



Full wwPDB EM Validation Report ⓘ

Dec 3, 2025 – 01:06 PM EST

PDB ID : 9P7R / pdb_00009p7r
EMDB ID : EMD-71351
Title : In situ structure of the sheathed FlaB flagellar filament in *Vibrio cholerae*
Authors : Guo, W.; Kumar, R.
Deposited on : 2025-06-21
Resolution : 3.16 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

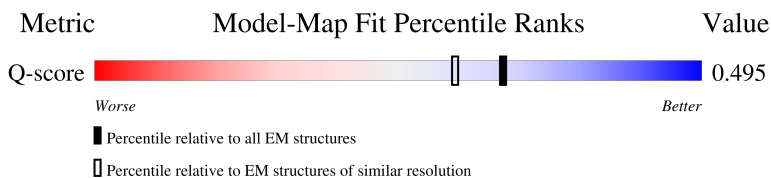
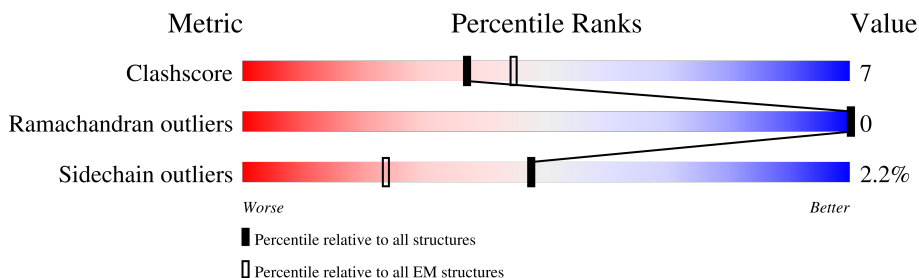
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 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.





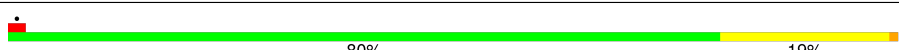
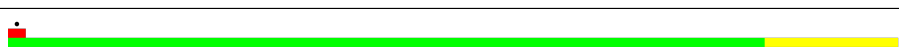

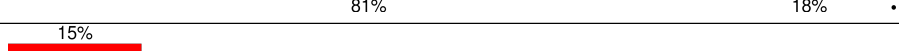
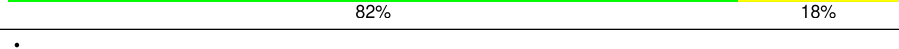





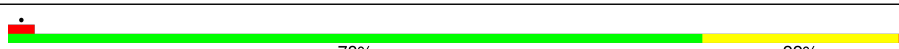


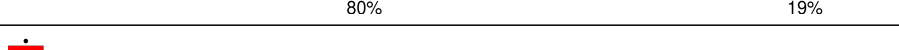








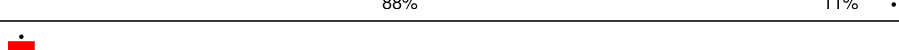
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	A1	376	<div> <div>23%</div> <div>83%</div> <div>17%</div> </div>
1	A2	376	<div> <div>88%</div> <div>12%</div> </div>
1	B2	376	<div> <div>86%</div> <div>14%</div> </div>
1	C2	376	<div> <div>85%</div> <div>14%</div> </div>


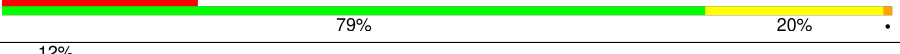

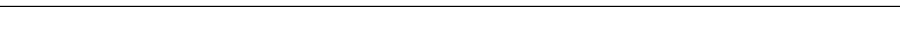
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Mol	Chain	Length	Quality of chain
1	D2	376	
1	E2	376	
1	F2	376	
1	G2	376	
1	H2	376	
1	I2	376	
1	J2	376	
1	K2	376	
1	L2	376	
1	M2	376	
1	N2	376	
1	O2	376	
1	P2	376	
1	Q2	376	
1	R2	376	
1	S2	376	
1	T2	376	
1	U2	376	
1	V2	376	
1	W2	376	
1	X2	376	
1	Y2	376	
1	Z2	376	
1	a2	376	
1	b2	376	

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Mol	Chain	Length	Quality of chain
1	c2	376	 9% 80% 19% •
1	d2	376	 22% 79% 20% •
1	e2	376	 12% 78% 22% •
1	f2	376	 6% 79% 20% •

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 91179 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 B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	A2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	B2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	C2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	D2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	E2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	F2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	G2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	H2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	I2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	J2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	K2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	L2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	M2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	N2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	O2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		
1	P2	376	Total	C	N	O	S	0	0
			2763	1656	509	586	12		

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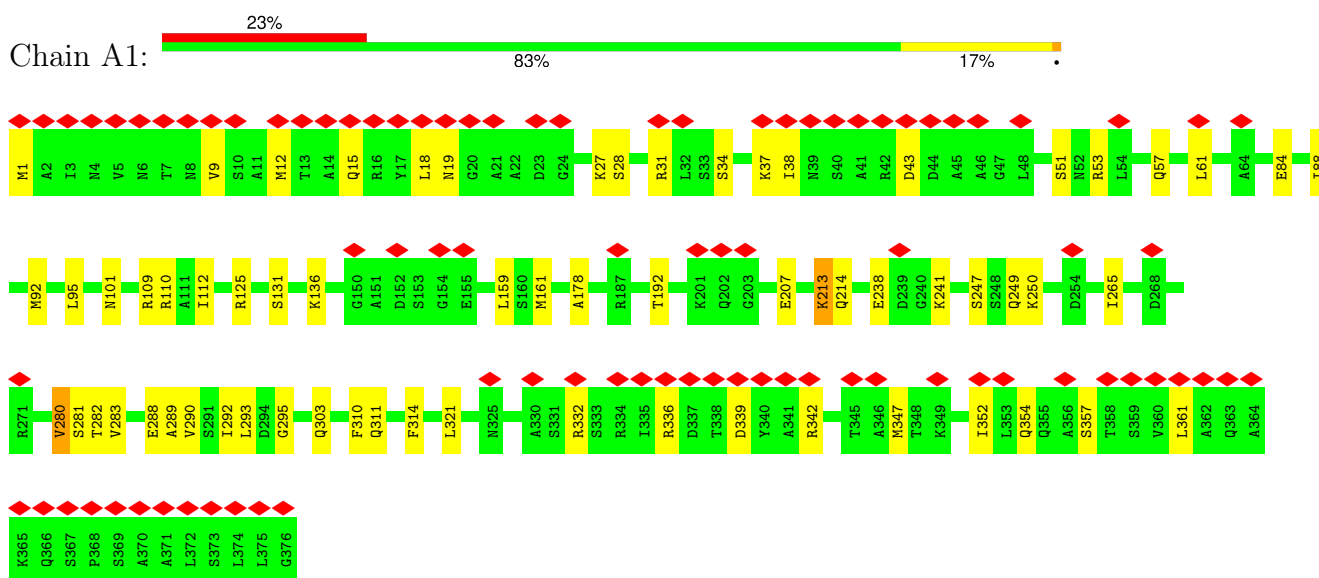
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	R2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	S2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	T2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	U2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	V2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	W2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	X2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	Y2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	Z2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	a2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	b2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	c2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
1	d2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0
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1	f2	376	Total 2763	C 1656	N 509	O 586	S 12	0	0

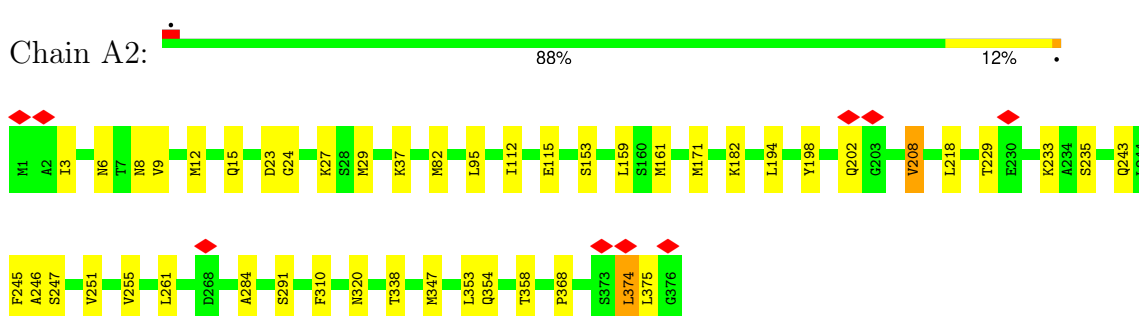
3 Residue-property plots

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.

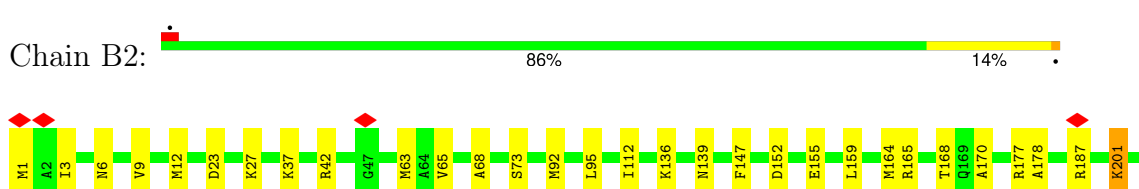
• Molecule 1: Flagellin B



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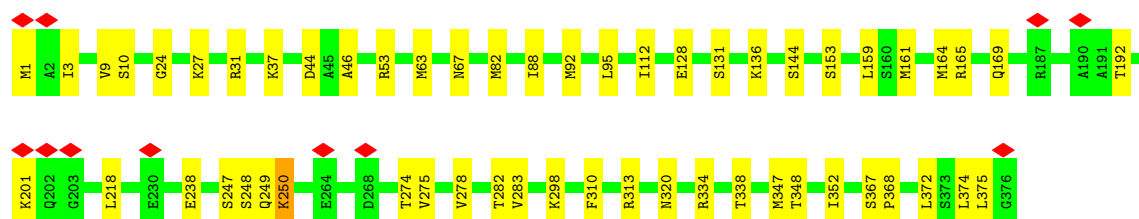
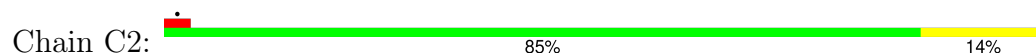


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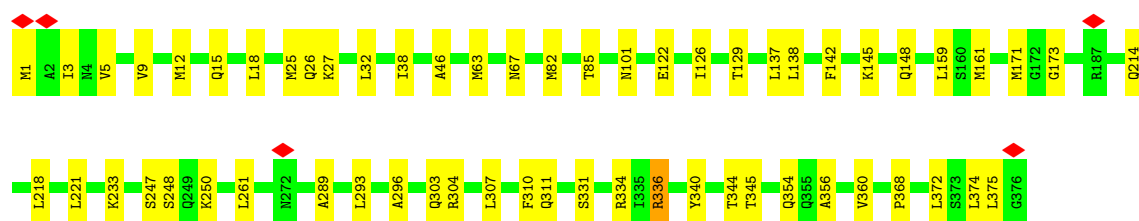
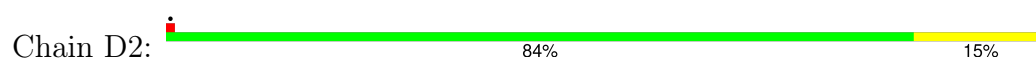




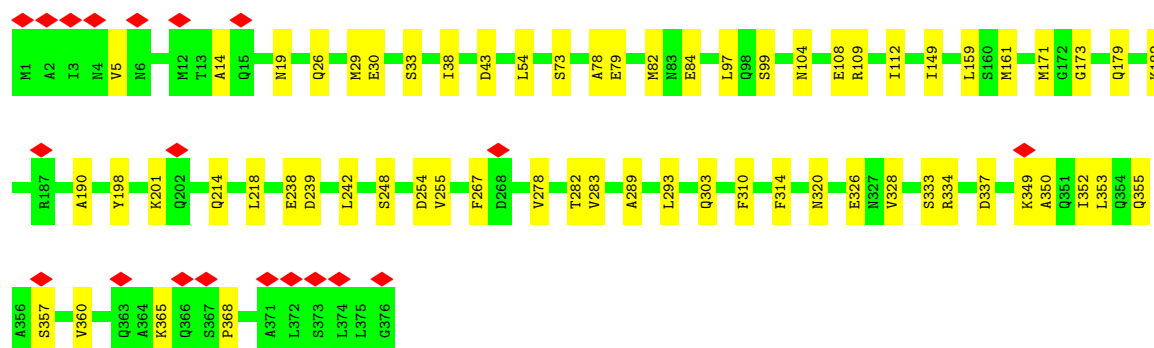
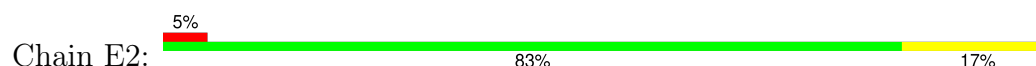
- Molecule 1: Flagellin B



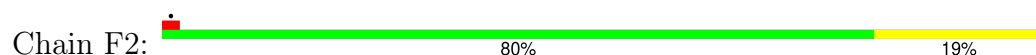
- Molecule 1: Flagellin B

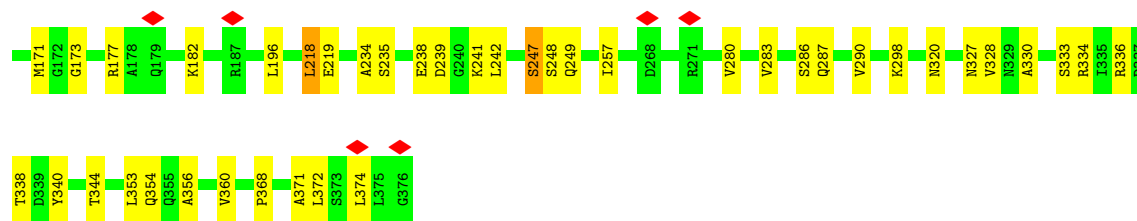


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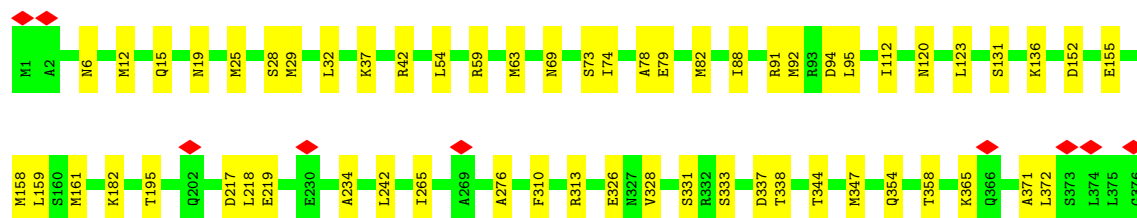
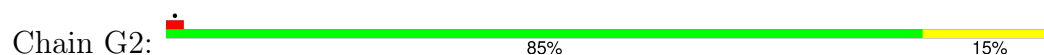


- Molecule 1: Flagellin B

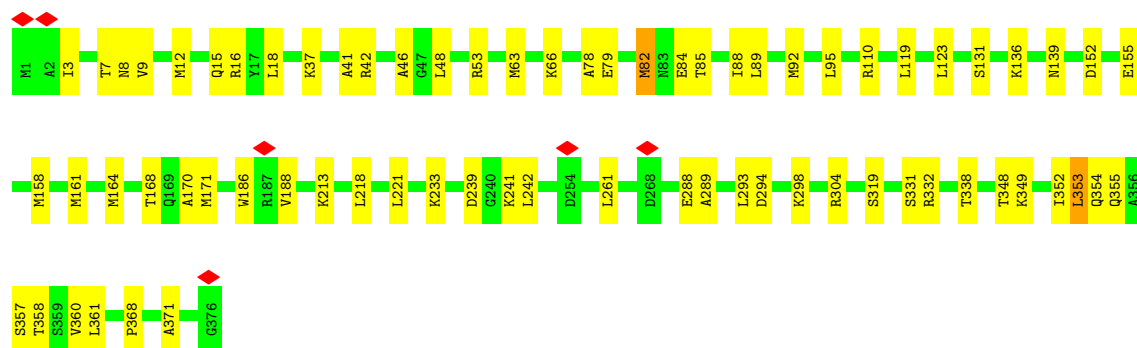
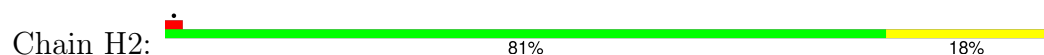




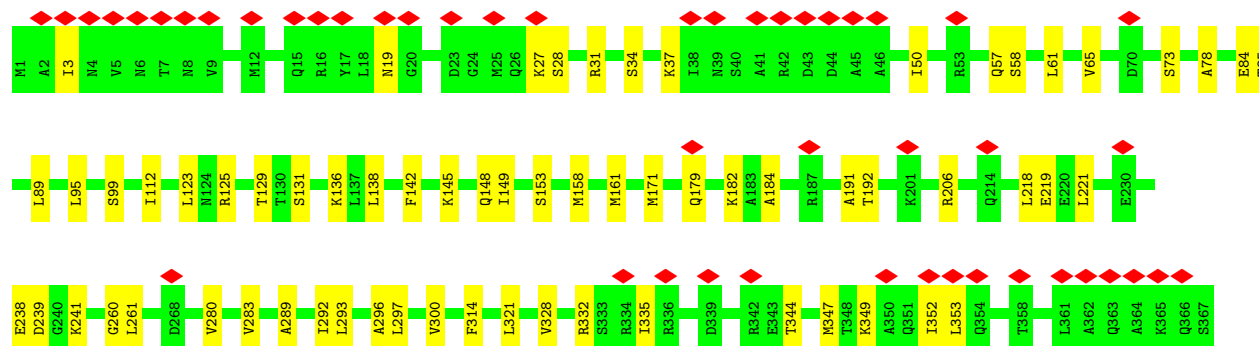
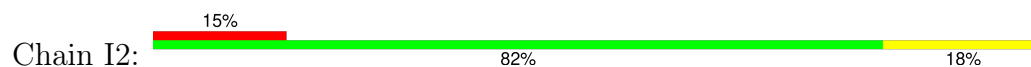
• Molecule 1: Flagellin B

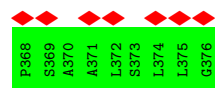


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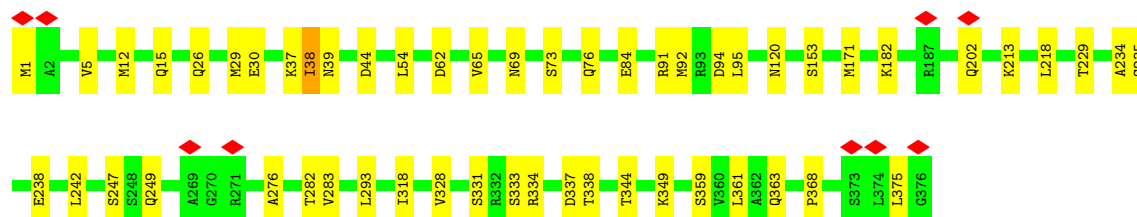
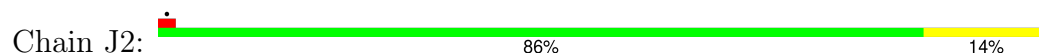


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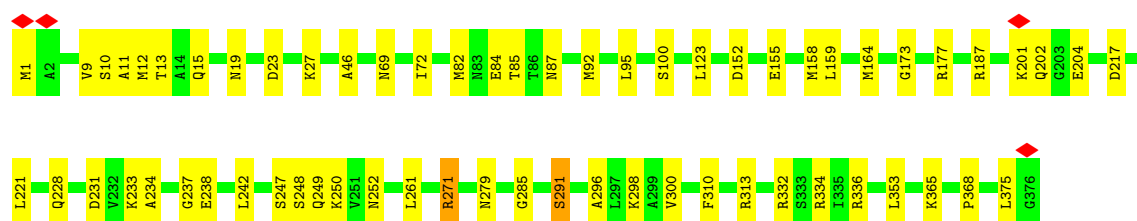
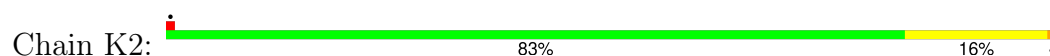




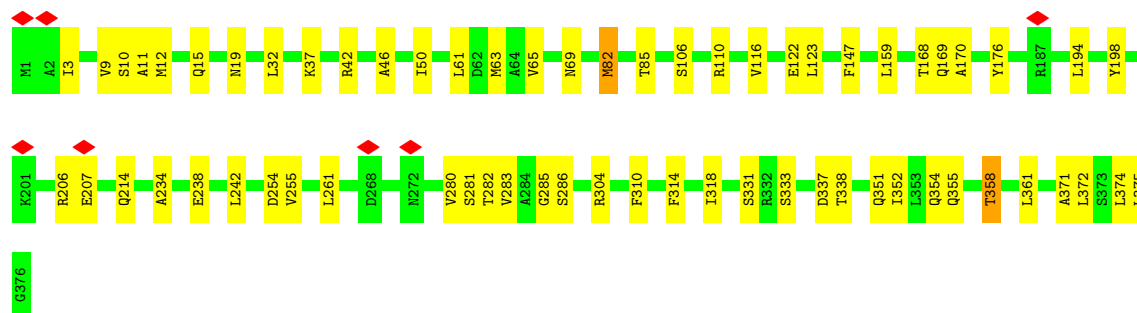
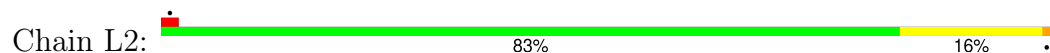
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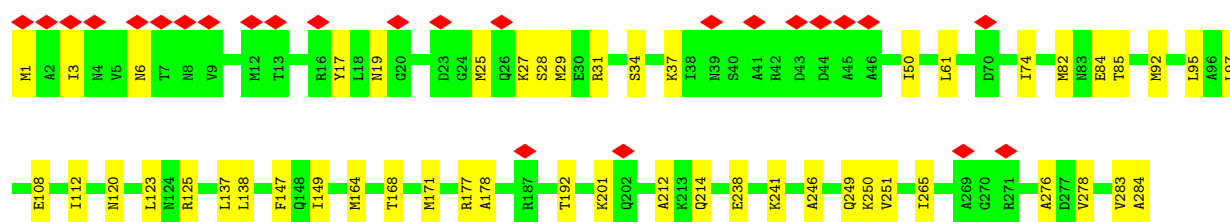
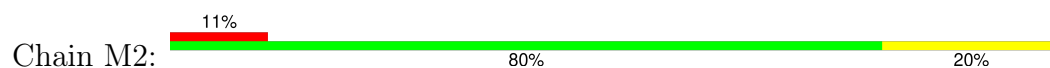
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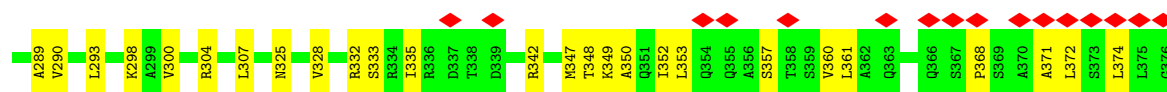


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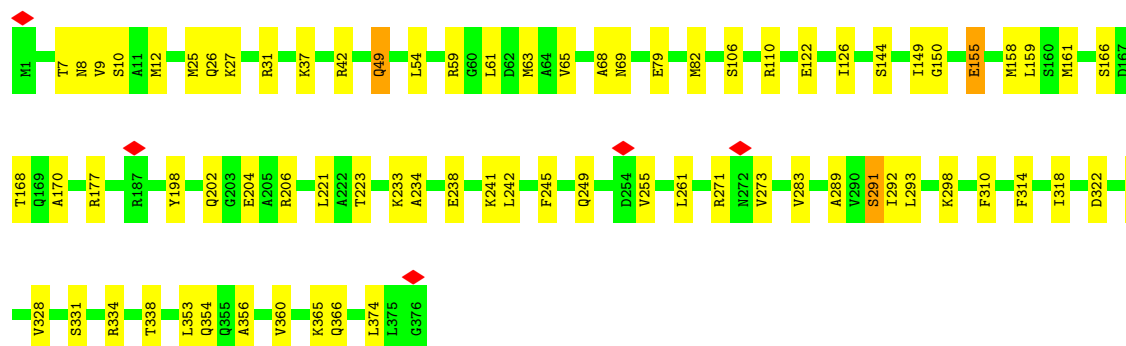
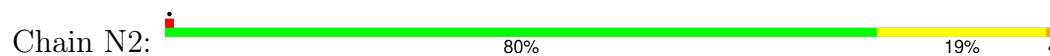


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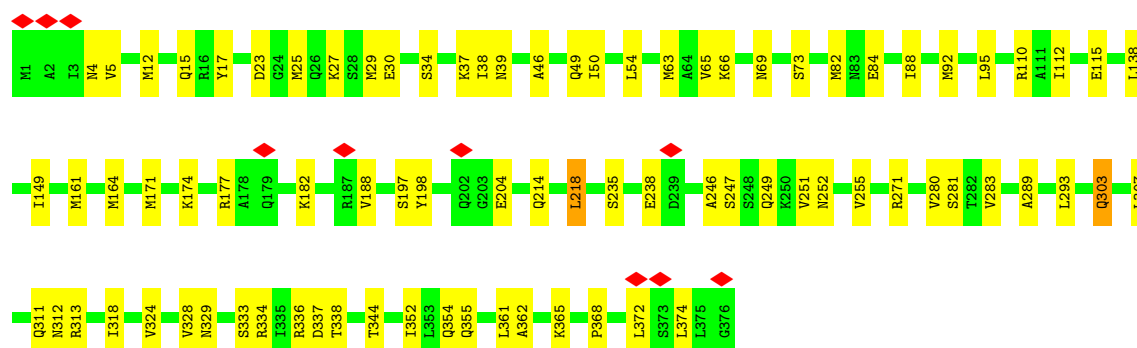
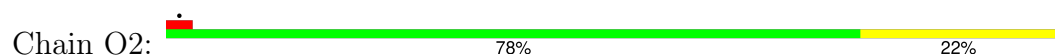




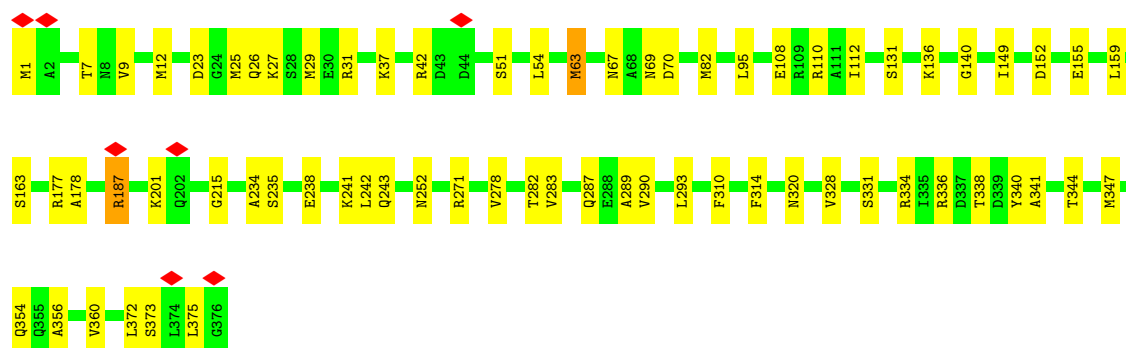
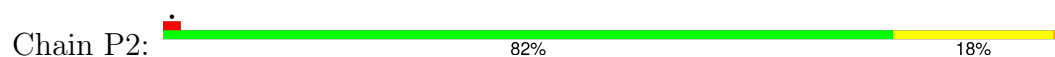
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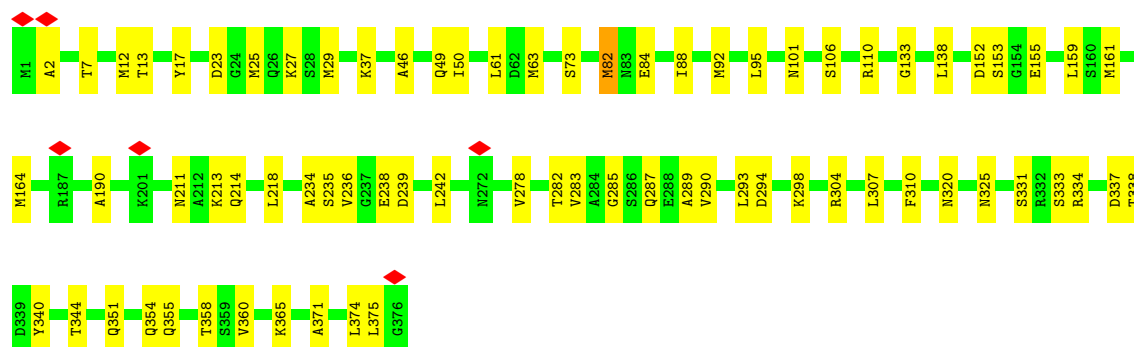


