8	Ag	324	Total	C	N	O	S	0	0
			2584	1641	440	495	8		
8	Ah	323	Total	C	N	O	S	0	0
			2577	1636	439	494	8		
8	Af	323	Total	C	N	O	S	0	0
			2571	1633	438	492	8		
8	Ae	324	Total	C	N	O	S	0	0
			2580	1638	439	495	8		
8	Ad	325	Total	C	N	O	S	0	0
			2592	1645	442	497	8		
8	Ac	323	Total	C	N	O	S	0	0
			2577	1636	439	494	8		
8	Aa	311	Total	C	N	O	S	0	0
			2487	1583	426	470	8		

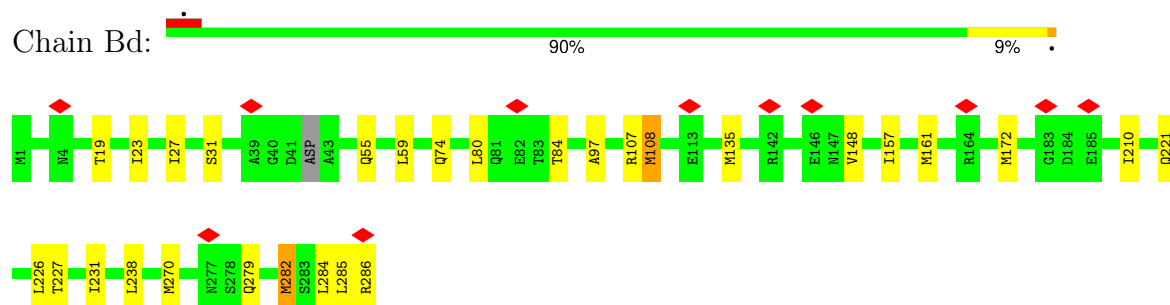
3 Residue-property plots [i](#)

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.

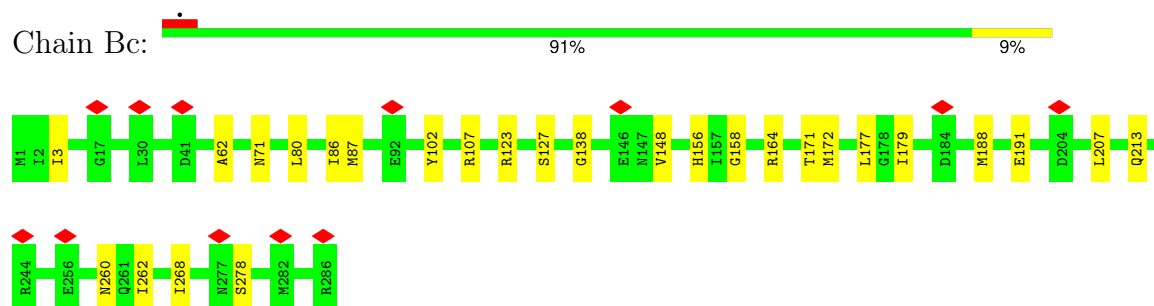
• Molecule 1: Flagellin



• Molecule 1: Flagellin

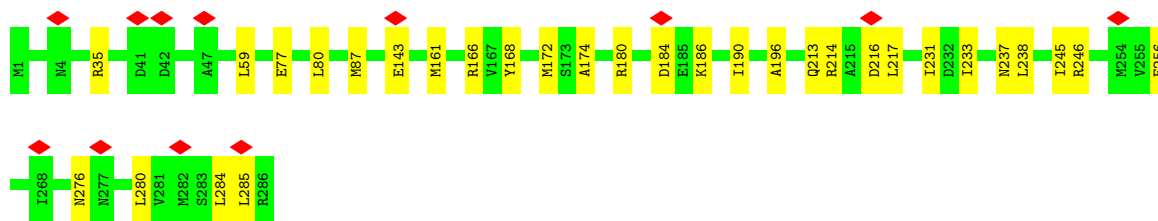


• Molecule 1: Flagellin

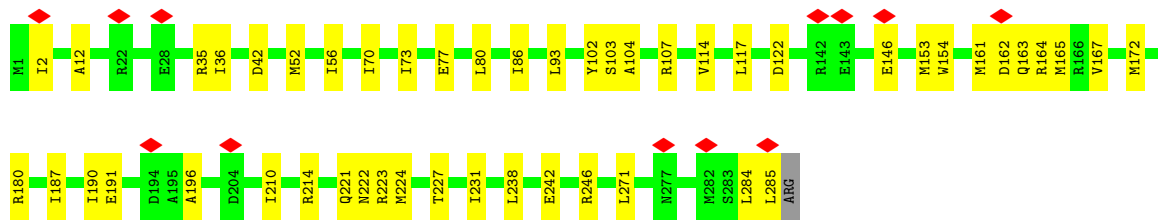
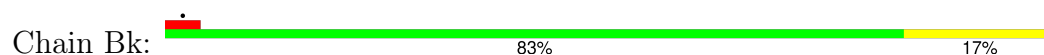


• Molecule 1: Flagellin

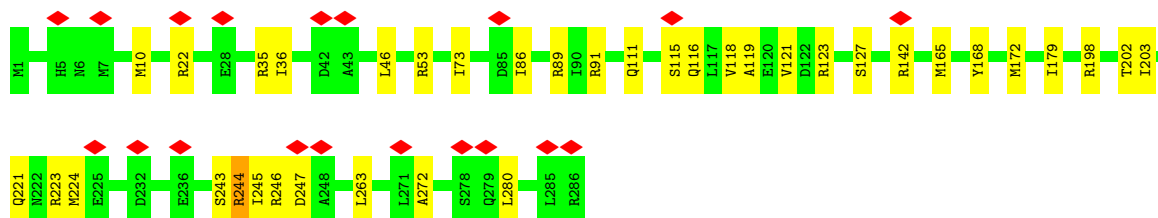
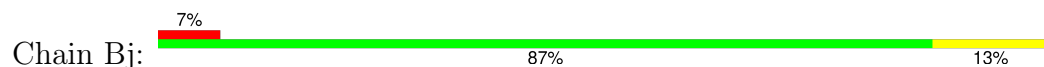




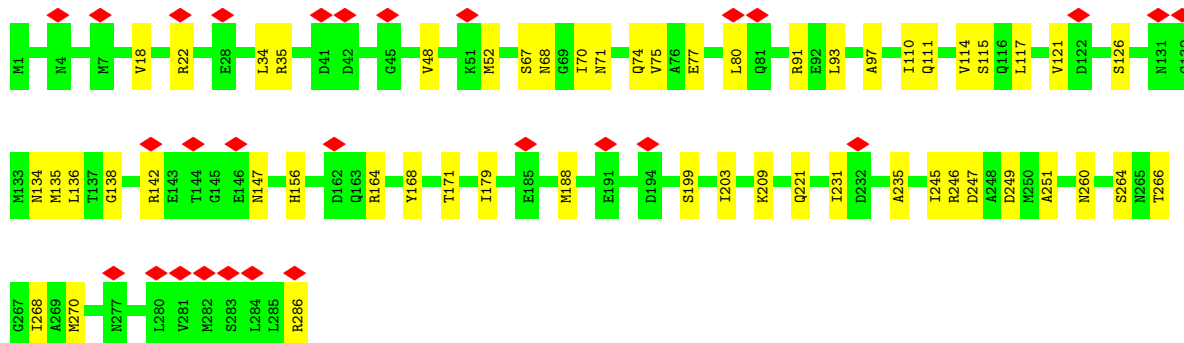
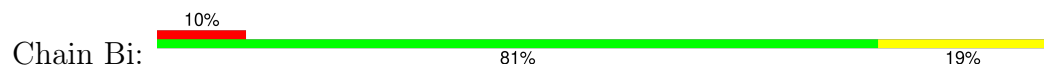
• Molecule 1: Flagellin



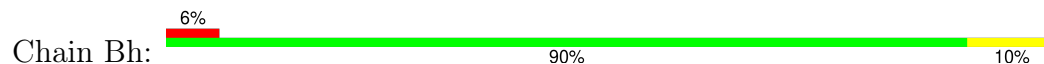
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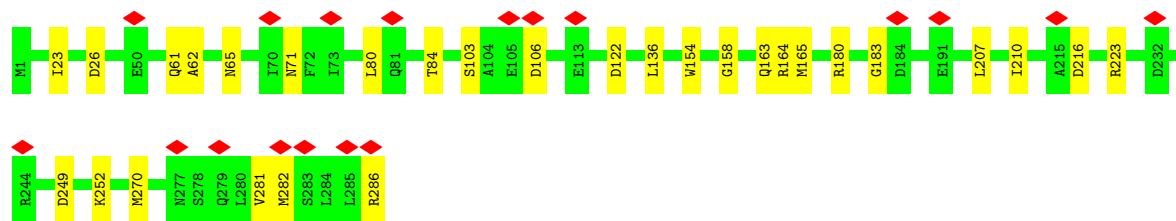


• Molecule 1: Flagellin

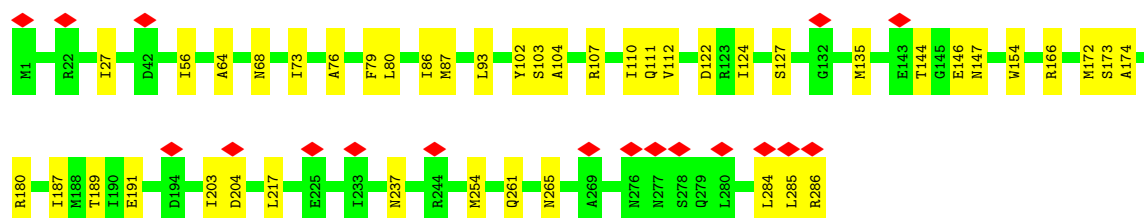
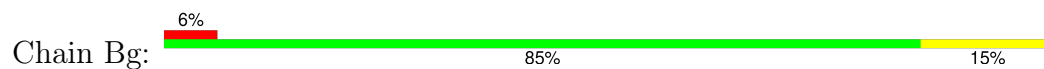


• Molecule 1: Flagellin

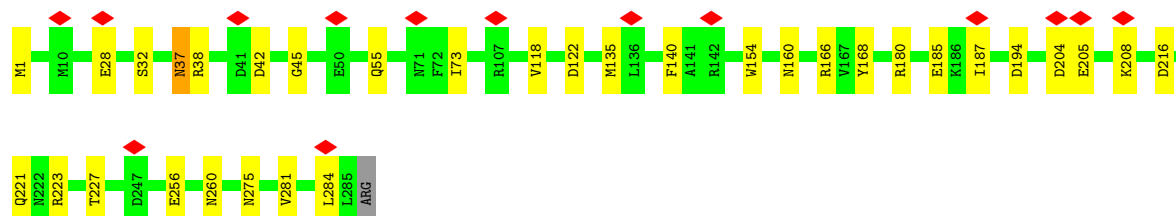




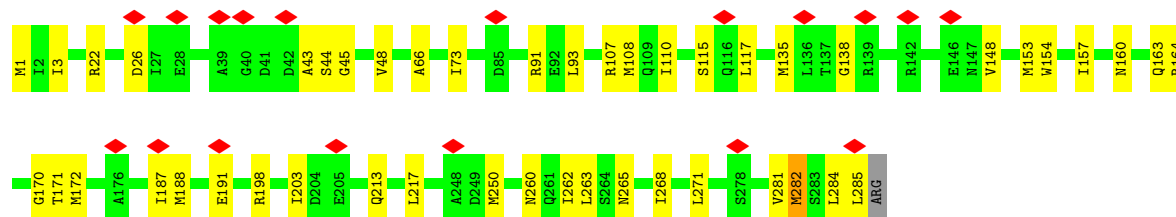
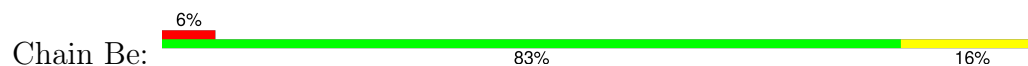
• Molecule 1: Flagellin



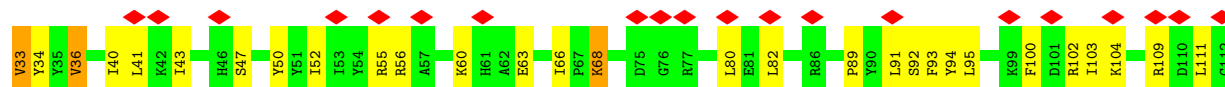
• Molecule 1: Flagellin

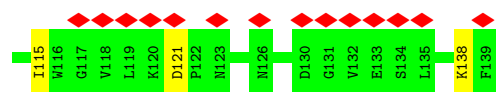


• Molecule 1: Flagellin

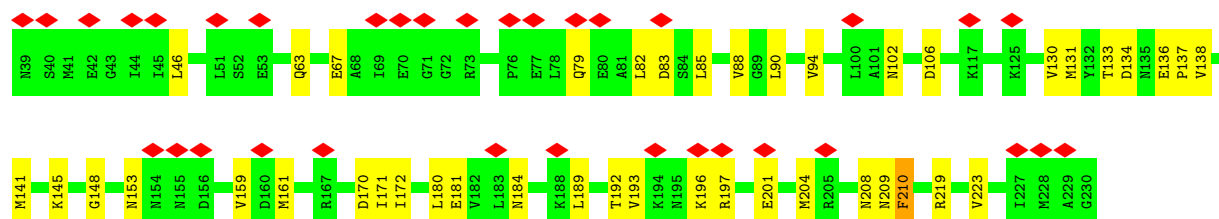
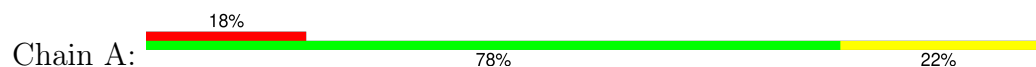


• Molecule 2: Flagellin

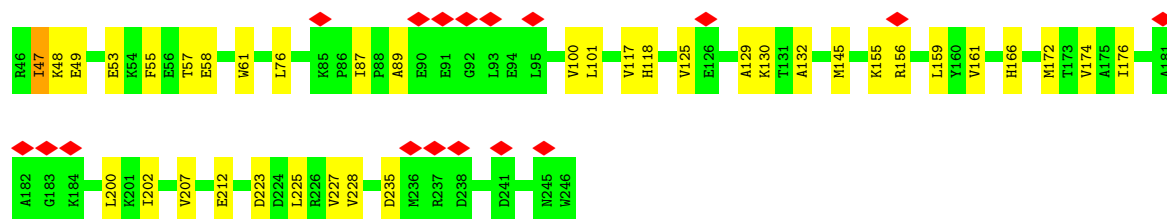
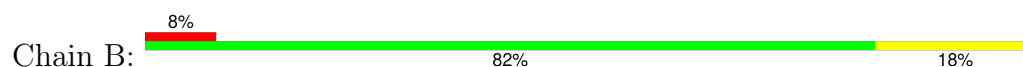




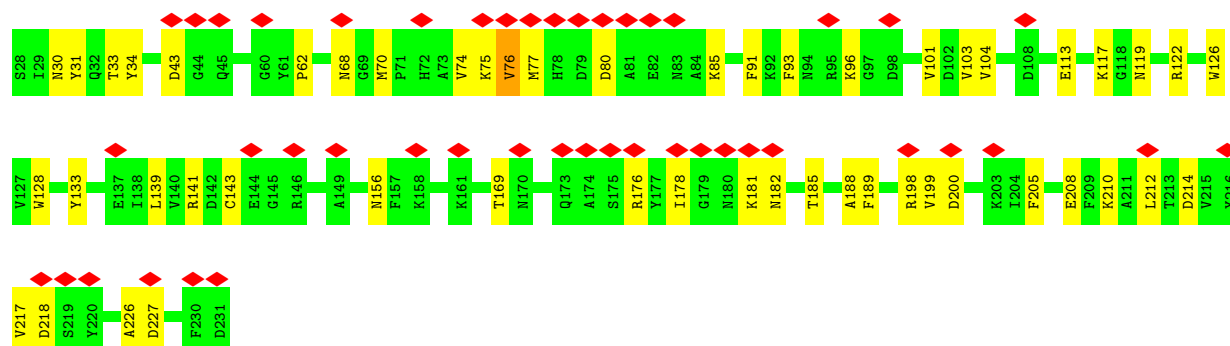
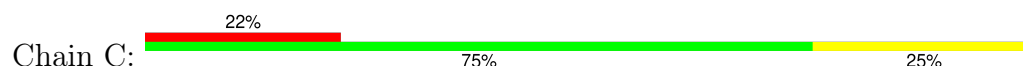
- Molecule 3: HEAT repeat domain-containing protein



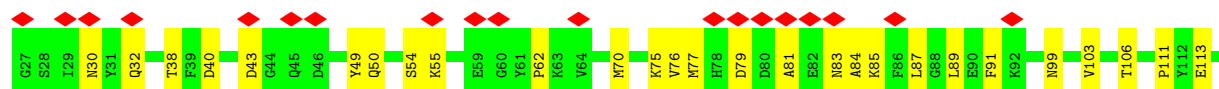
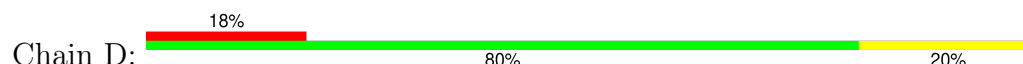
- Molecule 4: Flagellar filament outer layer protein FlaA, putative

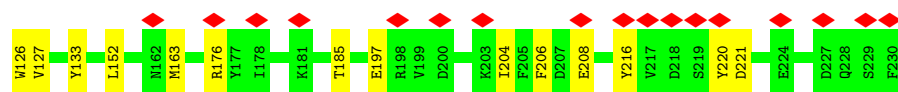


- Molecule 5: Flagellar filament outer layer protein FlaA, putative

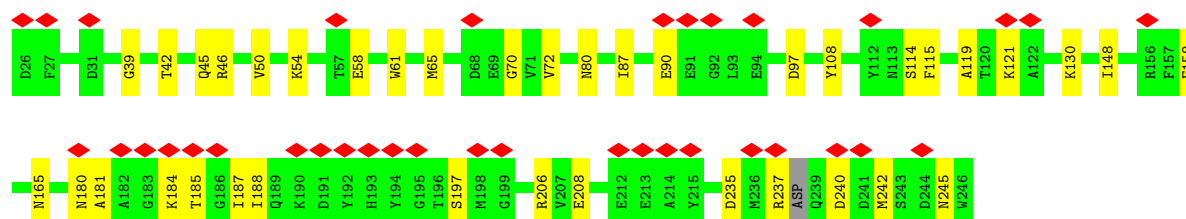
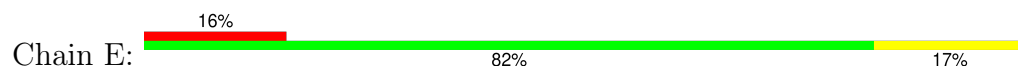


