



Full wwPDB EM Validation Report ⓘ

Oct 25, 2025 – 08:49 am BST

PDB ID : 9QGP / pdb_00009qgp
EMDB ID : EMD-53141
Title : Cryo-EM structure of the PIPVC1 sheath, 6-fold symmetrized (C6), in contracted state
Authors : Marin-Arraiza, L.; Taylor, N.M.I.
Deposited on : 2025-03-14
Resolution : 3.10 Å(reported)

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

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

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:

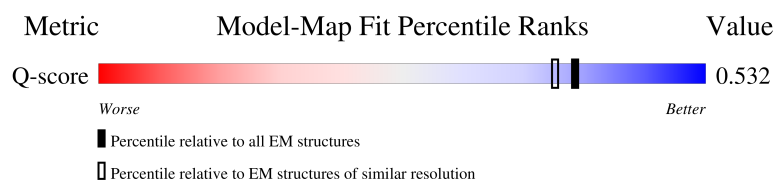
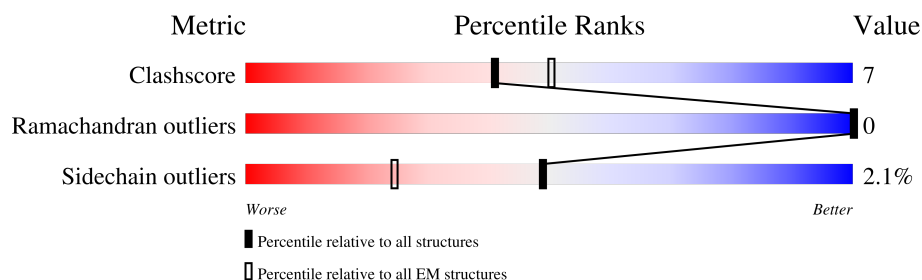
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.10 Å.

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





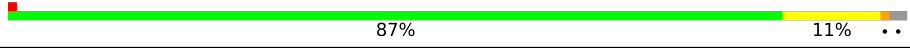



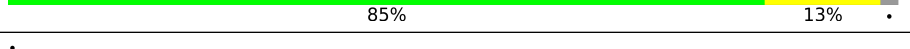
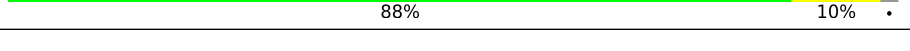
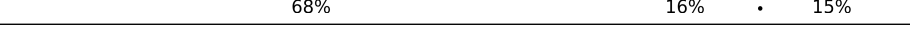
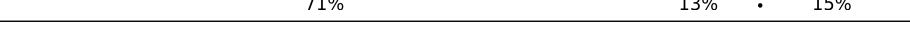
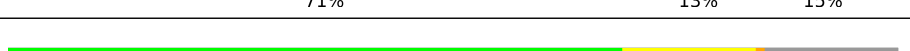



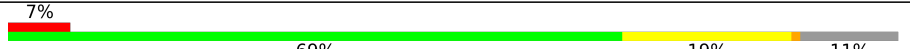





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	2A	354	
1	2B	354	
1	2C	354	
1	2D	354	

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Mol	Chain	Length	Quality of chain
1	2E	354	
1	2F	354	
1	2G	354	
1	2H	354	
1	2I	354	
1	2J	354	
1	2K	354	
1	2L	354	
2	3A	466	
2	3B	466	
2	3C	466	
2	3D	466	
2	3E	466	
2	3F	466	
3	4A	392	
3	4B	392	
3	4C	392	
3	4D	392	
3	4E	392	
3	4F	392	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 67578 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 Phage tail sheath family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2A	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2B	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2C	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2D	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2E	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2F	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2G	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2H	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2I	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2J	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2K	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		
1	2L	348	Total	C	N	O	S	0	0
			2704	1731	442	523	8		