• Molecule 1: Flagellin B




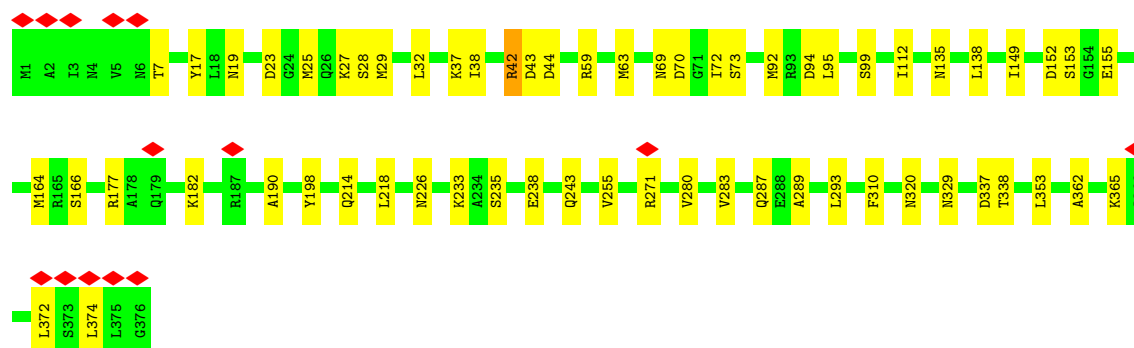
• Molecule 1: Flagellin B

Chain Q2:  80% 19%




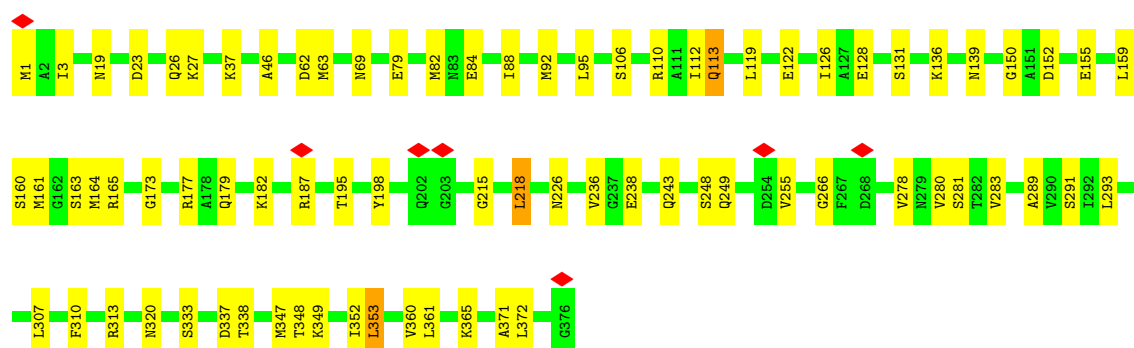
• Molecule 1: Flagellin B

Chain R2:  84% 16%




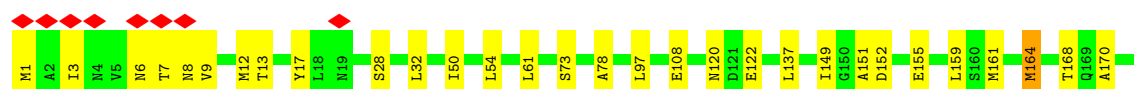
• Molecule 1: Flagellin B

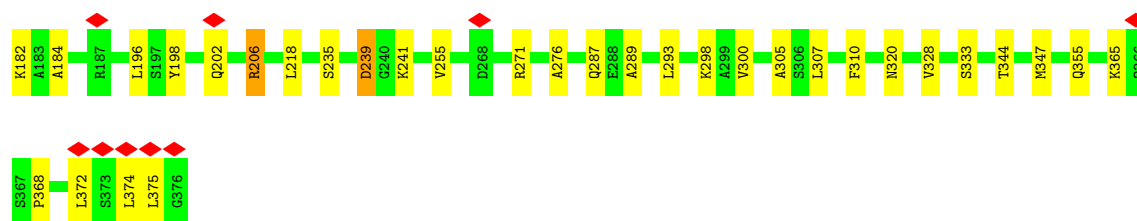
Chain S2:  79% 20%



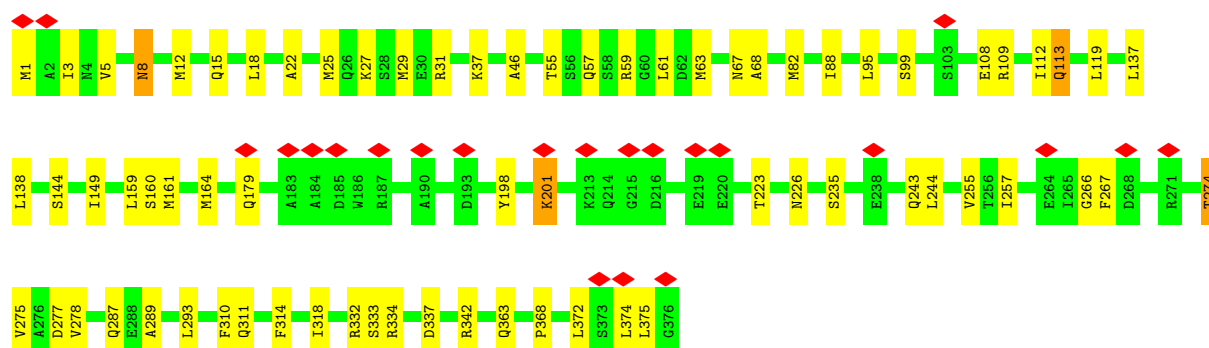
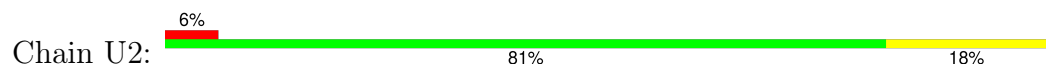
• Molecule 1: Flagellin B

Chain T2:  83% 16% 5%

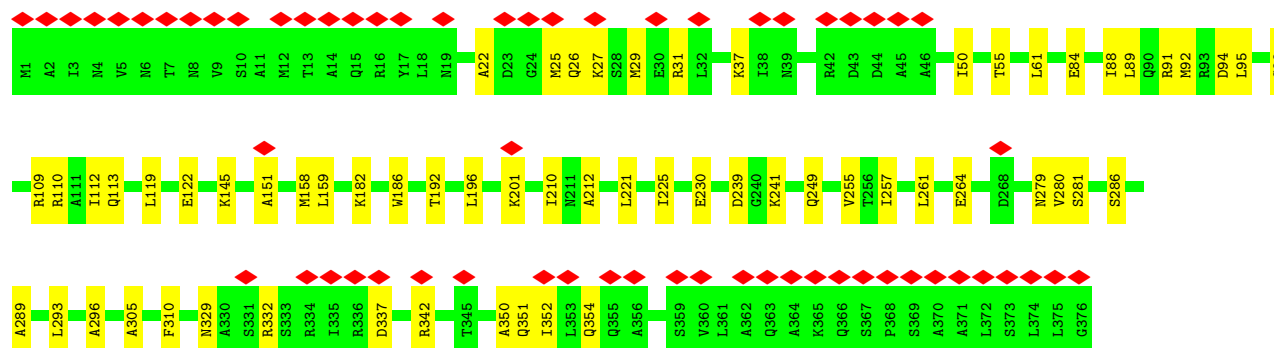
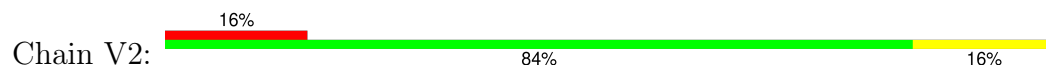




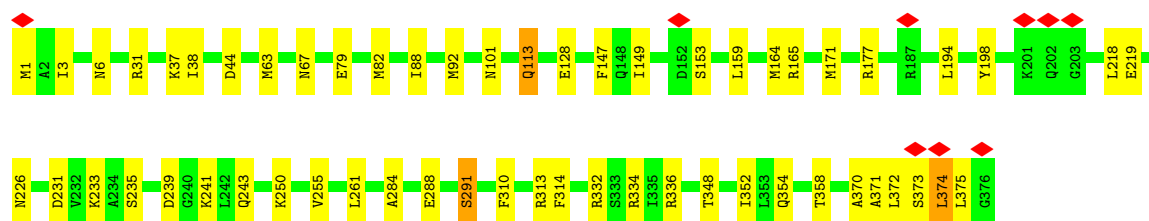
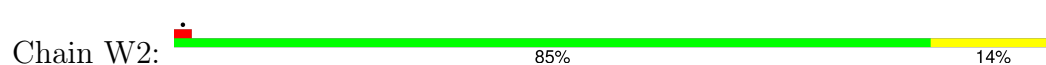
• Molecule 1: Flagellin B



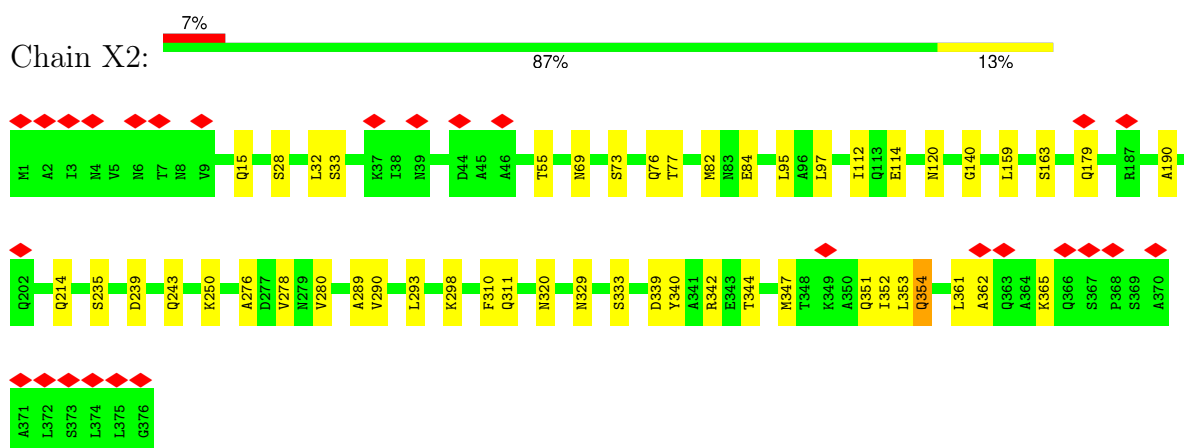
• Molecule 1: Flagellin B



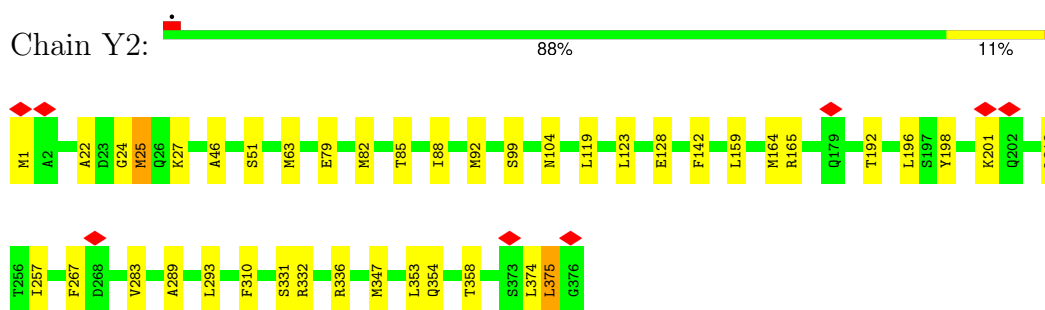
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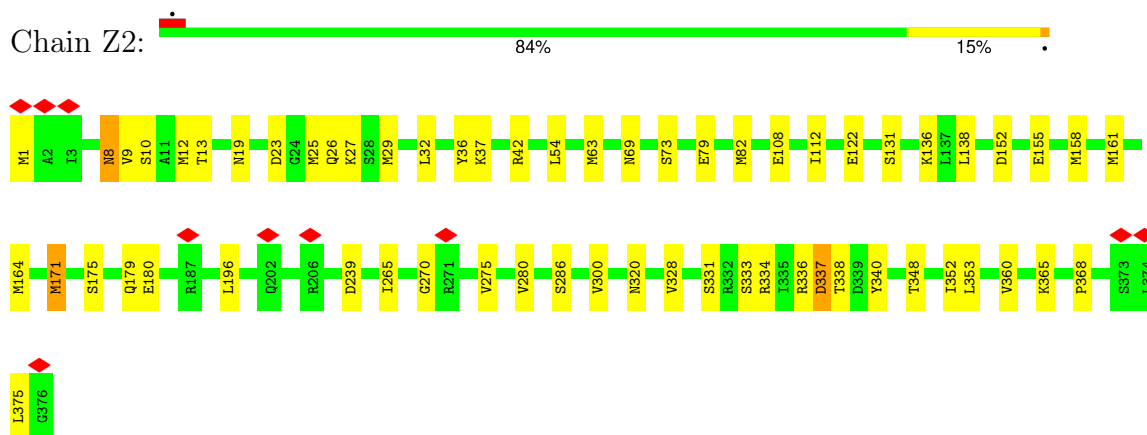
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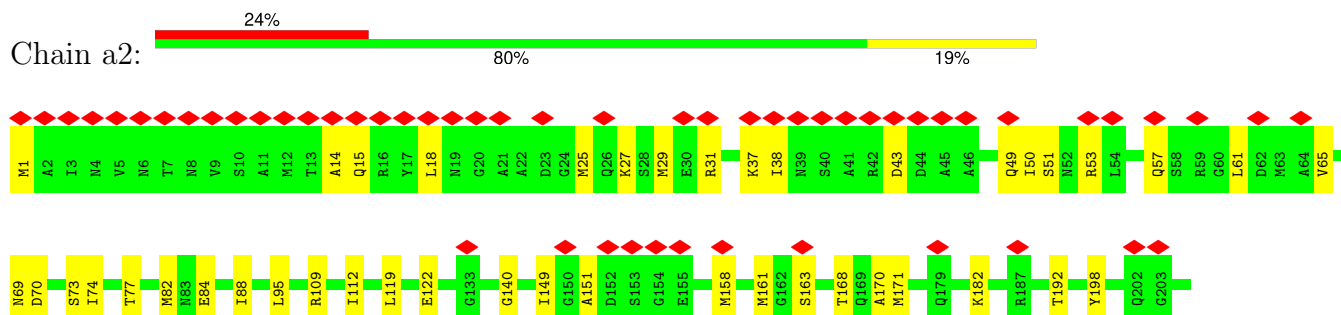
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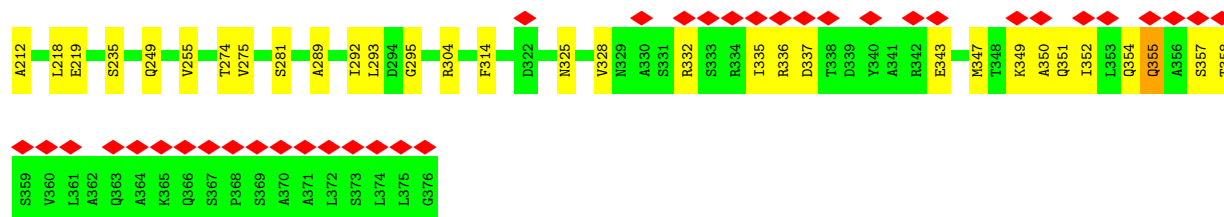


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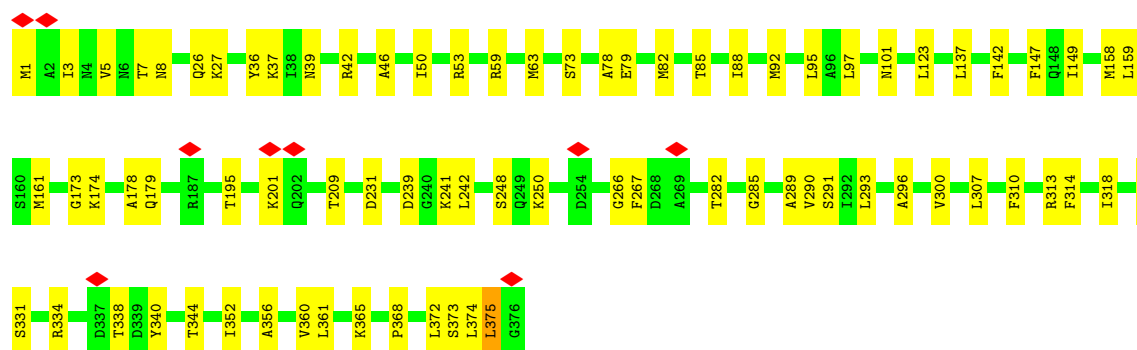
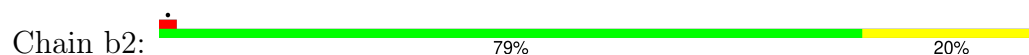


• Molecule 1: Flagellin B

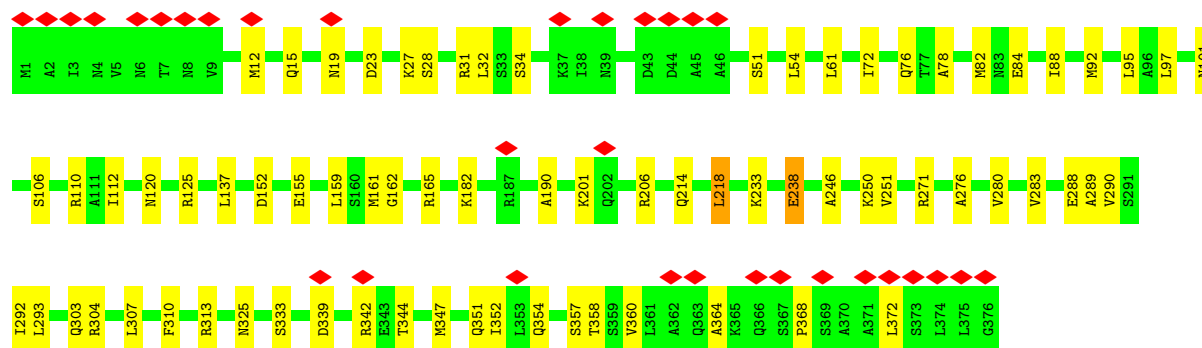
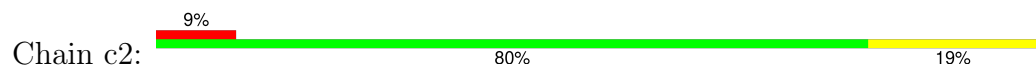




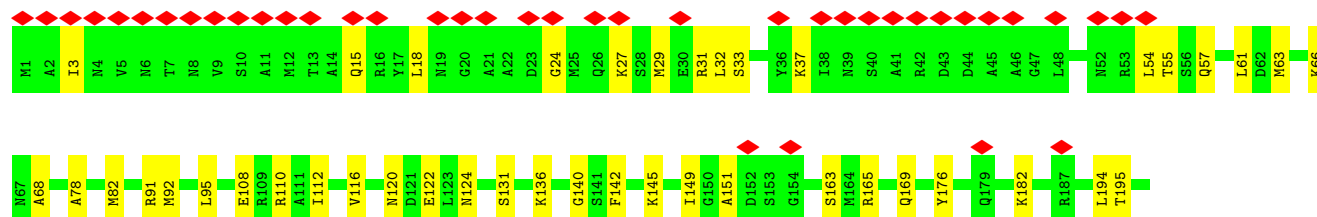
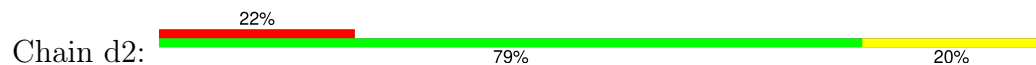
• Molecule 1: Flagellin B

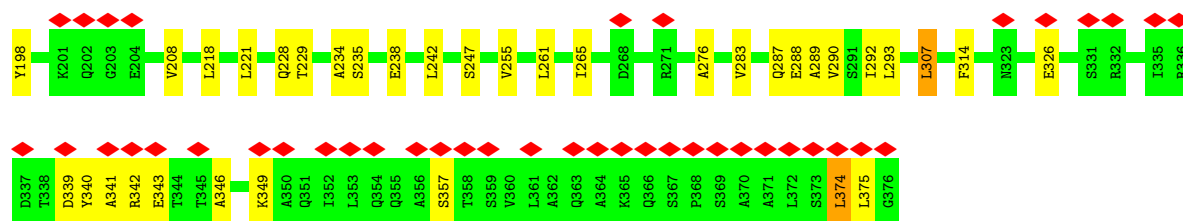


• Molecule 1: Flagellin B

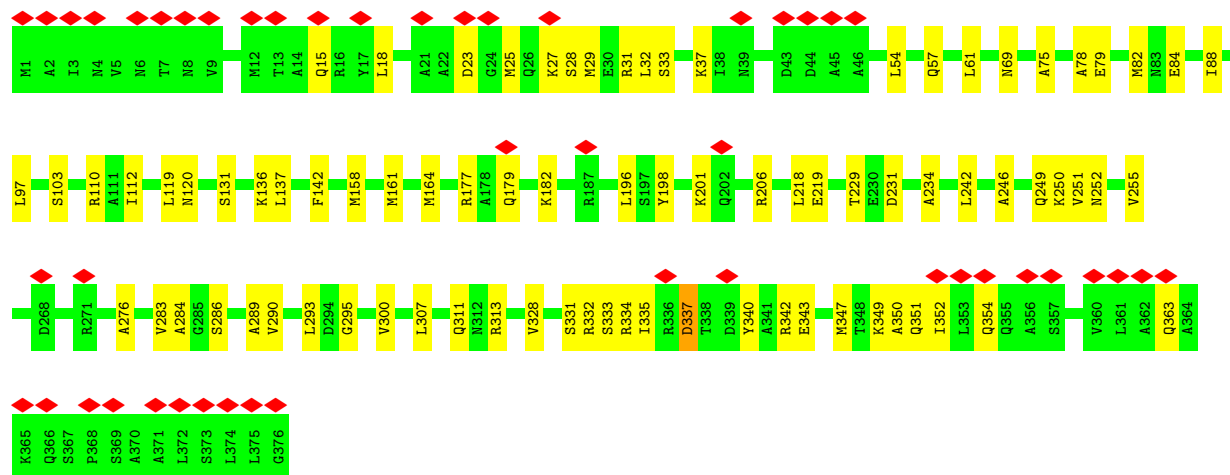
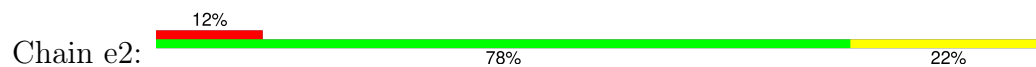


• Molecule 1: Flagellin B

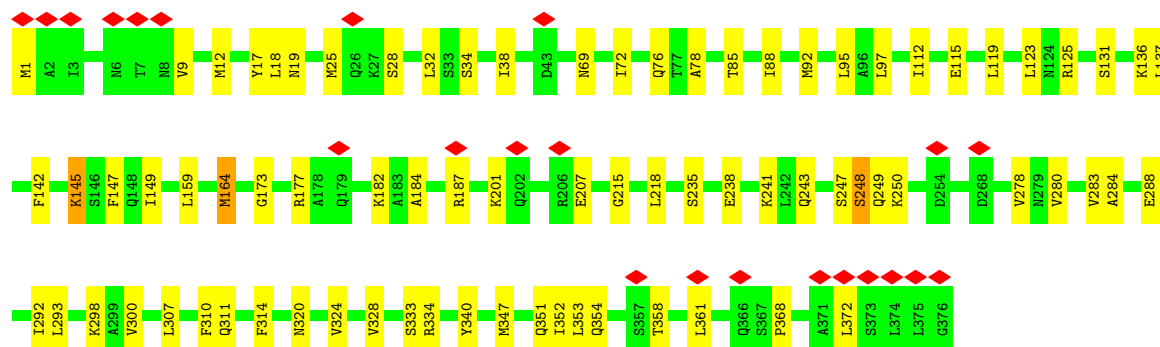
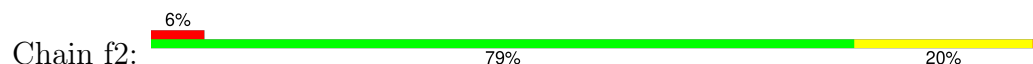