- Molecule 6: Flagellar filament outer layer protein FlaA, putative

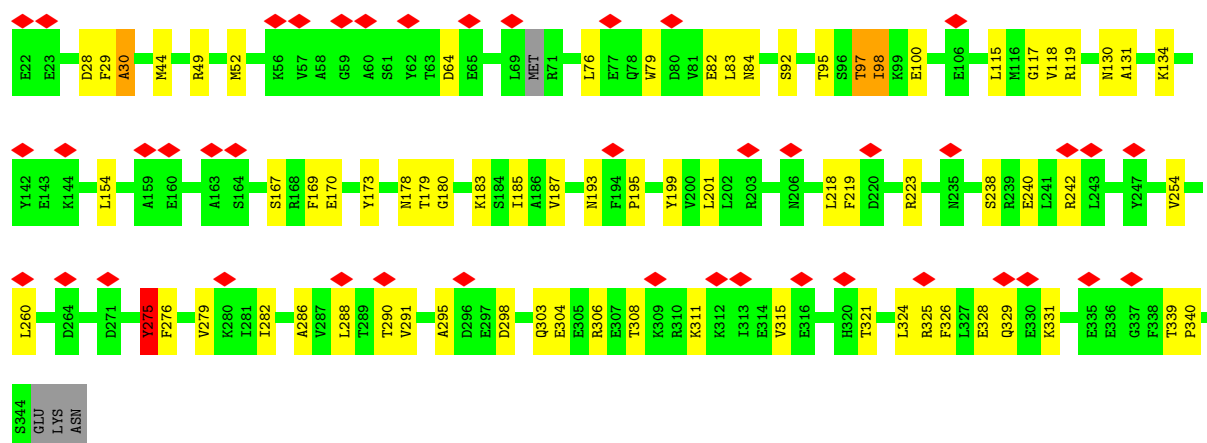
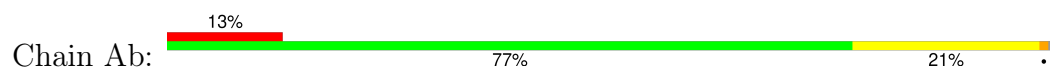




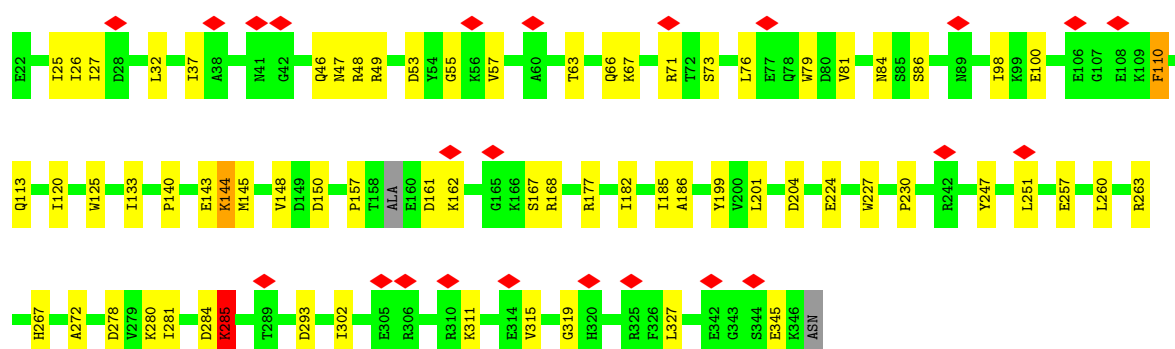
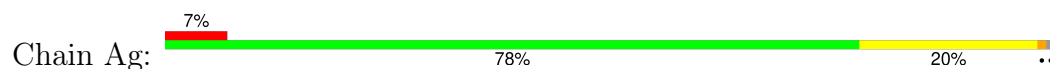
- Molecule 7: Flagellar filament outer layer protein FlaA, putative



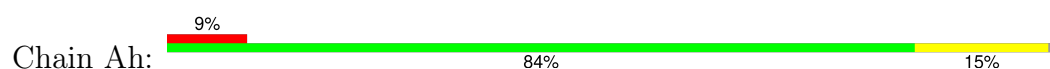
- Molecule 8: Flagellar filament outer layer protein

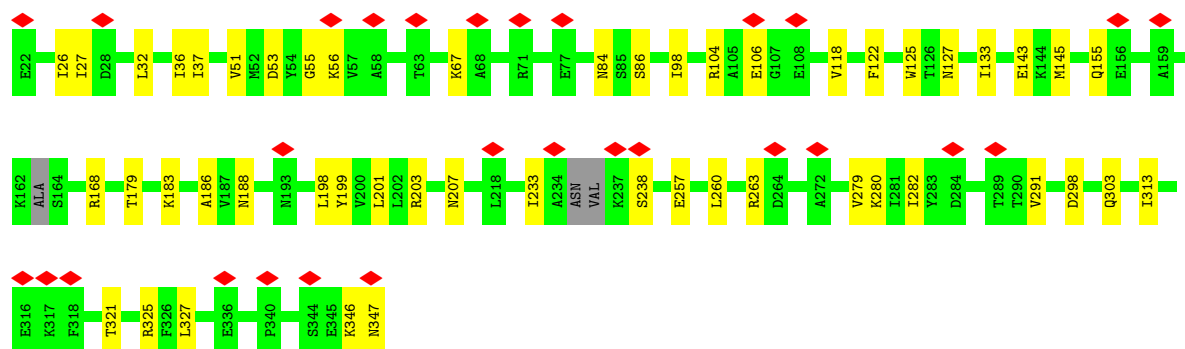


- Molecule 8: Flagellar filament outer layer protein



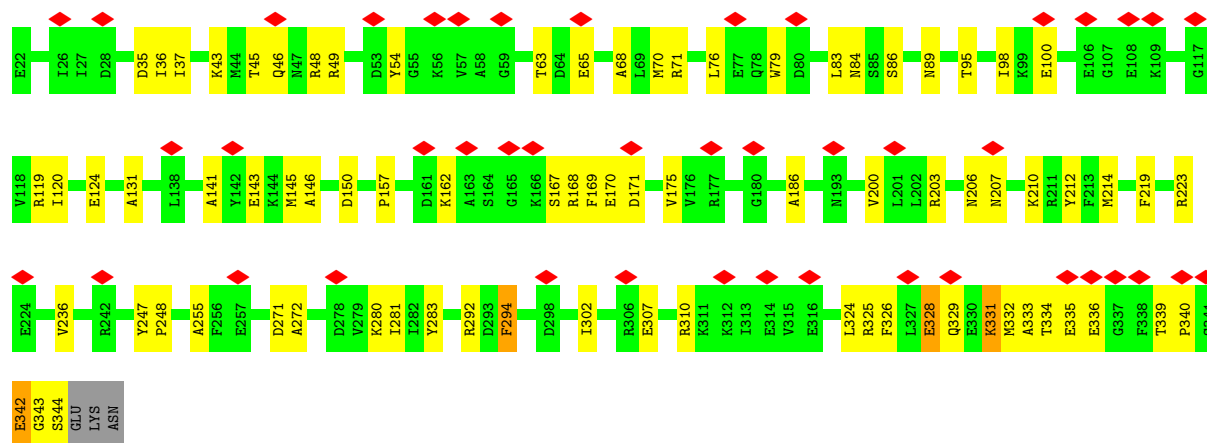
- Molecule 8: Flagellar filament outer layer protein





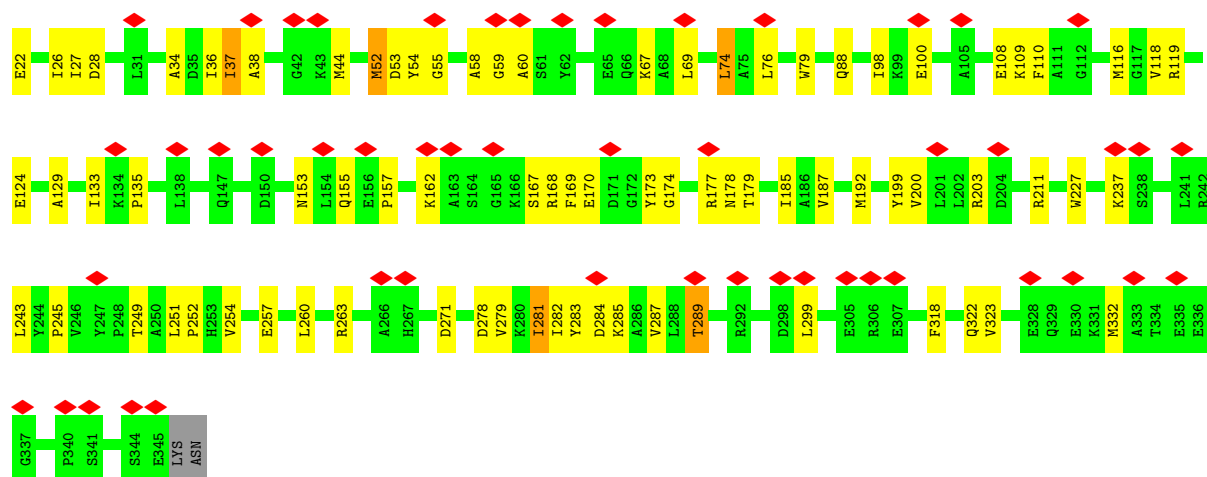
• Molecule 8: Flagellar filament outer layer protein

Chain Af: 13% 75% 23% ..



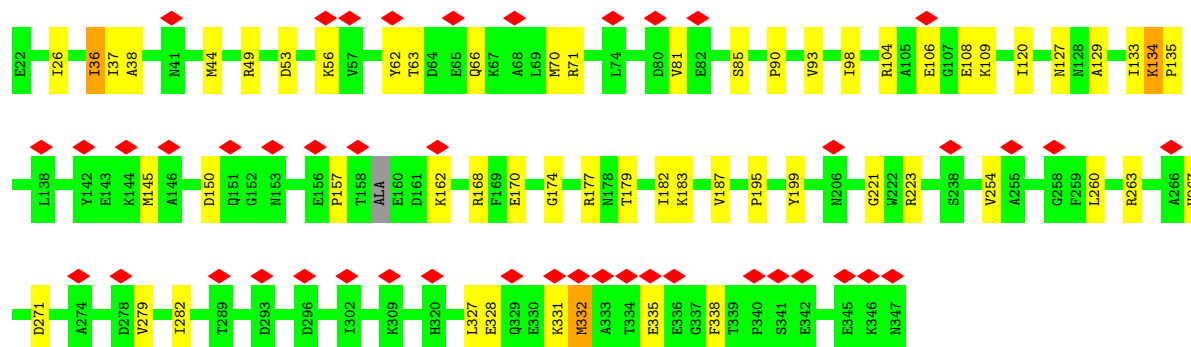
• Molecule 8: Flagellar filament outer layer protein

Chain Ae: 15% 75% 23% ..

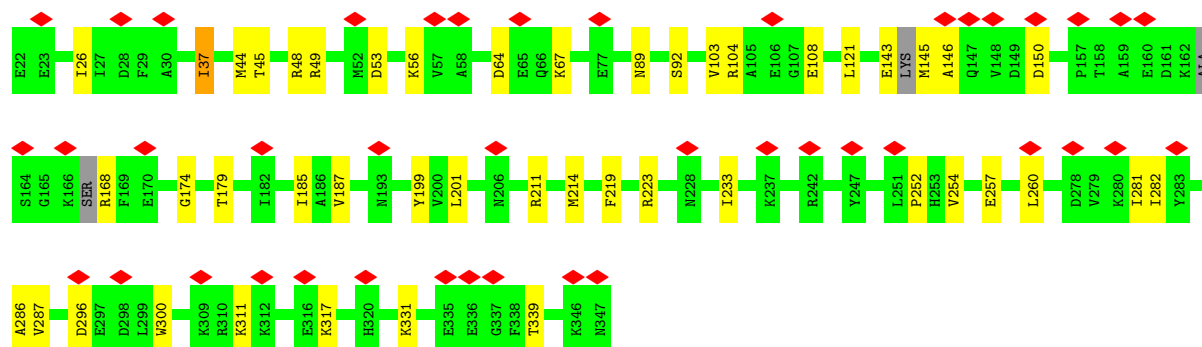
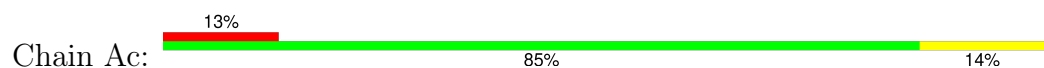


• Molecule 8: Flagellar filament outer layer protein

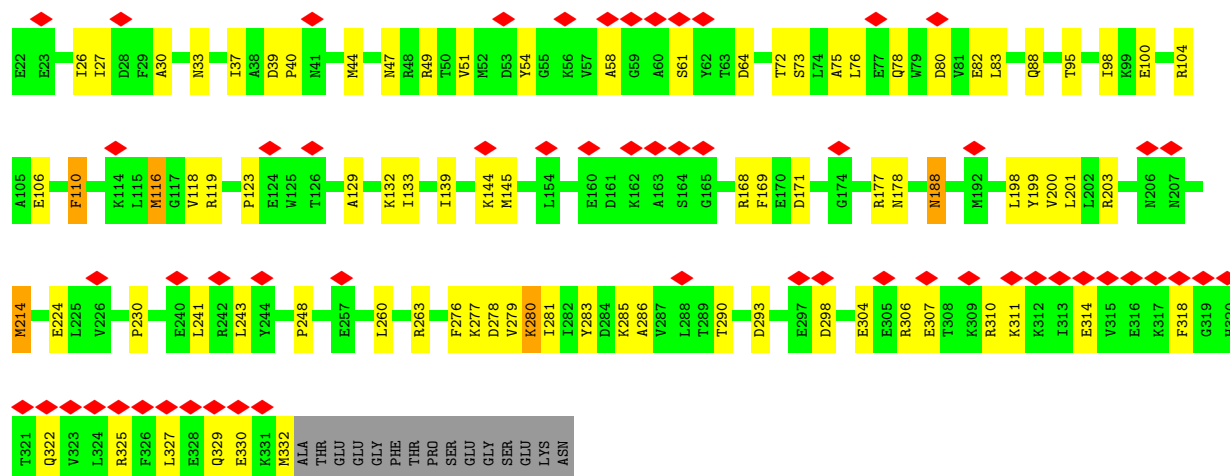
Chain Ad: 14% 82% 17% .



• Molecule 8: Flagellar filament outer layer protein



• Molecule 8: Flagellar filament outer layer protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	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	0.422	Depositor
Minimum map value	-0.266	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	384.47998, 384.47998, 384.47998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.068, 1.068, 1.068	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ba	0.20	0/2195	0.55	2/2945 (0.1%)
1	Bb	0.19	0/2195	0.50	0/2945
1	Bc	0.16	0/2195	0.43	0/2945
1	Bd	0.18	0/2186	0.48	2/2931 (0.1%)
1	Be	0.19	0/2183	0.57	4/2931 (0.1%)
1	Bf	0.19	0/2183	0.51	0/2931
1	Bg	0.19	0/2195	0.52	0/2945
1	Bh	0.19	0/2195	0.52	0/2945
1	Bi	0.19	0/2195	0.52	1/2945 (0.0%)
1	Bj	0.20	0/2195	0.53	0/2945
1	Bk	0.21	0/2183	0.55	0/2931
2	F	0.18	0/912	0.55	1/1231 (0.1%)
3	A	0.27	0/1508	0.60	2/2033 (0.1%)
4	B	0.20	0/1664	0.52	0/2249
5	C	0.23	0/1733	0.62	1/2351 (0.0%)
6	D	0.29	0/1729	0.63	1/2345 (0.0%)
7	E	0.22	0/1803	0.58	0/2438
8	Aa	0.28	0/2538	0.74	2/3432 (0.1%)
8	Ab	0.37	0/2615	0.78	6/3536 (0.2%)
8	Ac	0.24	0/2627	0.60	0/3548
8	Ad	0.23	0/2644	0.64	1/3573 (0.0%)
8	Ae	0.22	0/2633	0.61	1/3561 (0.0%)
8	Af	0.26	0/2624	0.68	1/3549 (0.0%)
8	Ag	0.21	0/2636	0.56	3/3562 (0.1%)
8	Ah	0.24	0/2628	0.59	0/3549
All	All	0.23	0/54394	0.59	28/73296 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

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Mol	Chain	#Chirality outliers	#Planarity outliers
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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Bj	0	1
8	Aa	0	1
8	Ab	0	1
8	Ae	0	1
8	Af	0	1
All	All	0	5

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Aa	280	LYS	N-CA-CB	-9.41	95.41	110.46
6	D	79	ASP	N-CA-C	-7.93	101.36	113.89
8	Ab	30	ALA	N-CA-C	-7.29	105.00	114.04
8	Aa	116	MET	N-CA-CB	6.15	119.80	110.45
2	F	68	LYS	CA-CB-CG	6.08	126.26	114.10
8	Af	342	GLU	CB-CA-C	-5.86	101.89	111.50
1	Ba	135	MET	CB-CG-SD	5.74	129.91	112.70
1	Bd	108	MET	CB-CG-SD	5.72	129.85	112.70
8	Ag	284	ASP	CA-C-N	5.65	132.33	121.54
8	Ag	284	ASP	C-N-CA	5.65	132.33	121.54
8	Ab	117	GLY	CA-C-N	-5.64	114.59	122.71
8	Ab	117	GLY	C-N-CA	-5.64	114.59	122.71
1	Be	135	MET	CB-CG-SD	5.52	129.27	112.70
1	Ba	285	LEU	N-CA-C	-5.47	108.38	114.62
8	Ag	144	LYS	CB-CG-CD	5.36	123.62	111.30
1	Bd	282	MET	CB-CG-SD	5.33	128.71	112.70
8	Ab	29	PHE	CA-CB-CG	5.33	119.13	113.80
1	Be	282	MET	CB-CG-SD	5.32	128.66	112.70
5	C	226	ALA	CB-CA-C	-5.22	110.13	117.23
8	Ae	74	LEU	CA-CB-CG	5.21	134.53	116.30
1	Bi	270	MET	CB-CG-SD	5.18	128.23	112.70
1	Be	135	MET	CA-CB-CG	5.16	124.42	114.10
8	Ab	275	TYR	CA-C-O	-5.11	115.79	121.51
8	Ad	332	MET	CB-CG-SD	5.09	127.98	112.70
8	Ab	44	MET	CB-CG-SD	5.07	127.91	112.70
1	Be	108	MET	CB-CG-SD	5.03	127.79	112.70
3	A	180	LEU	CA-C-N	-5.00	113.32	122.38
3	A	180	LEU	C-N-CA	-5.00	113.32	122.38

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	Aa	177	ARG	Peptide
8	Ab	119	ARG	Sidechain
8	Ae	52	MET	Peptide
8	Af	331	LYS	Peptide
1	Bj	244	ARG	Peptide

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	2182	0	2195	30	0
1	Bb	2182	0	2195	21	0
1	Bc	2182	0	2195	15	0
1	Bd	2174	0	2190	17	0
1	Be	2170	0	2182	25	0
1	Bf	2170	0	2182	22	0
1	Bg	2182	0	2195	27	0
1	Bh	2182	0	2195	19	0
1	Bi	2182	0	2195	32	0
1	Bj	2182	0	2195	27	0
1	Bk	2170	0	2182	30	0
2	F	887	0	898	21	0
3	A	1494	0	1538	28	0
4	B	1622	0	1579	23	0
5	C	1680	0	1592	30	0
6	D	1676	0	1591	23	0
7	E	1760	0	1705	26	0
8	Aa	2487	0	2459	60	0
8	Ab	2563	0	2518	40	0
8	Ac	2577	0	2527	29	0
8	Ad	2592	0	2547	34	0
8	Ae	2580	0	2534	55	0
8	Af	2571	0	2528	56	0
8	Ag	2584	0	2541	40	0
8	Ah	2577	0	2531	28	0
All	All	53608	0	53189	705	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 7.