- Molecule 2 is a protein called Phage tail sheath family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3A	395	Total	C	N	O	S	0	0
			3081	1962	515	594	10		
2	3B	395	Total	C	N	O	S	0	0
			3081	1962	515	594	10		
2	3C	395	Total	C	N	O	S	0	0
			3081	1962	515	594	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	3D	395	Total	C	N	O	S	0	0
			3081	1962	515	594	10		
2	3E	395	Total	C	N	O	S	0	0
			3081	1962	515	594	10		
2	3F	395	Total	C	N	O	S	0	0
			3081	1962	515	594	10		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3A	267	GLN	-	insertion	UNP A0A6L9JMV2
3A	268	LYS	-	insertion	UNP A0A6L9JMV2
3A	269	ILE	-	insertion	UNP A0A6L9JMV2
3A	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3B	267	GLN	-	insertion	UNP A0A6L9JMV2
3B	268	LYS	-	insertion	UNP A0A6L9JMV2
3B	269	ILE	-	insertion	UNP A0A6L9JMV2
3B	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3C	267	GLN	-	insertion	UNP A0A6L9JMV2
3C	268	LYS	-	insertion	UNP A0A6L9JMV2
3C	269	ILE	-	insertion	UNP A0A6L9JMV2
3C	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3D	267	GLN	-	insertion	UNP A0A6L9JMV2
3D	268	LYS	-	insertion	UNP A0A6L9JMV2
3D	269	ILE	-	insertion	UNP A0A6L9JMV2
3D	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3E	267	GLN	-	insertion	UNP A0A6L9JMV2
3E	268	LYS	-	insertion	UNP A0A6L9JMV2
3E	269	ILE	-	insertion	UNP A0A6L9JMV2
3E	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3F	267	GLN	-	insertion	UNP A0A6L9JMV2
3F	268	LYS	-	insertion	UNP A0A6L9JMV2
3F	269	ILE	-	insertion	UNP A0A6L9JMV2
3F	309	ILE	VAL	conflict	UNP A0A6L9JMV2

- Molecule 3 is a protein called Phage tail sheath family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4A	350	Total	C	N	O	S	0	0
			2774	1775	481	509	9		
3	4B	350	Total	C	N	O	S	0	0
			2774	1775	481	509	9		

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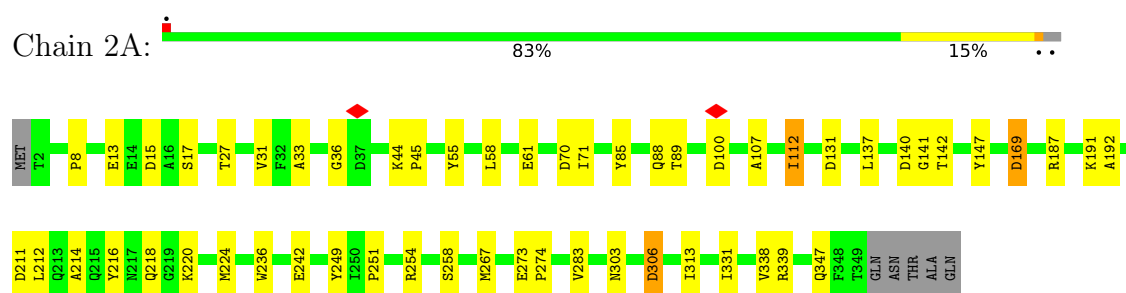
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	4C	350	Total	C	N	O	S	0	0
			2774	1775	481	509	9		
3	4D	350	Total	C	N	O	S	0	0
			2774	1775	481	509	9		
3	4E	350	Total	C	N	O	S	0	0
			2774	1775	481	509	9		
3	4F	350	Total	C	N	O	S	0	0
			2774	1775	481	509	9		

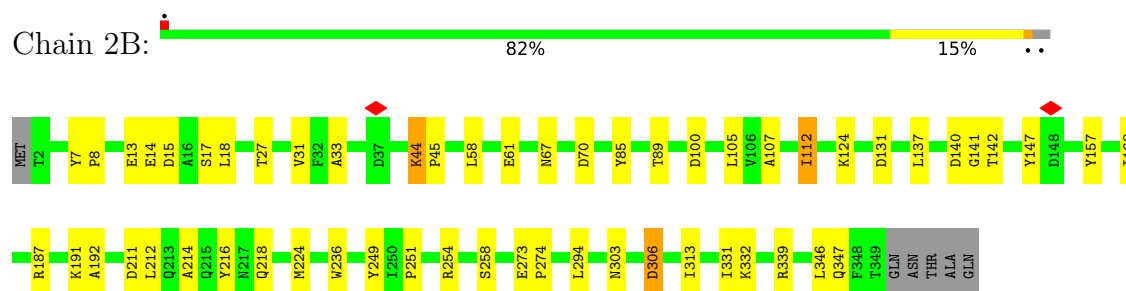
3 Residue-property plots

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.