• Molecule 1: Flagellin B



• Molecule 1: Flagellin B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	468618	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	0.650	Depositor
Minimum map value	-0.372	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	478.464, 478.464, 478.464	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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	A1	0.11	0/2779	0.32	0/3738
1	A2	0.09	0/2779	0.26	0/3738
1	B2	0.09	0/2779	0.26	0/3738
1	C2	0.10	0/2779	0.30	0/3738
1	D2	0.11	0/2779	0.29	0/3738
1	E2	0.12	0/2779	0.32	1/3738 (0.0%)
1	F2	0.11	0/2779	0.32	0/3738
1	G2	0.09	0/2779	0.26	0/3738
1	H2	0.09	0/2779	0.27	0/3738
1	I2	0.11	0/2779	0.29	0/3738
1	J2	0.10	0/2779	0.27	0/3738
1	K2	0.11	0/2779	0.31	0/3738
1	L2	0.11	0/2779	0.30	0/3738
1	M2	0.12	0/2779	0.32	0/3738
1	N2	0.09	0/2779	0.27	0/3738
1	O2	0.12	0/2779	0.32	0/3738
1	P2	0.10	0/2779	0.29	0/3738
1	Q2	0.10	0/2779	0.30	0/3738
1	R2	0.09	0/2779	0.26	0/3738
1	S2	0.11	0/2779	0.29	0/3738
1	T2	0.10	0/2779	0.28	0/3738
1	U2	0.10	0/2779	0.30	0/3738
1	V2	0.11	0/2779	0.30	0/3738
1	W2	0.11	0/2779	0.32	0/3738
1	X2	0.11	0/2779	0.29	0/3738
1	Y2	0.09	0/2779	0.28	0/3738
1	Z2	0.09	0/2779	0.27	0/3738
1	a2	0.12	0/2779	0.32	0/3738
1	b2	0.10	0/2779	0.28	0/3738
1	c2	0.10	0/2779	0.31	0/3738
1	d2	0.12	0/2779	0.34	0/3738
1	e2	0.11	0/2779	0.33	0/3738
1	f2	0.10	0/2779	0.29	0/3738
All	All	0.10	0/91707	0.30	1/123354 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E2	5	VAL	N-CA-C	-5.28	108.36	113.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	2763	0	2708	49	0
1	A2	2763	0	2708	33	0
1	B2	2763	0	2708	37	0
1	C2	2763	0	2708	45	0
1	D2	2763	0	2708	43	0
1	E2	2763	0	2708	43	0
1	F2	2763	0	2708	51	0
1	G2	2763	0	2708	47	0
1	H2	2763	0	2708	52	0
1	I2	2763	0	2708	45	0
1	J2	2763	0	2708	36	0
1	K2	2763	0	2708	45	0
1	L2	2763	0	2708	49	0
1	M2	2763	0	2708	58	0
1	N2	2763	0	2708	50	0
1	O2	2763	0	2708	56	0
1	P2	2763	0	2708	50	0
1	Q2	2763	0	2708	54	0
1	R2	2763	0	2708	45	0
1	S2	2763	0	2708	55	0
1	T2	2763	0	2708	43	0
1	U2	2763	0	2708	56	0
1	V2	2763	0	2708	42	0
1	W2	2763	0	2708	49	0
1	X2	2763	0	2708	39	0
1	Y2	2763	0	2708	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z2	2763	0	2708	52	0
1	a2	2763	0	2708	56	0
1	b2	2763	0	2708	63	0
1	c2	2763	0	2708	56	0
1	d2	2763	0	2708	56	0
1	e2	2763	0	2708	59	0
1	f2	2763	0	2708	53	0
All	All	91179	0	89364	1339	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 (1339) 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)
1:L2:374:LEU:HD12	1:L2:375:LEU:HG	1.51	0.92
1:P2:37:LYS:HG3	1:P2:338:THR:HA	1.60	0.84
1:G2:63:MET:HE2	1:e2:97:LEU:HB3	1.58	0.83
1:T2:120:ASN:HD21	1:T2:276:ALA:HA	1.45	0.81
1:Y2:374:LEU:HG	1:Y2:375:LEU:HG	1.61	0.81
1:F2:95:LEU:HD12	1:F2:112:ILE:HD12	1.61	0.80
1:D2:63:MET:HE2	1:E2:97:LEU:HB3	1.65	0.79
1:Z2:8:ASN:ND2	1:Z2:8:ASN:O	2.16	0.78
1:S2:182:LYS:HB2	1:S2:218:LEU:HD21	1.64	0.78
1:G2:120:ASN:HD21	1:G2:276:ALA:HA	1.50	0.77
1:E2:54:LEU:HD12	1:E2:328:VAL:HG13	1.66	0.76
1:Q2:344:THR:HB	1:W2:375:LEU:HD12	1.68	0.76
1:F2:327:ASN:HB3	1:X2:77:THR:HG22	1.66	0.75
1:U2:8:ASN:HD21	1:U2:368:PRO:HD3	1.52	0.75
1:W2:233:LYS:HD2	1:W2:291:SER:HB3	1.69	0.74
1:S2:37:LYS:HG3	1:S2:338:THR:HA	1.69	0.74
1:e2:29:MET:HA	1:e2:32:LEU:HB2	1.67	0.74
1:c2:28:SER:HA	1:c2:31:ARG:HD2	1.69	0.73
1:F2:57:GLN:HE21	1:F2:61:LEU:HD11	1.53	0.72
1:S2:371:ALA:HB1	1:Z2:340:TYR:HD2	1.53	0.72
1:V2:95:LEU:HB3	1:V2:112:ILE:HG23	1.72	0.72
1:c2:360:VAL:HG11	1:d2:33:SER:HB3	1.70	0.71
1:C2:31:ARG:HD3	1:C2:37:LYS:HA	1.72	0.71
1:O2:73:SER:HB3	1:Q2:331:SER:HB3	1.72	0.71
1:Q2:290:VAL:HB	1:W2:153:SER:HB3	1.71	0.71
1:H2:92:MET:HA	1:H2:95:LEU:HD12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J2:120:ASN:HD21	1:J2:276:ALA:HA	1.56	0.71
1:R2:112:ILE:HD11	1:Y2:46:ALA:HB2	1.73	0.70
1:C2:95:LEU:HD12	1:C2:112:ILE:HG23	1.74	0.70
1:V2:342:ARG:HH22	1:f2:19:ASN:HD21	1.37	0.70
1:L2:37:LYS:HG3	1:L2:338:THR:HA	1.73	0.69
1:c2:120:ASN:HD21	1:c2:276:ALA:HA	1.56	0.69
1:F2:63:MET:HE2	1:F2:63:MET:HA	1.75	0.69
1:d2:339:ASP:HB3	1:d2:342:ARG:HE	1.57	0.69
1:Q2:37:LYS:HG3	1:Q2:338:THR:HA	1.73	0.69
1:G2:42:ARG:HD3	1:e2:311:GLN:HB3	1.75	0.69
1:C2:159:LEU:HD21	1:C2:161:MET:HE2	1.74	0.69
1:D2:375:LEU:HD11	1:G2:365:LYS:HZ2	1.58	0.69
1:J2:37:LYS:HG3	1:J2:338:THR:HA	1.72	0.69
1:Z2:365:LYS:HD3	1:b2:375:LEU:HD21	1.75	0.69
1:A2:233:LYS:HD2	1:A2:291:SER:HB3	1.75	0.68
1:A1:290:VAL:HB	1:R2:153:SER:HB3	1.75	0.68
1:R2:238:GLU:HG3	1:R2:283:VAL:HG12	1.76	0.68
1:L2:358:THR:HB	1:W2:374:LEU:HD22	1.76	0.68
1:C2:247:SER:HB3	1:C2:250:LYS:HD2	1.76	0.68
1:O2:30:GLU:HG3	1:Q2:13:THR:HG21	1.76	0.68
1:P2:344:THR:HG23	1:P2:347:MET:HE3	1.76	0.68
1:G2:158:MET:HE2	1:e2:219:GLU:HG2	1.76	0.68
1:I2:50:ILE:HD11	1:I2:335:ILE:HG12	1.75	0.68
1:P2:375:LEU:HB3	1:c2:344:THR:HG21	1.76	0.67
1:U2:95:LEU:HD12	1:U2:112:ILE:HG23	1.77	0.67
1:H2:46:ALA:HB2	1:X2:112:ILE:HD11	1.75	0.67
1:F2:238:GLU:HG3	1:F2:283:VAL:HG12	1.76	0.67
1:G2:331:SER:HB3	1:T2:73:SER:HB3	1.77	0.67
1:A1:361:LEU:HD23	1:M2:374:LEU:HD11	1.77	0.67
1:C2:37:LYS:HG3	1:C2:338:THR:HA	1.77	0.67
1:W2:177:ARG:HH12	1:W2:241:LYS:HD3	1.60	0.67
1:O2:63:MET:HA	1:O2:66:LYS:HB3	1.77	0.67
1:O2:238:GLU:HG3	1:O2:283:VAL:HG12	1.75	0.66
1:S2:352:ILE:HG23	1:U2:372:LEU:HD23	1.77	0.66
1:b2:37:LYS:HG3	1:b2:338:THR:HA	1.76	0.66
1:S2:131:SER:HB3	1:S2:136:LYS:HD3	1.77	0.66
1:Z2:9:VAL:HA	1:Z2:12:MET:HE3	1.77	0.66
1:B2:165:ARG:HH21	1:J2:213:LYS:HD2	1.60	0.66
1:N2:27:LYS:HD3	1:N2:42:ARG:HH22	1.61	0.66
1:I2:182:LYS:HB2	1:I2:218:LEU:HD22	1.78	0.66
1:W2:63:MET:HE3	1:W2:63:MET:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c2:201:LYS:HB3	1:c2:250:LYS:HA	1.78	0.65
1:b2:201:LYS:HB3	1:b2:250:LYS:HA	1.78	0.65
1:H2:37:LYS:HG3	1:H2:338:THR:HA	1.77	0.65
1:O2:313:ARG:HH12	1:f2:125:ARG:HD3	1.61	0.65
1:E2:365:LYS:HE2	1:Z2:375:LEU:HD21	1.79	0.65
1:T2:372:LEU:HB2	1:e2:352:ILE:HG23	1.78	0.65
1:A2:29:MET:HG3	1:A2:347:MET:HE1	1.77	0.65
1:T2:168:THR:HG22	1:T2:170:ALA:H	1.62	0.65
1:Y2:201:LYS:HA	1:Y2:201:LYS:HE2	1.79	0.65
1:a2:25:MET:HB2	1:a2:29:MET:HE1	1.79	0.65
1:D2:331:SER:HB3	1:G2:73:SER:HB3	1.77	0.65
1:J2:344:THR:HB	1:Y2:375:LEU:HD22	1.79	0.65
1:J2:65:VAL:HG23	1:J2:318:ILE:HG12	1.79	0.64
1:Q2:371:ALA:HB1	1:X2:340:TYR:HD2	1.62	0.64
1:T2:182:LYS:HB2	1:T2:218:LEU:HD22	1.78	0.64
1:f2:173:GLY:HA2	1:f2:248:SER:HB2	1.79	0.64
1:A2:153:SER:HB3	1:P2:290:VAL:HB	1.79	0.64
1:c2:246:ALA:HB1	1:c2:251:VAL:HG11	1.79	0.64
1:B2:112:ILE:H	1:B2:112:ILE:HD12	1.62	0.64
1:a2:57:GLN:HE22	1:a2:328:VAL:HG21	1.61	0.64
1:E2:352:ILE:HG13	1:G2:372:LEU:HD23	1.79	0.64
1:Z2:63:MET:HA	1:Z2:63:MET:HE3	1.79	0.64
1:F2:320:ASN:HB2	1:X2:84:GLU:HG2	1.79	0.64
1:J2:375:LEU:HD21	1:R2:362:ALA:HA	1.80	0.63
1:I2:27:LYS:HD2	1:I2:28:SER:N	2.14	0.63
1:A1:9:VAL:HA	1:A1:12:MET:HG3	1.79	0.63
1:G2:25:MET:HG2	1:G2:29:MET:HE2	1.81	0.63
1:W2:149:ILE:HG21	1:W2:314:PHE:CE1	2.34	0.63
1:d2:120:ASN:HD21	1:d2:276:ALA:HA	1.62	0.63
1:X2:95:LEU:HD22	1:X2:112:ILE:HG13	1.79	0.63
1:a2:289:ALA:HA	1:a2:292:ILE:HD12	1.80	0.63
1:e2:120:ASN:HD21	1:e2:276:ALA:HA	1.61	0.63
1:M2:50:ILE:HD11	1:M2:335:ILE:HD13	1.81	0.63
1:U2:289:ALA:O	1:U2:293:LEU:HD12	1.99	0.63
1:e2:333:SER:HA	1:e2:337:ASP:HB2	1.81	0.63
1:H2:89:LEU:HD23	1:H2:293:LEU:HD23	1.80	0.63
1:F2:37:LYS:HG3	1:F2:338:THR:HA	1.80	0.63
1:e2:28:SER:HB3	1:e2:347:MET:HB2	1.80	0.63
1:Y2:25:MET:HE2	1:Y2:347:MET:HE1	1.80	0.62
1:K2:221:LEU:HD11	1:K2:261:LEU:HD21	1.81	0.62
1:W2:374:LEU:HG	1:W2:375:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D2:375:LEU:HD21	1:G2:365:LYS:HZ1	1.64	0.62
1:a2:57:GLN:HB2	1:a2:151:ALA:HB1	1.79	0.62
1:B2:37:LYS:HG3	1:B2:338:THR:HA	1.81	0.62
1:C2:63:MET:HE2	1:b2:97:LEU:HB3	1.81	0.62
1:I2:148:GLN:HE22	1:I2:153:SER:HA	1.63	0.62
1:K2:69:ASN:HB3	1:U2:334:ARG:HD2	1.81	0.62
1:E2:30:GLU:HG3	1:Z2:13:THR:HG21	1.80	0.62
1:I2:344:THR:HA	1:I2:347:MET:HG3	1.82	0.62
1:T2:8:ASN:HD21	1:T2:365:LYS:HA	1.64	0.62
1:A1:249:GLN:HE22	1:A1:295:GLY:HA2	1.65	0.62
1:A2:198:TYR:HB3	1:A2:255:VAL:HG22	1.80	0.62
1:F2:173:GLY:HA2	1:F2:248:SER:HB2	1.81	0.62
1:H2:289:ALA:O	1:H2:293:LEU:HD12	1.99	0.62
1:S2:113:GLN:HE21	1:S2:113:GLN:C	2.07	0.62
1:E2:26:GLN:HE22	1:Z2:10:SER:HB2	1.65	0.62
1:U2:99:SER:HB2	1:U2:112:ILE:HG21	1.82	0.62
1:A2:37:LYS:HG3	1:A2:338:THR:HA	1.82	0.62
1:C2:159:LEU:HD22	1:C2:310:PHE:HE1	1.65	0.62
1:L2:12:MET:HE1	1:O2:329:ASN:HD22	1.65	0.62
1:D2:25:MET:HE1	1:D2:354:GLN:OE1	1.99	0.61
1:Y2:332:ARG:HG2	1:Y2:332:ARG:HH11	1.65	0.61
1:c2:95:LEU:HB3	1:c2:112:ILE:HG23	1.82	0.61
1:B2:73:SER:HB3	1:Y2:331:SER:HB3	1.82	0.61
1:D2:344:THR:HB	1:U2:375:LEU:HD13	1.82	0.61
1:O2:84:GLU:HG2	1:Q2:320:ASN:HB2	1.81	0.61
1:A2:374:LEU:HD11	1:H2:361:LEU:HD23	1.81	0.61
1:b2:173:GLY:HA2	1:b2:248:SER:HB2	1.82	0.61
1:X2:120:ASN:HD21	1:X2:276:ALA:HA	1.63	0.61
1:P2:238:GLU:HG3	1:P2:283:VAL:HG12	1.81	0.61
1:I2:239:ASP:HB2	1:I2:241:LYS:HD2	1.82	0.61
1:R2:37:LYS:HG3	1:R2:338:THR:HA	1.83	0.61
1:b2:195:THR:HG22	1:b2:209:THR:HG23	1.82	0.61
1:c2:357:SER:HA	1:c2:360:VAL:HG12	1.83	0.61
1:A1:214:GLN:H	1:A1:214:GLN:CD	2.09	0.61
1:P2:234:ALA:HB1	1:P2:242:LEU:HD11	1.81	0.61
1:B2:42:ARG:HH22	1:R2:72:ILE:HG23	1.66	0.61
1:D2:27:LYS:N	1:D2:27:LYS:HD3	2.15	0.61
1:B2:360:VAL:HG13	1:P2:29:MET:HG2	1.82	0.61
1:W2:31:ARG:HD3	1:W2:37:LYS:HA	1.83	0.61
1:c2:271:ARG:HG3	1:c2:271:ARG:HH11	1.65	0.61
1:D2:171:MET:HE3	1:D2:296:ALA:HB1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P2:131:SER:HB3	1:P2:136:LYS:HD3	1.83	0.61
1:e2:110:ARG:H	1:e2:110:ARG:HD2	1.65	0.61
1:M2:125:ARG:HD2	1:T2:149:ILE:HD11	1.82	0.60
1:W2:38:ILE:HG12	1:W2:44:ASP:HB2	1.82	0.60
1:G2:313:ARG:HG3	1:T2:122:GLU:HG2	1.83	0.60
1:I2:238:GLU:HG3	1:I2:283:VAL:HG12	1.81	0.60
1:T2:9:VAL:HA	1:T2:12:MET:HE3	1.83	0.60
1:e2:25:MET:HE1	1:e2:351:GLN:HG2	1.82	0.60
1:H2:360:VAL:HG23	1:Q2:29:MET:HG2	1.83	0.60
1:e2:15:GLN:HA	1:e2:18:LEU:HB2	1.83	0.60
1:A2:95:LEU:HD11	1:A2:115:GLU:HG2	1.84	0.60
1:D2:46:ALA:HB2	1:e2:112:ILE:HG12	1.83	0.60
1:H2:3:ILE:HG12	1:H2:371:ALA:HB2	1.84	0.60
1:I2:131:SER:HB3	1:I2:136:LYS:HD3	1.83	0.60
1:S2:177:ARG:HG3	1:S2:243:GLN:HB3	1.83	0.60
1:f2:164:MET:HE3	1:f2:300:VAL:HG22	1.82	0.60
1:C2:3:ILE:HG22	1:b2:340:TYR:HB2	1.83	0.60
1:N2:158:MET:HE1	1:T2:184:ALA:HA	1.84	0.60
1:R2:95:LEU:HB3	1:R2:112:ILE:HG23	1.83	0.60
1:H2:42:ARG:HH11	1:H2:42:ARG:HG2	1.68	0.59
1:M2:177:ARG:HH12	1:M2:284:ALA:HB1	1.67	0.59
1:V2:92:MET:HB3	1:V2:293:LEU:HD13	1.84	0.59
1:A1:110:ARG:HH11	1:A1:281:SER:HB3	1.67	0.59
1:B2:164:MET:HE3	1:B2:300:VAL:HG22	1.83	0.59
1:A2:375:LEU:HD13	1:P2:344:THR:HB	1.85	0.59
1:E2:173:GLY:HA2	1:E2:248:SER:HB2	1.83	0.59
1:a2:82:MET:HG2	1:a2:304:ARG:HG3	1.83	0.59
1:G2:365:LYS:H	1:G2:365:LYS:HD3	1.67	0.59
1:K2:247:SER:HB3	1:K2:250:LYS:HE2	1.84	0.59
1:a2:51:SER:HB2	1:a2:336:ARG:HD3	1.85	0.59
1:a2:198:TYR:HB3	1:a2:255:VAL:HG22	1.84	0.59
1:G2:79:GLU:HA	1:G2:82:MET:HE3	1.84	0.59
1:K2:92:MET:HA	1:K2:95:LEU:HD12	1.85	0.59
1:Q2:7:THR:HG21	1:X2:333:SER:HB2	1.85	0.59
1:R2:92:MET:HB3	1:R2:293:LEU:HD13	1.85	0.58
1:U2:235:SER:HB3	1:U2:287:GLN:HB3	1.85	0.58
1:E2:33:SER:HB3	1:Z2:360:VAL:HG11	1.84	0.58
1:N2:63:MET:C	1:N2:63:MET:HE3	2.28	0.58
1:G2:37:LYS:HG3	1:G2:338:THR:HA	1.85	0.58
1:I2:95:LEU:HB3	1:I2:112:ILE:HG23	1.86	0.58
1:M2:177:ARG:HE	1:M2:241:LYS:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F2:177:ARG:HD3	1:F2:241:LYS:HD3	1.84	0.58
1:K2:69:ASN:O	1:K2:72:ILE:HG22	2.04	0.58
1:U2:149:ILE:HG21	1:U2:314:PHE:HE1	1.68	0.58
1:X2:351:GLN:HA	1:X2:354:GLN:HG3	1.83	0.58
1:d2:149:ILE:HG21	1:d2:314:PHE:HE2	1.67	0.58
1:J2:375:LEU:HD13	1:R2:365:LYS:HZ2	1.68	0.58
1:M2:249:GLN:HG2	1:M2:250:LYS:HG3	1.86	0.58
1:O2:149:ILE:HD11	1:f2:125:ARG:HD2	1.85	0.58
1:C2:375:LEU:HD13	1:b2:344:THR:HB	1.85	0.58
1:E2:320:ASN:HB2	1:e2:84:GLU:HG2	1.86	0.58
1:F2:31:ARG:HD3	1:F2:37:LYS:HA	1.85	0.58
1:f2:112:ILE:HG22	1:f2:280:VAL:HG21	1.86	0.58
1:D2:9:VAL:HA	1:D2:12:MET:HG3	1.84	0.58
1:M2:246:ALA:HB1	1:M2:251:VAL:HG21	1.86	0.58
1:a2:249:GLN:HE22	1:a2:295:GLY:HA2	1.69	0.58
1:d2:92:MET:HG2	1:d2:293:LEU:HD21	1.85	0.58
1:e2:142:PHE:HD2	1:e2:161:MET:HG3	1.69	0.58
1:L2:9:VAL:HA	1:L2:12:MET:HB2	1.86	0.58
1:Q2:340:TYR:HB2	1:W2:3:ILE:HG23	1.86	0.58
1:e2:54:LEU:HG	1:e2:328:VAL:HG13	1.85	0.57
1:F2:182:LYS:HB2	1:F2:218:LEU:HD22	1.86	0.57
1:K2:173:GLY:HA2	1:K2:248:SER:HB2	1.84	0.57
1:V2:26:GLN:HA	1:V2:29:MET:HE1	1.85	0.57
1:D2:214:GLN:CD	1:D2:214:GLN:H	2.12	0.57
1:D2:334:ARG:HD2	1:G2:69:ASN:HB3	1.86	0.57
1:E2:360:VAL:HG11	1:e2:33:SER:HB3	1.86	0.57
1:X2:112:ILE:HG22	1:X2:280:VAL:HG21	1.86	0.57
1:D2:374:LEU:HG	1:D2:375:LEU:HD12	1.85	0.57
1:K2:365:LYS:HZ1	1:U2:375:LEU:HD21	1.68	0.57
1:M2:120:ASN:HD21	1:M2:276:ALA:HA	1.69	0.57
1:Q2:92:MET:HB2	1:Q2:293:LEU:HD21	1.85	0.57
1:W2:149:ILE:HD13	1:W2:314:PHE:HE1	1.69	0.57
1:A1:238:GLU:HG3	1:A1:283:VAL:HG12	1.85	0.57
1:P2:25:MET:HE1	1:P2:354:GLN:OE1	2.04	0.57
1:L2:375:LEU:HD13	1:b2:365:LYS:HD2	1.87	0.57
1:N2:149:ILE:HD13	1:N2:314:PHE:HE1	1.70	0.57
1:F2:38:ILE:HG22	1:F2:43:ASP:HB2	1.85	0.57
1:J2:29:MET:HG2	1:N2:360:VAL:HG13	1.87	0.57
1:b2:374:LEU:HD23	1:b2:375:LEU:HB2	1.87	0.57
1:f2:177:ARG:HH12	1:f2:284:ALA:HB1	1.69	0.57
1:R2:182:LYS:HB2	1:R2:218:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W2:243:GLN:HE22	1:W2:284:ALA:HA	1.70	0.56
1:W2:370:ALA:O	1:W2:374:LEU:HB3	2.05	0.56
1:Z2:69:ASN:HB3	1:b2:334:ARG:HD2	1.85	0.56
1:E2:109:ARG:HH21	1:E2:283:VAL:HG22	1.70	0.56
1:N2:234:ALA:HB1	1:N2:242:LEU:HD11	1.87	0.56
1:O2:372:LEU:HD23	1:X2:352:ILE:HG13	1.88	0.56
1:b2:63:MET:HE2	1:f2:97:LEU:HB3	1.88	0.56
1:E2:190:ALA:HA	1:E2:214:GLN:HE22	1.70	0.56
1:I2:73:SER:HB3	1:f2:334:ARG:HH12	1.71	0.56
1:J2:334:ARG:HD2	1:R2:69:ASN:HB3	1.86	0.56
1:M2:361:LEU:HD23	1:T2:374:LEU:HD11	1.87	0.56
1:P2:31:ARG:HD3	1:P2:37:LYS:HA	1.88	0.56
1:V2:239:ASP:HB2	1:V2:241:LYS:HD2	1.87	0.56
1:A1:95:LEU:HB3	1:A1:112:ILE:HG23	1.86	0.56
1:A1:131:SER:HB3	1:A1:136:LYS:HD3	1.87	0.56
1:R2:23:ASP:HB3	1:R2:27:LYS:HZ1	1.71	0.56
1:f2:235:SER:HB2	1:f2:243:GLN:HE21	1.70	0.56
1:N2:198:TYR:HB3	1:N2:255:VAL:HG22	1.88	0.56
1:R2:38:ILE:HD11	1:R2:44:ASP:HB2	1.88	0.56
1:S2:136:LYS:HB3	1:S2:139:ASN:HD21	1.70	0.56
1:H2:349:LYS:HE2	1:W2:6:ASN:HA	1.87	0.56
1:K2:233:LYS:HD2	1:K2:291:SER:HB3	1.87	0.56
1:O2:324:VAL:O	1:O2:328:VAL:HG12	2.06	0.56
1:c2:112:ILE:HG22	1:c2:280:VAL:HG21	1.86	0.56
1:K2:201:LYS:HE2	1:K2:252:ASN:HB3	1.88	0.56
1:M2:342:ARG:HB2	1:M2:342:ARG:NH1	2.21	0.56
1:O2:198:TYR:HB3	1:O2:255:VAL:HG22	1.88	0.56
1:e2:27:LYS:HD3	1:e2:27:LYS:N	2.20	0.56
1:M2:352:ILE:HG13	1:R2:372:LEU:HD23	1.88	0.56
1:O2:188:VAL:HG23	1:O2:214:GLN:HA	1.88	0.56
1:D2:122:GLU:HG2	1:S2:313:ARG:HG3	1.89	0.55
1:L2:361:LEU:HD23	1:W2:374:LEU:HD11	1.86	0.55
1:S2:198:TYR:HB3	1:S2:255:VAL:HG22	1.88	0.55
1:Z2:73:SER:HB2	1:b2:331:SER:HB3	1.87	0.55
1:K2:365:LYS:NZ	1:U2:375:LEU:HD21	2.21	0.55
1:B2:168:THR:HG22	1:B2:170:ALA:H	1.71	0.55
1:Z2:164:MET:HE3	1:Z2:164:MET:HA	1.89	0.55
1:a2:61:LEU:HD12	1:a2:151:ALA:HB2	1.88	0.55
1:d2:142:PHE:HE2	1:d2:145:LYS:HD2	1.71	0.55
1:V2:55:THR:HG23	1:V2:332:ARG:HH22	1.71	0.55
1:Y2:198:TYR:HB3	1:Y2:255:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q2:289:ALA:O	1:Q2:293:LEU:HD12	2.06	0.55
1:S2:289:ALA:O	1:S2:293:LEU:HG	2.07	0.55
1:H2:331:SER:HB2	1:Q2:73:SER:HB3	1.87	0.55
1:I2:112:ILE:HG22	1:I2:280:VAL:HG21	1.88	0.55
1:T2:164:MET:HE1	1:T2:300:VAL:HA	1.87	0.55
1:c2:344:THR:HA	1:c2:347:MET:HG3	1.86	0.55
1:B2:187:ARG:HB3	1:B2:215:GLY:HA2	1.89	0.55
1:K2:12:MET:HA	1:K2:15:GLN:HE21	1.72	0.55
1:Z2:29:MET:HG2	1:b2:360:VAL:HG13	1.87	0.55
1:S2:82:MET:HE1	1:S2:307:LEU:HD13	1.89	0.55
1:C2:313:ARG:HG3	1:S2:122:GLU:HG2	1.89	0.55
1:C2:372:LEU:HB2	1:L2:352:ILE:HG23	1.88	0.55
1:N2:233:LYS:HD2	1:N2:291:SER:HB3	1.90	0.55
1:R2:177:ARG:HH11	1:R2:271:ARG:HH21	1.55	0.55
1:Y2:63:MET:N	1:Y2:63:MET:HE2	2.21	0.55
1:Z2:122:GLU:HG2	1:b2:313:ARG:HG3	1.89	0.55
1:D2:375:LEU:HD11	1:G2:365:LYS:NZ	2.22	0.54
1:E2:368:PRO:HB2	1:I2:352:ILE:HD13	1.89	0.54
1:O2:246:ALA:HB1	1:O2:251:VAL:HG21	1.88	0.54
1:A1:125:ARG:HD2	1:M2:149:ILE:HD11	1.89	0.54
1:H2:18:LEU:HD13	1:H2:357:SER:HB2	1.89	0.54
1:a2:69:ASN:HB3	1:e2:334:ARG:HD2	1.87	0.54
1:a2:347:MET:HE3	1:a2:347:MET:O	2.07	0.54
1:G2:371:ALA:HB1	1:e2:340:TYR:HD2	1.72	0.54
1:L2:354:GLN:O	1:L2:358:THR:HG22	2.07	0.54
1:Z2:79:GLU:HA	1:Z2:82:MET:HE3	1.89	0.54
1:a2:158:MET:HE3	1:a2:158:MET:HA	1.89	0.54
1:d2:95:LEU:HB3	1:d2:112:ILE:HG23	1.90	0.54
1:H2:88:ILE:HG23	1:H2:119:LEU:HD22	1.88	0.54
1:Q2:235:SER:HB3	1:Q2:287:GLN:HB3	1.89	0.54
1:b2:79:GLU:HA	1:b2:82:MET:HE3	1.89	0.54
1:F2:69:ASN:HB3	1:P2:334:ARG:HD2	1.89	0.54
1:Y2:88:ILE:HG23	1:Y2:119:LEU:HD22	1.89	0.54
1:b2:159:LEU:HB2	1:b2:310:PHE:CE1	2.43	0.54
1:d2:15:GLN:HA	1:d2:18:LEU:HD12	1.88	0.54
1:G2:333:SER:HA	1:G2:337:ASP:OD2	2.08	0.54
1:S2:164:MET:HE2	1:S2:300:VAL:HG22	1.89	0.54
1:U2:274:THR:H	1:U2:277:ASP:HB3	1.73	0.54