All (705) 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)
8:Af:340:PRO:C	8:Af:342:GLU:H	1.93	0.75
8:Af:342:GLU:O	8:Af:344:SER:N	2.19	0.75
8:Ab:79:TRP:HB2	8:Ab:98:ILE:HG21	1.67	0.74
8:Ac:187:VAL:HG22	8:Ac:214:MET:HE2	1.68	0.74
1:Ba:170:GLY:H	1:Ba:213:GLN:HE22	1.36	0.70
8:Af:340:PRO:HA	8:Af:342:GLU:HG3	1.74	0.69
8:Af:326:PHE:HA	8:Af:329:GLN:HB2	1.74	0.69
8:Aa:110:PHE:HD1	8:Aa:110:PHE:H	1.40	0.69
5:C:119:ASN:HB2	5:C:214:ASP:HB3	1.75	0.69
8:Ad:199:TYR:HB2	8:Ad:260:LEU:HB3	1.74	0.68
8:Aa:322:GLN:HE22	8:Aa:325:ARG:HD3	1.59	0.68
8:Ab:328:GLU:HA	8:Ab:331:LYS:HB3	1.76	0.67
8:Ac:199:TYR:HB2	8:Ac:260:LEU:HB3	1.76	0.67
8:Ae:52:MET:HB2	8:Ae:168:ARG:HH22	1.59	0.67
1:Bb:172:MET:HE1	1:Bb:213:GLN:HG2	1.75	0.67
1:Bc:179:ILE:HA	1:Bc:188:MET:HE3	1.75	0.67
8:Ae:26:ILE:HG22	8:Ae:27:ILE:HG13	1.75	0.67
8:Ah:122:PHE:HD1	8:Ah:263:ARG:HD2	1.59	0.66
8:Af:95:THR:HB	8:Af:119:ARG:HH21	1.60	0.66
1:Bj:111:GLN:NE2	1:Bj:115:SER:OG	2.28	0.66
8:Aa:145:MET:HA	8:Aa:168:ARG:HG3	1.78	0.66
8:Ab:199:TYR:HB2	8:Ab:260:LEU:HB3	1.78	0.65
8:Ag:199:TYR:HB2	8:Ag:260:LEU:HB3	1.78	0.65
1:Be:91:ARG:HB2	1:Be:203:ILE:HG21	1.79	0.65
8:Af:45:THR:HG22	8:Af:46:GLN:HG2	1.79	0.65
4:B:49:GLU:HB2	4:B:228:VAL:HG22	1.79	0.65
1:Ba:166:ARG:HE	1:Ba:168:TYR:HE1	1.46	0.64
8:Ab:339:THR:HG22	8:Ab:340:PRO:HD2	1.79	0.64
8:Aa:51:VAL:O	8:Aa:168:ARG:NH2	2.30	0.64
8:Ag:63:THR:HB	8:Ag:66:GLN:HG2	1.80	0.64
2:F:56:ARG:HH21	2:F:60:LYS:HD3	1.61	0.64
8:Ae:167:SER:HB3	8:Ae:170:GLU:HG3	1.80	0.64
8:Ab:178:ASN:HD21	8:Ab:286:ALA:H	1.46	0.64
8:Ae:169:PHE:HA	8:Ae:173:TYR:HB2	1.79	0.64
8:Aa:49:ARG:HH12	8:Aa:168:ARG:HG2	1.62	0.64
3:A:131:MET:HB3	3:A:161:MET:HE3	1.81	0.63
8:Af:203:ARG:NH2	8:Af:207:ASN:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bd:172:MET:HE1	1:Bd:210:ILE:HA	1.81	0.63
1:Be:172:MET:HE1	1:Be:213:GLN:HG2	1.81	0.63
8:Ah:118:VAL:HG11	8:Ah:133:ILE:HD13	1.79	0.63
8:Af:344:SER:HB3	8:Ae:110:PHE:CD1	2.33	0.63
8:Ag:263:ARG:NH1	8:Ag:267:HIS:O	2.31	0.62
1:Bk:223:ARG:NH1	1:Bj:116:GLN:OE1	2.32	0.62
3:A:193:VAL:O	3:A:196:LYS:NZ	2.33	0.62
5:C:113:GLU:HB3	5:C:185:THR:HB	1.80	0.62
8:Aa:26:ILE:HG22	8:Aa:27:ILE:HG22	1.80	0.62
1:Bi:188:MET:SD	1:Bi:199:SER:OG	2.57	0.62
8:Ah:143:GLU:OE2	8:Ah:168:ARG:NH2	2.32	0.62
8:Ae:185:ILE:HA	8:Ae:281:ILE:HG21	1.82	0.62
1:Ba:198:ARG:HH12	4:B:212:GLU:HG2	1.65	0.62
1:Bd:97:ALA:O	1:Bd:107:ARG:NH2	2.33	0.62
2:F:100:PHE:HZ	2:F:103:ILE:HB	1.64	0.62
8:Ab:82:GLU:OE1	8:Ab:134:LYS:NZ	2.33	0.62
8:Ad:63:THR:H	8:Ad:66:GLN:HE21	1.48	0.62
1:Bh:163:GLN:NE2	1:Bg:127:SER:OG	2.33	0.61
8:Ag:26:ILE:HG22	8:Ag:27:ILE:HG22	1.82	0.61
8:Af:210:LYS:NZ	8:Af:212:TYR:OH	2.33	0.61
8:Aa:281:ILE:HG12	8:Aa:283:TYR:HD1	1.65	0.61
6:D:50:GLN:HE21	6:D:106:THR:HG21	1.65	0.61
1:Bb:284:LEU:HD23	1:Bb:285:LEU:HB2	1.82	0.61
1:Bj:53:ARG:HH21	1:Bj:246:ARG:HD3	1.65	0.61
8:Ac:44:MET:SD	8:Ac:44:MET:N	2.73	0.61
5:C:217:VAL:HG21	6:D:76:VAL:HG21	1.83	0.61
6:D:106:THR:HG22	6:D:111:PRO:HA	1.83	0.61
8:Aa:332:MET:SD	8:Aa:332:MET:N	2.73	0.61
1:Bf:122:ASP:OD2	1:Bf:180:ARG:NH2	2.30	0.60
8:Ad:108:GLU:HG2	8:Ad:109:LYS:HG3	1.83	0.60
8:Aa:139:ILE:HG23	8:Aa:169:PHE:HD2	1.66	0.60
1:Bb:161:MET:SD	8:Ah:127:ASN:ND2	2.74	0.60
5:C:34:TYR:OH	5:C:117:LYS:NZ	2.34	0.60
7:E:65:MET:HB3	7:E:115:PHE:HA	1.83	0.60
3:A:136:GLU:OE2	4:B:130:LYS:NZ	2.35	0.60
1:Bk:146:GLU:HG3	5:C:176:ARG:HB3	1.84	0.60
4:B:87:ILE:HG22	4:B:89:ALA:H	1.67	0.60
8:Ah:199:TYR:HB2	8:Ah:260:LEU:HB3	1.84	0.59
8:Af:119:ARG:NH1	8:Af:271:ASP:OD2	2.35	0.59
1:Bb:80:LEU:HD21	1:Bb:172:MET:HE3	1.83	0.59
8:Aa:199:TYR:HB2	8:Aa:260:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bj:280:LEU:HD21	1:Bi:268:ILE:HG12	1.83	0.59
1:Ba:73:ILE:HG23	1:Ba:217:LEU:HD22	1.84	0.59
1:Bg:111:GLN:HE22	1:Bg:189:THR:HA	1.67	0.59
1:Bg:122:ASP:OD2	1:Bg:180:ARG:NH1	2.36	0.59
8:Ag:120:ILE:HB	8:Ag:272:ALA:HB3	1.85	0.59
8:Ab:92:SER:HA	8:Ab:95:THR:HG22	1.84	0.59
8:Ah:27:ILE:HD11	8:Ah:32:LEU:HD11	1.85	0.59
8:Ae:199:TYR:HB2	8:Ae:260:LEU:HB3	1.84	0.59
5:C:128:TRP:HB3	5:C:205:PHE:HB2	1.85	0.59
8:Ad:104:ARG:NH1	8:Ad:106:GLU:OE2	2.36	0.59
1:Bj:165:MET:SD	1:Bj:223:ARG:NH2	2.73	0.58
8:Aa:293:ASP:OD1	8:Aa:293:ASP:N	2.36	0.58
8:Ab:187:VAL:HG22	8:Ab:279:VAL:HG12	1.85	0.58
8:Ac:146:ALA:O	8:Ac:168:ARG:NH1	2.37	0.58
1:Bk:114:VAL:HG21	1:Bk:190:ILE:HD11	1.85	0.58
3:A:153:ASN:OD1	3:A:192:THR:OG1	2.20	0.58
8:Af:186:ALA:HB3	8:Af:280:LYS:HB2	1.86	0.58
5:C:143:CYS:O	5:C:182:ASN:ND2	2.35	0.58
8:Ab:193:ASN:ND2	8:Ab:218:LEU:O	2.36	0.58
1:Bb:166:ARG:HE	1:Bb:168:TYR:HE1	1.50	0.58
1:Bk:36:ILE:HD11	1:Bk:42:ASP:HB3	1.86	0.58
1:Bk:222:ASN:HD21	1:Bj:89:ARG:HH21	1.52	0.58
1:Bf:185:GLU:OE1	8:Ac:211:ARG:NH1	2.37	0.58
1:Bf:284:LEU:HD21	1:Be:271:LEU:HG	1.86	0.58
3:A:79:GLN:NE2	3:A:83:ASP:OD1	2.37	0.58
8:Ac:143:GLU:HG2	8:Ac:168:ARG:HG3	1.85	0.58
1:Bh:281:VAL:HG12	1:Bh:286:ARG:HE	1.68	0.57
8:Ac:89:ASN:OD1	8:Ac:92:SER:OG	2.22	0.57
1:Bi:18:VAL:HG13	1:Bi:22:ARG:HH21	1.69	0.57
5:C:139:LEU:HD12	5:C:188:ALA:HB3	1.86	0.57
8:Ae:98:ILE:HD11	8:Ae:133:ILE:HG13	1.86	0.57
1:Bi:97:ALA:HB2	1:Bi:110:ILE:HG21	1.86	0.57
1:Bh:80:LEU:HD21	1:Bh:136:LEU:HD11	1.86	0.57
3:A:94:VAL:HB	3:A:102:ASN:HD22	1.69	0.57
5:C:80:ASP:OD1	5:C:80:ASP:N	2.36	0.57
8:Ae:185:ILE:HG21	8:Ae:200:VAL:HG21	1.85	0.57
8:Ad:170:GLU:OE1	8:Ad:177:ARG:NH2	2.37	0.57
8:Af:203:ARG:HB3	8:Af:255:ALA:HB3	1.87	0.57
8:Aa:51:VAL:HG23	8:Aa:73:SER:HB3	1.87	0.57
1:Bh:80:LEU:HD12	1:Bh:210:ILE:HG23	1.86	0.57
1:Be:170:GLY:H	1:Be:213:GLN:HE22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ah:53:ASP:HB3	8:Ah:56:LYS:HG2	1.87	0.57
2:F:92:SER:HB2	2:F:104:LYS:HB3	1.86	0.57
8:Aa:76:LEU:HD12	8:Aa:100:GLU:HG3	1.85	0.57
8:Af:35:ASP:N	8:Af:46:GLN:O	2.38	0.57
8:Ag:53:ASP:OD2	8:Ag:71:ARG:NH1	2.37	0.56
8:Ae:203:ARG:HH21	8:Ae:257:GLU:HA	1.71	0.56
8:Aa:44:MET:N	8:Aa:44:MET:SD	2.78	0.56
1:Bj:118:VAL:HG13	1:Bj:179:ILE:HD12	1.87	0.56
1:Bi:138:GLY:HA3	1:Bi:171:THR:HG22	1.87	0.56
6:D:54:SER:OG	6:D:55:LYS:N	2.35	0.56
7:E:245:ASN:OD1	7:E:245:ASN:N	2.37	0.56
8:Ae:185:ILE:H	8:Ae:227:TRP:HB3	1.69	0.56
5:C:43:ASP:OD1	5:C:43:ASP:N	2.39	0.56
5:C:122:ARG:HD2	5:C:212:LEU:HB3	1.88	0.56
8:Ag:26:ILE:HG13	8:Ag:281:ILE:HG21	1.88	0.56
8:Ah:98:ILE:HG12	8:Ah:118:VAL:HG12	1.87	0.56
8:Ac:145:MET:SD	8:Ac:145:MET:N	2.79	0.56
8:Ac:179:THR:OG1	8:Ac:252:PRO:O	2.21	0.56
1:Bg:111:GLN:HE21	1:Bg:191:GLU:HG2	1.71	0.56
1:Bd:59:LEU:HB3	1:Bd:231:ILE:HG23	1.87	0.56
1:Bf:73:ILE:HG22	1:Bf:221:GLN:HE21	1.71	0.56
8:Ae:108:GLU:HG2	8:Ae:109:LYS:HG2	1.88	0.56
2:F:80:LEU:HD23	7:E:245:ASN:HD22	1.71	0.56
4:B:125:VAL:HG11	4:B:129:ALA:HB2	1.86	0.56
8:Ag:125:TRP:O	8:Ag:263:ARG:NH2	2.38	0.56
1:Ba:53:ARG:HA	1:Ba:56:ILE:HG22	1.88	0.56
1:Bb:35:ARG:NH2	1:Bb:245:ILE:O	2.39	0.56
6:D:70:MET:HE1	6:D:75:LYS:HA	1.87	0.56
8:Ah:203:ARG:NH2	8:Ah:257:GLU:OE2	2.39	0.56
8:Af:36:ILE:HD12	8:Af:37:ILE:HG13	1.86	0.56
1:Bf:194:ASP:OD2	8:Ad:85:SER:OG	2.24	0.55
4:B:161:VAL:HG12	4:B:174:VAL:HB	1.88	0.55
1:Ba:136:LEU:HD12	1:Ba:172:MET:HG2	1.88	0.55
8:Ab:179:THR:OG1	8:Ab:180:GLY:N	2.39	0.55
1:Be:3:ILE:HG21	1:Be:281:VAL:HG11	1.88	0.55
2:F:121:ASP:OD1	2:F:121:ASP:N	2.39	0.55
1:Bi:111:GLN:NE2	1:Bi:115:SER:OG	2.40	0.55
3:A:171:ILE:HG22	3:A:172:ILE:HG12	1.88	0.55
8:Af:292:ARG:HG3	8:Af:294:PHE:H	1.72	0.55
1:Ba:268:ILE:HG12	1:Bb:284:LEU:HD12	1.88	0.55
1:Bg:237:ASN:HD21	1:Bf:38:ARG:HH22	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:42:THR:HB	7:E:45:GLN:HG2	1.89	0.55
8:Ag:81:VAL:HG13	8:Ag:133:ILE:HG13	1.89	0.55
8:Aa:278:ASP:N	8:Aa:278:ASP:OD1	2.39	0.55
1:Be:26:ASP:OD2	1:Be:260:ASN:ND2	2.40	0.55
8:Ab:240:GLU:OE1	8:Ab:242:ARG:NH2	2.40	0.55
8:Ag:48:ARG:NH2	8:Ag:150:ASP:OD2	2.35	0.55
8:Ad:150:ASP:OD1	8:Ad:150:ASP:N	2.36	0.55
1:Bg:80:LEU:HD11	1:Bg:172:MET:HG3	1.88	0.54
1:Bj:91:ARG:HB2	1:Bj:203:ILE:HG21	1.88	0.54
8:Ag:84:ASN:ND2	8:Ag:86:SER:OG	2.40	0.54
8:Ad:145:MET:HA	8:Ad:168:ARG:HD3	1.88	0.54
1:Bc:123:ARG:O	1:Bc:127:SER:OG	2.25	0.54
8:Ah:303:GLN:O	8:Ah:303:GLN:NE2	2.40	0.54
1:Bk:107:ARG:HG2	1:Bk:191:GLU:HA	1.89	0.54
1:Ba:265:ASN:HA	1:Ba:268:ILE:HB	1.89	0.54
8:Ab:79:TRP:CB	8:Ab:98:ILE:HG21	2.36	0.54
5:C:208:GLU:OE1	5:C:210:LYS:NZ	2.36	0.54
8:Ae:53:ASP:OD2	8:Ae:55:GLY:N	2.37	0.54
8:Aa:110:PHE:CD1	8:Aa:110:PHE:N	2.75	0.54
3:A:90:LEU:HD11	3:A:134:ASP:HB2	1.90	0.54
8:Aa:178:ASN:HB2	8:Aa:286:ALA:HB3	1.89	0.54
8:Ab:321:THR:HG22	8:Ab:325:ARG:HE	1.72	0.54
1:Bb:77:GLU:HG2	1:Bb:214:ARG:HD2	1.89	0.53
8:Aa:118:VAL:HG11	8:Aa:133:ILE:HD13	1.90	0.53
6:D:133:TYR:H	6:D:197:GLU:HG2	1.74	0.53
6:D:87:LEU:HD23	6:D:206:PHE:HD2	1.73	0.53
8:Ah:55:GLY:O	8:Ah:67:LYS:NZ	2.36	0.53
8:Ac:26:ILE:O	8:Ac:174:GLY:N	2.41	0.53
8:Ac:108:GLU:N	8:Ac:108:GLU:OE1	2.40	0.53
1:Bi:34:LEU:HA	1:Bi:247:ASP:HA	1.89	0.53
1:Be:107:ARG:HB3	1:Be:191:GLU:HA	1.88	0.53
8:Ah:125:TRP:HE3	8:Ah:127:ASN:HD21	1.54	0.53
8:Aa:110:PHE:CZ	8:Aa:277:LYS:HG2	2.44	0.53
2:F:50:TYR:N	2:F:66:ILE:O	2.42	0.53
8:Ah:183:LYS:HB3	8:Ah:282:ILE:HB	1.90	0.53
8:Ah:186:ALA:HB3	8:Ah:280:LYS:HB2	1.89	0.53
1:Ba:86:ILE:HG23	1:Ba:117:LEU:HD22	1.91	0.53
2:F:43:ILE:HG13	2:F:52:ILE:HG12	1.90	0.53
3:A:197:ARG:NH1	3:A:201:GLU:OE2	2.41	0.53
1:Bb:184:ASP:HB3	1:Bb:186:LYS:HG3	1.90	0.53
3:A:184:ASN:OD1	3:A:219:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:53:GLU:HG3	4:B:55:PHE:H	1.74	0.53
8:Ag:247:TYR:HH	8:Ag:302:ILE:H	1.52	0.53
8:Af:333:ALA:HB3	8:Ae:284:ASP:HA	1.91	0.53
1:Bd:80:LEU:O	1:Bd:84:THR:OG1	2.27	0.53
1:Bj:121:VAL:HG11	1:Bj:179:ILE:HD11	1.91	0.53
1:Bf:55:GLN:HE22	1:Bf:160:ASN:HD21	1.57	0.53
8:Ae:36:ILE:HG13	8:Ae:37:ILE:HG12	1.90	0.53
1:Bk:86:ILE:HG23	1:Bk:117:LEU:HD22	1.91	0.53
1:Bi:266:THR:HG23	1:Bh:286:ARG:HD3	1.90	0.53
2:F:47:SER:O	2:F:68:LYS:NZ	2.42	0.52
8:Ab:324:LEU:HB3	8:Aa:241:LEU:HD12	1.91	0.52
5:C:76:VAL:HG23	5:C:77:MET:HE2	1.92	0.52
1:Bd:226:LEU:HD13	1:Bc:86:ILE:HG12	1.91	0.52
1:Bc:172:MET:HE1	1:Bc:213:GLN:HG2	1.91	0.52
8:Af:307:GLU:OE1	8:Af:310:ARG:NE	2.40	0.52
8:Ae:28:ASP:HA	8:Ae:278:ASP:HB3	1.91	0.52
1:Bh:122:ASP:OD2	1:Bh:180:ARG:NH2	2.38	0.52
8:Af:170:GLU:HB3	8:Af:175:VAL:HG23	1.90	0.52
8:Ae:287:VAL:HG22	8:Ae:289:THR:H	1.74	0.52
1:Bj:243:SER:O	1:Bj:247:ASP:N	2.41	0.52
1:Bd:279:GLN:HG2	1:Be:262:ILE:HD11	1.91	0.52
1:Bd:284:LEU:HD11	1:Bc:268:ILE:HD12	1.92	0.52
5:C:93:PHE:HB2	5:C:199:VAL:HB	1.91	0.52
8:Ag:227:TRP:HE1	8:Ag:230:PRO:HD3	1.75	0.52
1:Bf:28:GLU:O	1:Bf:32:SER:OG	2.27	0.52
1:Bk:80:LEU:HD21	1:Bk:172:MET:HG3	1.91	0.52
2:F:33:VAL:N	2:F:95:LEU:O	2.42	0.52
8:Ag:110:PHE:HB3	8:Ag:113:GLN:HG3	1.92	0.52
8:Af:247:TYR:OH	8:Af:292:ARG:NH1	2.43	0.52
8:Ae:157:PRO:O	8:Ae:162:LYS:NZ	2.41	0.52
8:Ac:201:LEU:HD11	8:Ac:260:LEU:HB2	1.91	0.52
1:Ba:26:ASP:OD2	1:Ba:260:ASN:ND2	2.43	0.52
7:E:240:ASP:OD1	7:E:240:ASP:N	2.36	0.52
8:Af:79:TRP:HB2	8:Af:98:ILE:HD13	1.92	0.52
8:Ad:183:LYS:HB3	8:Ad:282:ILE:HB	1.92	0.52
1:Bi:35:ARG:N	1:Bi:246:ARG:O	2.43	0.51
5:C:68:ASN:OD1	5:C:85:LYS:NZ	2.43	0.51
1:Bg:64:ALA:O	1:Bg:68:ASN:ND2	2.37	0.51
1:Bg:173:SER:OG	1:Bg:174:ALA:N	2.42	0.51
8:Ab:201:LEU:HD11	8:Ab:260:LEU:HB2	1.91	0.51
8:Af:328:GLU:HA	8:Af:331:LYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:93:LEU:HD22	1:Bg:110:ILE:HD11	1.93	0.51
6:D:220:TYR:HD1	6:D:221:ASP:H	1.56	0.51
8:Af:76:LEU:HD12	8:Af:100:GLU:HG3	1.93	0.51
1:Bb:143:GLU:N	1:Bb:143:GLU:OE2	2.44	0.51
1:Bh:165:MET:SD	1:Bh:223:ARG:NH2	2.82	0.51
8:Ad:53:ASP:HB3	8:Ad:56:LYS:HE3	1.93	0.51
1:Bk:80:LEU:HD22	1:Bk:210:ILE:HG23	1.93	0.51
1:Bj:198:ARG:NH2	1:Bj:202:THR:OG1	2.44	0.51
8:Ah:104:ARG:HE	8:Ah:106:GLU:HB2	1.76	0.51
8:Af:281:ILE:HG12	8:Af:283:TYR:HD2	1.76	0.51
8:Ad:81:VAL:HG22	8:Ad:133:ILE:HG12	1.93	0.51
8:Ab:295:ALA:HB3	8:Ab:298:ASP:HB3	1.93	0.51
8:Aa:178:ASN:HD21	8:Aa:285:LYS:HE2	1.75	0.51
3:A:138:VAL:HA	3:A:141:MET:HE2	1.93	0.51
8:Af:124:GLU:OE1	8:Af:124:GLU:N	2.43	0.51
8:Aa:139:ILE:O	8:Aa:203:ARG:NH2	2.44	0.51
8:Af:219:PHE:HB2	8:Af:223:ARG:HH21	1.75	0.51
1:Bf:166:ARG:NH1	1:Bf:168:TYR:OH	2.44	0.51
1:Be:115:SER:HA	1:Be:187:ILE:HG21	1.92	0.51
8:Ab:219:PHE:CG	8:Ab:223:ARG:HD2	2.46	0.51
8:Af:167:SER:OG	8:Af:168:ARG:N	2.40	0.51
7:E:54:LYS:HE3	7:E:97:ASP:HB2	1.93	0.50
8:Ad:26:ILE:O	8:Ad:174:GLY:N	2.44	0.50
1:Bk:122:ASP:OD2	1:Bk:180:ARG:NH1	2.45	0.50
8:Aa:80:ASP:OD1	8:Aa:80:ASP:N	2.44	0.50
1:Ba:35:ARG:N	1:Ba:246:ARG:O	2.38	0.50
1:Bj:73:ILE:HG21	1:Bj:221:GLN:HB2	1.92	0.50
8:Af:49:ARG:NH2	8:Af:145:MET:SD	2.84	0.50
8:Af:145:MET:HA	8:Af:168:ARG:HB2	1.93	0.50
8:Ad:36:ILE:HB	8:Ad:37:ILE:HD12	1.94	0.50
1:Bc:102:TYR:O	1:Bc:107:ARG:NH2	2.45	0.50
1:Be:73:ILE:HG23	1:Be:217:LEU:HD12	1.92	0.50
8:Ag:185:ILE:HG23	8:Ag:281:ILE:HB	1.94	0.50
8:Ae:59:GLY:O	8:Ae:67:LYS:NZ	2.39	0.50
8:Ad:134:LYS:NZ	8:Ad:135:PRO:O	2.44	0.50
8:Ad:179:THR:HG21	8:Ad:254:VAL:H	1.76	0.50
1:Bg:103:SER:OG	1:Bg:104:ALA:N	2.45	0.50
3:A:181:GLU:HA	3:A:184:ASN:HB2	1.93	0.50
4:B:132:ALA:HA	4:B:227:VAL:HA	1.94	0.50
8:Ae:178:ASN:HB3	8:Ae:285:LYS:HG2	1.94	0.50
8:Ac:179:THR:HG21	8:Ac:254:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:34:TYR:HE1	7:E:50:VAL:HG13	1.76	0.50
4:B:58:GLU:OE2	5:C:141:ARG:NH2	2.43	0.50
8:Af:157:PRO:O	8:Af:162:LYS:NZ	2.39	0.50
8:Ac:49:ARG:O	8:Ac:168:ARG:NH2	2.45	0.50
8:Aa:82:GLU:N	8:Aa:82:GLU:OE1	2.45	0.50
1:Ba:23:ILE:HD11	1:Ba:261:GLN:HA	1.94	0.50
5:C:133:TYR:HE1	5:C:156:ASN:HD22	1.60	0.50
7:E:39:GLY:O	7:E:130:LYS:NZ	2.44	0.50
8:Ad:90:PRO:HA	8:Ad:93:VAL:HG12	1.93	0.50
8:Aa:95:THR:OG1	8:Aa:119:ARG:NH1	2.45	0.50
5:C:33:THR:HG21	6:D:32:GLN:HA	1.94	0.49
8:Ag:27:ILE:HD11	8:Ag:32:LEU:HD11	1.93	0.49
1:Ba:107:ARG:HB3	1:Ba:191:GLU:HA	1.94	0.49
1:Bd:157:ILE:HD12	1:Bd:227:THR:HG21	1.94	0.49
1:Bk:73:ILE:HG21	1:Bk:221:GLN:HB2	1.93	0.49
1:Bk:102:TYR:HB2	1:Bk:107:ARG:HH21	1.77	0.49
1:Bh:207:LEU:HA	1:Bh:210:ILE:HD12	1.94	0.49
2:F:40:ILE:HD11	2:F:91:LEU:HD13	1.95	0.49
1:Bc:87:MET:HE2	1:Bc:177:LEU:HD13	1.94	0.49
8:Ab:326:PHE:HA	8:Ab:329:GLN:HG2	1.93	0.49
8:Ah:203:ARG:NH1	8:Ah:207:ASN:OD1	2.46	0.49
8:Af:344:SER:CB	8:Ae:110:PHE:H	2.25	0.49
8:Ac:185:ILE:HG23	8:Ac:281:ILE:HB	1.94	0.49
1:Bi:156:HIS:HA	1:Bi:164:ARG:HB3	1.94	0.49
3:A:106:ASP:OD1	3:A:106:ASP:N	2.44	0.49
6:D:113:GLU:HB3	6:D:185:THR:HB	1.94	0.49
1:Ba:198:ARG:NH1	4:B:212:GLU:HG2	2.27	0.49
1:Bi:91:ARG:HB2	1:Bi:203:ILE:HG21	1.94	0.49
2:F:102:ARG:HH22	7:E:237:ARG:HB3	1.76	0.49
7:E:197:SER:O	7:E:197:SER:OG	2.28	0.49
8:Ag:204:ASP:OD1	8:Ag:204:ASP:N	2.37	0.49
8:Ae:187:VAL:HG22	8:Ae:279:VAL:HG22	1.93	0.49
8:Ac:53:ASP:O	8:Ac:56:LYS:NZ	2.45	0.49
1:Ba:77:GLU:OE2	1:Ba:214:ARG:NH2	2.46	0.49
1:Bk:165:MET:SD	1:Bk:223:ARG:NH1	2.85	0.49
4:B:100:VAL:HG23	4:B:223:ASP:HB2	1.95	0.49
4:B:145:MET:HB2	4:B:207:VAL:HG22	1.94	0.49
6:D:38:THR:HG22	6:D:40:ASP:H	1.78	0.49
8:Aa:198:LEU:HD11	8:Aa:276:PHE:HE2	1.77	0.49
8:Af:37:ILE:O	8:Af:45:THR:N	2.44	0.49
3:A:141:MET:HE1	4:B:47:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ah:84:ASN:ND2	8:Ah:86:SER:OG	2.45	0.49
8:Ac:37:ILE:O	8:Ac:45:THR:OG1	2.31	0.49
8:Af:143:GLU:O	8:Af:167:SER:OG	2.30	0.48
8:Aa:75:ALA:HB3	8:Aa:78:GLN:HG2	1.94	0.48
8:Ad:81:VAL:HG23	8:Ad:98:ILE:HD11	1.94	0.48
8:Ac:64:ASP:HA	8:Ac:67:LYS:HG3	1.94	0.48
1:Bg:285:LEU:HB3	1:Bg:286:ARG:HD3	1.95	0.48
1:Bf:205:GLU:HA	1:Bf:208:LYS:HD2	1.95	0.48
4:B:76:LEU:HD23	4:B:101:LEU:HA	1.95	0.48
8:Ad:187:VAL:HG22	8:Ad:279:VAL:HG22	1.94	0.48
1:Bh:216:ASP:HA	1:Bg:112:VAL:HG11	1.95	0.48
7:E:61:TRP:HA	7:E:119:ALA:HA	1.95	0.48
7:E:180:ASN:HD21	7:E:184:LYS:HB2	1.78	0.48
1:Ba:265:ASN:HB3	1:Bb:280:LEU:HD21	1.96	0.48
1:Be:198:ARG:NH1	8:Ae:88:GLN:O	2.47	0.48
8:Ag:48:ARG:NE	8:Ag:148:VAL:O	2.46	0.48
8:Ad:328:GLU:HA	8:Ad:331:LYS:HB2	1.95	0.48
8:Af:84:ASN:ND2	8:Af:86:SER:OG	2.46	0.48
1:Bi:77:GLU:HA	1:Bi:80:LEU:HD23	1.95	0.48
1:Bg:144:THR:OG1	1:Bg:147:ASN:OD1	2.28	0.48
8:Ab:303:GLN:HA	8:Ab:306:ARG:HG3	1.95	0.48
1:Bb:213:GLN:HE21	1:Bb:217:LEU:HG	1.79	0.48
1:Bi:260:ASN:O	1:Bi:264:SER:N	2.47	0.48
1:Bh:183:GLY:HA3	8:Aa:230:PRO:HG2	1.95	0.48
3:A:90:LEU:HD12	3:A:130:VAL:HA	1.96	0.48
8:Ab:97:THR:OG1	8:Ab:98:ILE:N	2.47	0.48
1:Bi:71:ASN:O	1:Bi:75:VAL:HG12	2.14	0.48
6:D:81:ALA:C	6:D:83:ASN:N	2.70	0.48
8:Ae:58:ALA:HB3	8:Ae:323:VAL:HG11	1.95	0.48
1:Ba:78:ALA:HB2	1:Bb:237:ASN:HD22	1.79	0.47
1:Bf:223:ARG:O	1:Bf:227:THR:OG1	2.27	0.47
2:F:91:LEU:HG	2:F:103:ILE:HD11	1.95	0.47
8:Ab:76:LEU:HD12	8:Ab:100:GLU:HG2	1.96	0.47
8:Ad:38:ALA:HA	8:Ad:44:MET:HA	1.96	0.47
1:Bc:156:HIS:HA	1:Bc:164:ARG:HB3	1.96	0.47
1:Bi:126:SER:O	1:Bi:134:ASN:ND2	2.48	0.47
8:Ae:245:PRO:O	8:Ae:249:THR:OG1	2.28	0.47
8:Aa:310:ARG:HG2	8:Aa:314:GLU:HG2	1.96	0.47
1:Bc:107:ARG:HB3	1:Bc:191:GLU:HA	1.97	0.47
1:Bj:35:ARG:N	1:Bj:246:ARG:O	2.29	0.47
8:Ab:195:PRO:HG3	8:Ab:218:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ah:201:LEU:HB3	8:Ah:257:GLU:HB3	1.95	0.47
8:Ae:167:SER:OG	8:Ae:168:ARG:N	2.47	0.47