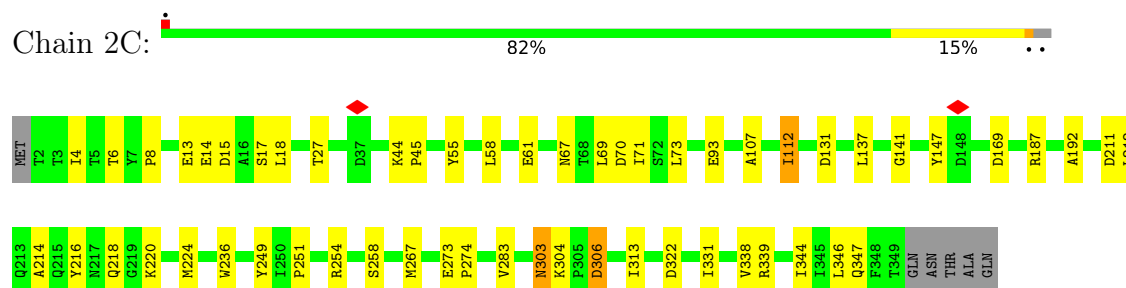
- Molecule 1: Phage tail sheath family protein



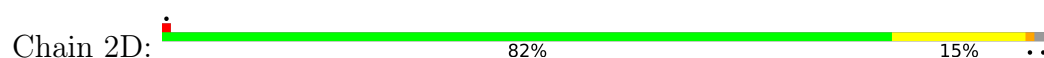
- Molecule 1: Phage tail sheath family protein

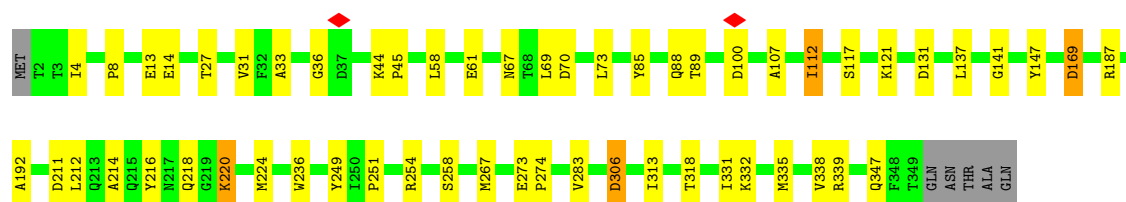


- Molecule 1: Phage tail sheath family protein

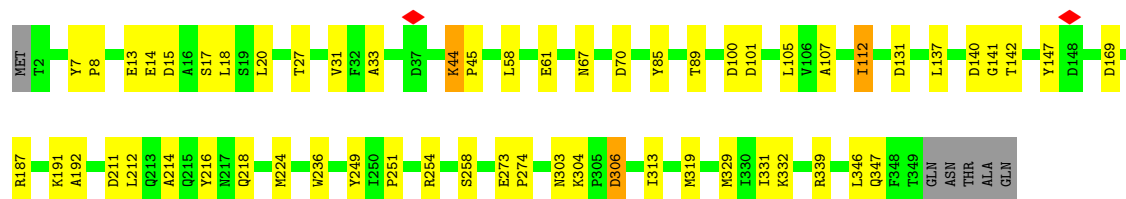
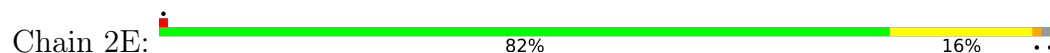