1:C2:159:LEU:HD13	1:C2:310:PHE:HD1	1.72	0.54
1:D2:82:MET:HG2	1:D2:304:ARG:HG3	1.89	0.54
1:I2:344:THR:HB	1:Z2:375:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P2:108:GLU:CD	1:P2:108:GLU:H	2.16	0.54
1:O2:289:ALA:O	1:O2:293:LEU:HG	2.08	0.54
1:O2:333:SER:HA	1:O2:337:ASP:OD2	2.08	0.54
1:a2:168:THR:HG22	1:a2:170:ALA:H	1.73	0.54
1:G2:152:ASP:O	1:G2:155:GLU:HG3	2.08	0.53
1:J2:91:ARG:HH21	1:J2:95:LEU:HD21	1.72	0.53
1:O2:362:ALA:HA	1:O2:365:LYS:HE2	1.89	0.53
1:P2:289:ALA:O	1:P2:293:LEU:HG	2.08	0.53
1:d2:234:ALA:HB1	1:d2:242:LEU:HD11	1.89	0.53
1:N2:49:GLN:HE22	1:T2:305:ALA:HB2	1.73	0.53
1:X2:235:SER:HB2	1:X2:243:GLN:HE21	1.73	0.53
1:F2:15:GLN:HA	1:F2:18:LEU:HB3	1.89	0.53
1:J2:333:SER:HA	1:J2:337:ASP:OD2	2.07	0.53
1:J2:344:THR:HG21	1:Y2:375:LEU:HB2	1.91	0.53
1:K2:187:ARG:HH12	1:K2:217:ASP:HB3	1.72	0.53
1:Y2:289:ALA:O	1:Y2:293:LEU:HG	2.07	0.53
1:e2:332:ARG:NH1	1:e2:332:ARG:HB3	2.24	0.53
1:L2:122:GLU:HG2	1:W2:313:ARG:HG3	1.90	0.53
1:L2:282:THR:HG23	1:L2:285:GLY:H	1.74	0.53
1:O2:352:ILE:HG23	1:b2:372:LEU:HD13	1.90	0.53
1:U2:27:LYS:O	1:U2:27:LYS:HD3	2.08	0.53
1:U2:257:ILE:HG21	1:U2:267:PHE:CD1	2.43	0.53
1:W2:374:LEU:HG	1:W2:375:LEU:CD2	2.38	0.53
1:A1:92:MET:HB3	1:A1:293:LEU:HD13	1.90	0.53
1:C2:46:ALA:HB1	1:Z2:108:GLU:HB3	1.88	0.53
1:O2:82:MET:HE1	1:O2:303:GLN:OE1	2.09	0.53
1:V2:99:SER:HB2	1:V2:112:ILE:HG13	1.90	0.53
1:Z2:138:LEU:HD13	1:Z2:164:MET:HG2	1.91	0.53
1:e2:27:LYS:HD3	1:e2:27:LYS:H	1.74	0.53
1:e2:97:LEU:HD22	1:e2:290:VAL:HG22	1.91	0.53
1:N2:159:LEU:HB2	1:N2:310:PHE:CE1	2.44	0.53
1:O2:54:LEU:HD22	1:O2:328:VAL:HG23	1.90	0.53
1:P2:356:ALA:O	1:P2:360:VAL:HG23	2.09	0.53
1:U2:22:ALA:HA	1:U2:25:MET:HE3	1.90	0.53
1:V2:25:MET:HE1	1:V2:351:GLN:HG2	1.89	0.53
1:E2:84:GLU:HG2	1:Z2:320:ASN:HB2	1.91	0.53
1:K2:234:ALA:HB1	1:K2:242:LEU:HD11	1.91	0.53
1:L2:63:MET:HE3	1:L2:63:MET:O	2.09	0.53
1:f2:92:MET:HB2	1:f2:293:LEU:HD21	1.90	0.53
1:E2:78:ALA:HB1	1:E2:161:MET:HE1	1.91	0.53
1:Q2:333:SER:HA	1:Q2:337:ASP:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T2:28:SER:O	1:T2:32:LEU:HD12	2.08	0.53
1:b2:282:THR:HG23	1:b2:285:GLY:H	1.73	0.53
1:c2:182:LYS:HB2	1:c2:218:LEU:HD22	1.91	0.53
1:H2:164:MET:HG3	1:H2:171:MET:HE3	1.89	0.52
1:K2:177:ARG:HH22	1:K2:237:GLY:HA3	1.73	0.52
1:M2:368:PRO:HB2	1:a2:352:ILE:HD13	1.91	0.52
1:O2:25:MET:HE1	1:O2:354:GLN:OE1	2.09	0.52
1:U2:149:ILE:HD13	1:U2:314:PHE:CE1	2.44	0.52
1:d2:63:MET:HA	1:d2:66:LYS:HB2	1.91	0.52
1:F2:368:PRO:HB2	1:c2:352:ILE:HG21	1.92	0.52
1:K2:159:LEU:HB2	1:K2:310:PHE:CE1	2.45	0.52
1:d2:142:PHE:CE2	1:d2:145:LYS:HD2	2.45	0.52
1:L2:314:PHE:O	1:L2:318:ILE:HD12	2.10	0.52
1:b2:3:ILE:HG22	1:f2:340:TYR:HB2	1.90	0.52
1:C2:63:MET:HE3	1:C2:63:MET:C	2.35	0.52
1:M2:289:ALA:O	1:M2:293:LEU:HD12	2.09	0.52
1:a2:192:THR:HB	1:a2:212:ALA:HB3	1.92	0.52
1:F2:249:GLN:HE21	1:F2:298:LYS:HD2	1.74	0.52
1:F2:344:THR:HG22	1:Q2:365:LYS:HE2	1.91	0.52
1:W2:38:ILE:HD12	1:W2:336:ARG:HA	1.91	0.52
1:d2:194:LEU:HB2	1:d2:261:LEU:HB3	1.90	0.52
1:O2:112:ILE:HG22	1:O2:280:VAL:HG21	1.91	0.52
1:W2:194:LEU:HB2	1:W2:261:LEU:HB3	1.90	0.52
1:d2:68:ALA:HB2	1:d2:149:ILE:HG22	1.91	0.52
1:e2:54:LEU:HD23	1:e2:332:ARG:HG2	1.91	0.52
1:D2:368:PRO:HB2	1:Z2:352:ILE:HG13	1.91	0.52
1:D2:101:ASN:HD22	1:U2:67:ASN:HB3	1.75	0.52
1:K2:365:LYS:HD3	1:U2:375:LEU:HD11	1.91	0.52
1:M2:95:LEU:HD12	1:M2:112:ILE:HG23	1.91	0.52
1:O2:374:LEU:HD11	1:f2:361:LEU:HD23	1.91	0.52
1:Q2:92:MET:HA	1:Q2:95:LEU:HD12	1.92	0.52
1:T2:61:LEU:HD23	1:T2:151:ALA:HB2	1.91	0.52
1:G2:95:LEU:HB3	1:G2:112:ILE:HG23	1.92	0.52
1:U2:159:LEU:HB2	1:U2:310:PHE:CE1	2.45	0.52
1:a2:332:ARG:HG3	1:a2:332:ARG:HH11	1.74	0.52
1:C2:159:LEU:HD13	1:C2:310:PHE:CD1	2.46	0.51
1:F2:104:ASN:HB3	1:F2:108:GLU:HB2	1.92	0.51
1:Q2:138:LEU:HD23	1:Q2:164:MET:HG2	1.91	0.51
1:M2:3:ILE:HG13	1:M2:371:ALA:HB1	1.93	0.51
1:c2:351:GLN:HA	1:c2:354:GLN:HE21	1.75	0.51
1:A2:12:MET:HA	1:A2:15:GLN:HE21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K2:332:ARG:HD2	1:K2:336:ARG:HG2	1.92	0.51
1:Q2:190:ALA:HA	1:Q2:214:GLN:HE22	1.76	0.51
1:a2:149:ILE:HG21	1:a2:314:PHE:HE1	1.74	0.51
1:Q2:61:LEU:HD13	1:Q2:325:ASN:HA	1.93	0.51
1:S2:333:SER:HA	1:S2:337:ASP:HB2	1.93	0.51
1:a2:88:ILE:HG23	1:a2:119:LEU:HD13	1.92	0.51
1:W2:332:ARG:HG2	1:W2:332:ARG:HH11	1.76	0.51
1:X2:289:ALA:O	1:X2:293:LEU:HG	2.11	0.51
1:c2:313:ARG:HG3	1:d2:122:GLU:OE2	2.10	0.51
1:A2:243:GLN:HE22	1:A2:284:ALA:HA	1.76	0.51
1:W2:82:MET:HG2	1:W2:164:MET:HE1	1.91	0.51
1:D2:356:ALA:O	1:D2:360:VAL:HG23	2.11	0.51
1:J2:54:LEU:HD22	1:J2:328:VAL:HG13	1.91	0.51
1:O2:37:LYS:HG3	1:O2:338:THR:HA	1.91	0.51
1:d2:288:GLU:O	1:d2:292:ILE:HG13	2.10	0.51
1:C2:82:MET:HG2	1:C2:164:MET:HE2	1.93	0.51
1:H2:42:ARG:HG2	1:H2:42:ARG:NH1	2.25	0.51
1:L2:375:LEU:HD12	1:O2:344:THR:HB	1.92	0.51
1:V2:61:LEU:HD12	1:V2:151:ALA:HB2	1.92	0.51
1:b2:53:ARG:HH12	1:f2:298:LYS:HD3	1.76	0.51
1:e2:182:LYS:HB2	1:e2:218:LEU:HD22	1.92	0.51
1:D2:137:LEU:HB2	1:D2:138:LEU:HD12	1.93	0.51
1:E2:334:ARG:HD2	1:e2:69:ASN:HB3	1.91	0.51
1:Q2:82:MET:HG2	1:Q2:304:ARG:HG3	1.92	0.51
1:V2:91:ARG:O	1:V2:95:LEU:HD22	2.10	0.51
1:a2:38:ILE:HG23	1:a2:43:ASP:HB2	1.93	0.51
1:f2:159:LEU:HB2	1:f2:310:PHE:CZ	2.46	0.51
1:A1:15:GLN:HA	1:A1:18:LEU:HD12	1.93	0.51
1:F2:340:TYR:CD2	1:H2:371:ALA:HB1	2.45	0.51
1:F2:374:LEU:HD11	1:X2:361:LEU:HD23	1.93	0.51
1:X2:190:ALA:HA	1:X2:214:GLN:HE22	1.75	0.51
1:G2:344:THR:HG21	1:K2:375:LEU:HB3	1.92	0.50
1:I2:112:ILE:HG13	1:b2:46:ALA:HB2	1.92	0.50
1:J2:361:LEU:HD23	1:N2:374:LEU:HD11	1.93	0.50
1:L2:116:VAL:HG21	1:L2:280:VAL:HG21	1.92	0.50
1:Q2:234:ALA:HB1	1:Q2:242:LEU:HD11	1.93	0.50
1:a2:61:LEU:HD22	1:a2:325:ASN:HB3	1.93	0.50
1:b2:158:MET:HE1	1:f2:184:ALA:HA	1.92	0.50
1:c2:61:LEU:HD13	1:c2:325:ASN:HA	1.94	0.50
1:c2:97:LEU:HD13	1:c2:290:VAL:HG21	1.93	0.50
1:E2:198:TYR:HB3	1:E2:255:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I2:142:PHE:CE2	1:I2:145:LYS:HE3	2.47	0.50
1:X2:342:ARG:NH1	1:X2:342:ARG:HB2	2.25	0.50
1:L2:168:THR:HG22	1:L2:170:ALA:H	1.77	0.50
1:M2:108:GLU:O	1:M2:112:ILE:HD12	2.11	0.50
1:S2:88:ILE:HG23	1:S2:119:LEU:HD12	1.92	0.50
1:S2:122:GLU:O	1:S2:126:ILE:HG12	2.11	0.50
1:e2:88:ILE:HG23	1:e2:119:LEU:HD22	1.93	0.50
1:O2:368:PRO:HB2	1:X2:352:ILE:HG12	1.92	0.50
1:Q2:12:MET:HE1	1:X2:329:ASN:HD22	1.75	0.50
1:b2:36:TYR:HB2	1:b2:39:ASN:ND2	2.27	0.50
1:A1:19:ASN:HA	1:M2:1:MET:H1	1.77	0.50
1:H2:213:LYS:HG3	1:W2:165:ARG:NH2	2.27	0.50
1:W2:149:ILE:HG21	1:W2:314:PHE:HE1	1.76	0.50
1:Y2:51:SER:HB2	1:Y2:336:ARG:HD2	1.92	0.50
1:a2:109:ARG:HB3	1:a2:281:SER:HA	1.93	0.50
1:f2:238:GLU:HG3	1:f2:283:VAL:HG12	1.92	0.50
1:f2:351:GLN:O	1:f2:354:GLN:HG3	2.11	0.50
1:A1:84:GLU:O	1:A1:88:ILE:HG13	2.12	0.50
1:L2:85:THR:HG23	1:L2:123:LEU:HD22	1.94	0.50
1:O2:355:GLN:HB2	1:b2:372:LEU:HD12	1.93	0.50
1:e2:350:ALA:O	1:e2:354:GLN:HG2	2.12	0.50
1:E2:289:ALA:O	1:E2:293:LEU:HG	2.12	0.50
1:P2:9:VAL:HA	1:P2:12:MET:HE3	1.92	0.50
1:C2:67:ASN:ND2	1:b2:101:ASN:HB2	2.27	0.50
1:D2:289:ALA:O	1:D2:293:LEU:HG	2.12	0.50
1:U2:12:MET:HA	1:U2:15:GLN:HE21	1.77	0.50
1:U2:333:SER:HA	1:U2:337:ASP:OD2	2.12	0.50
1:D2:32:LEU:HB3	1:S2:360:VAL:HG21	1.94	0.50
1:F2:247:SER:HB2	1:F2:249:GLN:OE1	2.12	0.50
1:H2:85:THR:HG23	1:H2:123:LEU:HD22	1.94	0.50
1:L2:333:SER:HA	1:L2:337:ASP:HB2	1.93	0.50
1:a2:122:GLU:OE2	1:e2:313:ARG:HG3	2.11	0.50
1:b2:92:MET:HA	1:b2:95:LEU:HD12	1.94	0.50
1:J2:73:SER:HB3	1:N2:331:SER:HB2	1.94	0.49
1:L2:159:LEU:HB2	1:L2:310:PHE:CE2	2.47	0.49
1:Q2:2:ALA:HB1	1:X2:339:ASP:HB2	1.93	0.49
1:V2:196:LEU:HD23	1:V2:257:ILE:HG12	1.94	0.49
1:L2:238:GLU:HG3	1:L2:283:VAL:HG12	1.95	0.49
1:Q2:152:ASP:O	1:Q2:155:GLU:HG3	2.12	0.49
1:S2:92:MET:HA	1:S2:95:LEU:HD12	1.94	0.49
1:a2:15:GLN:HA	1:a2:18:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f2:9:VAL:HA	1:f2:12:MET:HG3	1.93	0.49
1:G2:88:ILE:O	1:G2:92:MET:HG3	2.12	0.49
1:I2:58:SER:HA	1:I2:61:LEU:HD23	1.94	0.49
1:L2:46:ALA:O	1:L2:50:ILE:HG22	2.13	0.49
1:Q2:88:ILE:O	1:Q2:92:MET:HG3	2.12	0.49
1:C2:9:VAL:HG11	1:b2:330:ALA:HB2	1.93	0.49
1:I2:99:SER:HB3	1:I2:112:ILE:HD13	1.94	0.49
1:J2:5:VAL:HA	1:J2:368:PRO:HB3	1.95	0.49
1:K2:231:ASP:HA	1:K2:250:LYS:HE3	1.94	0.49
1:M2:372:LEU:HD11	1:a2:355:GLN:HG3	1.93	0.49
1:P2:63:MET:HE2	1:c2:97:LEU:HB3	1.94	0.49
1:R2:289:ALA:O	1:R2:293:LEU:HG	2.12	0.49
1:T2:50:ILE:O	1:T2:54:LEU:HD12	2.12	0.49
1:U2:113:GLN:HA	1:U2:113:GLN:NE2	2.27	0.49
1:X2:159:LEU:HB2	1:X2:310:PHE:CZ	2.48	0.49
1:d2:140:GLY:HA3	1:d2:163:SER:HB2	1.94	0.49
1:A2:375:LEU:HD11	1:P2:341:ALA:HA	1.94	0.49
1:T2:159:LEU:HB2	1:T2:310:PHE:CE1	2.48	0.49
1:a2:31:ARG:HG3	1:a2:37:LYS:HA	1.94	0.49
1:c2:238:GLU:HG3	1:c2:283:VAL:HG12	1.93	0.49
1:A1:352:ILE:HD13	1:c2:368:PRO:HB2	1.94	0.49
1:A2:159:LEU:HB2	1:A2:310:PHE:CE1	2.48	0.49
1:D2:161:MET:HG2	1:D2:307:LEU:HD11	1.93	0.49
1:G2:354:GLN:O	1:G2:358:THR:HG23	2.13	0.49
1:Q2:153:SER:HB2	1:X2:290:VAL:HB	1.94	0.49
1:R2:152:ASP:O	1:R2:155:GLU:HG3	2.13	0.49
1:U2:235:SER:HB2	1:U2:243:GLN:HG3	1.93	0.49
1:V2:91:ARG:O	1:V2:94:ASP:HB2	2.13	0.49
1:c2:161:MET:HE3	1:c2:307:LEU:HD21	1.94	0.49
1:c2:360:VAL:HG23	1:d2:29:MET:HE3	1.93	0.49
1:e2:31:ARG:HG2	1:e2:37:LYS:HA	1.94	0.49
1:A2:194:LEU:HB2	1:A2:261:LEU:HB3	1.95	0.49
1:F2:234:ALA:HB1	1:F2:242:LEU:HD11	1.93	0.49
1:H2:41:ALA:HB2	1:H2:48:LEU:HD22	1.93	0.49
1:I2:78:ALA:HB1	1:I2:138:LEU:HD21	1.95	0.49
1:R2:149:ILE:HD11	1:c2:125:ARG:HD2	1.95	0.49
1:U2:274:THR:HG22	1:U2:275:VAL:H	1.78	0.49
1:H2:168:THR:HG22	1:H2:170:ALA:H	1.78	0.49
1:L2:110:ARG:NH1	1:L2:281:SER:HB3	2.27	0.49
1:M2:97:LEU:HD13	1:M2:290:VAL:HG21	1.94	0.49
1:Q2:340:TYR:CD2	1:W2:371:ALA:HB1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c2:23:ASP:O	1:c2:27:LYS:HG2	2.13	0.49
1:e2:246:ALA:HB1	1:e2:251:VAL:HG21	1.94	0.49
1:A1:31:ARG:HD2	1:A1:37:LYS:O	2.13	0.49
1:A1:61:LEU:HD12	1:A1:321:LEU:HB3	1.93	0.49
1:P2:7:THR:HG21	1:c2:333:SER:HB2	1.92	0.49
1:P2:159:LEU:HB2	1:P2:310:PHE:CE1	2.47	0.49
1:b2:289:ALA:O	1:b2:293:LEU:HG	2.13	0.49
1:N2:61:LEU:O	1:N2:65:VAL:HG23	2.13	0.49
1:O2:368:PRO:HB2	1:X2:352:ILE:HG21	1.94	0.49
1:S2:82:MET:HG2	1:S2:164:MET:HE1	1.94	0.49
1:W2:159:LEU:HB2	1:W2:310:PHE:CZ	2.47	0.49
1:M2:112:ILE:HD12	1:M2:112:ILE:H	1.78	0.48
1:M2:357:SER:HA	1:M2:360:VAL:HG12	1.95	0.48
1:d2:3:ILE:HG21	1:d2:374:LEU:HD21	1.95	0.48
1:A1:289:ALA:O	1:A1:293:LEU:HG	2.13	0.48
1:C2:334:ARG:HD2	1:S2:69:ASN:HB3	1.95	0.48
1:V2:159:LEU:HB2	1:V2:310:PHE:CE1	2.48	0.48
1:V2:289:ALA:O	1:V2:293:LEU:HG	2.13	0.48
1:b2:374:LEU:O	1:b2:375:LEU:HD22	2.14	0.48
1:f2:88:ILE:HG23	1:f2:119:LEU:HD22	1.95	0.48
1:E2:19:ASN:HB3	1:Z2:1:MET:H2	1.79	0.48
1:M2:214:GLN:OE1	1:M2:214:GLN:HA	2.12	0.48
1:P2:241:LYS:HE2	1:P2:241:LYS:HB3	1.63	0.48
1:U2:31:ARG:HG2	1:U2:37:LYS:HA	1.95	0.48
1:Z2:26:GLN:OE1	1:b2:1:MET:HG3	2.13	0.48
1:Z2:36:TYR:HA	1:Z2:337:ASP:HA	1.94	0.48
1:I2:171:MET:HE3	1:I2:296:ALA:HB1	1.95	0.48
1:I2:289:ALA:O	1:I2:293:LEU:HG	2.14	0.48
1:M2:164:MET:HE1	1:M2:300:VAL:HA	1.96	0.48
1:N2:37:LYS:HG3	1:N2:338:THR:HA	1.95	0.48
1:Q2:23:ASP:O	1:Q2:27:LYS:HD2	2.13	0.48
1:R2:112:ILE:HG22	1:R2:280:VAL:HG21	1.96	0.48
1:c2:12:MET:HA	1:c2:15:GLN:HE21	1.78	0.48
1:c2:354:GLN:O	1:c2:358:THR:HG23	2.14	0.48
1:A1:112:ILE:HG22	1:A1:280:VAL:HG21	1.96	0.48
1:B2:165:ARG:NH2	1:J2:213:LYS:HD2	2.26	0.48
1:B2:365:LYS:HE2	1:Y2:375:LEU:HD23	1.94	0.48
1:G2:112:ILE:HG13	1:U2:46:ALA:HB2	1.96	0.48
1:I2:27:LYS:O	1:I2:31:ARG:HG3	2.14	0.48
1:J2:1:MET:N	1:R2:19:ASN:HB3	2.28	0.48
1:T2:7:THR:HG22	1:a2:332:ARG:HH21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e2:234:ALA:HB1	1:e2:242:LEU:HD11	1.95	0.48
1:A2:95:LEU:HD22	1:A2:112:ILE:HG23	1.96	0.48
1:J2:234:ALA:HB1	1:J2:242:LEU:HD11	1.95	0.48
1:L2:207:GLU:HA	1:L2:207:GLU:OE2	2.13	0.48
1:P2:54:LEU:HD22	1:P2:328:VAL:HG13	1.95	0.48
1:S2:161:MET:HB3	1:S2:161:MET:HE2	1.69	0.48
1:T2:368:PRO:HB2	1:e2:352:ILE:HD13	1.96	0.48
1:b2:372:LEU:HD23	1:b2:373:SER:H	1.78	0.48
1:d2:221:LEU:HD11	1:d2:261:LEU:HD21	1.96	0.48
1:F2:153:SER:HB3	1:d2:290:VAL:HB	1.96	0.48
1:U2:88:ILE:HG23	1:U2:119:LEU:HD22	1.94	0.48
1:e2:198:TYR:HB3	1:e2:255:VAL:HG22	1.96	0.48
1:E2:161:MET:HE2	1:E2:161:MET:HB3	1.67	0.48
1:H2:355:GLN:HA	1:H2:358:THR:HG22	1.96	0.48
1:I2:61:LEU:O	1:I2:65:VAL:HG23	2.14	0.48
1:L2:280:VAL:HG13	1:L2:286:SER:HB3	1.95	0.48
1:P2:27:LYS:HB3	1:P2:31:ARG:HH12	1.79	0.48
1:P2:235:SER:HB3	1:P2:287:GLN:HB3	1.96	0.48
1:E2:182:LYS:HB2	1:E2:218:LEU:HD22	1.96	0.48
1:K2:365:LYS:O	1:K2:368:PRO:HD2	2.13	0.48
1:T2:198:TYR:HB3	1:T2:255:VAL:HG22	1.95	0.48
1:Y2:347:MET:O	1:Y2:347:MET:HE3	2.13	0.48
1:d2:288:GLU:OE1	1:d2:288:GLU:HA	2.13	0.48
1:A1:112:ILE:HD12	1:A1:112:ILE:H	1.79	0.48
1:B2:177:ARG:HA	1:B2:177:ARG:HD3	1.71	0.48
1:F2:152:ASP:O	1:F2:155:GLU:HG3	2.14	0.48
1:I2:219:GLU:HG2	1:Z2:158:MET:SD	2.54	0.48
1:T2:239:ASP:HB2	1:T2:241:LYS:HE3	1.96	0.48
1:c2:159:LEU:HB2	1:c2:310:PHE:CZ	2.48	0.48
1:B2:6:ASN:HA	1:J2:349:LYS:HD2	1.95	0.47
1:D2:63:MET:HE1	1:D2:67:ASN:ND2	2.29	0.47
1:E2:242:LEU:HD23	1:E2:267:PHE:HZ	1.77	0.47
1:O2:365:LYS:HE3	1:Q2:375:LEU:HD23	1.96	0.47
1:d2:238:GLU:HG3	1:d2:283:VAL:HG12	1.95	0.47
1:C2:46:ALA:HB2	1:Z2:112:ILE:HG13	1.95	0.47
1:D2:345:THR:HA	1:K2:365:LYS:HD2	1.96	0.47
1:G2:182:LYS:HB2	1:G2:218:LEU:HD22	1.95	0.47
1:K2:85:THR:HG23	1:K2:123:LEU:HD22	1.97	0.47
1:O2:95:LEU:HB3	1:O2:112:ILE:HG23	1.95	0.47
1:S2:173:GLY:HA2	1:S2:248:SER:HB2	1.96	0.47
1:U2:159:LEU:HD12	1:U2:160:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V2:352:ILE:HD13	1:f2:368:PRO:HB2	1.95	0.47
1:V2:352:ILE:HG23	1:f2:372:LEU:HD23	1.96	0.47
1:b2:36:TYR:HB2	1:b2:39:ASN:HD21	1.80	0.47
1:d2:91:ARG:O	1:d2:95:LEU:HD12	2.13	0.47
1:F2:219:GLU:HG3	1:H2:158:MET:HG3	1.95	0.47
1:O2:88:ILE:O	1:O2:92:MET:HG3	2.14	0.47
1:R2:38:ILE:HD13	1:R2:43:ASP:HB2	1.95	0.47
1:W2:372:LEU:HD23	1:W2:373:SER:H	1.79	0.47
1:Y2:63:MET:HE2	1:Y2:63:MET:H	1.77	0.47
1:f2:25:MET:HE1	1:f2:354:GLN:HG2	1.96	0.47
1:J2:84:GLU:HA	1:J2:84:GLU:OE1	2.13	0.47
1:O2:69:ASN:HB3	1:Q2:334:ARG:HD2	1.97	0.47
1:U2:179:GLN:HE21	1:U2:266:GLY:HA3	1.78	0.47
1:c2:190:ALA:HA	1:c2:214:GLN:HE22	1.79	0.47
1:d2:108:GLU:O	1:d2:112:ILE:HG12	2.13	0.47
1:d2:339:ASP:H	1:d2:342:ARG:NH2	2.12	0.47
1:A1:28:SER:HB3	1:A1:347:MET:HB3	1.97	0.47
1:I2:34:SER:HB3	1:f2:17:TYR:CE2	2.50	0.47
1:K2:10:SER:HB2	1:N2:26:GLN:HG3	1.95	0.47
1:O2:29:MET:HG3	1:Q2:360:VAL:HG22	1.96	0.47
1:W2:147:PHE:HE1	1:W2:159:LEU:HB3	1.79	0.47
1:a2:95:LEU:HB3	1:a2:112:ILE:HG23	1.96	0.47
1:b2:42:ARG:HH12	1:f2:76:GLN:HG3	1.79	0.47
1:S2:372:LEU:HB2	1:b2:352:ILE:HG23	1.96	0.47
1:e2:249:GLN:HG2	1:e2:250:LYS:HG3	1.96	0.47
1:A1:27:LYS:HD3	1:A1:27:LYS:N	2.28	0.47
1:F2:78:ALA:HB1	1:F2:161:MET:HE1	1.97	0.47
1:N2:63:MET:HE2	1:T2:97:LEU:HB3	1.97	0.47
1:O2:334:ARG:HD2	1:f2:69:ASN:HB3	1.96	0.47
1:P2:201:LYS:HA	1:P2:252:ASN:ND2	2.30	0.47
1:Q2:82:MET:HG2	1:Q2:304:ARG:CG	2.45	0.47
1:S2:110:ARG:NH1	1:S2:281:SER:HB3	2.29	0.47
1:T2:289:ALA:O	1:T2:293:LEU:HG	2.14	0.47
1:W2:88:ILE:O	1:W2:92:MET:HG3	2.14	0.47
1:Y2:24:GLY:HA2	1:Y2:27:LYS:HZ2	1.79	0.47
1:Y2:88:ILE:O	1:Y2:92:MET:HG3	2.15	0.47
1:Z2:161:MET:HE3	1:Z2:161:MET:HB2	1.84	0.47
1:b2:314:PHE:O	1:b2:318:ILE:HD13	2.15	0.47
1:A1:101:ASN:HD21	1:R2:70:ASP:HB2	1.80	0.47
1:D2:1:MET:N	1:G2:19:ASN:HB3	2.29	0.47
1:H2:152:ASP:O	1:H2:155:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O2:38:ILE:HD11	1:O2:336:ARG:HB2	1.96	0.47
1:P2:178:ALA:HB3	1:P2:241:LYS:HB2	1.97	0.47
1:d2:182:LYS:HB2	1:d2:218:LEU:HG	1.96	0.47
1:e2:164:MET:HE1	1:e2:300:VAL:HG22	1.96	0.47
1:f2:177:ARG:HD2	1:f2:241:LYS:HD3	1.97	0.47
1:C2:1:MET:N	1:S2:19:ASN:HB3	2.30	0.47
1:F2:360:VAL:HG11	1:X2:33:SER:HB3	1.95	0.47
1:N2:150:GLY:HA3	1:N2:155:GLU:HB2	1.95	0.47
1:Q2:84:GLU:HA	1:Q2:84:GLU:OE1	2.14	0.47
1:U2:25:MET:O	1:U2:29:MET:HG3	2.15	0.47
1:Z2:336:ARG:HG2	1:Z2:336:ARG:HH11	1.80	0.47
1:I2:85:THR:HG23	1:I2:123:LEU:HD22	1.97	0.47
1:R2:226:ASN:HD21	1:R2:233:LYS:HD3	1.79	0.47
1:U2:201:LYS:HD2	1:U2:201:LYS:HA	1.68	0.47
1:Z2:333:SER:HA	1:Z2:337:ASP:OD2	2.15	0.47
1:a2:31:ARG:HD3	1:a2:37:LYS:HA	1.97	0.47
1:d2:32:LEU:HD12	1:d2:340:TYR:HE1	1.80	0.47
1:A1:18:LEU:HG	1:A1:357:SER:HB3	1.97	0.46
1:D2:85:THR:OG1	1:D2:126:ILE:HG21	2.14	0.46
1:F2:73:SER:HB3	1:P2:331:SER:HB2	1.97	0.46
1:J2:238:GLU:HG3	1:J2:283:VAL:HG12	1.97	0.46
1:P2:187:ARG:HG2	1:P2:215:GLY:HA2	1.97	0.46
1:V2:230:GLU:HA	1:V2:230:GLU:OE1	2.14	0.46
1:a2:61:LEU:O	1:a2:65:VAL:HG12	2.15	0.46
1:a2:325:ASN:HA	1:a2:328:VAL:HG12	1.97	0.46
1:c2:28:SER:O	1:c2:32:LEU:HD22	2.14	0.46
1:A1:38:ILE:HG22	1:A1:43:ASP:HB2	1.95	0.46
1:M2:164:MET:SD	1:M2:300:VAL:HG22	2.55	0.46
1:N2:8:ASN:HD21	1:N2:365:LYS:HA	1.81	0.46
1:V2:192:THR:HB	1:V2:212:ALA:HB3	1.97	0.46
1:W2:372:LEU:HD23	1:W2:373:SER:N	2.30	0.46
1:A2:374:LEU:HG	1:A2:375:LEU:CD2	2.46	0.46
1:D2:360:VAL:HG13	1:G2:29:MET:HG2	1.97	0.46
1:H2:12:MET:O	1:H2:16:ARG:HB2	2.15	0.46
1:L2:318:ILE:HD12	1:L2:318:ILE:H	1.80	0.46
1:A1:38:ILE:HD11	1:A1:336:ARG:HD3	1.96	0.46