8:Ae:199:TYR:HE2	8:Ae:211:ARG:HD3	1.78	0.47
8:Ac:104:ARG:H	8:Ac:104:ARG:HD2	1.79	0.47
1:Bd:27:ILE:O	1:Bd:31:SER:OG	2.29	0.47
1:Bj:36:ILE:HG21	1:Bj:46:LEU:HD13	1.95	0.47
6:D:127:VAL:HG21	6:D:163:MET:HE2	1.96	0.47
8:Ah:298:ASP:OD1	8:Ah:298:ASP:N	2.40	0.47
1:Bk:103:SER:OG	1:Bk:104:ALA:N	2.48	0.47
8:Ae:179:THR:HG22	8:Ae:283:TYR:HD2	1.79	0.47
1:Bk:56:ILE:HD11	1:Bk:238:LEU:HB3	1.96	0.47
1:Bk:227:THR:O	1:Bk:231:ILE:HD12	2.15	0.47
1:Bg:261:GLN:O	1:Bg:265:ASN:ND2	2.47	0.47
1:Bf:256:GLU:O	1:Bf:260:ASN:ND2	2.48	0.47
5:C:103:VAL:HB	5:C:189:PHE:HB2	1.97	0.47
6:D:30:ASN:HD22	6:D:216:TYR:HA	1.80	0.47
8:Ab:179:THR:HG21	8:Ab:254:VAL:HG13	1.96	0.47
8:Af:43:LYS:HE3	8:Af:43:LYS:HB3	1.67	0.47
8:Af:48:ARG:HH12	8:Af:150:ASP:HA	1.80	0.47
8:Af:63:THR:HG22	8:Af:65:GLU:H	1.79	0.47
8:Af:335:GLU:HG2	8:Af:336:GLU:HG2	1.96	0.47
8:Ae:76:LEU:HD22	8:Ae:116:MET:HB2	1.96	0.47
8:Ae:98:ILE:HG12	8:Ae:118:VAL:HG12	1.96	0.47
1:Bb:59:LEU:HB3	1:Bb:231:ILE:HG23	1.97	0.47
1:Bj:244:ARG:HH11	1:Bi:67:SER:HB3	1.80	0.47
8:Ab:52:MET:HG2	8:Ab:169:PHE:HZ	1.78	0.47
8:Ab:275:TYR:C	8:Ab:276:PHE:CD1	2.93	0.47
8:Ab:288:LEU:HB3	8:Ab:290:THR:HG23	1.97	0.47
8:Af:333:ALA:HB1	8:Ae:22:GLU:HG2	1.97	0.47
8:Aa:129:ALA:HB3	8:Aa:263:ARG:HB3	1.96	0.47
4:B:129:ALA:HB3	4:B:200:LEU:HD21	1.95	0.47
5:C:218:ASP:N	5:C:218:ASP:OD1	2.47	0.47
8:Aa:30:ALA:O	8:Aa:33:ASN:ND2	2.48	0.47
1:Ba:102:TYR:HB3	1:Ba:106:ASP:HB2	1.98	0.46
1:Be:154:TRP:HB3	1:Be:164:ARG:HB3	1.95	0.46
5:C:74:VAL:HG13	5:C:76:VAL:H	1.80	0.46
6:D:62:PRO:HB3	6:D:91:PHE:HB3	1.95	0.46
1:Ba:118:VAL:HG21	1:Ba:187:ILE:HG23	1.96	0.46
1:Be:45:GLY:HA2	1:Be:48:VAL:HB	1.97	0.46
2:F:94:TYR:HB2	2:F:102:ARG:HB2	1.96	0.46
8:Af:83:LEU:HD13	8:Af:131:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ae:74:LEU:HD13	8:Ae:169:PHE:HE2	1.80	0.46
1:Bj:86:ILE:HG21	1:Bj:121:VAL:HG23	1.97	0.46
1:Be:43:ALA:O	1:Be:45:GLY:N	2.48	0.46
8:Af:141:ALA:HA	8:Af:175:VAL:HG11	1.97	0.46
1:Bd:55:GLN:HE21	1:Bd:238:LEU:HD21	1.79	0.46
1:Bi:74:GLN:HE21	1:Bi:221:GLN:HE21	1.62	0.46
6:D:89:LEU:HB2	6:D:204:ILE:HG22	1.97	0.46
8:Ag:49:ARG:O	8:Ag:168:ARG:NH1	2.48	0.46
8:Ae:53:ASP:OD2	8:Ae:54:TYR:N	2.49	0.46
1:Bk:52:MET:HG2	1:Bk:242:GLU:HB2	1.97	0.46
8:Ah:104:ARG:HG3	8:Ah:106:GLU:H	1.80	0.46
8:Ae:177:ARG:HB3	8:Ae:251:LEU:HD23	1.96	0.46
1:Ba:143:GLU:OE1	4:B:155:LYS:NZ	2.44	0.46
1:Bb:190:ILE:HG22	1:Bb:196:ALA:HA	1.98	0.46
1:Bk:190:ILE:HG22	1:Bk:196:ALA:HA	1.98	0.46
1:Bf:135:MET:HA	1:Bf:140:PHE:HE2	1.81	0.46
3:A:204:MET:O	3:A:208:ASN:HB2	2.16	0.46
8:Ag:46:GLN:OE1	8:Ag:73:SER:N	2.48	0.46
8:Ae:38:ALA:HA	8:Ae:44:MET:HA	1.98	0.46
8:Aa:47:ASN:OD1	8:Aa:49:ARG:N	2.48	0.46
1:Bj:172:MET:HB2	1:Bj:172:MET:HE2	1.81	0.46
1:Bi:147:ASN:HD21	1:Bi:171:THR:HG21	1.81	0.46
2:F:89:PRO:HG2	2:F:115:ILE:HG21	1.98	0.46
7:E:121:LYS:HD3	7:E:121:LYS:HA	1.82	0.46
8:Ad:332:MET:HE3	8:Ad:332:MET:HA	1.97	0.46
8:Ac:48:ARG:NH2	8:Ac:150:ASP:OD1	2.49	0.46
1:Be:93:LEU:HD12	1:Be:110:ILE:HG23	1.96	0.46
6:D:126:TRP:HD1	6:D:208:GLU:HB3	1.80	0.46
8:Ab:275:TYR:O	8:Ab:276:PHE:CD1	2.69	0.46
8:Ae:34:ALA:HB1	8:Ae:44:MET:HB2	1.97	0.46
8:Aa:49:ARG:NH1	8:Aa:168:ARG:HG2	2.30	0.46
8:Aa:83:LEU:O	8:Aa:88:GLN:NE2	2.49	0.46
8:Aa:200:VAL:HG11	8:Aa:279:VAL:HG11	1.98	0.46
1:Bh:103:SER:OG	1:Bh:106:ASP:OD2	2.34	0.45
4:B:235:ASP:OD1	4:B:235:ASP:N	2.49	0.45
1:Bk:163:GLN:NE2	1:Bj:127:SER:OG	2.49	0.45
6:D:152:LEU:HG	6:D:163:MET:HE3	1.98	0.45
8:Ag:182:ILE:HD12	8:Ag:281:ILE:HD11	1.98	0.45
8:Ah:321:THR:HG22	8:Ah:325:ARG:HE	1.81	0.45
8:Ae:79:TRP:CD1	8:Ae:135:PRO:HA	2.51	0.45
8:Ad:129:ALA:HB3	8:Ad:263:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bh:61:GLN:NE2	1:Bh:65:ASN:OD1	2.49	0.45
7:E:46:ARG:NH1	7:E:235:ASP:OD2	2.49	0.45
8:Ah:36:ILE:HD11	8:Ah:51:VAL:HG21	1.98	0.45
8:Ad:37:ILE:HD12	8:Ad:37:ILE:H	1.82	0.45
1:Bg:146:GLU:N	1:Bg:146:GLU:OE2	2.50	0.45
8:Ah:26:ILE:HB	8:Ah:279:VAL:HB	1.98	0.45
8:Ae:179:THR:OG1	8:Ae:252:PRO:O	2.24	0.45
1:Ba:141:ALA:HB3	1:Ba:149:VAL:HG12	1.98	0.45
1:Bk:284:LEU:HA	1:Bj:272:ALA:HB2	1.98	0.45
1:Bh:282:MET:SD	1:Bh:286:ARG:NH2	2.83	0.45
8:Ag:293:ASP:OD1	8:Ag:293:ASP:N	2.49	0.45
8:Ae:153:ASN:ND2	8:Ae:155:GLN:OE1	2.49	0.45
8:Aa:26:ILE:HD11	8:Aa:281:ILE:HD12	1.98	0.45
3:A:148:GLY:HA2	3:A:189:LEU:HD11	1.98	0.45
8:Ab:238:SER:O	8:Ab:238:SER:OG	2.23	0.45
8:Ac:296:ASP:HA	8:Ac:300:TRP:HD1	1.82	0.45
3:A:153:ASN:HD22	3:A:153:ASN:HA	1.57	0.45
8:Af:37:ILE:HD12	8:Af:46:GLN:HG3	1.99	0.45
8:Ae:124:GLU:N	8:Ae:124:GLU:OE1	2.49	0.45
1:Ba:133:MET:SD	1:Ba:139:ARG:NH2	2.89	0.45
1:Bc:278:SER:O	1:Bc:278:SER:OG	2.35	0.45
1:Bg:254:MET:HE1	1:Bf:275:ASN:HD22	1.82	0.45
1:Bf:118:VAL:HG21	1:Bf:187:ILE:HG23	1.99	0.45
5:C:31:TYR:HD1	5:C:212:LEU:HG	1.82	0.45
8:Ae:26:ILE:O	8:Ae:174:GLY:N	2.49	0.45
8:Ad:195:PRO:HB2	8:Ad:267:HIS:CD2	2.52	0.45
8:Aa:33:ASN:H	8:Aa:47:ASN:HD22	1.64	0.45
1:Ba:262:ILE:O	1:Ba:266:THR:OG1	2.26	0.45
1:Bi:35:ARG:NH2	1:Bi:245:ILE:O	2.50	0.45
1:Bf:1:MET:HE2	1:Bf:281:VAL:HG22	1.98	0.45
1:Bf:204:ASP:O	1:Bf:208:LYS:HG3	2.17	0.45
1:Bh:249:ASP:HB3	1:Bh:252:LYS:HB3	1.99	0.44
2:F:36:VAL:HG23	2:F:93:PHE:HB2	1.98	0.44
1:Ba:99:ASN:O	1:Ba:107:ARG:NH2	2.49	0.44
1:Bh:23:ILE:HA	1:Bh:26:ASP:HB2	1.98	0.44
1:Be:250:MET:HE3	1:Be:250:MET:HB2	1.90	0.44
8:Ab:167:SER:N	8:Ab:170:GLU:OE1	2.47	0.44
8:Ab:201:LEU:HD21	8:Ab:260:LEU:HD22	1.99	0.44
8:Ae:119:ARG:NH1	8:Ae:271:ASP:OD2	2.50	0.44
1:Bi:142:ARG:HD3	1:Bi:168:TYR:CD2	2.52	0.44
8:Ab:49:ARG:HG2	8:Ab:173:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ag:140:PRO:HB3	8:Ag:311:LYS:HE2	1.99	0.44
1:Be:22:ARG:HH22	1:Be:263:LEU:HD22	1.83	0.44
3:A:63:GLN:O	3:A:67:GLU:HG3	2.18	0.44
3:A:159:VAL:HG21	3:A:193:VAL:HG22	1.99	0.44
8:Af:340:PRO:C	8:Af:342:GLU:N	2.59	0.44
8:Ac:317:LYS:HB3	8:Ac:317:LYS:HE2	1.60	0.44
8:Aa:314:GLU:O	8:Aa:318:PHE:HB2	2.17	0.44
1:Bh:154:TRP:CE3	1:Bh:164:ARG:HD2	2.53	0.44
8:Ad:223:ARG:HE	8:Ad:223:ARG:HB3	1.60	0.44
8:Aa:54:TYR:HE1	8:Aa:72:THR:HG22	1.83	0.44
1:Bd:270:MET:HE2	1:Bd:270:MET:HB3	1.66	0.44
1:Bc:62:ALA:HB1	1:Bc:158:GLY:H	1.82	0.44
1:Be:138:GLY:HA3	1:Be:171:THR:HG23	2.00	0.44
3:A:145:LYS:HB2	3:A:181:GLU:HG3	1.99	0.44
8:Ae:170:GLU:OE2	8:Ae:177:ARG:N	2.50	0.44
8:Ac:201:LEU:HB2	8:Ac:257:GLU:HB3	2.00	0.44
8:Aa:281:ILE:HG12	8:Aa:283:TYR:CD1	2.51	0.44
1:Bc:71:ASN:OD1	1:Bc:71:ASN:N	2.51	0.44
1:Bj:224:MET:HE2	1:Bj:224:MET:HB2	1.95	0.44
2:F:94:TYR:HE2	2:F:104:LYS:HB2	1.83	0.44
3:A:219:ARG:O	3:A:223:VAL:HG23	2.18	0.44
8:Ag:145:MET:HB2	8:Ag:161:ASP:HB3	2.00	0.44
8:Ag:201:LEU:HB3	8:Ag:257:GLU:HB3	1.99	0.44
8:Ae:318:PHE:CE1	8:Ae:322:GLN:HG3	2.53	0.44
8:Aa:132:LYS:HE3	8:Aa:201:LEU:HD12	1.99	0.44
7:E:80:ASN:ND2	7:E:97:ASP:O	2.50	0.44
8:Ae:278:ASP:N	8:Ae:278:ASP:OD1	2.49	0.44
4:B:118:HIS:CE1	4:B:156:ARG:HH22	2.36	0.44
8:Ag:177:ARG:HH11	8:Ag:251:LEU:HD23	1.82	0.44
8:Ah:313:ILE:HD13	8:Ah:313:ILE:HA	1.88	0.44
8:Af:247:TYR:HB2	8:Af:248:PRO:HD3	2.00	0.44
8:Ad:335:GLU:OE1	8:Ad:335:GLU:N	2.50	0.44
1:Bg:56:ILE:H	1:Bg:56:ILE:HG13	1.66	0.43
4:B:172:MET:HB3	4:B:172:MET:HE2	1.69	0.43
5:C:200:ASP:OD1	5:C:200:ASP:N	2.50	0.43
7:E:65:MET:HE2	7:E:72:VAL:HG23	2.00	0.43
1:Bd:108:MET:HE2	1:Bd:108:MET:HA	2.00	0.43
1:Bd:282:MET:HE2	1:Bd:286:ARG:HE	1.81	0.43
1:Be:284:LEU:HD23	1:Be:285:LEU:HG	2.00	0.43
3:A:46:LEU:HD23	3:A:46:LEU:HA	1.87	0.43
6:D:84:ALA:C	6:D:85:LYS:HG3	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ad:70:MET:C	8:Ad:71:ARG:HH11	2.26	0.43
1:Bc:262:ILE:HD13	1:Bc:262:ILE:HA	1.92	0.43
1:Bi:268:ILE:H	1:Bi:268:ILE:HD12	1.83	0.43
4:B:166:HIS:CE1	4:B:172:MET:HE1	2.53	0.43
6:D:49:TYR:HD2	6:D:103:VAL:HG12	1.83	0.43
7:E:148:ILE:HD11	7:E:206:ARG:HB2	2.01	0.43
8:Ae:60:ALA:HB3	8:Ad:221:GLY:HA3	2.00	0.43
8:Ad:157:PRO:HB2	8:Ad:162:LYS:HE3	2.00	0.43
1:Bc:138:GLY:HA3	1:Bc:171:THR:HG22	1.99	0.43
8:Ad:331:LYS:NZ	8:Ac:287:VAL:HA	2.34	0.43
8:Aa:58:ALA:HA	8:Aa:61:SER:HB2	1.98	0.43
1:Bh:62:ALA:HB1	1:Bh:158:GLY:H	1.84	0.43
4:B:53:GLU:CD	4:B:61:TRP:HE1	2.27	0.43
8:Af:170:GLU:OE1	8:Af:171:ASP:N	2.51	0.43
8:Ac:311:LYS:HB2	8:Ac:311:LYS:HE3	1.70	0.43
8:Aa:123:PRO:O	8:Aa:263:ARG:NH2	2.50	0.43
1:Bd:135:MET:HE2	1:Bd:135:MET:HB3	1.89	0.43
8:Ag:79:TRP:HB2	8:Ag:98:ILE:HD13	2.01	0.43
8:Aa:98:ILE:HD11	8:Aa:116:MET:HB2	1.99	0.43
8:Aa:224:GLU:OE1	8:Aa:280:LYS:HE3	2.18	0.43
1:Bk:154:TRP:HB3	1:Bk:164:ARG:HD2	2.01	0.43
1:Bg:73:ILE:HG13	1:Bg:217:LEU:HB3	2.00	0.43
8:Af:54:TYR:CE1	8:Af:70:MET:HE2	2.54	0.43
1:Bb:276:ASN:OD1	1:Bb:276:ASN:N	2.52	0.43
1:Bf:154:TRP:CZ2	1:Bf:166:ARG:HD2	2.54	0.43
3:A:90:LEU:HD13	3:A:133:THR:HB	2.00	0.43
8:Ag:55:GLY:O	8:Ag:67:LYS:NZ	2.47	0.43
8:Ac:121:LEU:HD23	8:Ac:121:LEU:HA	1.87	0.43
3:A:85:LEU:HA	3:A:88:VAL:HG23	2.01	0.42
8:Ad:49:ARG:NH1	8:Ad:168:ARG:HG3	2.34	0.42
1:Bk:70:ILE:HD13	1:Bk:70:ILE:HA	1.83	0.42
1:Be:153:MET:HB2	1:Be:153:MET:HE2	1.72	0.42
6:D:43:ASP:OD1	6:D:43:ASP:N	2.40	0.42
7:E:58:GLU:HG2	8:Aa:327:LEU:HD21	2.01	0.42
8:Ag:25:ILE:HG21	8:Ag:278:ASP:HB2	2.00	0.42
8:Ag:143:GLU:O	8:Ag:167:SER:OG	2.28	0.42
1:Bb:87:MET:HE2	1:Bb:87:MET:HB2	1.68	0.42
1:Bj:119:ALA:O	1:Bj:123:ARG:N	2.49	0.42
1:Bj:142:ARG:HG3	1:Bj:168:TYR:CE2	2.54	0.42
1:Bi:249:ASP:OD1	1:Bi:251:ALA:N	2.52	0.42
1:Bh:270:MET:HE1	1:Bg:27:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Aa:39:ASP:OD1	8:Aa:40:PRO:HD2	2.19	0.42
1:Bk:12:ALA:HB3	1:Bk:271:LEU:HD13	2.01	0.42
1:Bh:71:ASN:OD1	1:Bh:71:ASN:N	2.48	0.42
1:Bg:87:MET:HG3	1:Bg:203:ILE:HG23	2.01	0.42
1:Bg:187:ILE:HD12	1:Bg:187:ILE:HA	1.84	0.42
7:E:70:GLY:HA2	7:E:108:TYR:CZ	2.54	0.42
8:Ag:327:LEU:HD13	8:Ag:327:LEU:HA	1.94	0.42
1:Bk:35:ARG:N	1:Bk:246:ARG:O	2.46	0.42
1:Bk:153:MET:HG2	1:Bk:167:VAL:HG12	2.00	0.42
7:E:148:ILE:HG12	7:E:158:GLU:HG2	2.01	0.42
7:E:185:THR:HG22	7:E:188:ILE:HD11	2.00	0.42
8:Ag:186:ALA:HB1	8:Ag:224:GLU:HG3	2.02	0.42
8:Af:120:ILE:HB	8:Af:272:ALA:HB3	2.02	0.42
8:Af:344:SER:C	8:Ae:109:LYS:NZ	2.78	0.42
1:Bd:19:THR:O	1:Bd:23:ILE:HG13	2.19	0.42
1:Bb:174:ALA:HB3	1:Bb:180:ARG:HE	1.85	0.42
1:Bb:233:ILE:HD13	1:Bb:233:ILE:HA	1.89	0.42
1:Bi:135:MET:HG2	1:Bi:136:LEU:HD22	2.00	0.42
1:Bg:102:TYR:O	1:Bg:107:ARG:NH2	2.53	0.42
5:C:62:PRO:HB3	5:C:91:PHE:HB3	2.00	0.42
8:Af:200:VAL:HG23	8:Af:214:MET:HE1	2.02	0.42
8:Ad:81:VAL:HG11	8:Ad:120:ILE:HG13	2.00	0.42
1:Bi:48:VAL:HG22	1:Bi:52:MET:HE3	2.01	0.42
1:Bf:55:GLN:HE22	1:Bf:160:ASN:ND2	2.16	0.42
8:Af:120:ILE:O	8:Af:272:ALA:N	2.53	0.42
1:Bk:221:GLN:HA	1:Bk:224:MET:HB2	2.01	0.42
8:Ag:47:ASN:OD1	8:Ag:48:ARG:N	2.53	0.42
8:Aa:104:ARG:HD2	8:Aa:106:GLU:HB2	2.01	0.42
1:Ba:247:ASP:OD1	1:Ba:247:ASP:N	2.53	0.42
1:Bb:35:ARG:N	1:Bb:246:ARG:O	2.39	0.42
1:Be:160:ASN:HB2	1:Be:163:GLN:HE21	1.85	0.42
5:C:70:MET:HE3	5:C:74:VAL:HG23	2.02	0.42
7:E:87:ILE:HB	7:E:90:GLU:HB2	2.02	0.42
8:Ag:76:LEU:HB2	8:Ag:100:GLU:HG3	2.02	0.42
8:Aa:298:ASP:OD1	8:Aa:298:ASP:N	2.49	0.42
1:Bj:244:ARG:HH12	1:Bi:71:ASN:HD21	1.68	0.41
1:Bf:223:ARG:HG3	1:Be:117:LEU:HD23	2.01	0.41
8:Af:49:ARG:HH12	8:Af:169:PHE:H	1.67	0.41
1:Bg:76:ALA:HB2	1:Bg:135:MET:SD	2.59	0.41
1:Bf:37:ASN:OD1	1:Bf:37:ASN:N	2.53	0.41
3:A:210:PHE:HD1	3:A:210:PHE:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ab:275:TYR:C	8:Ab:276:PHE:CG	2.98	0.41
1:Bi:209:LYS:HE3	1:Bi:209:LYS:HB2	1.89	0.41
3:A:170:ASP:OD2	3:A:209:ASN:ND2	2.54	0.41
8:Ab:304:GLU:O	8:Ab:308:THR:OG1	2.34	0.41
8:Ae:36:ILE:HD12	8:Ae:37:ILE:H	1.85	0.41
1:Bk:2:ILE:HD13	1:Bk:2:ILE:HA	1.88	0.41
1:Bf:42:ASP:OD1	1:Bf:45:GLY:N	2.45	0.41
1:Be:282:MET:HA	1:Be:282:MET:HE2	2.01	0.41
8:Ab:311:LYS:O	8:Ab:315:VAL:HG22	2.19	0.41
8:Ag:186:ALA:O	8:Ag:280:LYS:N	2.52	0.41
8:Ae:76:LEU:HD12	8:Ae:100:GLU:HG3	2.02	0.41
8:Ac:219:PHE:CG	8:Ac:223:ARG:HD2	2.56	0.41
8:Aa:214:MET:HE3	8:Aa:214:MET:HB3	1.80	0.41
1:Bc:207:LEU:HD23	1:Bc:207:LEU:HA	1.91	0.41
4:B:202:ILE:HG21	4:B:225:LEU:HD21	2.03	0.41
5:C:30:ASN:HD22	5:C:30:ASN:C	2.29	0.41
8:Ab:28:ASP:C	8:Ab:30:ALA:H	2.28	0.41
8:Ab:83:LEU:HD13	8:Ab:131:ALA:HB2	2.02	0.41
8:Ag:37:ILE:HD13	8:Ag:37:ILE:HA	1.87	0.41
8:Ag:157:PRO:O	8:Ag:162:LYS:NZ	2.53	0.41
8:Ae:69:LEU:HD23	8:Ae:69:LEU:HA	1.91	0.41
8:Aa:64:ASP:OD1	8:Aa:64:ASP:N	2.43	0.41
1:Ba:27:ILE:HD13	1:Ba:27:ILE:HA	1.90	0.41
1:Ba:117:LEU:HD23	1:Ba:117:LEU:HA	1.94	0.41
1:Ba:172:MET:HE2	1:Ba:172:MET:HB2	1.79	0.41
1:Bk:161:MET:HG2	1:Bk:162:ASP:OD2	2.21	0.41
1:Bg:111:GLN:NE2	1:Bg:191:GLU:HG2	2.36	0.41
6:D:76:VAL:HG13	6:D:77:MET:HG3	2.03	0.41
8:Ag:144:LYS:HA	8:Ag:144:LYS:HE3	2.03	0.41
8:Ag:315:VAL:O	8:Ag:319:GLY:N	2.43	0.41
8:Ah:145:MET:HA	8:Ah:168:ARG:HB2	2.03	0.41
8:Af:325:ARG:HH22	8:Ae:237:LYS:HE3	1.86	0.41
8:Ae:169:PHE:O	8:Ae:174:GLY:N	2.53	0.41
8:Ad:62:TYR:CE1	8:Ad:327:LEU:HD11	2.55	0.41
1:Bk:77:GLU:HG3	1:Bk:214:ARG:HD2	2.01	0.41
8:Af:68:ALA:HA	8:Af:71:ARG:HH21	1.84	0.41
8:Ae:179:THR:HG21	8:Ae:254:VAL:HG22	2.03	0.41
8:Aa:144:LYS:HE3	8:Aa:144:LYS:HA	2.03	0.41
8:Aa:248:PRO:O	8:Aa:306:ARG:NH2	2.43	0.41
1:Bb:238:LEU:HD23	1:Bb:238:LEU:HA	1.93	0.41
1:Bj:244:ARG:NH1	1:Bi:71:ASN:HD21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:GLU:O	2:F:138:LYS:NZ	2.40	0.41
2:F:82:LEU:HD21	2:F:109:ARG:HG3	2.03	0.41
3:A:136:GLU:HA	3:A:137:PRO:HD3	1.92	0.41
8:Aa:188:ASN:HB2	8:Aa:277:LYS:HB3	2.01	0.41
1:Bd:282:MET:HE3	1:Bd:282:MET:HA	2.02	0.41
1:Bk:93:LEU:HD13	1:Bk:114:VAL:HG23	2.02	0.41
1:Be:265:ASN:HA	1:Be:268:ILE:HD12	2.03	0.41
4:B:159:LEU:HD11	4:B:176:ILE:HD13	2.02	0.41
8:Ah:188:ASN:OD1	8:Ah:188:ASN:N	2.52	0.41
8:Af:146:ALA:HA	8:Af:157:PRO:HB3	2.02	0.41
8:Aa:311:LYS:HE3	8:Aa:311:LYS:HB3	1.90	0.41
1:Bi:70:ILE:H	1:Bi:70:ILE:HG13	1.70	0.41
1:Bi:93:LEU:HD12	1:Bi:114:VAL:HG23	2.02	0.41
1:Bg:86:ILE:H	1:Bg:86:ILE:HG13	1.68	0.41
2:F:56:ARG:HH11	2:F:138:LYS:HB2	1.86	0.41
6:D:176:ARG:HH12	7:E:181:ALA:H	1.69	0.41
8:Ab:84:ASN:N	8:Ab:130:ASN:O	2.54	0.41
8:Ah:346:LYS:HD2	8:Ah:346:LYS:HA	1.91	0.41
8:Af:324:LEU:HD11	8:Ae:243:LEU:HB3	2.03	0.41
8:Aa:188:ASN:OD1	8:Aa:188:ASN:N	2.51	0.41
8:Aa:304:GLU:HA	8:Aa:307:GLU:HB2	2.01	0.41
8:Aa:329:GLN:HB3	8:Aa:330:GLU:H	1.69	0.41
1:Bi:121:VAL:HG11	1:Bi:179:ILE:HD11	2.02	0.40
1:Bi:231:ILE:O	1:Bi:235:ALA:N	2.47	0.40
1:Bg:79:PHE:HB3	1:Bg:124:ILE:HG23	2.02	0.40
1:Be:66:ALA:HB2	1:Be:157:ILE:HG22	2.02	0.40
5:C:75:LYS:HG2	5:C:126:TRP:CH2	2.56	0.40
7:E:242:MET:HE2	7:E:242:MET:HB2	1.89	0.40
8:Af:332:MET:O	8:Af:334:THR:N	2.54	0.40
8:Ac:331:LYS:HA	8:Ac:331:LYS:HD2	1.77	0.40
1:Bd:74:GLN:HE21	1:Bd:221:GLN:HE22	1.68	0.40
1:Bj:36:ILE:HD12	1:Bj:246:ARG:HA	2.02	0.40
1:Bg:154:TRP:CE2	1:Bg:166:ARG:HB2	2.56	0.40
5:C:96:LYS:HE3	5:C:198:ARG:HA	2.03	0.40
5:C:178:ILE:H	5:C:178:ILE:HG12	1.77	0.40
8:Ab:240:GLU:H	8:Ab:240:GLU:HG2	1.56	0.40
8:Ae:129:ALA:HB3	8:Ae:263:ARG:HD3	2.03	0.40
8:Aa:277:LYS:HG3	8:Aa:278:ASP:OD1	2.22	0.40
1:Ba:51:LYS:HB3	1:Ba:51:LYS:HE2	1.84	0.40
8:Ag:285:LYS:HA	8:Ag:285:LYS:HD3	1.89	0.40
8:Af:294:PHE:HD1	8:Af:294:PHE:HA	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ba:249:ASP:HB3	1:Ba:252:LYS:HB3	2.04	0.40
1:Bj:245:ILE:HD11	1:Bi:68:ASN:HD21	1.86	0.40
8:Ab:185:ILE:HD13	8:Ab:185:ILE:HA	1.90	0.40
8:Ad:338:PHE:CE1	8:Ac:282:ILE:HG12	2.56	0.40
8:Aa:171:ASP:N	8:Aa:171:ASP:OD1	2.55	0.40
1:Bj:22:ARG:HH22	1:Bj:263:LEU:HD13	1.86	0.40
2:F:41:LEU:HD21	2:F:55:ARG:HB2	2.02	0.40
5:C:181:LYS:NZ	5:C:227:ASP:OD2	2.45	0.40
7:E:114:SER:HB3	7:E:208:GLU:HG2	2.02	0.40
7:E:165:ASN:OD1	7:E:165:ASN:N	2.55	0.40
8:Ab:183:LYS:HB3	8:Ab:282:ILE:HB	2.03	0.40
8:Ah:327:LEU:HD23	8:Ah:327:LEU:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ba	284/286 (99%)	276 (97%)	8 (3%)	0	100	100
1	Bb	284/286 (99%)	279 (98%)	5 (2%)	0	100	100
1	Bc	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
1	Bd	281/286 (98%)	281 (100%)	0	0	100	100
1	Be	283/286 (99%)	276 (98%)	6 (2%)	1 (0%)	30	61
1	Bf	283/286 (99%)	276 (98%)	7 (2%)	0	100	100
1	Bg	284/286 (99%)	278 (98%)	6 (2%)	0	100	100
1	Bh	284/286 (99%)	275 (97%)	9 (3%)	0	100	100
1	Bi	284/286 (99%)	279 (98%)	5 (2%)	0	100	100
1	Bj	284/286 (99%)	274 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bk	283/286 (99%)	277 (98%)	6 (2%)	0	100	100
2	F	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
3	A	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
4	B	199/201 (99%)	178 (89%)	19 (10%)	2 (1%)	12	42
5	C	202/204 (99%)	186 (92%)	15 (7%)	1 (0%)	24	56
6	D	202/204 (99%)	181 (90%)	21 (10%)	0	100	100
7	E	216/221 (98%)	202 (94%)	13 (6%)	1 (0%)	24	56
8	Aa	309/326 (95%)	277 (90%)	31 (10%)	1 (0%)	36	66
8	Ab	318/326 (98%)	279 (88%)	38 (12%)	1 (0%)	36	66
8	Ac	315/326 (97%)	282 (90%)	31 (10%)	2 (1%)	21	52
8	Ad	321/326 (98%)	290 (90%)	29 (9%)	2 (1%)	21	52
8	Ae	322/326 (99%)	291 (90%)	30 (9%)	1 (0%)	36	66
8	Af	321/326 (98%)	291 (91%)	28 (9%)	2 (1%)	21	52
8	Ag	320/326 (98%)	294 (92%)	24 (8%)	2 (1%)	21	52
8	Ah	317/326 (97%)	292 (92%)	21 (7%)	4 (1%)	9	37
All	All	6775/6883 (98%)	6382 (94%)	373 (6%)	20 (0%)	37	66