1:A2:202:GLN:NE2	1:H2:110:ARG:HH21	2.12	0.46
1:M2:84:GLU:HG2	1:T2:320:ASN:HB2	1.96	0.46
1:Q2:46:ALA:HA	1:Q2:49:GLN:HG3	1.96	0.46
1:T2:235:SER:HB3	1:T2:287:GLN:HB3	1.96	0.46
1:Y2:92:MET:HB2	1:Y2:293:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y2:257:ILE:HG21	1:Y2:267:PHE:CD2	2.50	0.46
1:c2:19:ASN:O	1:c2:23:ASP:HB2	2.16	0.46
1:A2:9:VAL:HA	1:A2:12:MET:HE3	1.98	0.46
1:B2:201:LYS:HD2	1:B2:201:LYS:HA	1.74	0.46
1:D2:3:ILE:HD12	1:D2:3:ILE:HA	1.82	0.46
1:F2:340:TYR:HD2	1:H2:371:ALA:HB1	1.81	0.46
1:K2:164:MET:HE1	1:K2:300:VAL:HG22	1.97	0.46
1:T2:54:LEU:HD23	1:T2:328:VAL:HG13	1.98	0.46
1:a2:25:MET:HE3	1:a2:350:ALA:HB1	1.97	0.46
1:d2:176:TYR:CZ	1:d2:255:VAL:HG12	2.51	0.46
1:A2:235:SER:HB2	1:A2:243:GLN:HG3	1.98	0.46
1:M2:137:LEU:HB2	1:M2:138:LEU:HD12	1.97	0.46
1:M2:192:THR:HB	1:M2:212:ALA:HB3	1.97	0.46
1:S2:348:THR:O	1:S2:352:ILE:HG12	2.16	0.46
1:Y2:201:LYS:HE2	1:Y2:252:ASN:HD22	1.79	0.46
1:Z2:152:ASP:O	1:Z2:155:GLU:HG3	2.15	0.46
1:Z2:348:THR:O	1:Z2:352:ILE:HG12	2.15	0.46
1:d2:374:LEU:HD12	1:d2:375:LEU:HG	1.97	0.46
1:f2:18:LEU:HD21	1:f2:358:THR:HG23	1.97	0.46
1:f2:78:ALA:HB2	1:f2:137:LEU:HD13	1.98	0.46
1:H2:53:ARG:HD2	1:Q2:133:GLY:O	2.15	0.46
1:T2:161:MET:HE3	1:T2:307:LEU:HD21	1.97	0.46
1:U2:149:ILE:HG21	1:U2:314:PHE:CE1	2.50	0.46
1:V2:84:GLU:HG2	1:X2:320:ASN:HB2	1.97	0.46
1:e2:249:GLN:HE22	1:e2:295:GLY:HA2	1.81	0.46
1:E2:159:LEU:HB2	1:E2:310:PHE:CE2	2.50	0.46
1:N2:25:MET:HE1	1:N2:354:GLN:OE1	2.15	0.46
1:N2:298:LYS:HB2	1:N2:298:LYS:HE2	1.73	0.46
1:S2:159:LEU:HB2	1:S2:310:PHE:CE1	2.50	0.46
1:U2:342:ARG:HA	1:U2:342:ARG:HD3	1.62	0.46
1:W2:354:GLN:O	1:W2:358:THR:HG22	2.16	0.46
1:X2:76:GLN:HE21	1:X2:311:GLN:HE22	1.63	0.46
1:a2:73:SER:O	1:a2:77:THR:HG22	2.15	0.46
1:e2:229:THR:HG22	1:e2:231:ASP:H	1.81	0.46
1:f2:142:PHE:CE1	1:f2:145:LYS:HD2	2.51	0.46
1:B2:333:SER:HA	1:B2:337:ASP:HB2	1.97	0.46
1:G2:234:ALA:HB1	1:G2:242:LEU:HD11	1.98	0.46
1:H2:46:ALA:HB2	1:X2:112:ILE:CD1	2.43	0.46
1:U2:198:TYR:HB3	1:U2:255:VAL:HG22	1.96	0.46
1:Z2:27:LYS:HD2	1:Z2:42:ARG:HH12	1.80	0.46
1:a2:274:THR:HG22	1:a2:275:VAL:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d2:31:ARG:HH11	1:d2:37:LYS:HG3	1.81	0.46
1:E2:149:ILE:HD13	1:E2:314:PHE:CE1	2.51	0.46
1:F2:334:ARG:HD2	1:X2:69:ASN:HB3	1.98	0.46
1:I2:149:ILE:HG21	1:I2:314:PHE:CE1	2.50	0.46
1:L2:10:SER:HB3	1:b2:26:GLN:HG2	1.98	0.46
1:N2:273:VAL:HG23	1:N2:292:ILE:HD11	1.98	0.46
1:S2:1:MET:HE1	1:Z2:334:ARG:HG2	1.98	0.46
1:T2:178:ALA:HB3	1:T2:241:LYS:HB2	1.98	0.46
1:A2:218:LEU:HD12	1:A2:218:LEU:HA	1.78	0.45
1:H2:332:ARG:HG2	1:H2:332:ARG:HH11	1.81	0.45
1:U2:159:LEU:HG	1:U2:161:MET:HE2	1.98	0.45
1:d2:32:LEU:HD12	1:d2:340:TYR:CE1	2.51	0.45
1:f2:182:LYS:HB2	1:f2:218:LEU:HD12	1.98	0.45
1:A1:288:GLU:O	1:A1:292:ILE:HG13	2.16	0.45
1:F2:235:SER:HB3	1:F2:287:GLN:HB3	1.98	0.45
1:J2:238:GLU:OE2	1:J2:282:THR:HB	2.16	0.45
1:K2:19:ASN:HB3	1:U2:1:MET:N	2.31	0.45
1:K2:46:ALA:HB1	1:T2:108:GLU:HB3	1.97	0.45
1:L2:32:LEU:HD23	1:L2:32:LEU:HA	1.83	0.45
1:L2:358:THR:OG1	1:W2:374:LEU:HB2	2.16	0.45
1:M2:74:ILE:HD12	1:M2:147:PHE:HE2	1.81	0.45
1:O2:361:LEU:HD23	1:Q2:374:LEU:HD11	1.98	0.45
1:W2:113:GLN:HE21	1:W2:113:GLN:C	2.24	0.45
1:b2:149:ILE:HG21	1:b2:314:PHE:CE1	2.50	0.45
1:c2:364:ALA:HB2	1:d2:29:MET:HE2	1.99	0.45
1:B2:348:THR:HA	1:B2:351:GLN:HG3	1.98	0.45
1:C2:1:MET:H2	1:S2:19:ASN:HB3	1.82	0.45
1:E2:357:SER:HA	1:E2:360:VAL:HG12	1.97	0.45
1:N2:7:THR:HG21	1:T2:333:SER:HB2	1.98	0.45
1:P2:95:LEU:HB3	1:P2:112:ILE:HG23	1.99	0.45
1:S2:152:ASP:O	1:S2:155:GLU:HG3	2.17	0.45
1:b2:46:ALA:O	1:b2:50:ILE:HG22	2.16	0.45
1:e2:342:ARG:HE	1:e2:342:ARG:HB2	1.61	0.45
1:A1:192:THR:HG21	1:A1:214:GLN:HE21	1.80	0.45
1:C2:88:ILE:O	1:C2:92:MET:HG3	2.17	0.45
1:G2:12:MET:HA	1:G2:15:GLN:HE21	1.81	0.45
1:O2:46:ALA:O	1:O2:50:ILE:HG12	2.17	0.45
1:T2:375:LEU:HD13	1:T2:375:LEU:O	2.16	0.45
1:V2:113:GLN:HE22	1:V2:279:ASN:HA	1.81	0.45
1:B2:92:MET:HA	1:B2:95:LEU:HD12	1.97	0.45
1:G2:78:ALA:HB1	1:G2:161:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M2:328:VAL:O	1:M2:332:ARG:HG2	2.17	0.45
1:Q2:354:GLN:O	1:Q2:358:THR:HG23	2.16	0.45
1:Z2:37:LYS:HG3	1:Z2:338:THR:HA	1.99	0.45
1:a2:182:LYS:HB2	1:a2:218:LEU:HD22	1.99	0.45
1:a2:351:GLN:O	1:a2:354:GLN:HG3	2.17	0.45
1:c2:288:GLU:O	1:c2:292:ILE:HG13	2.16	0.45
1:E2:14:ALA:HB1	1:E2:360:VAL:HG13	1.98	0.45
1:I2:84:GLU:HG2	1:f2:320:ASN:HB2	1.99	0.45
1:I2:344:THR:HG21	1:Z2:375:LEU:HB3	1.99	0.45
1:M2:31:ARG:HD3	1:M2:37:LYS:HA	1.99	0.45
1:V2:280:VAL:HG13	1:V2:286:SER:HB3	1.99	0.45
1:b2:42:ARG:NH2	1:f2:72:ILE:HG23	2.32	0.45
1:c2:78:ALA:HB2	1:c2:137:LEU:HD13	1.98	0.45
1:d2:61:LEU:HD12	1:d2:151:ALA:HB2	1.99	0.45
1:f2:307:LEU:C	1:f2:311:GLN:HE21	2.24	0.45
1:A2:6:ASN:HA	1:B2:349:LYS:HE2	1.98	0.45
1:L2:65:VAL:HB	1:L2:318:ILE:HG23	1.99	0.45
1:N2:177:ARG:HD2	1:N2:241:LYS:HD3	1.99	0.45
1:W2:239:ASP:HB2	1:W2:241:LYS:HD2	1.99	0.45
1:c2:162:GLY:H	1:c2:303:GLN:NE2	2.15	0.45
1:C2:274:THR:HG22	1:C2:275:VAL:H	1.82	0.45
1:E2:112:ILE:HD11	1:S2:46:ALA:HB2	1.98	0.45
1:L2:82:MET:HG2	1:L2:304:ARG:HG3	1.97	0.45
1:T2:6:ASN:HA	1:e2:349:LYS:NZ	2.32	0.45
1:A1:109:ARG:HB3	1:A1:281:SER:HA	1.99	0.45
1:B2:23:ASP:O	1:B2:27:LYS:HG3	2.17	0.45
1:E2:108:GLU:O	1:E2:112:ILE:HG12	2.16	0.45
1:F2:330:ALA:HB2	1:H2:9:VAL:HG21	1.98	0.45
1:I2:3:ILE:HD12	1:I2:3:ILE:O	2.16	0.45
1:N2:161:MET:HE2	1:N2:161:MET:HB3	1.78	0.45
1:Q2:164:MET:HE2	1:Q2:164:MET:HB2	1.58	0.45
1:a2:27:LYS:HD2	1:a2:27:LYS:HA	1.64	0.45
1:b2:161:MET:HE3	1:b2:307:LEU:HD21	1.99	0.45
1:A1:18:LEU:HB3	1:M2:1:MET:SD	2.57	0.45
1:D2:159:LEU:HB2	1:D2:310:PHE:CE1	2.52	0.45
1:G2:12:MET:HA	1:G2:15:GLN:NE2	2.32	0.45
1:L2:374:LEU:O	1:L2:375:LEU:HD23	2.17	0.45
1:O2:138:LEU:HB3	1:O2:164:MET:HB2	1.99	0.45
1:C2:348:THR:O	1:C2:352:ILE:HG22	2.18	0.44
1:G2:32:LEU:HD23	1:G2:32:LEU:HA	1.83	0.44
1:H2:355:GLN:HB2	1:W2:372:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M2:61:LEU:HD13	1:M2:325:ASN:HA	1.99	0.44
1:Q2:106:SER:O	1:Q2:110:ARG:HG2	2.17	0.44
1:W2:198:TYR:HB3	1:W2:255:VAL:HG22	1.99	0.44
1:X2:73:SER:O	1:X2:77:THR:HG23	2.17	0.44
1:Z2:25:MET:HG2	1:Z2:29:MET:HE2	2.00	0.44
1:c2:72:ILE:O	1:c2:76:GLN:HG3	2.18	0.44
1:B2:65:VAL:HG13	1:B2:318:ILE:HD12	1.99	0.44
1:B2:159:LEU:HB2	1:B2:310:PHE:CE1	2.52	0.44
1:C2:275:VAL:O	1:C2:278:VAL:HG12	2.16	0.44
1:H2:221:LEU:HD21	1:H2:261:LEU:HD21	1.99	0.44
1:L2:198:TYR:HB3	1:L2:255:VAL:HG22	1.98	0.44
1:M2:82:MET:HG2	1:M2:304:ARG:HG3	1.99	0.44
1:M2:201:LYS:HA	1:M2:201:LYS:HD3	1.57	0.44
1:S2:3:ILE:HG12	1:S2:371:ALA:HB2	1.99	0.44
1:T2:7:THR:HG23	1:a2:337:ASP:OD2	2.16	0.44
1:Y2:196:LEU:HD23	1:Y2:257:ILE:HD12	2.00	0.44
1:C2:131:SER:HB3	1:C2:136:LYS:HD3	2.00	0.44
1:K2:271:ARG:H	1:K2:271:ARG:HE	1.63	0.44
1:L2:375:LEU:HD21	1:b2:361:LEU:HG	1.99	0.44
1:M2:348:THR:OG1	1:R2:365:LYS:HE2	2.17	0.44
1:O2:92:MET:HB2	1:O2:293:LEU:HD13	1.99	0.44
1:P2:149:ILE:HG21	1:P2:314:PHE:CE1	2.51	0.44
1:Q2:161:MET:HE3	1:Q2:307:LEU:HD11	1.98	0.44
1:S2:238:GLU:OE2	1:S2:283:VAL:HG12	2.17	0.44
1:V2:31:ARG:HH11	1:V2:37:LYS:HG3	1.82	0.44
1:V2:182:LYS:HD3	1:V2:186:TRP:CD2	2.52	0.44
1:W2:226:ASN:C	1:W2:226:ASN:HD22	2.26	0.44
1:Y2:142:PHE:HE2	1:Y2:159:LEU:HD23	1.81	0.44
1:Z2:164:MET:HE2	1:Z2:300:VAL:HG22	1.99	0.44
1:a2:18:LEU:HD13	1:a2:357:SER:HB2	2.00	0.44
1:b2:88:ILE:O	1:b2:92:MET:HG3	2.17	0.44
1:c2:339:ASP:HB3	1:c2:342:ARG:HB3	1.99	0.44
1:C2:144:SER:HA	1:C2:159:LEU:O	2.17	0.44
1:H2:353:LEU:HD13	1:H2:353:LEU:HA	1.88	0.44
1:I2:328:VAL:O	1:I2:332:ARG:HG2	2.17	0.44
1:M2:6:ASN:HA	1:a2:349:LYS:NZ	2.32	0.44
1:M2:352:ILE:HG23	1:R2:372:LEU:HD23	2.00	0.44
1:R2:42:ARG:HE	1:R2:42:ARG:HB3	1.55	0.44
1:U2:15:GLN:HA	1:U2:18:LEU:HB3	1.99	0.44
1:U2:235:SER:HB2	1:U2:243:GLN:HE21	1.82	0.44
1:X2:298:LYS:HB2	1:X2:298:LYS:HE3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z2:19:ASN:HB3	1:b2:1:MET:H2	1.83	0.44
1:a2:31:ARG:HG2	1:a2:343:GLU:OE1	2.17	0.44
1:b2:7:THR:HG21	1:f2:333:SER:HB2	1.98	0.44
1:d2:31:ARG:HD3	1:d2:37:LYS:HA	1.98	0.44
1:A1:213:LYS:HD2	1:c2:165:ARG:NH1	2.33	0.44
1:I2:125:ARG:O	1:I2:129:THR:HG23	2.17	0.44
1:K2:279:ASN:O	1:K2:285:GLY:HA3	2.18	0.44
1:U2:57:GLN:HE21	1:U2:61:LEU:HD11	1.83	0.44
1:Z2:280:VAL:HG12	1:Z2:286:SER:HA	1.99	0.44
1:d2:307:LEU:HD12	1:d2:307:LEU:HA	1.83	0.44
1:A2:353:LEU:HD23	1:A2:353:LEU:HA	1.86	0.44
1:E2:350:ALA:HA	1:E2:353:LEU:HD23	1.99	0.44
1:L2:11:ALA:O	1:L2:15:GLN:HG2	2.17	0.44
1:L2:206:ARG:HD2	1:L2:206:ARG:HA	1.82	0.44
1:M2:349:LYS:O	1:M2:353:LEU:HD23	2.17	0.44
1:P2:238:GLU:OE1	1:P2:282:THR:HB	2.18	0.44
1:Q2:298:LYS:HB2	1:Q2:298:LYS:NZ	2.32	0.44
1:R2:190:ALA:HA	1:R2:214:GLN:HE22	1.82	0.44
1:R2:320:ASN:HB2	1:c2:84:GLU:HG3	1.99	0.44
1:S2:218:LEU:HB3	1:S2:236:VAL:HG21	1.99	0.44
1:U2:108:GLU:O	1:U2:112:ILE:HG12	2.17	0.44
1:V2:329:ASN:O	1:V2:332:ARG:HG2	2.18	0.44
1:Z2:171:MET:HB3	1:Z2:275:VAL:HG23	2.00	0.44
1:b2:231:ASP:HA	1:b2:250:LYS:HD3	1.99	0.44
1:B2:23:ASP:OD2	1:Y2:1:MET:HB2	2.18	0.44
1:K2:334:ARG:HD2	1:N2:69:ASN:HB3	1.98	0.44
1:L2:42:ARG:HB2	1:L2:42:ARG:NH1	2.33	0.44
1:O2:365:LYS:H	1:O2:365:LYS:HG2	1.62	0.44
1:S2:23:ASP:HB3	1:S2:27:LYS:NZ	2.32	0.44
1:B2:1:MET:HE2	1:P2:26:GLN:NE2	2.33	0.44
1:B2:136:LYS:HB3	1:B2:139:ASN:HD21	1.81	0.44
1:B2:147:PHE:HE1	1:B2:159:LEU:HB3	1.83	0.44
1:I2:31:ARG:HH21	1:I2:37:LYS:HG3	1.83	0.44
1:J2:38:ILE:HD12	1:J2:44:ASP:HB3	1.99	0.44
1:J2:153:SER:HB3	1:M2:290:VAL:HB	1.99	0.44
1:K2:202:GLN:HB2	1:K2:204:GLU:OE1	2.18	0.44
1:M2:25:MET:O	1:M2:29:MET:HE2	2.17	0.44
1:N2:9:VAL:HA	1:N2:12:MET:HB2	1.99	0.44
1:T2:152:ASP:O	1:T2:155:GLU:HG3	2.18	0.44
1:f2:324:VAL:O	1:f2:328:VAL:HG23	2.18	0.44
1:A2:23:ASP:O	1:A2:27:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B2:63:MET:HE2	1:R2:94:ASP:OD2	2.18	0.44
1:D2:372:LEU:HB2	1:Z2:352:ILE:HG23	2.00	0.44
1:L2:194:LEU:HB2	1:L2:261:LEU:HD23	1.99	0.44
1:L2:234:ALA:HB1	1:L2:242:LEU:HD11	1.99	0.44
1:A1:51:SER:HB2	1:A1:336:ARG:HH11	1.82	0.43
1:B2:249:GLN:HE21	1:B2:299:ALA:HB2	1.83	0.43
1:F2:3:ILE:HD13	1:F2:3:ILE:HA	1.86	0.43
1:G2:159:LEU:HB2	1:G2:310:PHE:CE1	2.53	0.43
1:H2:15:GLN:HA	1:H2:18:LEU:HB3	2.00	0.43
1:P2:152:ASP:O	1:P2:155:GLU:HG3	2.18	0.43
1:V2:109:ARG:HB3	1:V2:281:SER:HA	1.99	0.43
1:Z2:54:LEU:HD22	1:Z2:328:VAL:HG13	2.00	0.43
1:a2:219:GLU:OE2	1:a2:219:GLU:HA	2.17	0.43
1:b2:8:ASN:HD21	1:b2:368:PRO:HD3	1.83	0.43
1:A2:354:GLN:O	1:A2:358:THR:HG22	2.18	0.43
1:C2:63:MET:HE1	1:C2:67:ASN:ND2	2.33	0.43
1:F2:112:ILE:HG22	1:F2:280:VAL:HG21	2.00	0.43
1:K2:249:GLN:HE21	1:K2:298:LYS:HB3	1.84	0.43
1:O2:177:ARG:HH11	1:O2:271:ARG:HH12	1.66	0.43
1:R2:28:SER:O	1:R2:32:LEU:HD12	2.18	0.43
1:W2:159:LEU:HB2	1:W2:310:PHE:CE2	2.53	0.43
1:W2:231:ASP:HA	1:W2:250:LYS:HD3	1.99	0.43
1:Z2:131:SER:HB3	1:Z2:136:LYS:HD3	2.00	0.43
1:c2:152:ASP:O	1:c2:155:GLU:HG3	2.18	0.43
1:c2:289:ALA:O	1:c2:293:LEU:HG	2.18	0.43
1:e2:177:ARG:HH12	1:e2:284:ALA:HB1	1.82	0.43
1:A1:27:LYS:HD3	1:A1:27:LYS:H	1.82	0.43
1:I2:19:ASN:HA	1:f2:1:MET:H2	1.83	0.43
1:S2:150:GLY:HA3	1:S2:155:GLU:HB2	2.00	0.43
1:S2:353:LEU:HD13	1:S2:353:LEU:HA	1.90	0.43
1:W2:171:MET:HE3	1:W2:171:MET:HB3	1.77	0.43
1:X2:342:ARG:HB2	1:X2:342:ARG:HH11	1.83	0.43
1:d2:18:LEU:HG	1:d2:357:SER:HB3	2.01	0.43
1:d2:339:ASP:O	1:d2:343:GLU:HB2	2.18	0.43
1:e2:252:ASN:OD1	1:e2:252:ASN:C	2.62	0.43
1:A2:3:ILE:HG22	1:P2:340:TYR:HB2	2.00	0.43
1:A2:24:GLY:HA2	1:A2:27:LYS:HE3	2.00	0.43
1:G2:326:GLU:CD	1:K2:13:THR:HG22	2.43	0.43
1:H2:239:ASP:HB2	1:H2:241:LYS:HE3	1.99	0.43
1:Q2:375:LEU:HG	1:X2:344:THR:HB	2.01	0.43
1:R2:235:SER:HB3	1:R2:287:GLN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W2:310:PHE:CE1	1:W2:314:PHE:HE2	2.37	0.43
1:Y2:353:LEU:HD23	1:Y2:353:LEU:HA	1.80	0.43
1:a2:149:ILE:HG21	1:a2:314:PHE:CE1	2.52	0.43
1:c2:112:ILE:CG2	1:c2:280:VAL:HG21	2.49	0.43
1:f2:131:SER:HB3	1:f2:136:LYS:HE3	2.00	0.43
1:M2:25:MET:HG2	1:M2:350:ALA:HB1	2.01	0.43
1:N2:79:GLU:HA	1:N2:82:MET:HE2	2.00	0.43
1:P2:70:ASP:HB2	1:c2:101:ASN:HD21	1.84	0.43
1:S2:159:LEU:HD12	1:S2:160:SER:N	2.33	0.43
1:Z2:175:SER:O	1:Z2:270:GLY:HA2	2.18	0.43
1:b2:296:ALA:O	1:b2:300:VAL:HG23	2.18	0.43
1:A1:339:ASP:OD2	1:A1:342:ARG:HB2	2.19	0.43
1:C2:128:GLU:OE2	1:C2:165:ARG:HD2	2.18	0.43
1:F2:25:MET:HE2	1:F2:25:MET:HB3	1.75	0.43
1:G2:28:SER:HB3	1:G2:347:MET:HB2	2.01	0.43
1:N2:249:GLN:HE22	1:N2:298:LYS:HB3	1.83	0.43
1:Q2:238:GLU:HG3	1:Q2:283:VAL:HG22	2.00	0.43
1:S2:128:GLU:OE2	1:S2:165:ARG:HD2	2.19	0.43
1:S2:136:LYS:HB3	1:S2:139:ASN:ND2	2.32	0.43
1:a2:274:THR:HG22	1:a2:275:VAL:H	1.83	0.43
1:A2:8:ASN:ND2	1:A2:368:PRO:HD3	2.33	0.43
1:A2:374:LEU:C	1:A2:375:LEU:HD23	2.44	0.43
1:C2:320:ASN:HB2	1:S2:84:GLU:HG3	2.00	0.43
1:F2:371:ALA:HB1	1:d2:340:TYR:CD2	2.53	0.43
1:G2:217:ASP:OD2	1:G2:217:ASP:C	2.62	0.43
1:M2:178:ALA:HB3	1:M2:241:LYS:HB3	2.01	0.43
1:O2:49:GLN:HE21	1:V2:305:ALA:HB2	1.84	0.43
1:O2:182:LYS:HB2	1:O2:218:LEU:HD22	1.99	0.43
1:S2:113:GLN:O	1:S2:113:GLN:NE2	2.36	0.43
1:S2:365:LYS:HB2	1:S2:365:LYS:HE2	1.79	0.43
1:E2:171:MET:HE3	1:E2:171:MET:HB2	1.94	0.43
1:W2:348:THR:O	1:W2:352:ILE:HG12	2.18	0.43
1:a2:161:MET:HB3	1:a2:161:MET:HE2	1.68	0.43
1:b2:242:LEU:HD23	1:b2:267:PHE:HZ	1.82	0.43
1:c2:88:ILE:O	1:c2:92:MET:HG3	2.19	0.43
1:A1:12:MET:HA	1:A1:15:GLN:HG2	2.00	0.43
1:B2:12:MET:HE1	1:R2:329:ASN:HB3	2.01	0.43
1:E2:360:VAL:HG23	1:e2:29:MET:HB2	2.01	0.43
1:G2:54:LEU:HD22	1:G2:328:VAL:HG13	2.00	0.43
1:G2:131:SER:HB3	1:G2:136:LYS:HD3	2.01	0.43
1:J2:69:ASN:HB3	1:N2:334:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M2:238:GLU:HG3	1:M2:283:VAL:HG12	2.01	0.43
1:N2:42:ARG:H	1:N2:42:ARG:HG3	1.67	0.43
1:N2:202:GLN:HB2	1:N2:204:GLU:OE1	2.18	0.43
1:P2:201:LYS:HD2	1:P2:252:ASN:HD22	1.83	0.43
1:W2:235:SER:HB2	1:W2:243:GLN:HG3	2.01	0.43
1:Y2:82:MET:HE2	1:Y2:82:MET:HB2	1.96	0.43
1:b2:78:ALA:HB2	1:b2:137:LEU:HD13	2.01	0.43
1:b2:85:THR:HG23	1:b2:123:LEU:HD22	2.01	0.43
1:c2:12:MET:HA	1:c2:15:GLN:NE2	2.33	0.43
1:d2:198:TYR:HD1	1:d2:255:VAL:HG23	1.84	0.43
1:A1:38:ILE:HD12	1:A1:38:ILE:O	2.18	0.43
1:C2:153:SER:HB2	1:b2:290:VAL:HB	2.01	0.43
1:F2:25:MET:HE1	1:F2:354:GLN:CD	2.43	0.43
1:H2:186:TRP:CH2	1:H2:188:VAL:HG12	2.54	0.43
1:I2:89:LEU:HD12	1:I2:293:LEU:HB3	2.00	0.43
1:M2:347:MET:HE3	1:M2:348:THR:N	2.33	0.43
1:N2:221:LEU:HD11	1:N2:261:LEU:HD21	2.01	0.43
1:N2:245:PHE:CD2	1:N2:291:SER:HB2	2.54	0.43
1:N2:289:ALA:O	1:N2:293:LEU:HG	2.18	0.43
1:U2:55:THR:HB	1:U2:332:ARG:HH21	1.84	0.43
1:U2:179:GLN:NE2	1:U2:266:GLY:HA3	2.34	0.43
1:V2:350:ALA:O	1:V2:354:GLN:HG2	2.18	0.43
1:c2:206:ARG:HD2	1:c2:206:ARG:HA	1.89	0.43
1:c2:271:ARG:HG3	1:c2:271:ARG:NH1	2.34	0.43
1:c2:351:GLN:HA	1:c2:354:GLN:NE2	2.33	0.43
1:e2:78:ALA:HB2	1:e2:137:LEU:HD13	2.01	0.43
1:f2:347:MET:HE3	1:f2:347:MET:HB3	1.78	0.43
1:A1:53:ARG:O	1:A1:57:GLN:HG3	2.19	0.42
1:E2:278:VAL:HG21	1:E2:293:LEU:HD21	2.01	0.42
1:H2:298:LYS:HA	1:H2:298:LYS:HD3	1.88	0.42
1:I2:61:LEU:HD12	1:I2:321:LEU:HD22	2.01	0.42
1:J2:30:GLU:HG2	1:J2:39:ASN:HD22	1.84	0.42
1:N2:54:LEU:HD22	1:N2:328:VAL:HG13	2.00	0.42
1:N2:144:SER:HA	1:N2:159:LEU:O	2.19	0.42
1:N2:149:ILE:HG21	1:N2:314:PHE:CE1	2.54	0.42
1:O2:23:ASP:O	1:O2:27:LYS:HG2	2.19	0.42
1:V2:88:ILE:HG23	1:V2:119:LEU:HD22	2.01	0.42
1:c2:106:SER:O	1:c2:110:ARG:HG2	2.19	0.42
1:f2:28:SER:O	1:f2:32:LEU:HD22	2.19	0.42
1:C2:238:GLU:OE2	1:C2:283:VAL:HG12	2.18	0.42
1:D2:126:ILE:HD13	1:S2:320:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K2:313:ARG:HG3	1:N2:122:GLU:HG2	2.01	0.42
1:M2:28:SER:HB3	1:M2:347:MET:HB3	2.01	0.42
1:O2:252:ASN:OD1	1:O2:252:ASN:C	2.62	0.42
1:S2:187:ARG:HB3	1:S2:215:GLY:HA2	2.01	0.42
1:S2:347:MET:HB3	1:S2:347:MET:HE3	1.78	0.42
1:a2:355:GLN:HA	1:a2:358:THR:OG1	2.19	0.42
1:d2:289:ALA:HA	1:d2:292:ILE:HD12	2.01	0.42
1:A2:245:PHE:CD2	1:A2:291:SER:HB2	2.54	0.42
1:B2:1:MET:HB2	1:P2:23:ASP:OD1	2.19	0.42
1:C2:367:SER:OG	1:C2:368:PRO:HD3	2.19	0.42
1:F2:16:ARG:HH21	1:d2:326:GLU:HG3	1.85	0.42
1:G2:219:GLU:HG3	1:K2:158:MET:HG2	2.01	0.42
1:K2:23:ASP:O	1:K2:27:LYS:HG3	2.20	0.42
1:R2:135:ASN:C	1:R2:135:ASN:HD22	2.27	0.42
1:R2:177:ARG:HD2	1:R2:271:ARG:NH2	2.34	0.42
1:W2:79:GLU:HA	1:W2:82:MET:HE3	2.01	0.42
1:Z2:368:PRO:HB2	1:f2:352:ILE:HG21	2.01	0.42
1:a2:289:ALA:O	1:a2:293:LEU:HG	2.19	0.42
1:f2:38:ILE:HD12	1:f2:38:ILE:O	2.20	0.42
1:A1:19:ASN:HA	1:M2:1:MET:HG2	2.01	0.42
1:A1:311:GLN:HA	1:A1:314:PHE:HD1	1.84	0.42
1:E2:218:LEU:HD12	1:E2:218:LEU:HA	1.85	0.42
1:F2:356:ALA:O	1:F2:360:VAL:HG12	2.20	0.42
1:H2:8:ASN:HD22	1:H2:368:PRO:HD3	1.84	0.42
1:H2:78:ALA:O	1:H2:82:MET:HE2	2.19	0.42
1:K2:164:MET:HB3	1:K2:164:MET:HE3	1.77	0.42
1:V2:110:ARG:H	1:V2:110:ARG:HD3	1.84	0.42
1:c2:51:SER:HA	1:c2:54:LEU:HD12	2.01	0.42
1:d2:131:SER:HB3	1:d2:136:LYS:HD2	2.02	0.42
1:B2:361:LEU:HD23	1:Y2:374:LEU:HD11	2.00	0.42
1:C2:159:LEU:HD22	1:C2:310:PHE:CE1	2.50	0.42
1:E2:38:ILE:HG23	1:E2:43:ASP:HB2	2.01	0.42
1:H2:79:GLU:HA	1:H2:82:MET:HB2	2.02	0.42
1:I2:191:ALA:HB1	1:I2:260:GLY:HA3	2.01	0.42
1:K2:9:VAL:O	1:K2:13:THR:HG23	2.19	0.42