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Be	44	SER
5	C	76	VAL
8	Ag	285	LYS
4	B	47	ILE
8	Ab	291	VAL
8	Af	343	GLY
8	Ac	286	ALA
8	Ad	36	ILE
4	B	48	LYS
7	E	187	ILE
8	Ah	37	ILE
8	Ah	155	GLN
8	Af	236	VAL
8	Ad	182	ILE
8	Ag	110	PHE
8	Ac	37	ILE
8	Aa	37	ILE

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Mol	Chain	Res	Type
8	Ah	238	SER
8	Ah	233	ILE
8	Ae	37	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	230/230 (100%)	229 (100%)	1 (0%)	84	82
1	Bb	230/230 (100%)	228 (99%)	2 (1%)	70	76
1	Bc	230/230 (100%)	226 (98%)	4 (2%)	53	69
1	Bd	229/230 (100%)	226 (99%)	3 (1%)	61	72
1	Be	229/230 (100%)	226 (99%)	3 (1%)	61	72
1	Bf	229/230 (100%)	227 (99%)	2 (1%)	70	76
1	Bg	230/230 (100%)	228 (99%)	2 (1%)	70	76
1	Bh	230/230 (100%)	229 (100%)	1 (0%)	84	82
1	Bi	230/230 (100%)	228 (99%)	2 (1%)	70	76
1	Bj	230/230 (100%)	229 (100%)	1 (0%)	84	82
1	Bk	229/230 (100%)	227 (99%)	2 (1%)	70	76
2	F	94/94 (100%)	91 (97%)	3 (3%)	34	59
3	A	166/166 (100%)	164 (99%)	2 (1%)	63	73
4	B	171/171 (100%)	169 (99%)	2 (1%)	63	73
5	C	177/177 (100%)	174 (98%)	3 (2%)	53	69
6	D	176/176 (100%)	175 (99%)	1 (1%)	78	80
7	E	186/187 (100%)	186 (100%)	0	100	100
8	Aa	261/273 (96%)	256 (98%)	5 (2%)	50	67
8	Ab	269/273 (98%)	262 (97%)	7 (3%)	40	63
8	Ac	271/273 (99%)	268 (99%)	3 (1%)	65	74
8	Ad	273/273 (100%)	270 (99%)	3 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Ae	271/273 (99%)	265 (98%)	6 (2%)	45	65
8	Af	270/273 (99%)	264 (98%)	6 (2%)	45	65
8	Ag	272/273 (100%)	269 (99%)	3 (1%)	65	74
8	Ah	271/273 (99%)	267 (98%)	4 (2%)	57	71
All	All	5654/5685 (100%)	5583 (99%)	71 (1%)	59	72