1:K2:84:GLU:OE2	1:K2:84:GLU:HA	2.19	0.42
1:M2:307:LEU:HD23	1:M2:307:LEU:HA	1.89	0.42
1:N2:31:ARG:HD3	1:N2:37:LYS:HA	2.00	0.42
1:N2:271:ARG:H	1:N2:271:ARG:HD2	1.83	0.42
1:Q2:164:MET:HG3	1:Q2:164:MET:O	2.19	0.42
1:R2:17:TYR:CE2	1:c2:34:SER:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U2:244:LEU:HD23	1:U2:267:PHE:CE2	2.54	0.42
1:a2:61:LEU:CD1	1:a2:151:ALA:HB2	2.49	0.42
1:a2:82:MET:HG2	1:a2:304:ARG:CG	2.48	0.42
1:d2:235:SER:HB3	1:d2:287:GLN:HB3	2.02	0.42
1:A1:159:LEU:HB2	1:A1:310:PHE:CE2	2.54	0.42
1:B2:68:ALA:HB3	1:B2:318:ILE:HD11	2.01	0.42
1:C2:63:MET:HE1	1:C2:67:ASN:HD22	1.85	0.42
1:H2:136:LYS:HB3	1:H2:139:ASN:HD21	1.85	0.42
1:I2:184:ALA:HA	1:Z2:158:MET:HE2	2.01	0.42
1:I2:297:LEU:HA	1:I2:300:VAL:HG22	2.01	0.42
1:K2:12:MET:HE3	1:K2:12:MET:HB2	1.93	0.42
1:L2:3:ILE:HG13	1:L2:371:ALA:HB2	2.02	0.42
1:M2:19:ASN:OD1	1:M2:19:ASN:C	2.61	0.42
1:M2:348:THR:O	1:M2:352:ILE:HD13	2.19	0.42
1:N2:206:ARG:HE	1:N2:206:ARG:HB2	1.77	0.42
1:P2:51:SER:HB2	1:P2:336:ARG:HD2	2.02	0.42
1:P2:372:LEU:HD12	1:P2:373:SER:N	2.34	0.42
1:R2:374:LEU:HD12	1:c2:358:THR:HG22	1.99	0.42
1:T2:344:THR:HA	1:T2:347:MET:HG2	2.01	0.42
1:U2:109:ARG:HA	1:U2:112:ILE:HG12	2.00	0.42
1:V2:27:LYS:HB2	1:V2:31:ARG:HH21	1.85	0.42
1:a2:14:ALA:O	1:a2:18:LEU:HD22	2.19	0.42
1:a2:84:GLU:O	1:a2:88:ILE:HG13	2.19	0.42
1:F2:286:SER:O	1:F2:290:VAL:HG23	2.20	0.42
1:L2:61:LEU:O	1:L2:65:VAL:HG13	2.19	0.42
1:L2:331:SER:HB2	1:b2:73:SER:HB3	2.01	0.42
1:P2:152:ASP:OD1	1:c2:233:LYS:HD2	2.19	0.42
1:Q2:218:LEU:HD12	1:Q2:236:VAL:HG13	2.01	0.42
1:V2:22:ALA:HA	1:V2:354:GLN:HE22	1.83	0.42
1:V2:293:LEU:HA	1:V2:296:ALA:HB3	2.01	0.42
1:X2:278:VAL:HG21	1:X2:293:LEU:HD21	2.00	0.42
1:b2:356:ALA:O	1:b2:360:VAL:HG23	2.20	0.42
1:f2:288:GLU:O	1:f2:292:ILE:HG13	2.20	0.42
1:F2:57:GLN:O	1:F2:61:LEU:HG	2.20	0.42
1:M2:92:MET:HB3	1:M2:293:LEU:HD21	2.02	0.42
1:Q2:63:MET:HE2	1:X2:97:LEU:HB3	2.02	0.42
1:S2:179:GLN:HE22	1:S2:266:GLY:HA3	1.84	0.42
1:Y2:218:LEU:HD12	1:Y2:218:LEU:HA	1.79	0.42
1:a2:50:ILE:HD11	1:a2:335:ILE:HG21	2.02	0.42
1:e2:79:GLU:HA	1:e2:82:MET:HB2	2.02	0.42
1:e2:289:ALA:O	1:e2:293:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f2:187:ARG:HB3	1:f2:215:GLY:HA2	2.01	0.42
1:D2:221:LEU:HD21	1:D2:261:LEU:HD21	2.02	0.42
1:E2:73:SER:HB3	1:Z2:331:SER:HB2	2.02	0.42
1:F2:8:ASN:O	1:F2:12:MET:HG3	2.20	0.42
1:F2:19:ASN:HB2	1:P2:1:MET:N	2.34	0.42
1:H2:218:LEU:HD11	1:H2:242:LEU:HB2	2.01	0.42
1:H2:319:SER:HB3	1:Q2:84:GLU:OE2	2.19	0.42
1:I2:206:ARG:HD2	1:I2:206:ARG:HA	1.72	0.42
1:L2:19:ASN:HB3	1:W2:1:MET:N	2.34	0.42
1:O2:307:LEU:C	1:O2:311:GLN:HE21	2.28	0.42
1:P2:375:LEU:HD23	1:P2:375:LEU:HA	1.88	0.42
1:Y2:79:GLU:HA	1:Y2:82:MET:HE2	2.01	0.42
1:Y2:99:SER:HA	1:Y2:104:ASN:HD22	1.85	0.42
1:A1:27:LYS:HB2	1:A1:31:ARG:HH21	1.84	0.42
1:C2:310:PHE:C	1:C2:310:PHE:CD2	2.98	0.42
1:K2:11:ALA:O	1:K2:15:GLN:HG2	2.20	0.42
1:L2:42:ARG:HG3	1:O2:312:ASN:OD1	2.20	0.42
1:P2:110:ARG:H	1:P2:110:ARG:HG2	1.70	0.42
1:R2:99:SER:HB2	1:R2:112:ILE:HG21	2.01	0.42
1:V2:27:LYS:HD3	1:V2:31:ARG:NH2	2.35	0.42
1:Y2:85:THR:HG23	1:Y2:123:LEU:HD22	2.01	0.42
1:Z2:179:GLN:HG3	1:Z2:180:GLU:HG2	2.02	0.42
1:a2:49:GLN:HB3	1:a2:53:ARG:HH22	1.85	0.42
1:e2:23:ASP:O	1:e2:27:LYS:HG2	2.19	0.42
1:e2:218:LEU:HD12	1:e2:218:LEU:HA	1.80	0.42
1:f2:147:PHE:HE1	1:f2:159:LEU:HB3	1.85	0.42
1:A1:159:LEU:HD13	1:A1:310:PHE:CD2	2.55	0.41
1:D2:142:PHE:CE1	1:D2:145:LYS:HB2	2.55	0.41
1:G2:6:ASN:HB2	1:e2:337:ASP:OD2	2.20	0.41
1:I2:142:PHE:CE1	1:I2:161:MET:HE3	2.55	0.41
1:J2:247:SER:HB2	1:J2:249:GLN:HE21	1.85	0.41
1:L2:176:TYR:CZ	1:L2:255:VAL:HB	2.55	0.41
1:V2:112:ILE:HG21	1:V2:280:VAL:HG11	2.02	0.41
1:X2:347:MET:HE2	1:X2:351:GLN:OE1	2.20	0.41
1:Y2:22:ALA:O	1:Y2:25:MET:HG2	2.20	0.41
1:Z2:23:ASP:O	1:Z2:27:LYS:HG3	2.20	0.41
1:e2:57:GLN:O	1:e2:61:LEU:HG	2.20	0.41
1:f2:149:ILE:HD13	1:f2:314:PHE:HE2	1.85	0.41
1:A2:374:LEU:O	1:A2:375:LEU:HD23	2.20	0.41
1:E2:79:GLU:HA	1:E2:82:MET:HB2	2.02	0.41
1:G2:91:ARG:O	1:G2:95:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J2:359:SER:O	1:J2:363:GLN:HG3	2.20	0.41
1:K2:296:ALA:O	1:K2:300:VAL:HG23	2.20	0.41
1:O2:4:ASN:HD21	1:V2:337:ASP:HB3	1.85	0.41
1:U2:27:LYS:HD3	1:U2:27:LYS:C	2.45	0.41
1:W2:177:ARG:NH1	1:W2:241:LYS:HB2	2.35	0.41
1:X2:15:GLN:HB2	1:d2:341:ALA:HB1	2.02	0.41
1:A1:178:ALA:O	1:A1:241:LYS:HE3	2.20	0.41
1:D2:27:LYS:HD3	1:D2:27:LYS:H	1.85	0.41
1:H2:82:MET:HG2	1:H2:304:ARG:HG3	2.02	0.41
1:J2:26:GLN:HG2	1:N2:10:SER:HB3	2.03	0.41
1:L2:106:SER:O	1:L2:110:ARG:HD3	2.20	0.41
1:O2:65:VAL:HG23	1:O2:318:ILE:HG12	2.03	0.41
1:O2:161:MET:HE3	1:O2:161:MET:HB3	2.00	0.41
1:S2:112:ILE:HG22	1:S2:280:VAL:HG21	2.03	0.41
1:X2:353:LEU:HD23	1:X2:353:LEU:HA	1.82	0.41
1:Z2:353:LEU:HD23	1:Z2:353:LEU:HA	1.94	0.41
1:d2:208:VAL:HG11	1:d2:229:THR:HG21	2.02	0.41
1:f2:88:ILE:O	1:f2:92:MET:HG3	2.20	0.41
1:A1:247:SER:HB3	1:A1:250:LYS:HE2	2.01	0.41
1:F2:84:GLU:HG3	1:P2:320:ASN:HB2	2.02	0.41
1:I2:219:GLU:OE2	1:I2:219:GLU:HA	2.21	0.41
1:L2:69:ASN:HB3	1:W2:334:ARG:HD2	2.03	0.41
1:Q2:351:GLN:O	1:Q2:355:GLN:HG3	2.20	0.41
1:S2:106:SER:O	1:S2:110:ARG:HD3	2.20	0.41
1:V2:92:MET:HE3	1:V2:92:MET:HB2	1.90	0.41
1:V2:210:ILE:HG21	1:V2:225:ILE:HG12	2.02	0.41
1:b2:174:LYS:H	1:b2:174:LYS:HG2	1.66	0.41
1:b2:179:GLN:NE2	1:b2:266:GLY:HA3	2.35	0.41
1:A2:161:MET:HE2	1:A2:161:MET:HB3	1.86	0.41
1:A2:320:ASN:HB2	1:H2:84:GLU:HG2	2.02	0.41
1:D2:38:ILE:HD12	1:D2:336:ARG:HA	2.02	0.41
1:F2:131:SER:HB3	1:F2:136:LYS:HD2	2.02	0.41
1:I2:57:GLN:O	1:I2:61:LEU:HD22	2.20	0.41
1:I2:349:LYS:O	1:I2:353:LEU:HD23	2.20	0.41
1:J2:92:MET:HA	1:J2:95:LEU:HD12	2.03	0.41
1:S2:62:ASP:HB3	1:S2:63:MET:HE2	2.03	0.41
1:S2:349:LYS:HG3	1:U2:5:VAL:O	2.20	0.41
1:U2:374:LEU:HD12	1:U2:375:LEU:HB2	2.03	0.41
1:X2:84:GLU:OE2	1:X2:84:GLU:HA	2.21	0.41
1:a2:29:MET:HG3	1:e2:363:GLN:NE2	2.34	0.41
1:e2:23:ASP:HA	1:e2:27:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B2:233:LYS:HE3	1:B2:233:LYS:HB2	1.92	0.41
1:C2:347:MET:HE3	1:C2:347:MET:HB3	1.84	0.41
1:E2:333:SER:HA	1:E2:337:ASP:HB2	2.01	0.41
1:J2:182:LYS:HB2	1:J2:218:LEU:HD22	2.02	0.41
1:N2:159:LEU:HD13	1:N2:310:PHE:CD1	2.56	0.41
1:O2:17:TYR:CE1	1:f2:34:SER:HB3	2.55	0.41
1:V2:221:LEU:HD21	1:V2:261:LEU:HD21	2.03	0.41
1:e2:131:SER:HB3	1:e2:136:LYS:HD3	2.03	0.41
1:A1:207:GLU:OE1	1:A1:207:GLU:HA	2.19	0.41
1:B2:334:ARG:HD2	1:P2:69:ASN:HB3	2.03	0.41
1:C2:274:THR:HG22	1:C2:275:VAL:N	2.36	0.41
1:E2:238:GLU:OE1	1:E2:282:THR:HB	2.20	0.41
1:G2:59:ARG:HE	1:G2:59:ARG:HB3	1.76	0.41
1:M2:34:SER:HB3	1:T2:17:TYR:CE2	2.56	0.41
1:O2:174:LYS:HE2	1:O2:174:LYS:HB2	1.89	0.41
1:P2:42:ARG:HG2	1:P2:42:ARG:HH11	1.85	0.41
1:R2:23:ASP:HB3	1:R2:27:LYS:NZ	2.33	0.41
1:T2:9:VAL:O	1:T2:13:THR:HG23	2.21	0.41
1:Y2:354:GLN:O	1:Y2:358:THR:HG22	2.21	0.41
1:Z2:29:MET:HE3	1:Z2:29:MET:HB2	1.86	0.41
1:a2:140:GLY:HA3	1:a2:163:SER:HB2	2.03	0.41
1:d2:288:GLU:HG3	1:d2:292:ILE:HD11	2.02	0.41
1:B2:152:ASP:O	1:B2:155:GLU:HG3	2.20	0.41
1:B2:206:ARG:HD3	1:B2:206:ARG:HA	1.91	0.41
1:G2:94:ASP:OD1	1:G2:94:ASP:C	2.63	0.41
1:J2:12:MET:HA	1:J2:15:GLN:NE2	2.36	0.41
1:J2:92:MET:HE2	1:J2:293:LEU:HD21	2.02	0.41
1:L2:214:GLN:CD	1:L2:214:GLN:H	2.29	0.41
1:M2:27:LYS:O	1:M2:31:ARG:HG3	2.20	0.41
1:O2:110:ARG:NH1	1:O2:281:SER:HB3	2.36	0.41
1:R2:235:SER:HB2	1:R2:243:GLN:HE21	1.86	0.41
1:T2:206:ARG:HD2	1:T2:206:ARG:HA	1.85	0.41
1:U2:68:ALA:HB3	1:U2:318:ILE:HD11	2.03	0.41
1:U2:137:LEU:HB2	1:U2:138:LEU:HD22	2.02	0.41
1:b2:142:PHE:CD2	1:b2:161:MET:HG3	2.56	0.41
1:f2:201:LYS:HB3	1:f2:250:LYS:HA	2.02	0.41
1:A1:34:SER:HB3	1:M2:17:TYR:CZ	2.56	0.41
1:C2:169:GLN:OE1	1:C2:169:GLN:HA	2.21	0.41
1:C2:218:LEU:HD12	1:C2:218:LEU:HA	1.79	0.41
1:C2:374:LEU:HD11	1:S2:361:LEU:HD23	2.03	0.41
1:D2:15:GLN:HA	1:D2:18:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G2:74:ILE:HD11	1:e2:103:SER:HA	2.01	0.41
1:H2:92:MET:HB3	1:H2:293:LEU:HD21	2.02	0.41
1:H2:131:SER:HB3	1:H2:136:LYS:HE2	2.03	0.41
1:H2:294:ASP:O	1:H2:298:LYS:HG2	2.20	0.41
1:I2:289:ALA:HA	1:I2:292:ILE:HD12	2.01	0.41
1:K2:336:ARG:HE	1:K2:336:ARG:HB2	1.74	0.41
1:K2:353:LEU:HD23	1:K2:353:LEU:HA	1.92	0.41
1:L2:351:GLN:O	1:L2:355:GLN:HG3	2.20	0.41
1:N2:168:THR:HG22	1:N2:170:ALA:H	1.85	0.41
1:O2:12:MET:HA	1:O2:15:GLN:NE2	2.36	0.41
1:O2:95:LEU:CD1	1:O2:115:GLU:HG2	2.51	0.41
1:O2:247:SER:OG	1:O2:249:GLN:HG3	2.21	0.41
1:Q2:101:ASN:HD22	1:W2:67:ASN:CG	2.28	0.41
1:R2:198:TYR:HB3	1:R2:255:VAL:HG22	2.01	0.41
1:T2:164:MET:SD	1:T2:300:VAL:HG22	2.61	0.41
1:T2:218:LEU:HD12	1:T2:218:LEU:HA	1.77	0.41
1:U2:144:SER:HA	1:U2:159:LEU:O	2.19	0.41
1:U2:223:THR:HA	1:U2:226:ASN:ND2	2.36	0.41
1:X2:140:GLY:HA3	1:X2:163:SER:HB2	2.02	0.41
1:Y2:310:PHE:CD1	1:Y2:310:PHE:C	2.98	0.41
1:c2:82:MET:HG2	1:c2:304:ARG:HG3	2.02	0.41
1:c2:201:LYS:HD2	1:c2:250:LYS:HA	2.02	0.41
1:d2:24:GLY:HA2	1:d2:27:LYS:HD2	2.02	0.41
1:d2:124:ASN:HB3	1:d2:165:ARG:HH12	1.85	0.41
1:e2:331:SER:O	1:e2:335:ILE:HG22	2.21	0.41
1:f2:85:THR:HG23	1:f2:123:LEU:HD22	2.02	0.41
1:A2:208:VAL:HG11	1:A2:229:THR:HG21	2.03	0.41
1:B2:178:ALA:O	1:B2:241:LYS:HE3	2.21	0.41
1:C2:249:GLN:HE21	1:C2:298:LYS:HB3	1.85	0.41
1:E2:104:ASN:HB2	1:E2:109:ARG:NH1	2.35	0.41
1:M2:74:ILE:HD12	1:M2:147:PHE:CE2	2.55	0.41
1:Q2:159:LEU:HB2	1:Q2:310:PHE:CE1	2.56	0.41
1:U2:318:ILE:HD13	1:U2:318:ILE:HA	1.87	0.41
1:X2:362:ALA:HA	1:X2:365:LYS:NZ	2.36	0.41
1:a2:332:ARG:C	1:a2:332:ARG:HD2	2.46	0.41
1:d2:346:ALA:HA	1:d2:349:LYS:HG2	2.03	0.41
1:f2:95:LEU:HD11	1:f2:115:GLU:HG2	2.03	0.41
1:f2:238:GLU:HG3	1:f2:283:VAL:CG1	2.51	0.41
1:A1:161:MET:HE3	1:A1:161:MET:HB2	1.91	0.40
1:D2:233:LYS:HB3	1:D2:233:LYS:HE2	1.59	0.40
1:D2:375:LEU:HD21	1:G2:365:LYS:NZ	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E2:349:LYS:HE3	1:G2:6:ASN:HA	2.04	0.40
1:E2:360:VAL:CG2	1:e2:29:MET:HB2	2.51	0.40
1:F2:54:LEU:HD22	1:F2:328:VAL:HG23	2.02	0.40
1:J2:94:ASP:OD2	1:J2:94:ASP:C	2.64	0.40
1:J2:331:SER:HB2	1:R2:73:SER:HB2	2.03	0.40
1:M2:178:ALA:O	1:M2:241:LYS:HD2	2.21	0.40
1:N2:61:LEU:HD13	1:N2:325:ASN:HA	2.03	0.40
1:O2:34:SER:HB3	1:Q2:17:TYR:CZ	2.56	0.40
1:R2:159:LEU:HD22	1:R2:310:PHE:CE2	2.56	0.40
1:R2:218:LEU:HD12	1:R2:218:LEU:HA	1.80	0.40
1:T2:298:LYS:HB2	1:T2:298:LYS:HE3	1.76	0.40
1:U2:59:ARG:O	1:U2:63:MET:HG2	2.21	0.40
1:V2:89:LEU:HD23	1:V2:89:LEU:HA	1.89	0.40
1:W2:128:GLU:OE2	1:W2:165:ARG:HD2	2.20	0.40
1:X2:28:SER:O	1:X2:32:LEU:HG	2.21	0.40
1:b2:27:LYS:HE2	1:b2:27:LYS:HB2	1.63	0.40
1:b2:147:PHE:HE1	1:b2:159:LEU:HB3	1.86	0.40
1:b2:178:ALA:HB3	1:b2:241:LYS:HB3	2.03	0.40
1:b2:374:LEU:HD23	1:b2:375:LEU:N	2.36	0.40
1:c2:161:MET:HE2	1:c2:161:MET:HB3	1.95	0.40
1:d2:27:LYS:HE2	1:d2:27:LYS:HB3	1.69	0.40
1:d2:92:MET:SD	1:d2:116:VAL:HG13	2.61	0.40
1:A1:110:ARG:NH1	1:A1:281:SER:HB3	2.33	0.40
1:A1:332:ARG:HD2	1:A1:336:ARG:HB2	2.03	0.40
1:B2:3:ILE:HG23	1:B2:3:ILE:O	2.21	0.40
1:F2:2:ALA:HB1	1:d2:339:ASP:HB2	2.03	0.40
1:F2:5:VAL:HA	1:F2:368:PRO:HB3	2.02	0.40
1:G2:123:LEU:HD23	1:G2:123:LEU:HA	1.91	0.40
1:H2:348:THR:O	1:H2:352:ILE:HG12	2.22	0.40
1:I2:221:LEU:HD21	1:I2:261:LEU:HD21	2.03	0.40
1:M2:168:THR:HB	1:M2:171:MET:HG3	2.03	0.40
1:N2:106:SER:O	1:N2:110:ARG:HG2	2.22	0.40
1:P2:235:SER:HB2	1:P2:243:GLN:HE21	1.85	0.40
1:Q2:282:THR:HG23	1:Q2:285:GLY:H	1.87	0.40
1:T2:241:LYS:HB3	1:T2:241:LYS:HE2	1.85	0.40
1:U2:375:LEU:HD23	1:U2:375:LEU:HA	1.79	0.40
1:V2:50:ILE:HD12	1:V2:50:ILE:HA	1.91	0.40
1:d2:110:ARG:H	1:d2:110:ARG:HG2	1.66	0.40
1:e2:75:ALA:HB1	1:e2:307:LEU:HD22	2.03	0.40
1:e2:286:SER:O	1:e2:290:VAL:HG23	2.21	0.40
1:A2:246:ALA:HB1	1:A2:251:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:24:GLY:HA2	1:C2:27:LYS:NZ	2.36	0.40
1:C2:44:ASP:OD2	1:C2:44:ASP:C	2.64	0.40
1:D2:247:SER:OG	1:D2:250:LYS:HB2	2.21	0.40
1:D2:340:TYR:HB2	1:U2:3:ILE:HG23	2.03	0.40
1:E2:349:LYS:O	1:E2:353:LEU:HD22	2.20	0.40
1:F2:333:SER:HB2	1:H2:7:THR:OG1	2.20	0.40
1:H2:82:MET:HE2	1:H2:82:MET:HB2	1.85	0.40
1:K2:152:ASP:O	1:K2:155:GLU:HG3	2.21	0.40
1:L2:147:PHE:HE1	1:L2:159:LEU:HB3	1.87	0.40
1:N2:238:GLU:HG3	1:N2:283:VAL:HG22	2.02	0.40
1:N2:356:ALA:O	1:N2:360:VAL:HG23	2.21	0.40
1:P2:63:MET:HE1	1:P2:67:ASN:ND2	2.37	0.40
1:P2:201:LYS:HA	1:P2:201:LYS:HD2	1.85	0.40
1:T2:78:ALA:HB2	1:T2:137:LEU:HD13	2.03	0.40
1:U2:257:ILE:HD13	1:U2:257:ILE:HA	1.97	0.40
1:Z2:32:LEU:HD23	1:Z2:340:TYR:CD1	2.57	0.40
1:b2:59:ARG:O	1:b2:63:MET:HB2	2.21	0.40
1:d2:339:ASP:H	1:d2:342:ARG:HH21	1.68	0.40
1:e2:201:LYS:HD3	1:e2:201:LYS:HA	1.78	0.40
1:e2:343:GLU:OE2	1:e2:343:GLU:HA	2.21	0.40
1:H2:63:MET:SD	1:H2:66:LYS:HE3	2.61	0.40
1:Q2:46:ALA:O	1:Q2:50:ILE:HG22	2.20	0.40
1:R2:138:LEU:HB3	1:R2:164:MET:HB2	2.04	0.40
1:S2:179:GLN:NE2	1:S2:266:GLY:HA3	2.37	0.40
1:Y2:128:GLU:OE2	1:Y2:165:ARG:HD2	2.21	0.40
1:a2:70:ASP:O	1:a2:74:ILE:HG13	2.22	0.40
1:d2:54:LEU:HA	1:d2:57:GLN:HG3	2.03	0.40
1:d2:78:ALA:O	1:d2:82:MET:HG2	2.21	0.40
1:D2:129:THR:HB	1:S2:155:GLU:OE1	2.21	0.40
1:D2:173:GLY:HA2	1:D2:248:SER:HB2	2.02	0.40
1:E2:99:SER:HB2	1:E2:112:ILE:HG13	2.04	0.40
1:F2:161:MET:HE3	1:F2:161:MET:HB3	1.57	0.40
1:F2:196:LEU:HD23	1:F2:257:ILE:HG23	2.04	0.40
1:K2:1:MET:HG2	1:N2:26:GLN:OE1	2.20	0.40
1:M2:85:THR:HG23	1:M2:123:LEU:HD22	2.02	0.40
1:N2:68:ALA:HB3	1:N2:318:ILE:HD11	2.03	0.40
1:P2:140:GLY:HA3	1:P2:163:SER:HB2	2.04	0.40
1:R2:59:ARG:O	1:R2:63:MET:HG2	2.22	0.40
1:V2:113:GLN:NE2	1:V2:279:ASN:HA	2.36	0.40
1:V2:201:LYS:H	1:V2:201:LYS:HG3	1.52	0.40
1:Z2:73:SER:CB	1:b2:331:SER:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f2:247:SER:OG	1:f2:249:GLN:HG3	2.22	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	A1	374/376 (100%)	371 (99%)	3 (1%)	0	100	100
1	A2	374/376 (100%)	370 (99%)	4 (1%)	0	100	100
1	B2	374/376 (100%)	371 (99%)	3 (1%)	0	100	100
1	C2	374/376 (100%)	372 (100%)	2 (0%)	0	100	100
1	D2	374/376 (100%)	368 (98%)	6 (2%)	0	100	100
1	E2	374/376 (100%)	371 (99%)	3 (1%)	0	100	100
1	F2	374/376 (100%)	364 (97%)	10 (3%)	0	100	100
1	G2	374/376 (100%)	367 (98%)	7 (2%)	0	100	100
1	H2	374/376 (100%)	367 (98%)	7 (2%)	0	100	100
1	I2	374/376 (100%)	373 (100%)	1 (0%)	0	100	100
1	J2	374/376 (100%)	369 (99%)	5 (1%)	0	100	100
1	K2	374/376 (100%)	367 (98%)	7 (2%)	0	100	100
1	L2	374/376 (100%)	371 (99%)	3 (1%)	0	100	100
1	M2	374/376 (100%)	372 (100%)	2 (0%)	0	100	100
1	N2	374/376 (100%)	372 (100%)	2 (0%)	0	100	100
1	O2	374/376 (100%)	371 (99%)	3 (1%)	0	100	100
1	P2	374/376 (100%)	365 (98%)	9 (2%)	0	100	100
1	Q2	374/376 (100%)	367 (98%)	7 (2%)	0	100	100
1	R2	374/376 (100%)	371 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S2	374/376 (100%)	369 (99%)	5 (1%)	0	100	100
1	T2	374/376 (100%)	369 (99%)	5 (1%)	0	100	100
1	U2	374/376 (100%)	370 (99%)	4 (1%)	0	100	100
1	V2	374/376 (100%)	371 (99%)	3 (1%)	0	100	100
1	W2	374/376 (100%)	369 (99%)	5 (1%)	0	100	100
1	X2	374/376 (100%)	370 (99%)	4 (1%)	0	100	100
1	Y2	374/376 (100%)	369 (99%)	5 (1%)	0	100	100
1	Z2	374/376 (100%)	368 (98%)	6 (2%)	0	100	100
1	a2	374/376 (100%)	372 (100%)	2 (0%)	0	100	100
1	b2	374/376 (100%)	369 (99%)	5 (1%)	0	100	100
1	c2	374/376 (100%)	372 (100%)	2 (0%)	0	100	100
1	d2	374/376 (100%)	372 (100%)	2 (0%)	0	100	100
1	e2	374/376 (100%)	372 (100%)	2 (0%)	0	100	100
1	f2	374/376 (100%)	371 (99%)	3 (1%)	0	100	100
All	All	12342/12408 (100%)	12202 (99%)	140 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	A2	291/291 (100%)	285 (98%)	6 (2%)	48	71
1	B2	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	C2	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	D2	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	E2	291/291 (100%)	283 (97%)	8 (3%)	40	65
1	F2	291/291 (100%)	282 (97%)	9 (3%)	35	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G2	291/291 (100%)	289 (99%)	2 (1%)	81	90
1	H2	291/291 (100%)	285 (98%)	6 (2%)	48	71
1	I2	291/291 (100%)	288 (99%)	3 (1%)	73	85
1	J2	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	K2	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	L2	291/291 (100%)	286 (98%)	5 (2%)	56	75
1	M2	291/291 (100%)	287 (99%)	4 (1%)	62	80
1	N2	291/291 (100%)	281 (97%)	10 (3%)	32	60
1	O2	291/291 (100%)	283 (97%)	8 (3%)	40	65
1	P2	291/291 (100%)	285 (98%)	6 (2%)	48	71
1	Q2	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	R2	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	S2	291/291 (100%)	280 (96%)	11 (4%)	28	56
1	T2	291/291 (100%)	282 (97%)	9 (3%)	35	62
1	U2	291/291 (100%)	282 (97%)	9 (3%)	35	62
1	V2	291/291 (100%)	285 (98%)	6 (2%)	48	71
1	W2	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	X2	291/291 (100%)	284 (98%)	7 (2%)	44	68
1	Y2	291/291 (100%)	286 (98%)	5 (2%)	56	75
1	Z2	291/291 (100%)	285 (98%)	6 (2%)	48	71
1	a2	291/291 (100%)	287 (99%)	4 (1%)	62	80
1	b2	291/291 (100%)	287 (99%)	4 (1%)	62	80
1	c2	291/291 (100%)	288 (99%)	3 (1%)	73	85
1	d2	291/291 (100%)	283 (97%)	8 (3%)	40	65
1	e2	291/291 (100%)	285 (98%)	6 (2%)	48	71
1	f2	291/291 (100%)	285 (98%)	6 (2%)	48	71
All	All	9603/9603 (100%)	9389 (98%)	214 (2%)	47	70

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	1	MET
1	A1	213	LYS

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Mol	Chain	Res	Type
1	A1	265	ILE
1	A1	280	VAL
1	A1	282	THR
1	A1	303	GLN
1	A1	354	GLN
1	A2	82	MET
1	A2	171	MET
1	A2	182	LYS
1	A2	208	VAL
1	A2	247	SER
1	A2	374	LEU
1	B2	9	VAL
1	B2	201	LYS
1	B2	351	GLN
1	B2	353	LEU
1	B2	366	GLN
1	B2	372	LEU
1	B2	373	SER
1	C2	10	SER
1	C2	53	ARG
1	C2	192	THR
1	C2	201	LYS
1	C2	248	SER
1	C2	250	LYS
1	C2	282	THR
1	D2	5	VAL
1	D2	26	GLN
1	D2	148	GLN
1	D2	218	LEU
1	D2	303	GLN
1	D2	311	GLN
1	D2	336	ARG
1	E2	29	MET
1	E2	179	GLN
1	E2	201	LYS
1	E2	239	ASP
1	E2	254	ASP
1	E2	303	GLN
1	E2	326	GLU
1	E2	355	GLN
1	F2	38	ILE
1	F2	42	ARG

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Mol	Chain	Res	Type
1	F2	171	MET
1	F2	218	LEU
1	F2	239	ASP
1	F2	247	SER
1	F2	336	ARG
1	F2	353	LEU
1	F2	372	LEU
1	G2	195	THR
1	G2	265	ILE
1	H2	82	MET
1	H2	161	MET
1	H2	233	LYS
1	H2	288	GLU
1	H2	353	LEU
1	H2	354	GLN
1	I2	158	MET
1	I2	179	GLN
1	I2	192	THR
1	J2	38	ILE
1	J2	62	ASP
1	J2	76	GLN
1	J2	171	MET
1	J2	202	GLN
1	J2	229	THR
1	J2	235	SER
1	K2	82	MET
1	K2	87	ASN
1	K2	100	SER
1	K2	228	GLN
1	K2	238	GLU
1	K2	271	ARG
1	K2	291	SER
1	L2	82	MET
1	L2	169	GLN
1	L2	254	ASP
1	L2	358	THR
1	L2	372	LEU
1	M2	265	ILE
1	M2	278	VAL
1	M2	298	LYS
1	M2	333	SER
1	N2	49	GLN

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Mol	Chain	Res	Type
1	N2	59	ARG
1	N2	126	ILE
1	N2	155	GLU
1	N2	166	SER
1	N2	223	THR
1	N2	291	SER
1	N2	322	ASP
1	N2	353	LEU
1	N2	366	GLN
1	O2	5	VAL
1	O2	39	ASN
1	O2	171	MET
1	O2	197	SER
1	O2	204	GLU
1	O2	218	LEU
1	O2	235	SER
1	O2	303	GLN
1	P2	63	MET
1	P2	82	MET
1	P2	177	ARG
1	P2	187	ARG
1	P2	271	ARG
1	P2	278	VAL
1	Q2	25	MET
1	Q2	82	MET
1	Q2	211	ASN
1	Q2	213	LYS
1	Q2	239	ASP
1	Q2	278	VAL
1	Q2	294	ASP
1	R2	7	THR
1	R2	25	MET
1	R2	29	MET
1	R2	42	ARG
1	R2	166	SER
1	R2	337	ASP
1	R2	353	LEU
1	S2	26	GLN
1	S2	79	GLU
1	S2	113	GLN
1	S2	163	SER
1	S2	195	THR

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Mol	Chain	Res	Type
1	S2	218	LEU
1	S2	226	ASN
1	S2	249	GLN
1	S2	278	VAL
1	S2	291	SER
1	S2	353	LEU
1	T2	1	MET
1	T2	3	ILE
1	T2	164	MET
1	T2	196	LEU
1	T2	202	GLN
1	T2	206	ARG
1	T2	239	ASP
1	T2	271	ARG
1	T2	355	GLN
1	U2	8	ASN
1	U2	82	MET
1	U2	113	GLN
1	U2	164	MET
1	U2	201	LYS
1	U2	274	THR
1	U2	278	VAL
1	U2	311	GLN
1	U2	363	GLN
1	V2	122	GLU
1	V2	145	LYS
1	V2	158	MET
1	V2	249	GLN
1	V2	255	VAL
1	V2	264	GLU
1	W2	101	ASN
1	W2	113	GLN
1	W2	218	LEU
1	W2	219	GLU
1	W2	288	GLU
1	W2	291	SER
1	W2	374	LEU
1	X2	55	THR
1	X2	82	MET
1	X2	114	GLU
1	X2	179	GLN
1	X2	239	ASP

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Mol	Chain	Res	Type
1	X2	250	LYS
1	X2	354	GLN
1	Y2	25	MET
1	Y2	164	MET
1	Y2	192	THR
1	Y2	283	VAL
1	Y2	375	LEU
1	Z2	8	ASN
1	Z2	171	MET
1	Z2	196	LEU
1	Z2	239	ASP
1	Z2	265	ILE
1	Z2	337	ASP
1	a2	1	MET
1	a2	171	MET
1	a2	235	SER
1	a2	355	GLN
1	b2	5	VAL
1	b2	239	ASP
1	b2	291	SER
1	b2	375	LEU
1	c2	218	LEU
1	c2	238	GLU
1	c2	372	LEU
1	d2	55	THR
1	d2	169	GLN
1	d2	195	THR
1	d2	228	GLN
1	d2	247	SER
1	d2	265	ILE
1	d2	307	LEU
1	d2	374	LEU
1	e2	158	MET
1	e2	179	GLN
1	e2	196	LEU
1	e2	206	ARG
1	e2	283	VAL
1	e2	337	ASP
1	f2	145	LYS
1	f2	164	MET
1	f2	207	GLU
1	f2	248	SER

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Mol	Chain	Res	Type
1	f2	278	VAL
1	f2	353	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	135	ASN
1	A1	249	GLN
1	A1	272	ASN
1	A1	320	ASN
1	A2	15	GLN
1	A2	87	ASN
1	A2	113	GLN
1	A2	211	ASN
1	B2	6	ASN
1	B2	76	GLN
1	B2	101	ASN
1	B2	243	GLN
1	B2	325	ASN
1	C2	101	ASN
1	C2	320	ASN
1	C2	323	ASN
1	D2	67	ASN
1	D2	98	GLN
1	D2	320	ASN
1	D2	363	GLN
1	E2	19	ASN
1	E2	26	GLN
1	E2	69	ASN
1	E2	214	GLN
1	F2	76	GLN
1	F2	243	GLN
1	F2	320	ASN
1	F2	327	ASN
1	G2	15	GLN
1	G2	120	ASN
1	G2	272	ASN
1	G2	279	ASN
1	G2	303	GLN
1	G2	354	GLN
1	H2	39	ASN
1	I2	67	ASN

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Mol	Chain	Res	Type
1	I2	76	GLN
1	I2	148	GLN
1	I2	279	ASN
1	J2	98	GLN
1	J2	120	ASN
1	K2	179	GLN
1	K2	202	GLN
1	K2	311	GLN
1	K2	351	GLN
1	K2	355	GLN
1	K2	366	GLN
1	L2	6	ASN
1	L2	15	GLN
1	L2	211	ASN
1	M2	8	ASN
1	M2	69	ASN
1	M2	87	ASN
1	M2	90	GLN
1	M2	243	GLN
1	M2	363	GLN
1	N2	67	ASN
1	N2	249	GLN
1	O2	90	GLN
1	O2	113	GLN
1	O2	179	GLN
1	O2	200	ASN
1	P2	4	ASN
1	P2	98	GLN
1	P2	120	ASN
1	P2	252	ASN
1	P2	272	ASN
1	Q2	15	GLN
1	Q2	214	GLN
1	Q2	279	ASN
1	Q2	287	GLN
1	Q2	363	GLN
1	R2	87	ASN
1	R2	179	GLN
1	S2	15	GLN
1	S2	272	ASN
1	S2	320	ASN
1	S2	325	ASN

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Mol	Chain	Res	Type
1	T2	120	ASN
1	T2	211	ASN
1	T2	323	ASN
1	U2	8	ASN
1	U2	15	GLN
1	U2	39	ASN
1	U2	57	GLN
1	U2	87	ASN
1	U2	303	GLN
1	U2	363	GLN
1	V2	113	GLN
1	V2	279	ASN
1	W2	15	GLN
1	W2	87	ASN
1	W2	90	GLN
1	W2	179	GLN
1	W2	200	ASN
1	W2	252	ASN
1	W2	272	ASN
1	X2	76	GLN
1	X2	120	ASN
1	X2	179	GLN
1	X2	214	GLN
1	X2	366	GLN
1	Y2	113	GLN
1	Y2	252	ASN
1	Y2	303	GLN
1	Y2	323	ASN
1	Y2	327	ASN
1	Z2	15	GLN
1	Z2	214	GLN
1	Z2	272	ASN
1	Z2	323	ASN
1	Z2	366	GLN
1	a2	26	GLN
1	a2	179	GLN
1	a2	249	GLN
1	a2	272	ASN
1	a2	327	ASN
1	b2	39	ASN
1	b2	87	ASN
1	b2	148	GLN

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Mol	Chain	Res	Type
1	b2	272	ASN
1	b2	323	ASN
1	c2	15	GLN
1	c2	19	ASN
1	c2	120	ASN
1	c2	214	GLN
1	d2	113	GLN
1	d2	120	ASN
1	d2	320	ASN
1	e2	120	ASN
1	e2	329	ASN
1	e2	363	GLN
1	f2	15	GLN
1	f2	120	ASN
1	f2	214	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.

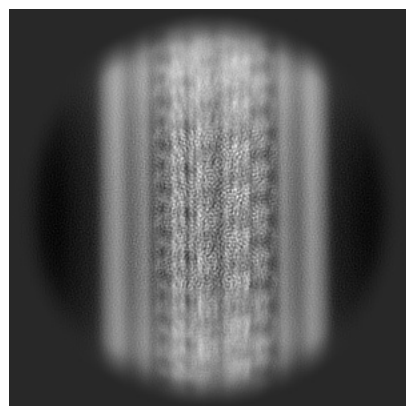
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71351. These allow visual inspection of the internal detail of the map and identification of artifacts.

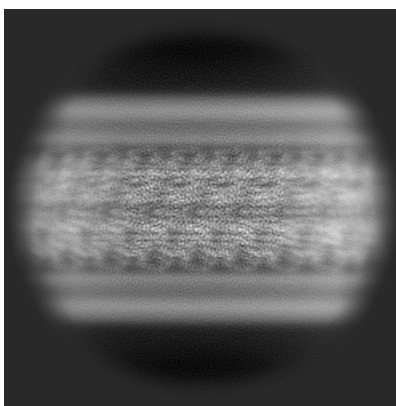
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

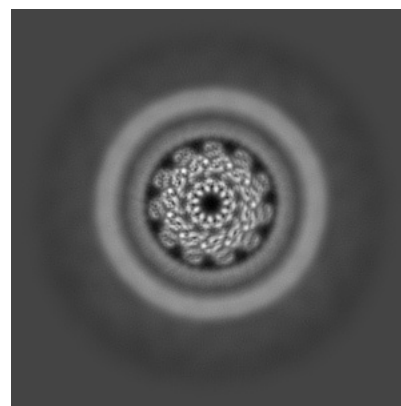
6.1.1 Primary map



X

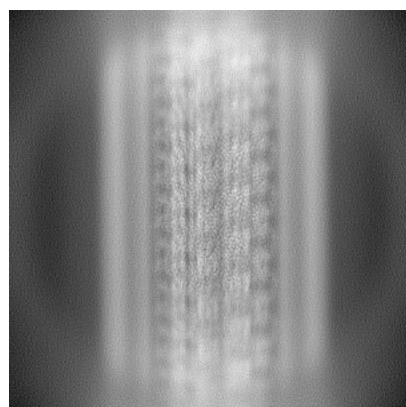


Y

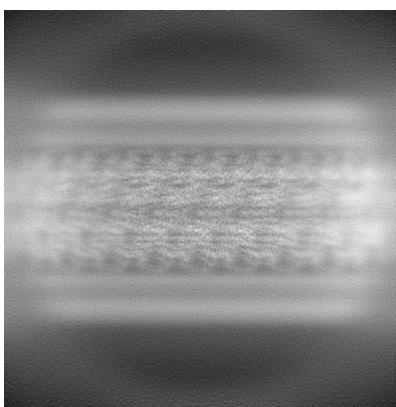


Z

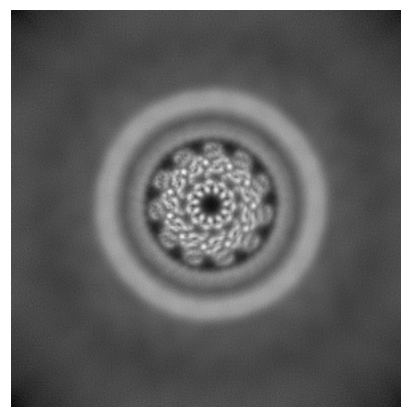
6.1.2 Raw map



X



Y

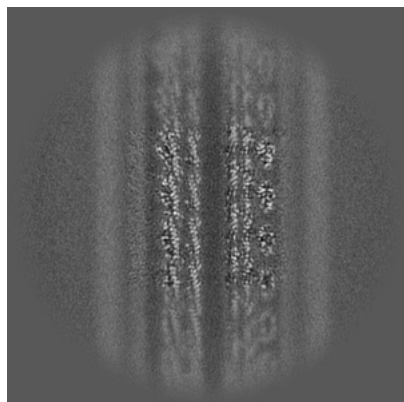


Z

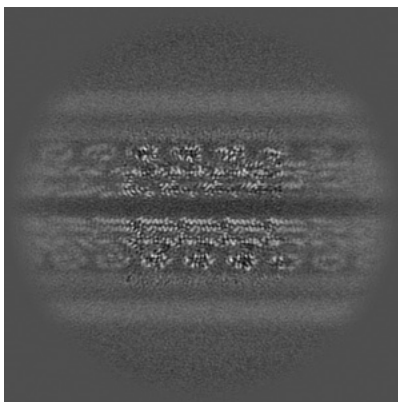
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

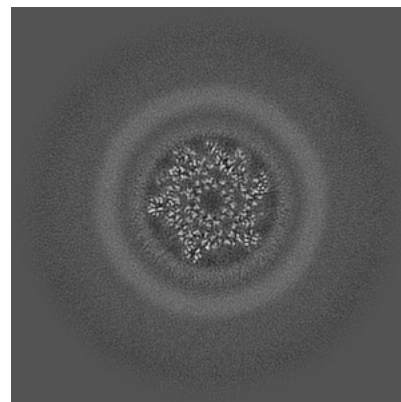
6.2.1 Primary map



X Index: 224

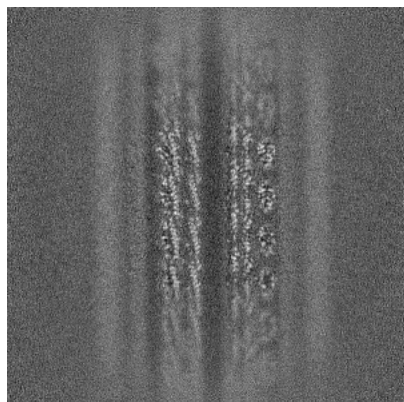


Y Index: 224

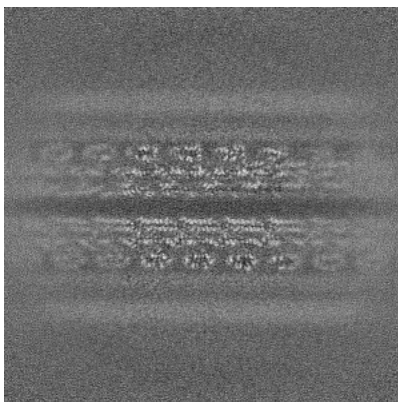


Z Index: 224

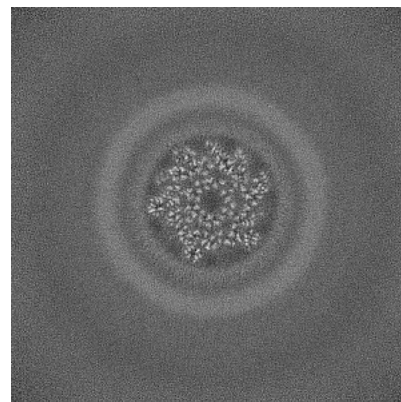
6.2.2 Raw map



X Index: 224



Y Index: 224

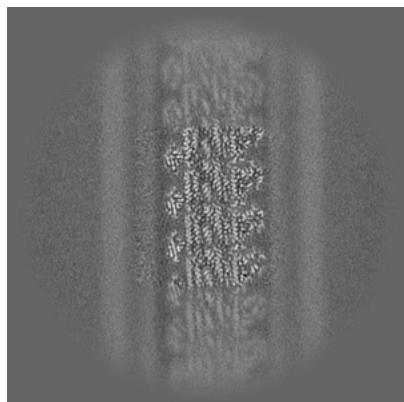


Z Index: 224

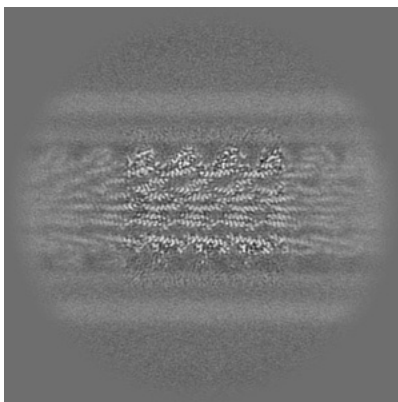
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

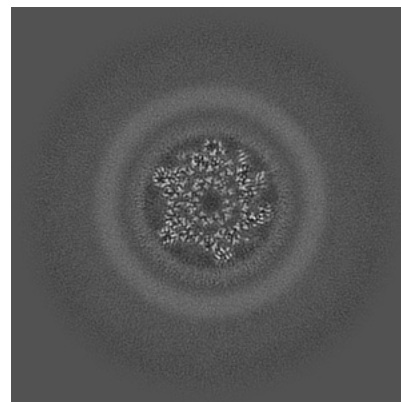
6.3.1 Primary map



X Index: 263

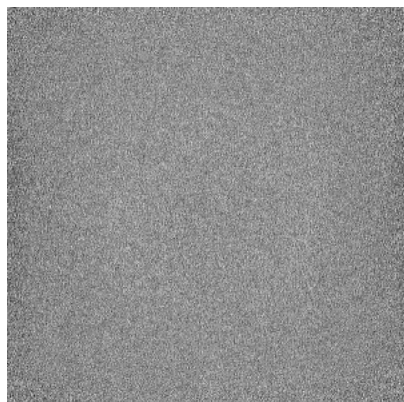


Y Index: 212

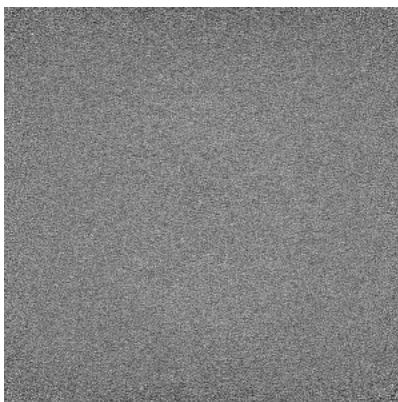


Z Index: 245

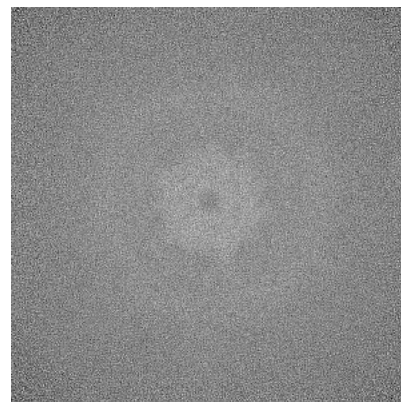
6.3.2 Raw map



X Index: 0



Y Index: 0

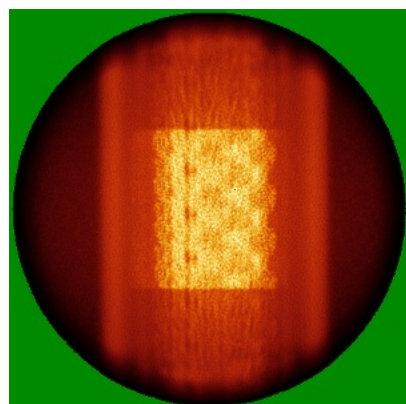


Z Index: 447

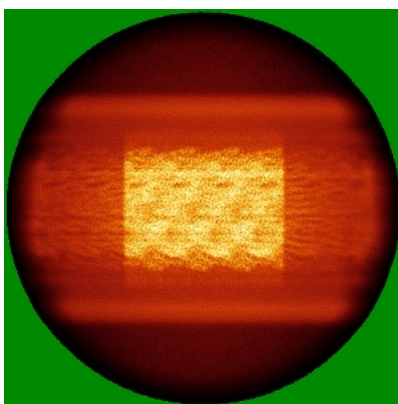
The images above show the largest variance slices of the map in three orthogonal directions.

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

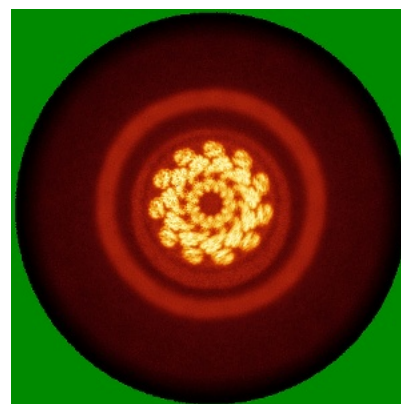
6.4.1 Primary map



X

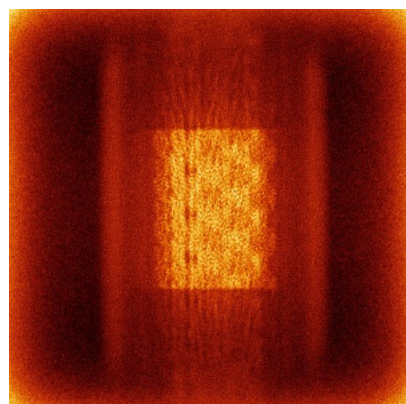


Y

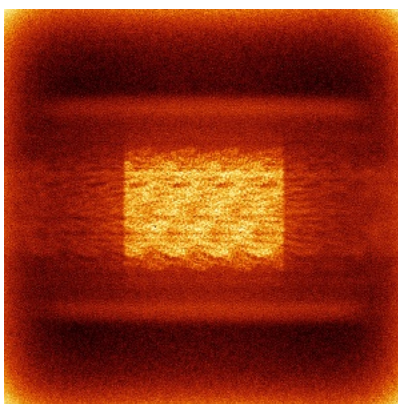


Z

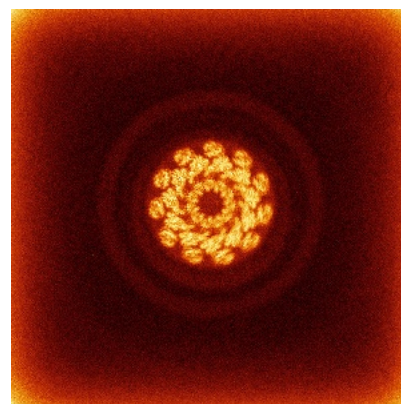
6.4.2 Raw map



X



Y

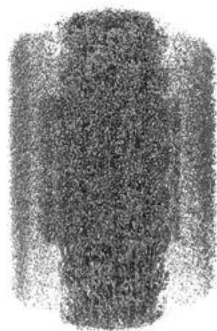


Z

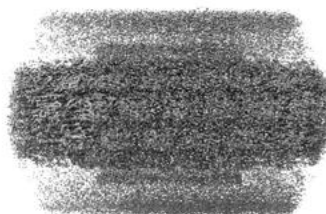
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

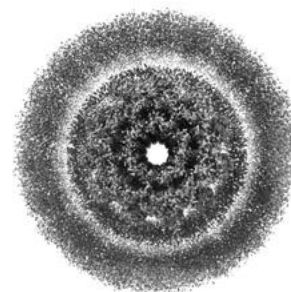
6.5.1 Primary map



X



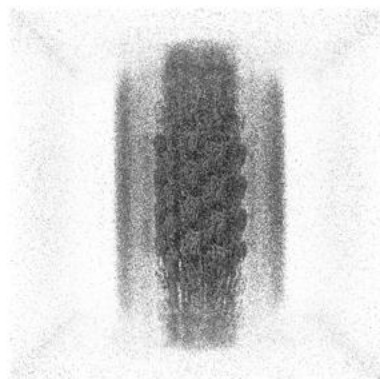
Y



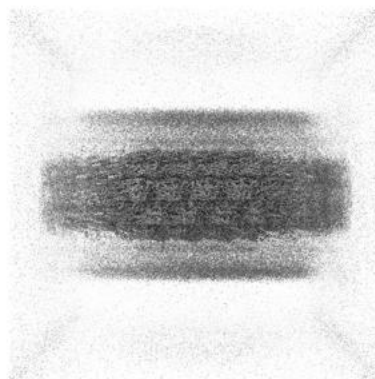
Z

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.