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ba	23	ILE
1	Bd	148	VAL
1	Bd	161	MET
1	Bd	285	LEU
1	Bc	3	ILE
1	Bc	80	LEU
1	Bc	148	VAL
1	Bc	260	ASN
1	Bb	216	ASP
1	Bb	256	GLU
1	Bk	187	ILE
1	Bk	285	LEU
1	Bj	10	MET
1	Bi	117	LEU
1	Bi	286	ARG
1	Bh	84	THR
1	Bg	204	ASP
1	Bg	284	LEU
1	Bf	37	ASN
1	Bf	216	ASP
1	Be	1	MET
1	Be	148	VAL
1	Be	188	MET
2	F	33	VAL
2	F	36	VAL
2	F	111	LEU
3	A	82	LEU
3	A	210	PHE
4	B	57	THR
4	B	117	VAL
5	C	101	VAL
5	C	104	VAL

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Mol	Chain	Res	Type
5	C	169	THR
6	D	99	ASN
8	Ab	64	ASP
8	Ab	97	THR
8	Ab	98	ILE
8	Ab	115	LEU
8	Ab	118	VAL
8	Ab	154	LEU
8	Ab	275	TYR
8	Ag	57	VAL
8	Ag	285	LYS
8	Ag	345	GLU
8	Ah	179	THR
8	Ah	198	LEU
8	Ah	291	VAL
8	Ah	347	ASN
8	Af	89	ASN
8	Af	206	ASN
8	Af	294	PHE
8	Af	302	ILE
8	Af	328	GLU
8	Af	339	THR
8	Ae	192	MET
8	Ae	281	ILE
8	Ae	282	ILE
8	Ae	289	THR
8	Ae	299	LEU
8	Ae	332	MET
8	Ad	127	ASN
8	Ad	134	LYS
8	Ad	271	ASP
8	Ac	103	VAL
8	Ac	233	ILE
8	Ac	339	THR
8	Aa	110	PHE
8	Aa	188	ASN
8	Aa	214	MET
8	Aa	243	LEU
8	Aa	290	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ba	16	GLN
1	Ba	68	ASN
1	Ba	71	ASN
1	Ba	213	GLN
1	Ba	253	GLN
1	Ba	260	ASN
1	Ba	261	GLN
1	Bd	5	HIS
1	Bd	55	GLN
1	Bd	71	ASN
1	Bd	74	GLN
1	Bd	237	ASN
1	Bd	253	GLN
1	Bc	5	HIS
1	Bc	16	GLN
1	Bc	131	ASN
1	Bc	147	ASN
1	Bb	5	HIS
1	Bb	213	GLN
1	Bb	237	ASN
1	Bk	16	GLN
1	Bk	68	ASN
1	Bk	74	GLN
1	Bk	111	GLN
1	Bk	134	ASN
1	Bk	163	GLN
1	Bk	260	ASN
1	Bk	265	ASN
1	Bk	276	ASN
1	Bj	5	HIS
1	Bj	6	ASN
1	Bj	55	GLN
1	Bj	68	ASN
1	Bj	211	ASN
1	Bj	253	GLN
1	Bi	37	ASN
1	Bi	71	ASN
1	Bi	74	GLN
1	Bi	111	GLN
1	Bi	129	GLN
1	Bi	134	ASN
1	Bi	147	ASN
1	Bi	156	HIS

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Mol	Chain	Res	Type
1	Bi	163	GLN
1	Bi	211	ASN
1	Bi	213	GLN
1	Bi	222	ASN
1	Bi	253	GLN
1	Bh	20	ASN
1	Bh	60	ASN
1	Bh	96	GLN
1	Bh	111	GLN
1	Bh	147	ASN
1	Bh	197	ASN
1	Bh	211	ASN
1	Bh	253	GLN
1	Bg	5	HIS
1	Bg	20	ASN
1	Bg	37	ASN
1	Bg	65	ASN
1	Bg	111	GLN
1	Bg	160	ASN
1	Bg	211	ASN
1	Bg	237	ASN
1	Bg	279	GLN
1	Bf	5	HIS
1	Bf	6	ASN
1	Bf	13	GLN
1	Bf	74	GLN
1	Bf	109	GLN
1	Bf	160	ASN
1	Bf	211	ASN
1	Bf	221	GLN
1	Bf	261	GLN
1	Bf	277	ASN
1	Be	55	GLN
1	Be	65	ASN
1	Be	68	ASN
1	Be	129	GLN
1	Be	163	GLN
1	Be	211	ASN
1	Be	253	GLN
3	A	153	ASN
3	A	166	ASN
4	B	180	ASN

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Mol	Chain	Res	Type
4	B	193	HIS
5	C	30	ASN
5	C	121	HIS
5	C	182	ASN
6	D	50	GLN
7	E	80	ASN
7	E	180	ASN
7	E	239	GLN
8	Ab	188	ASN
8	Ab	196	HIS
8	Ag	33	ASN
8	Ag	78	GLN
8	Ag	88	GLN
8	Ag	207	ASN
8	Ah	196	HIS
8	Af	193	ASN
8	Af	303	GLN
8	Ae	41	ASN
8	Ae	84	ASN
8	Ae	322	GLN
8	Ad	47	ASN
8	Ad	66	GLN
8	Ad	205	GLN
8	Ad	267	HIS
8	Ac	33	ASN
8	Ac	147	GLN
8	Ac	178	ASN
8	Ac	193	ASN
8	Ac	196	HIS
8	Ac	229	ASN
8	Ac	329	GLN
8	Aa	127	ASN
8	Aa	147	GLN
8	Aa	151	GLN
8	Aa	178	ASN
8	Aa	322	GLN

5.3.3 RNA ⓘ

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.

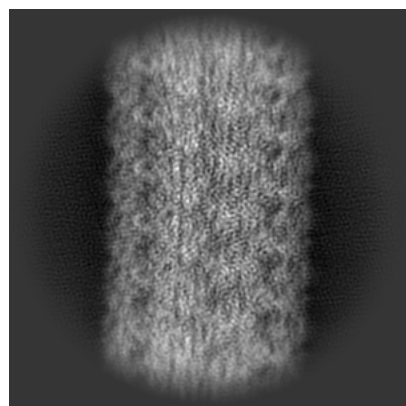
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75374. These allow visual inspection of the internal detail of the map and identification of artifacts.