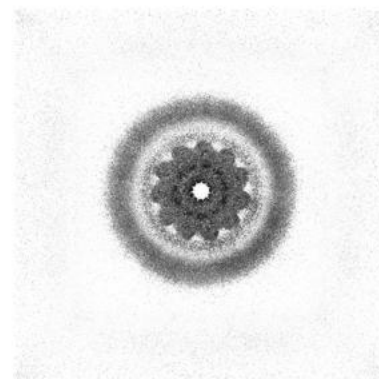
6.5.2 Raw map



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.

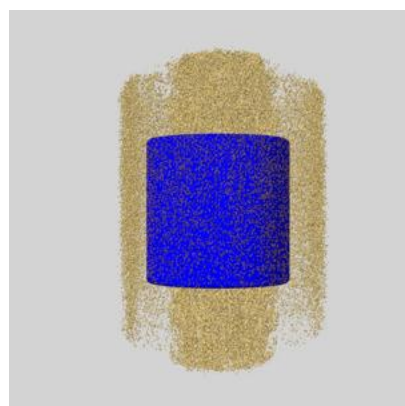
6.6 Mask visualisation [i](#)

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

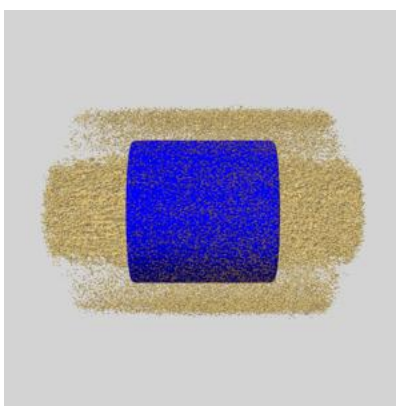
A mask typically either:

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

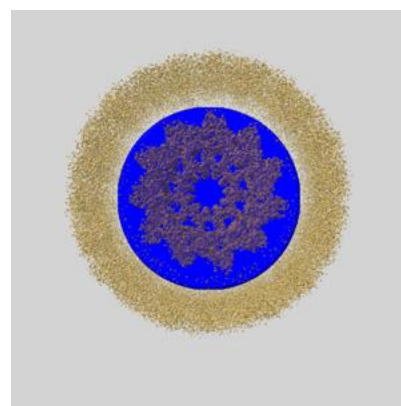
6.6.1 emd_71351_msk_1.map [i](#)



X



Y

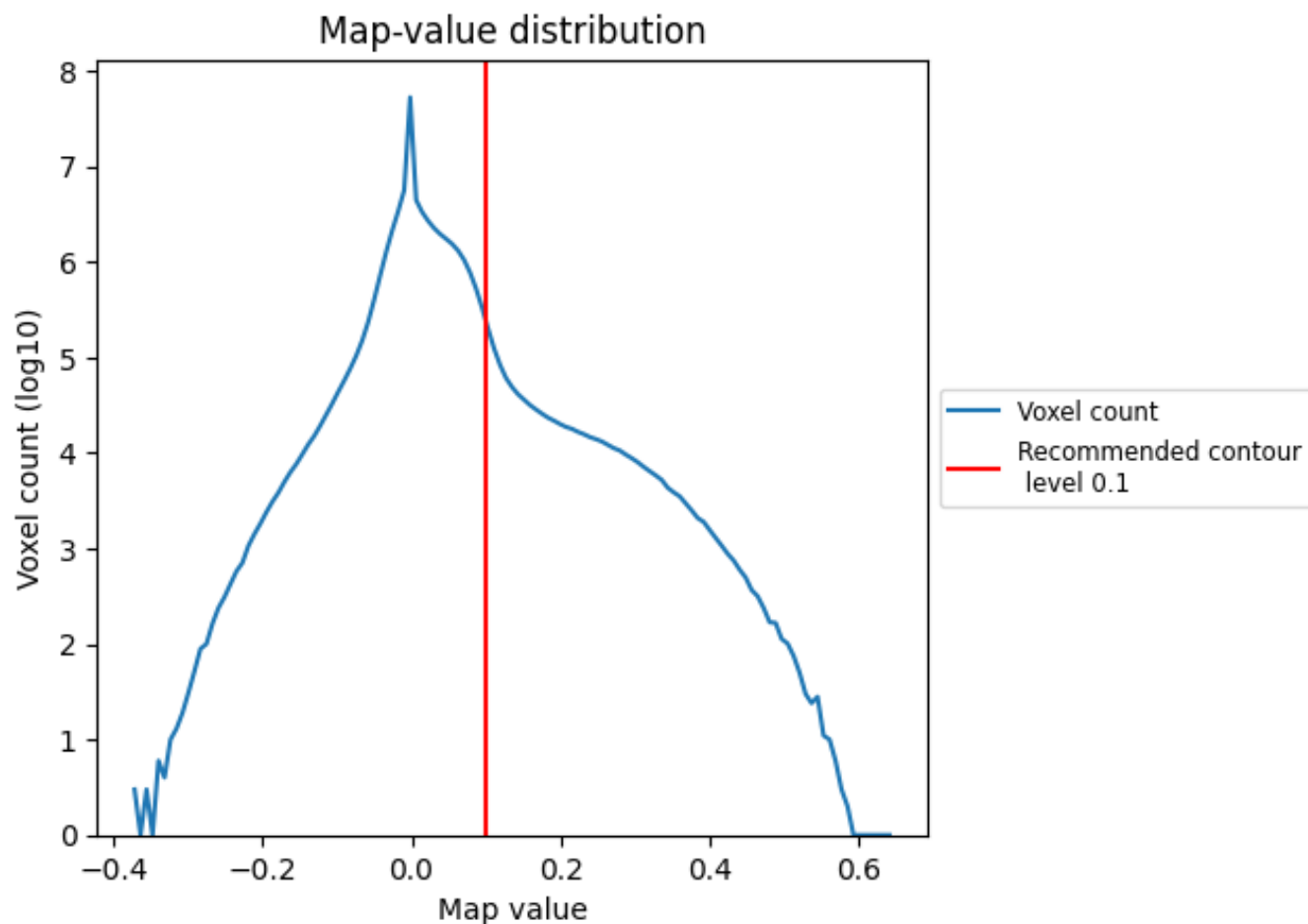


Z

7 Map analysis [i](#)

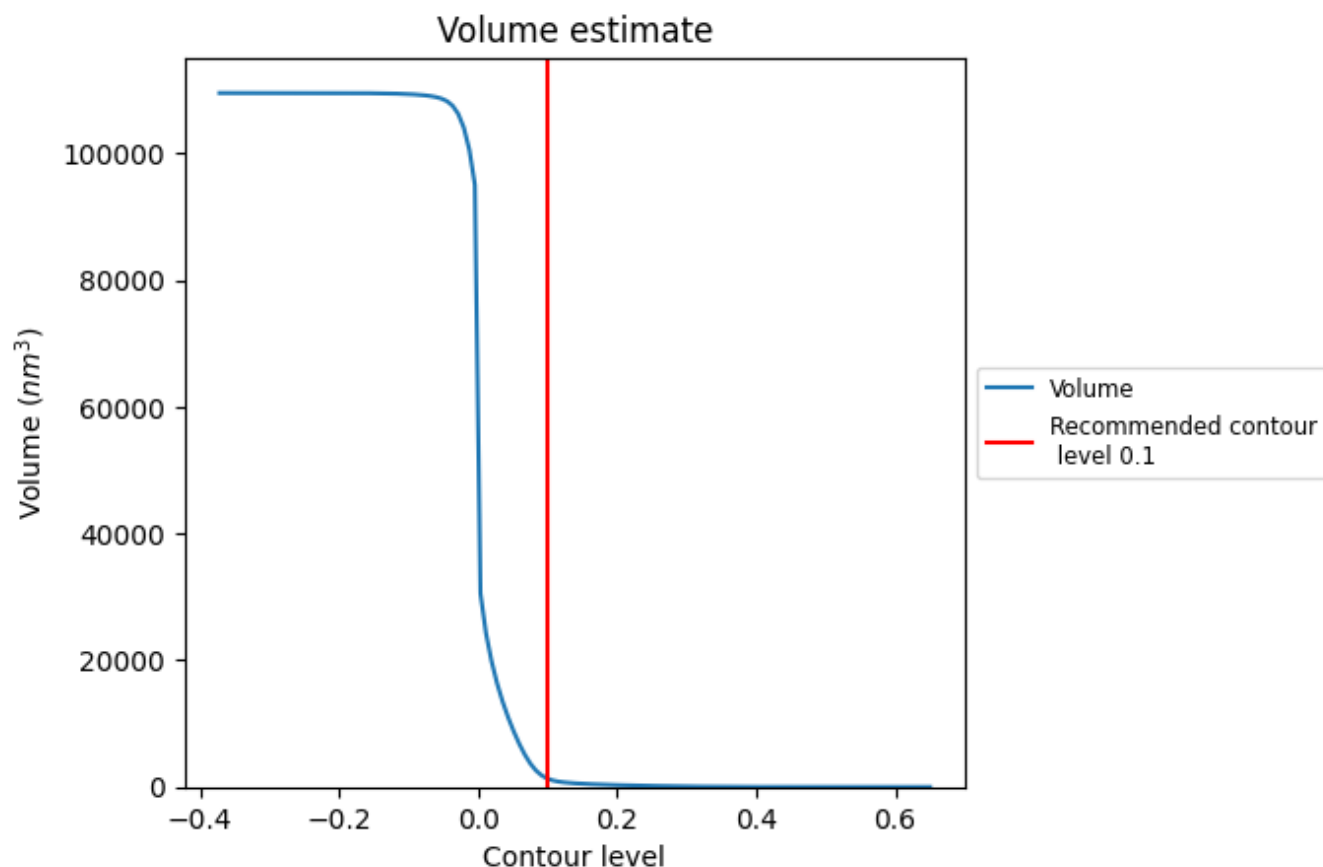
This section contains the results of statistical analysis of the map.

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.

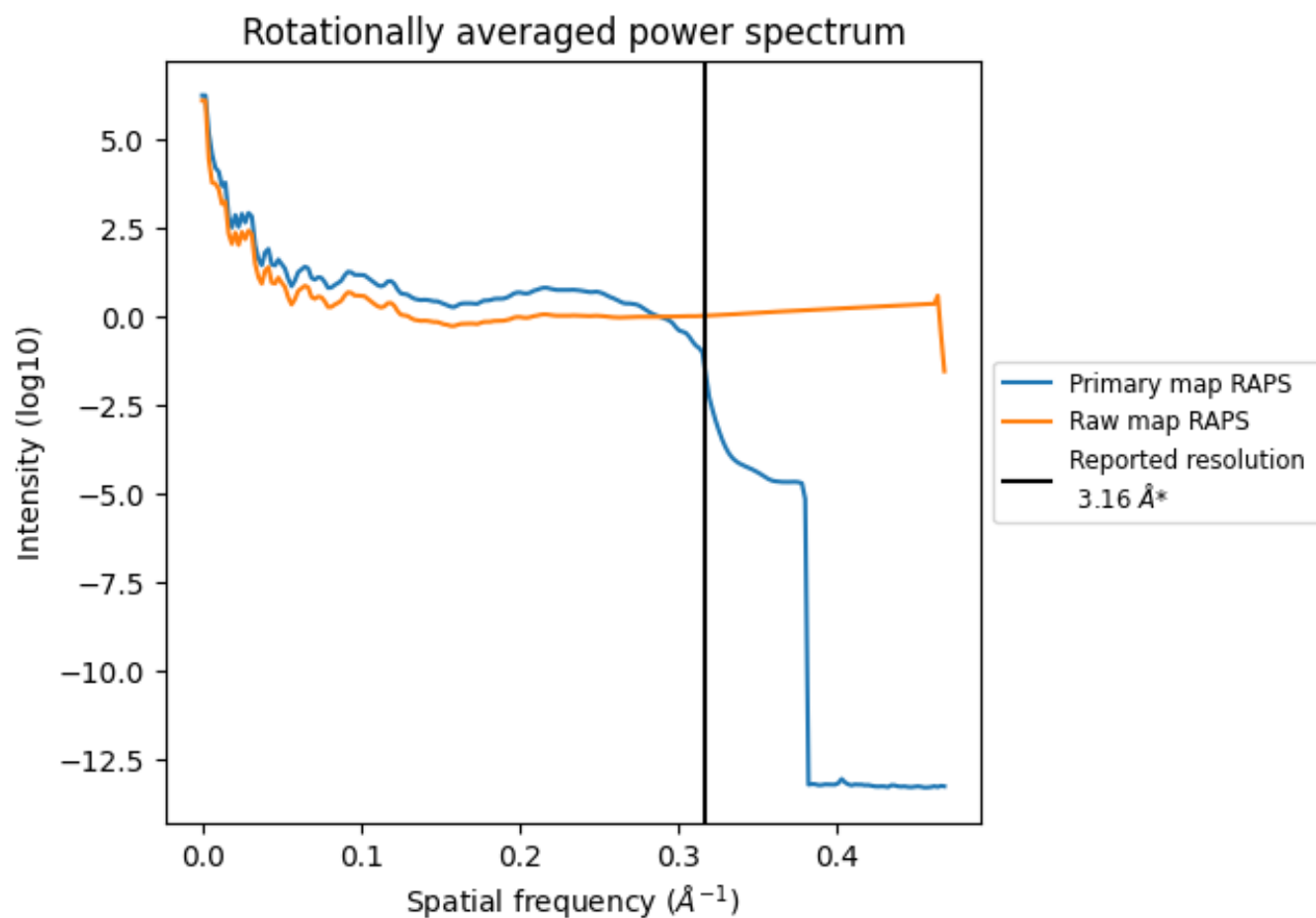
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1310 nm^3 ; this corresponds to an approximate mass of 1183 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 ⓘ

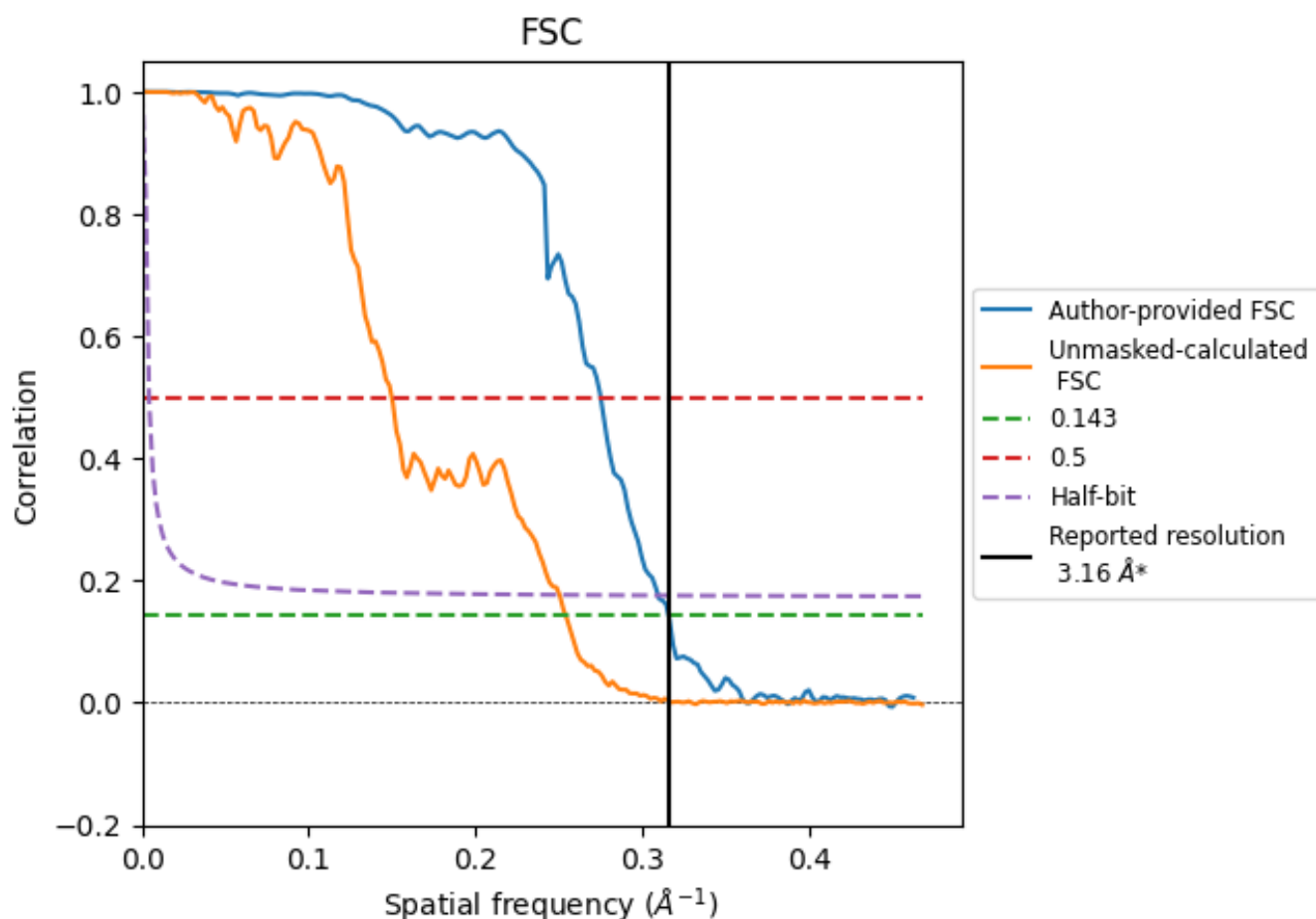


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

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 0.316 \AA^{-1}

8.2 Resolution estimates [i](#)

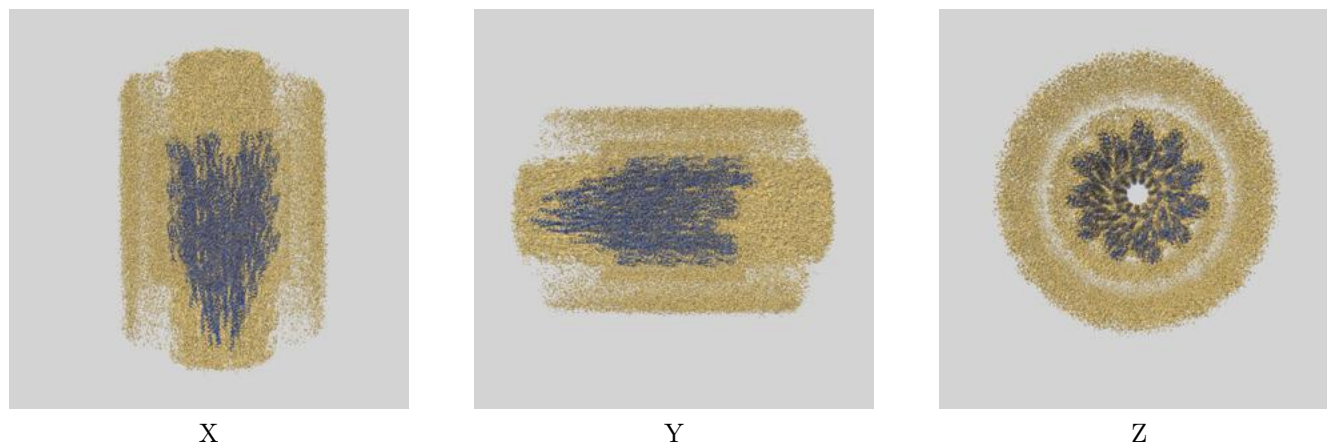
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.63	3.23
Unmasked-calculated*	3.94	6.68	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.16 by more than 10 %

9 Map-model fit [i](#)

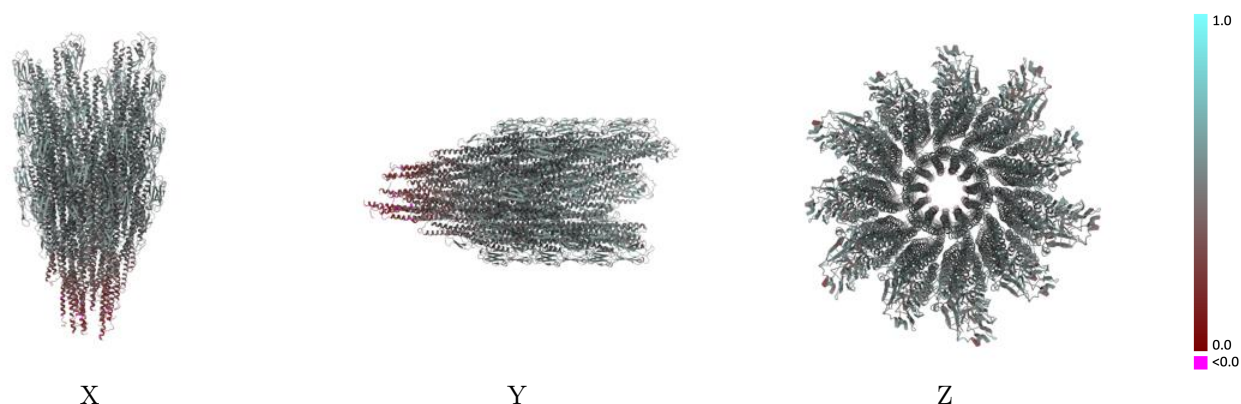
This section contains information regarding the fit between EMDB map EMD-71351 and PDB model 9P7R. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



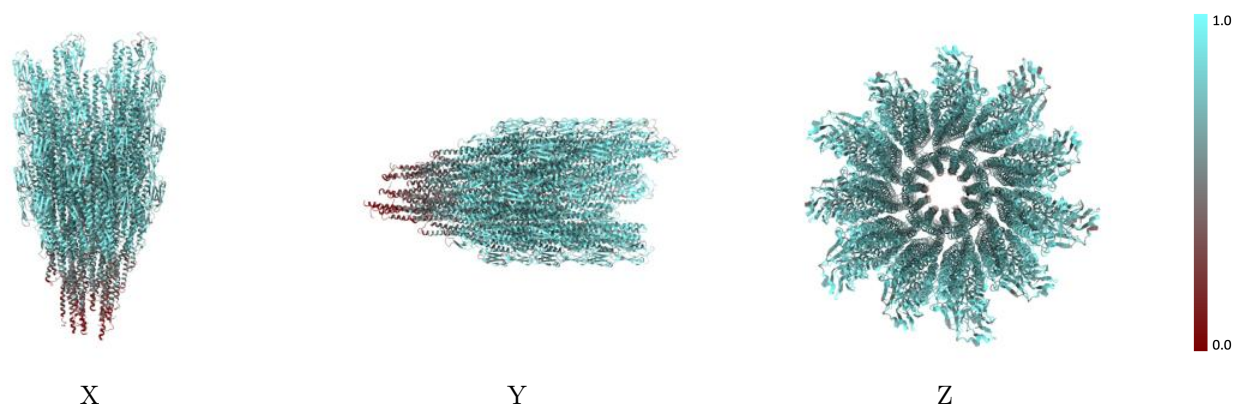
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



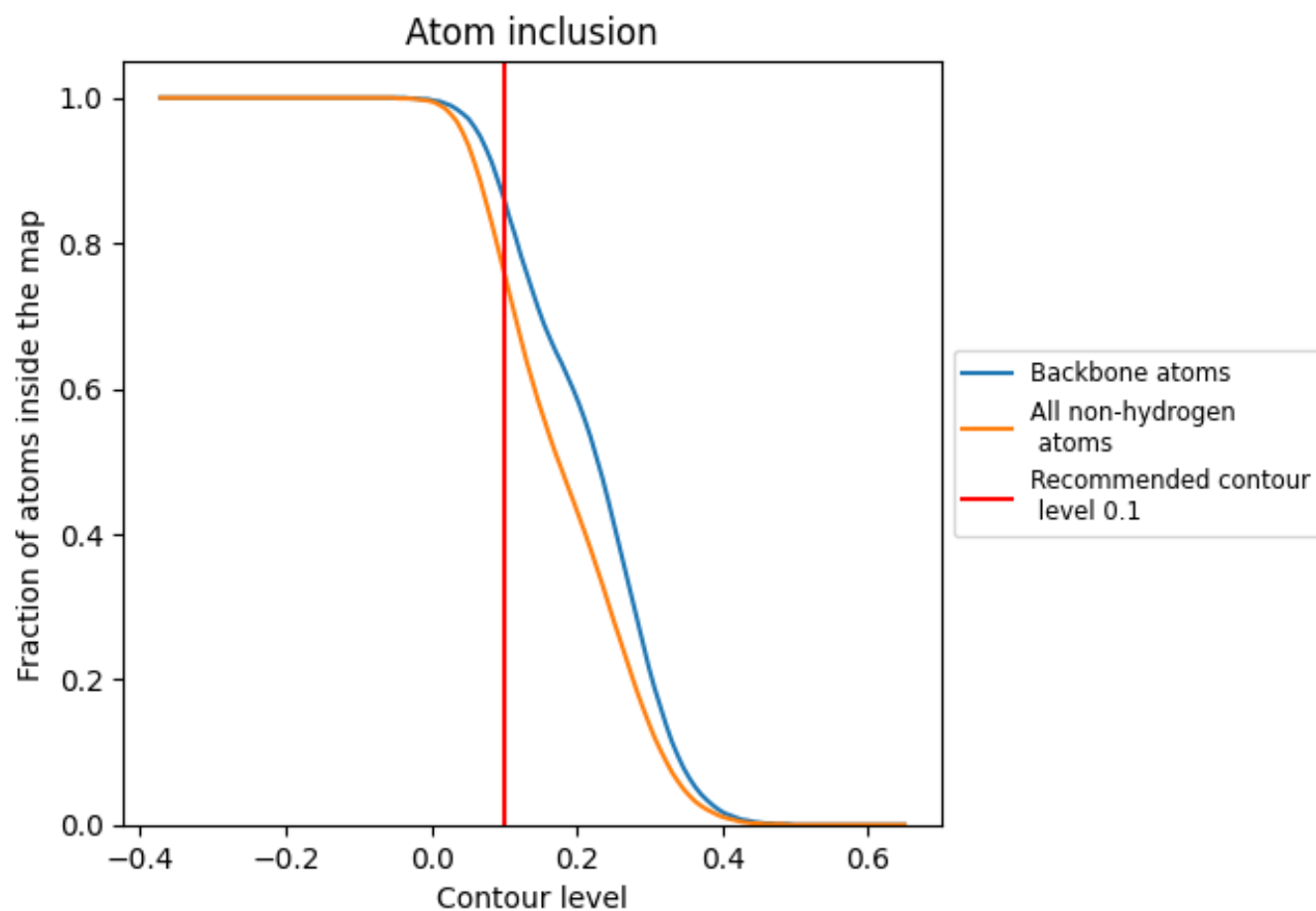
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 76% 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	 0.7600	 0.4950
A1	 0.6250	 0.4230
A2	 0.8080	 0.5120
B2	 0.7950	 0.5140
C2	 0.7840	 0.4990
D2	 0.8000	 0.5160
E2	 0.7660	 0.4990
F2	 0.7790	 0.5040
G2	 0.7880	 0.5130
H2	 0.8050	 0.5180
I2	 0.6890	 0.4610
J2	 0.8020	 0.5150
K2	 0.8070	 0.5120
L2	 0.8070	 0.5140
M2	 0.7100	 0.4730
N2	 0.8070	 0.5180
O2	 0.7840	 0.5100
P2	 0.8000	 0.5170
Q2	 0.8010	 0.5190
R2	 0.7720	 0.5080
S2	 0.8010	 0.5130
T2	 0.7650	 0.5020
U2	 0.7740	 0.4980
V2	 0.6690	 0.4560
W2	 0.8050	 0.5040
X2	 0.7430	 0.4880
Y2	 0.7970	 0.5100
Z2	 0.7810	 0.5120
a2	 0.6030	 0.4190
b2	 0.8030	 0.5160
c2	 0.7270	 0.4840
d2	 0.6410	 0.4380
e2	 0.6960	 0.4650
f2	 0.7530	 0.4930