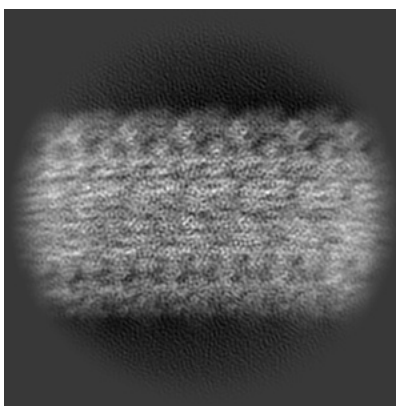
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

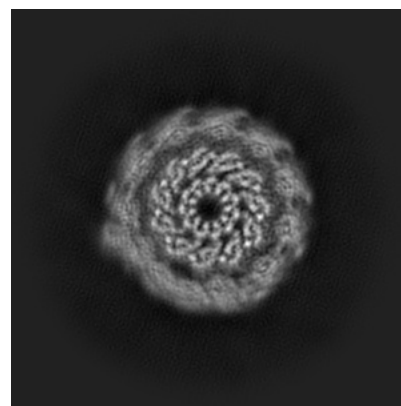
6.1.1 Primary map



X

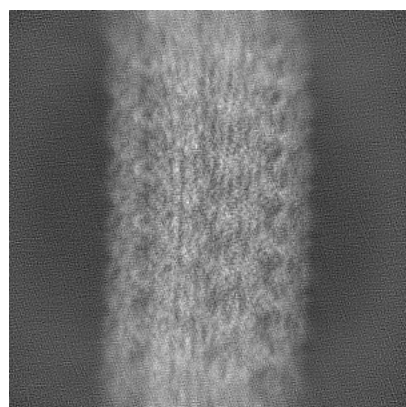


Y

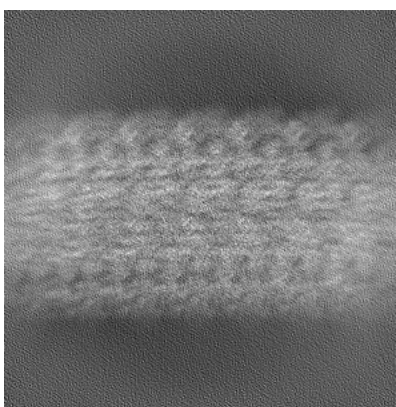


Z

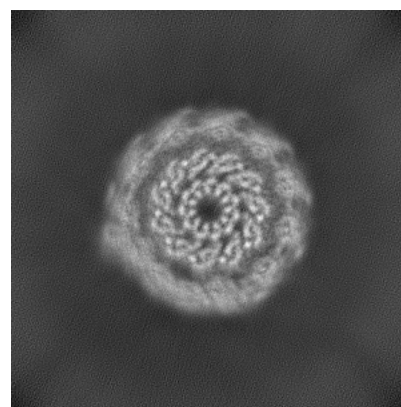
6.1.2 Raw map



X



Y

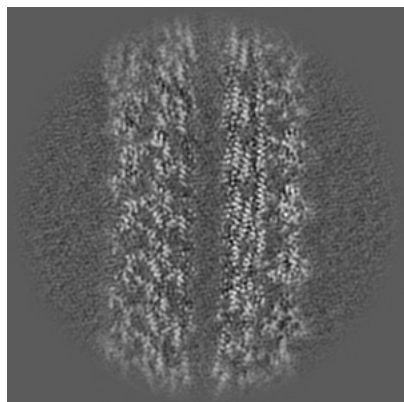


Z

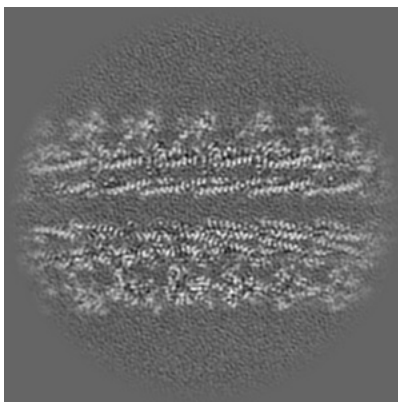
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

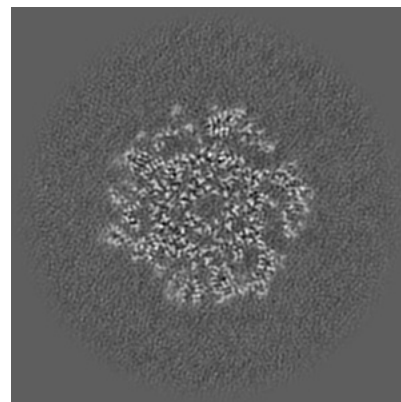
6.2.1 Primary map



X Index: 180

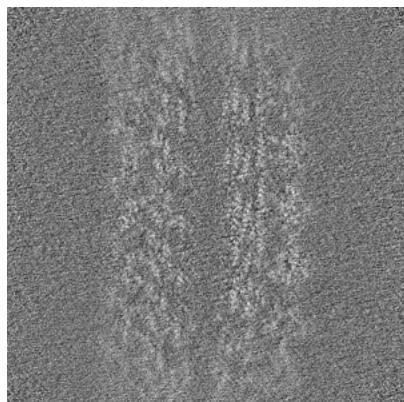


Y Index: 180

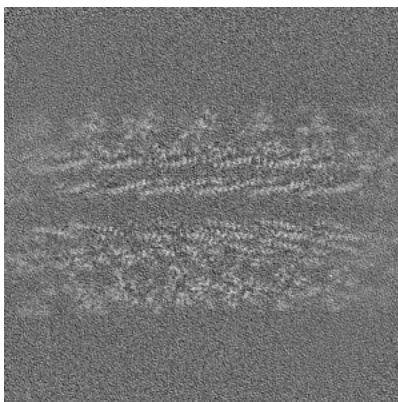


Z Index: 180

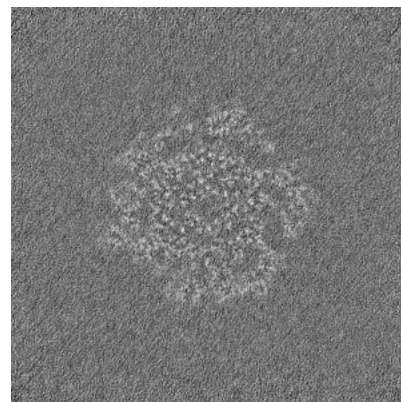
6.2.2 Raw map



X Index: 180



Y Index: 180

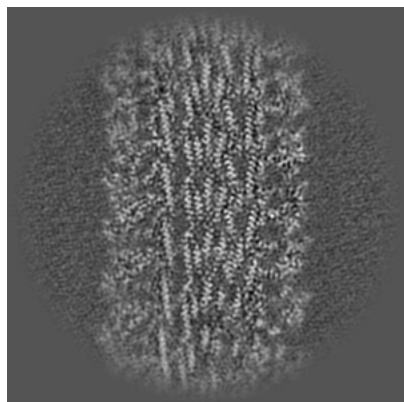


Z Index: 180

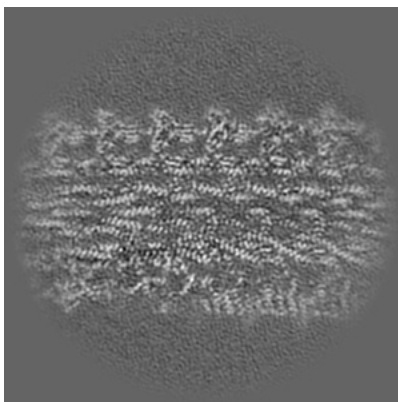
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

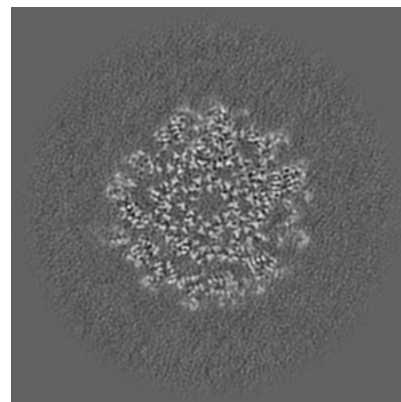
6.3.1 Primary map



X Index: 195

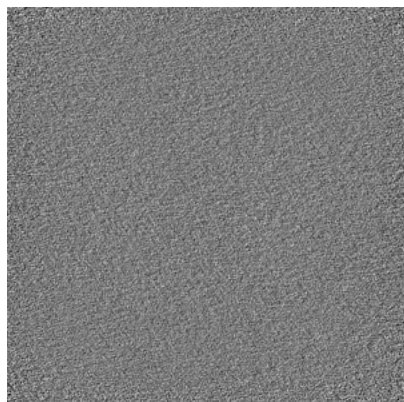


Y Index: 162

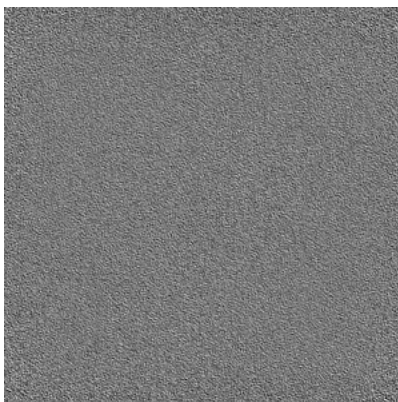


Z Index: 170

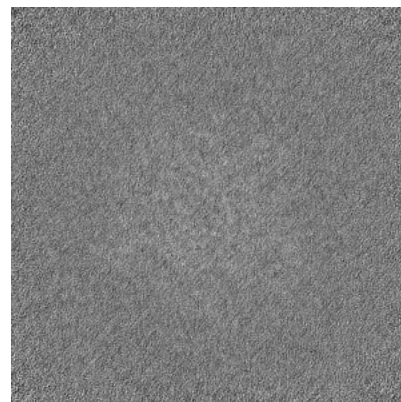
6.3.2 Raw map



X Index: 0



Y Index: 0

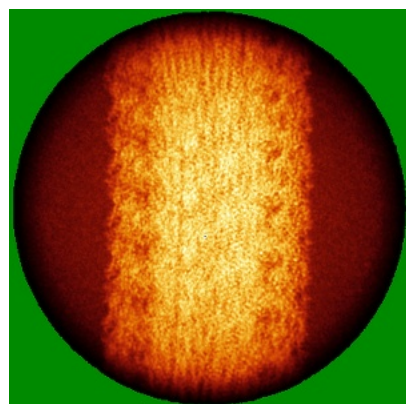


Z Index: 0

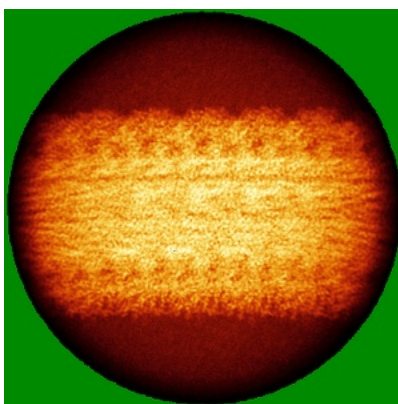
The images above show the largest variance slices of the map in three orthogonal directions.

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

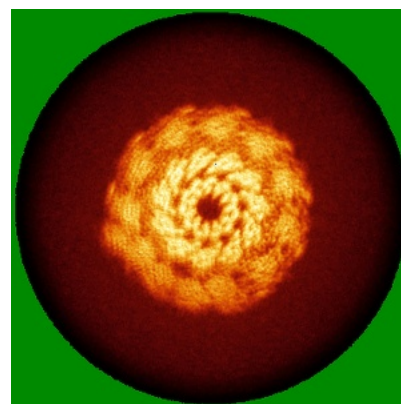
6.4.1 Primary map



X

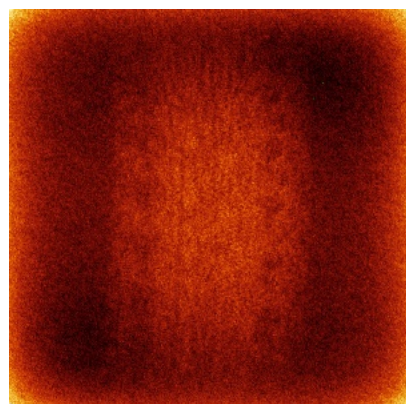


Y

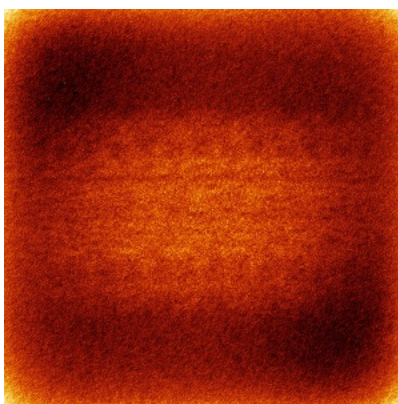


Z

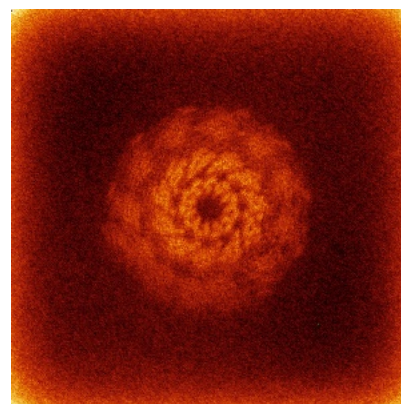
6.4.2 Raw map



X



Y

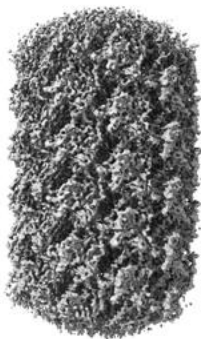


Z

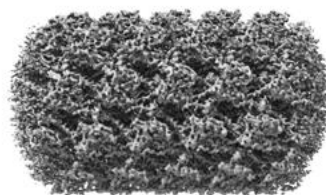
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



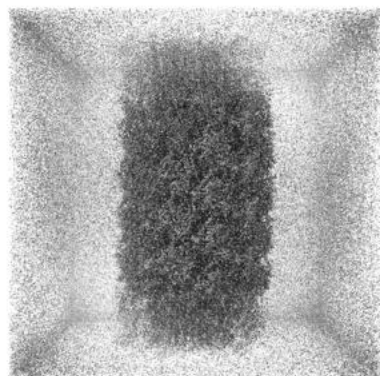
Y



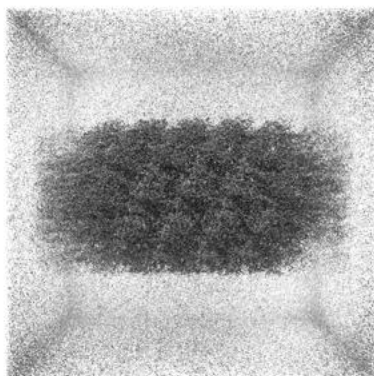
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

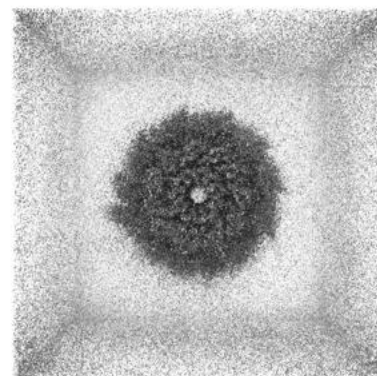
6.5.2 Raw map



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.

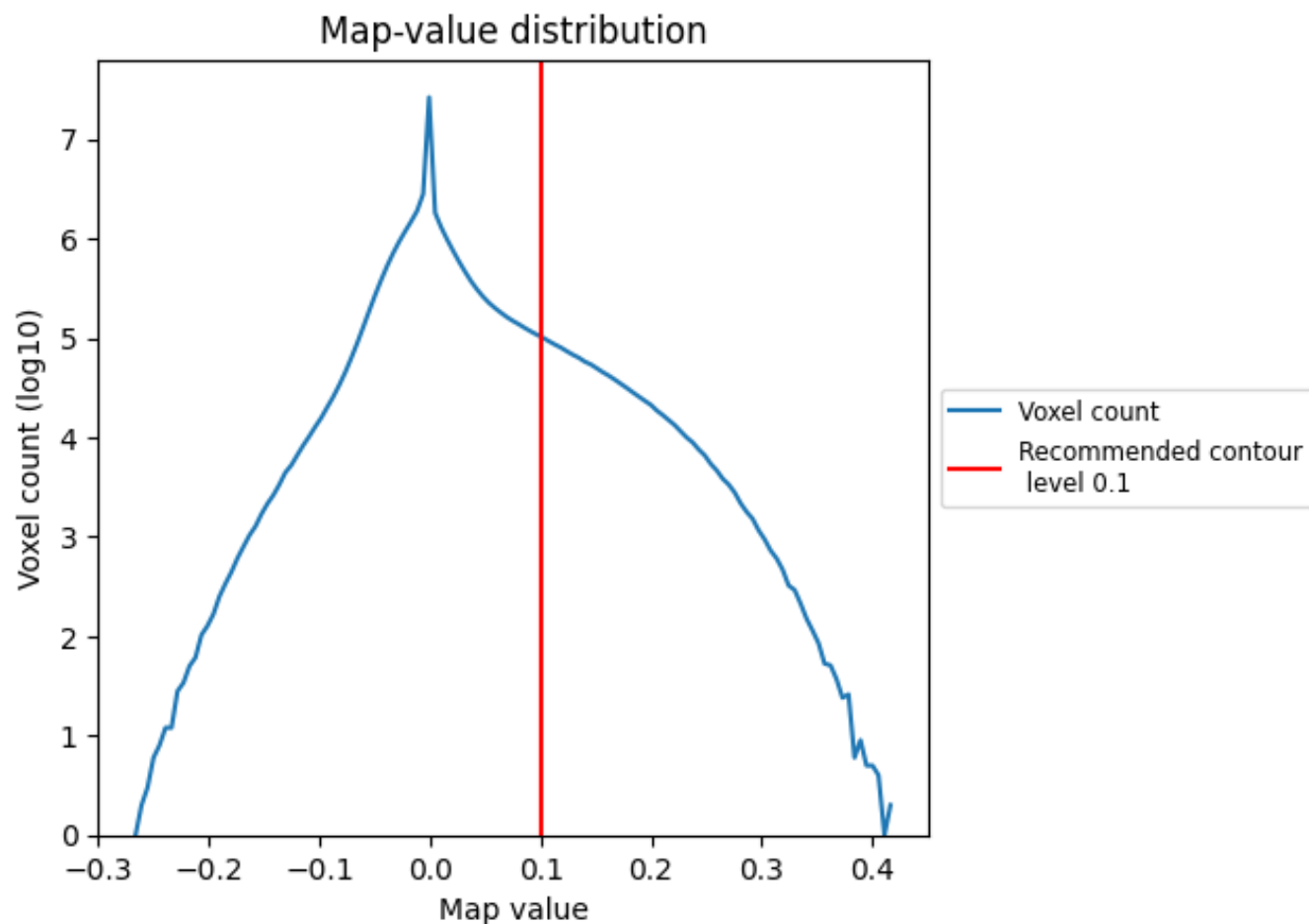
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

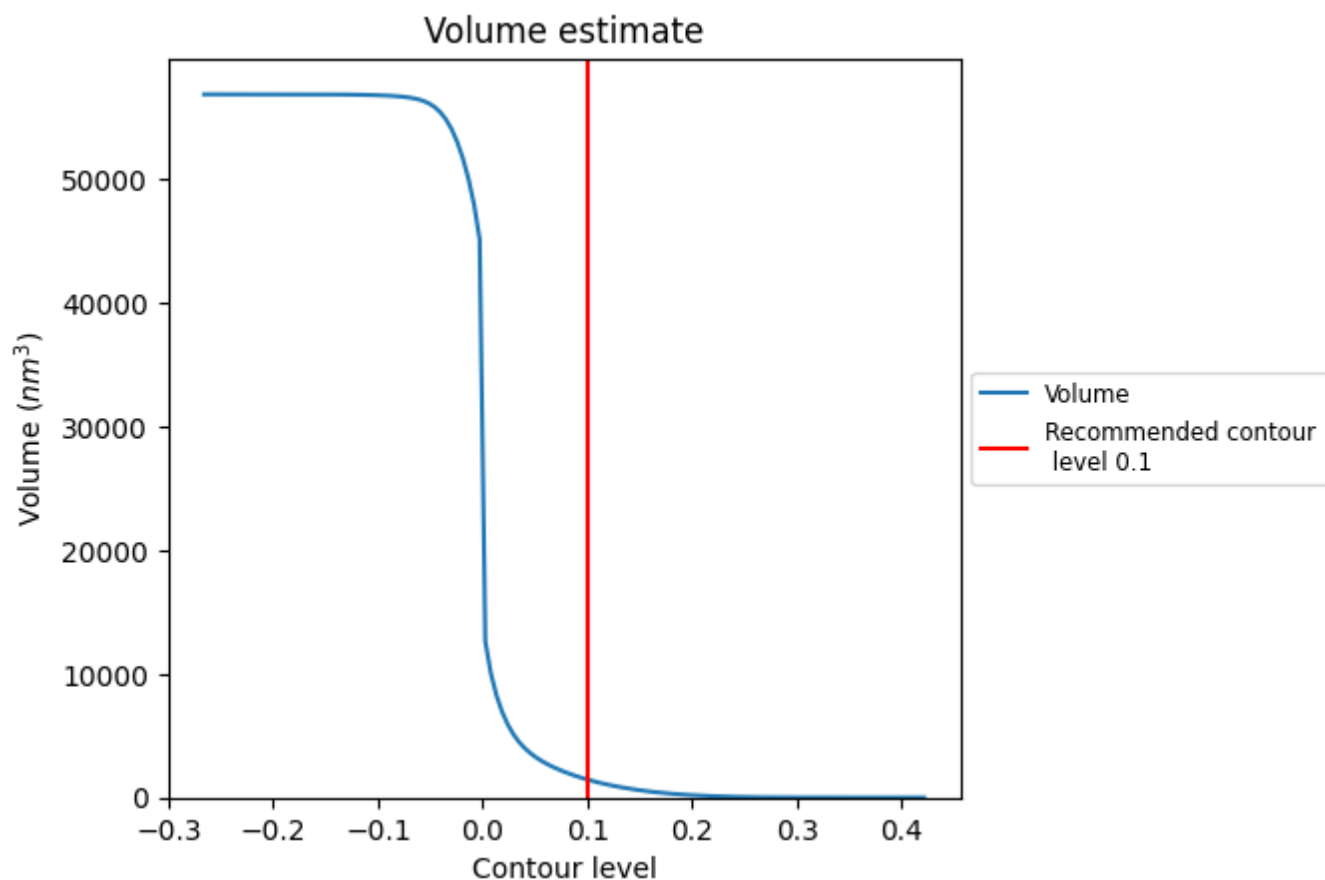
This section contains the results of statistical analysis of the map.

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.

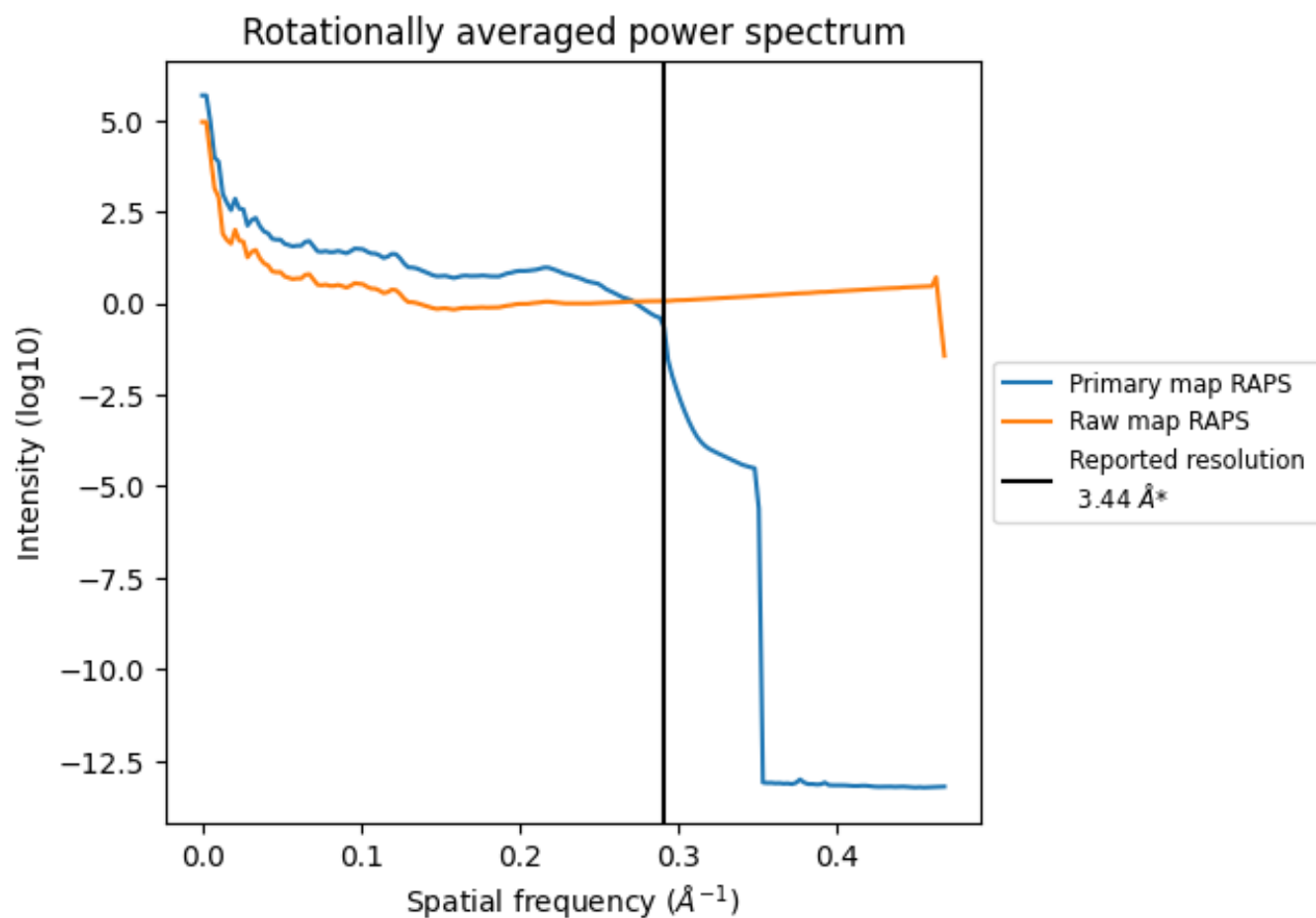
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1458 nm³; this corresponds to an approximate mass of 1317 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 ⓘ

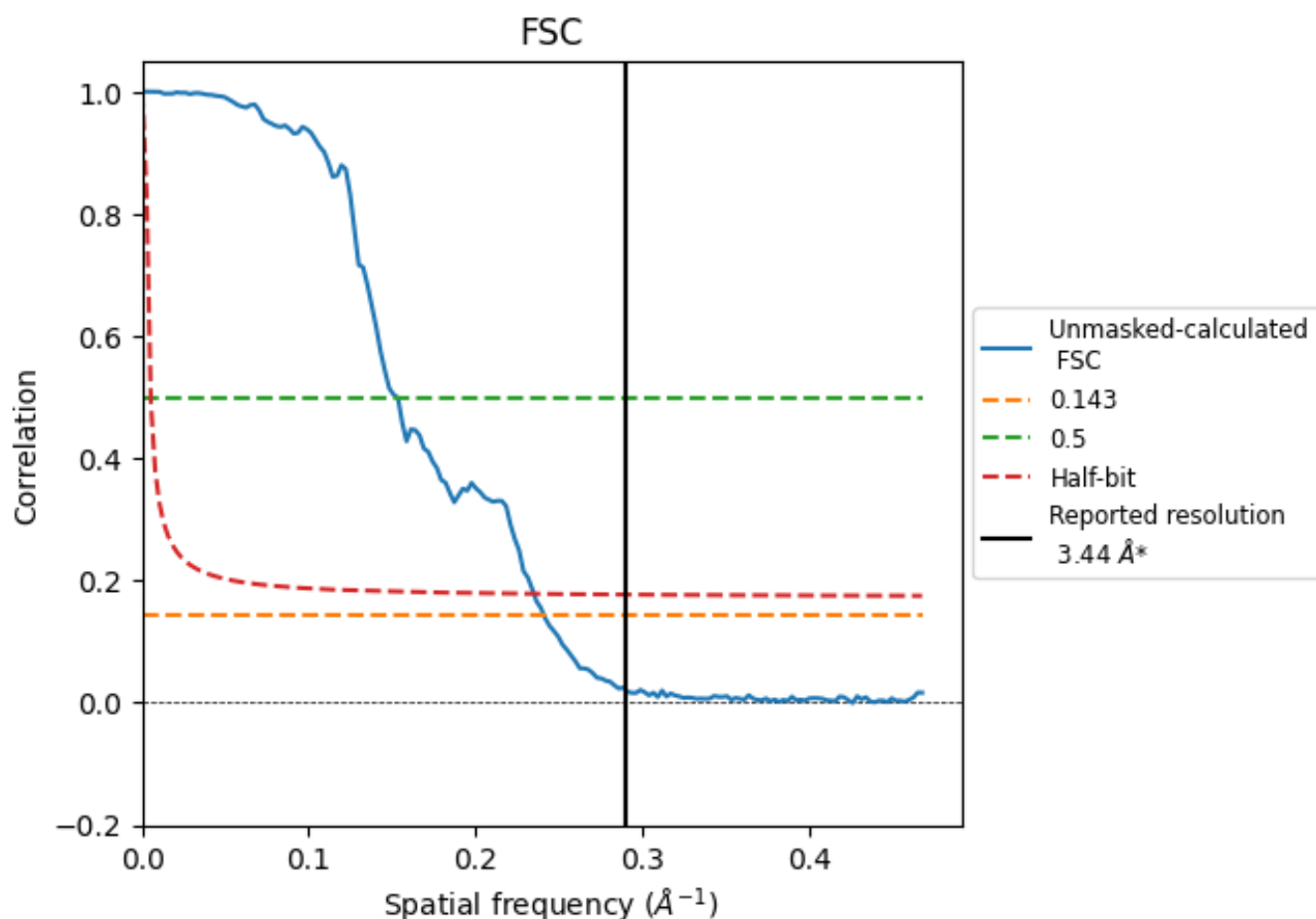


*Reported resolution corresponds to spatial frequency of 0.291 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.291 \AA^{-1}

8.2 Resolution estimates [i](#)

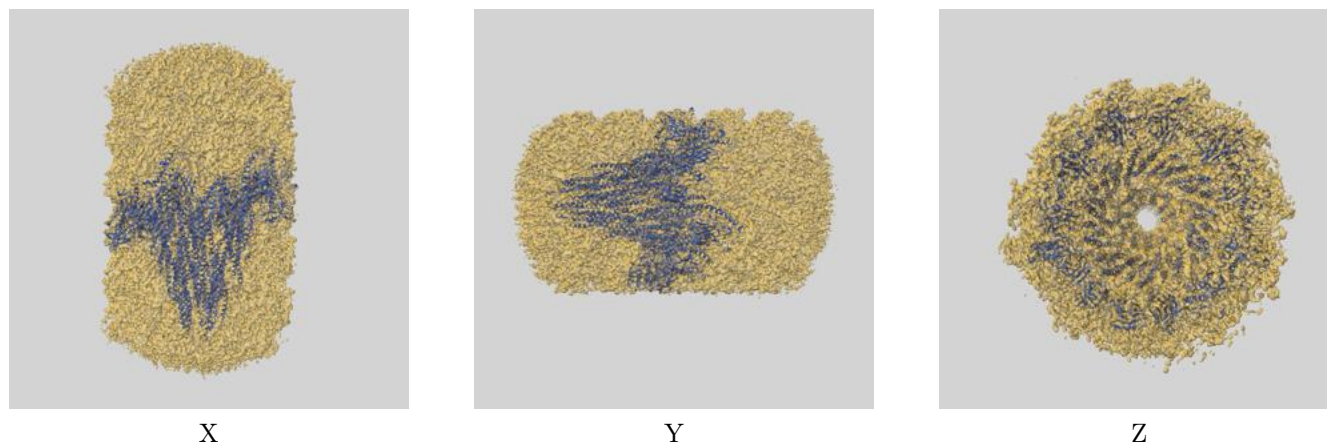
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	6.54	4.25

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

9 Map-model fit [i](#)

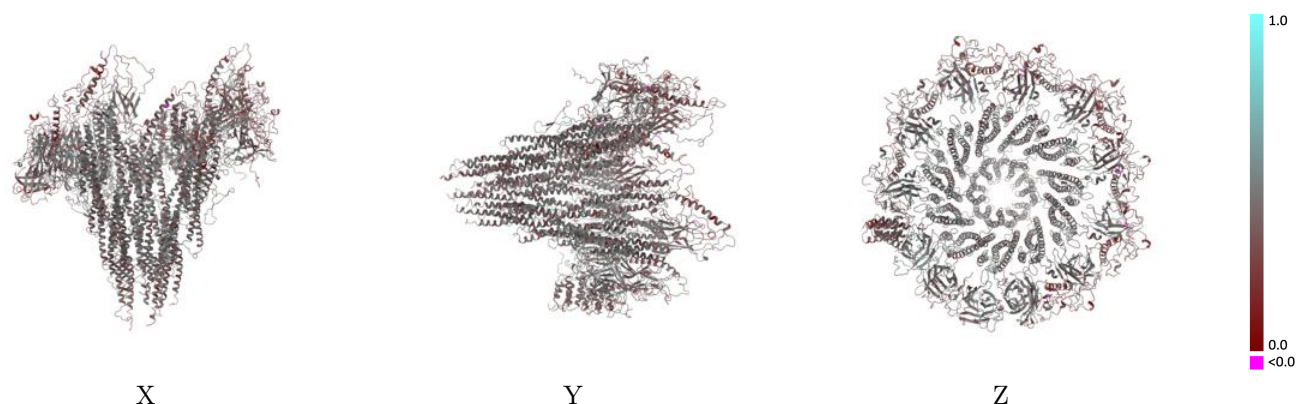
This section contains information regarding the fit between EMDB map EMD-75374 and PDB model 10PL. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



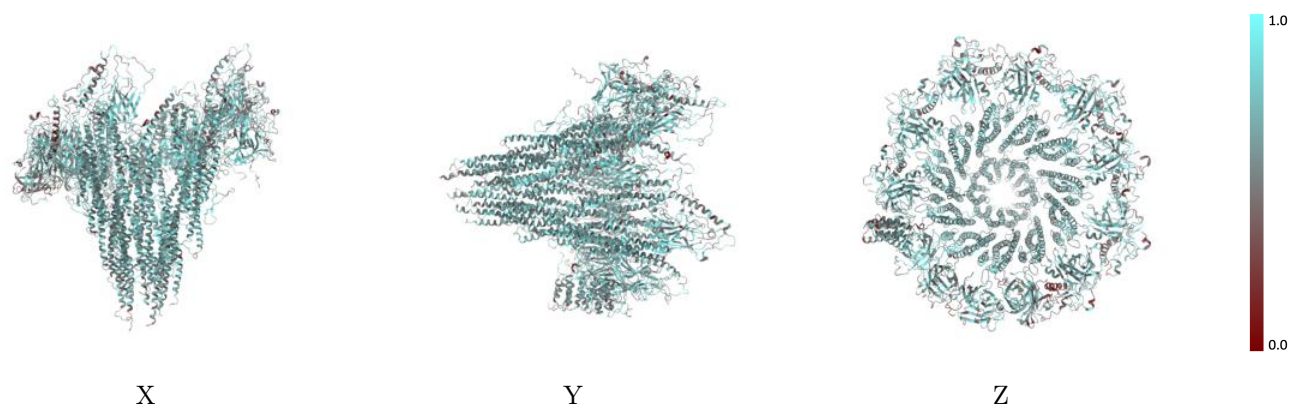
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



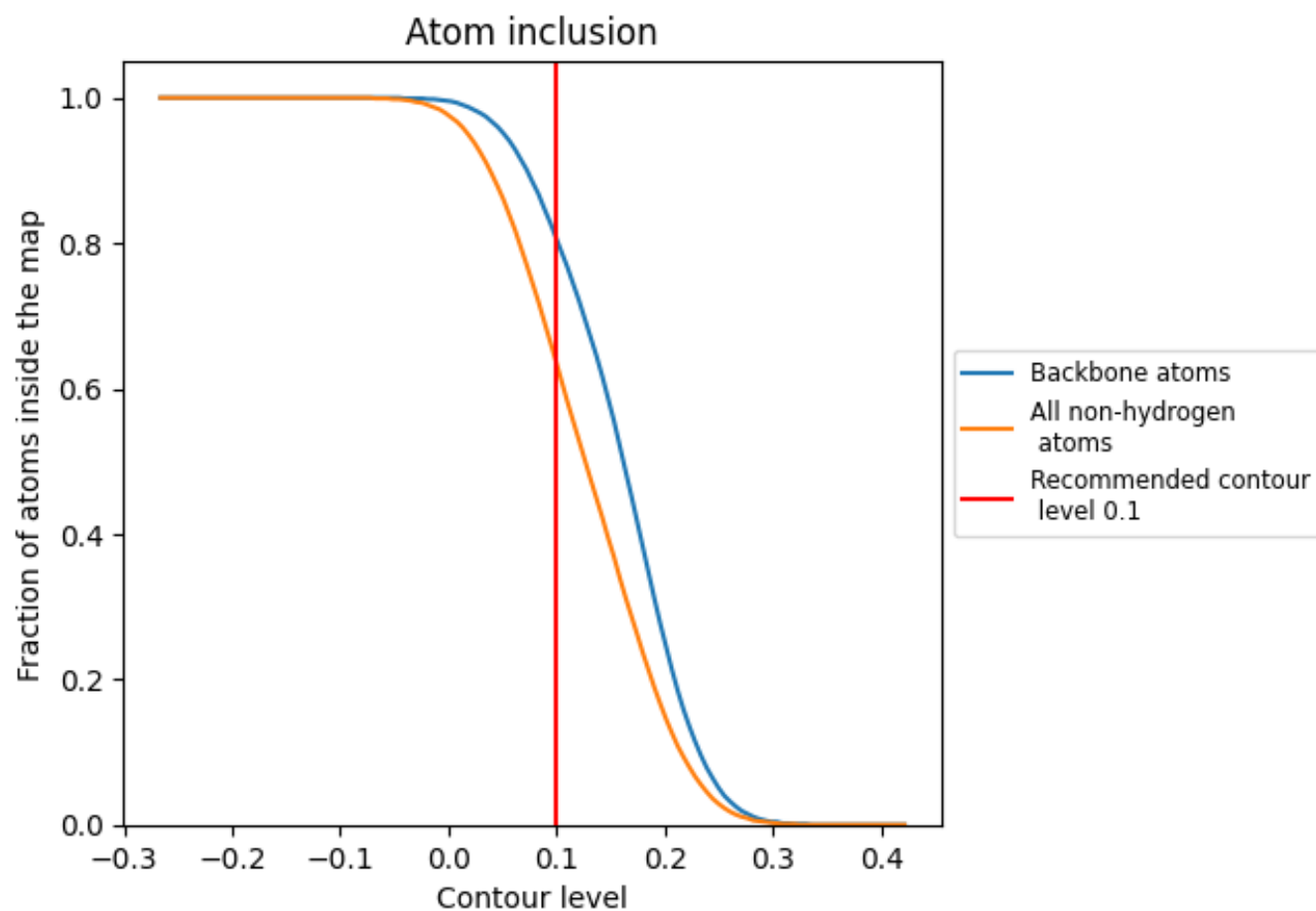
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 64% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6350	 0.4160
A	 0.5710	 0.3790
Aa	 0.5850	 0.3880
Ab	 0.6160	 0.3820
Ac	 0.6350	 0.3850
Ad	 0.6210	 0.3750
Ae	 0.6230	 0.3700
Af	 0.6190	 0.3880
Ag	 0.6520	 0.4090
Ah	 0.6420	 0.4140
B	 0.6710	 0.4490
Ba	 0.6710	 0.4470
Bb	 0.6710	 0.4600
Bc	 0.6690	 0.4380
Bd	 0.6710	 0.4370
Be	 0.6700	 0.4260
Bf	 0.6760	 0.4450
Bg	 0.6570	 0.4400
Bh	 0.6590	 0.4450
Bi	 0.6220	 0.4240
Bj	 0.6430	 0.4390
Bk	 0.6650	 0.4540
C	 0.5800	 0.4150
D	 0.6080	 0.4190
E	 0.5780	 0.4310
F	 0.5010	 0.3590