- Molecule 1: Phage tail sheath family protein

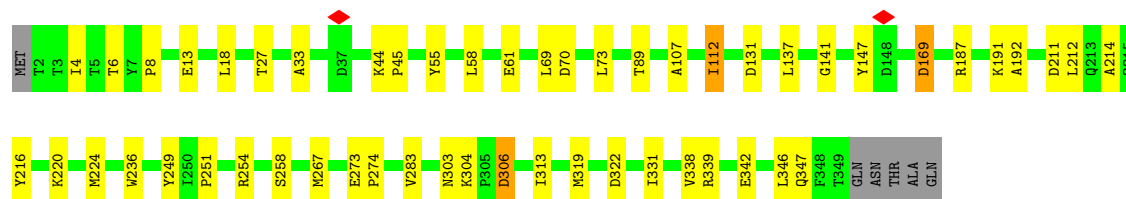
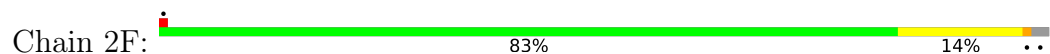




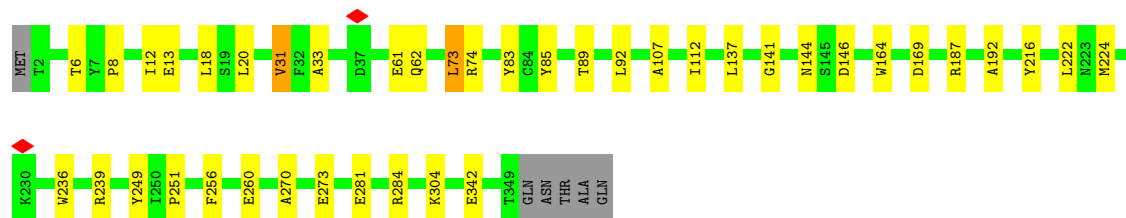
- Molecule 1: Phage tail sheath family protein



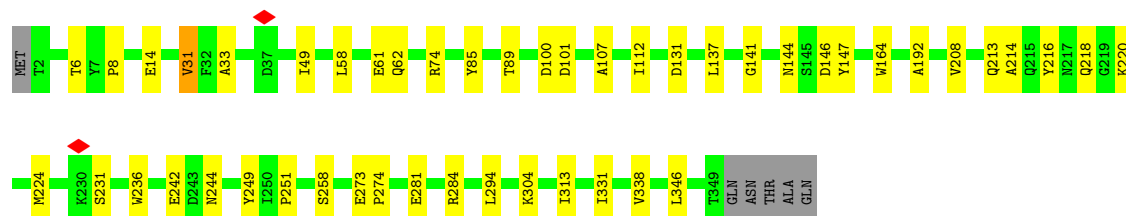
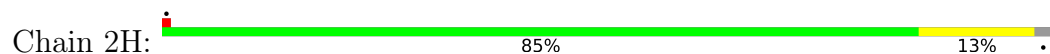
- Molecule 1: Phage tail sheath family protein



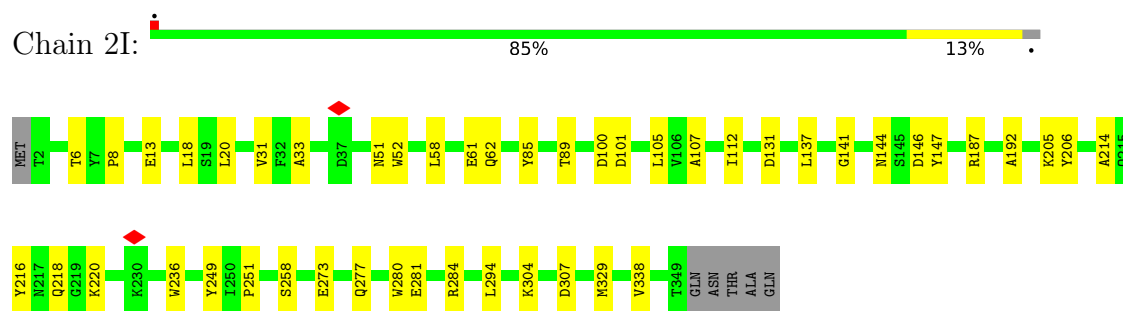
- Molecule 1: Phage tail sheath family protein



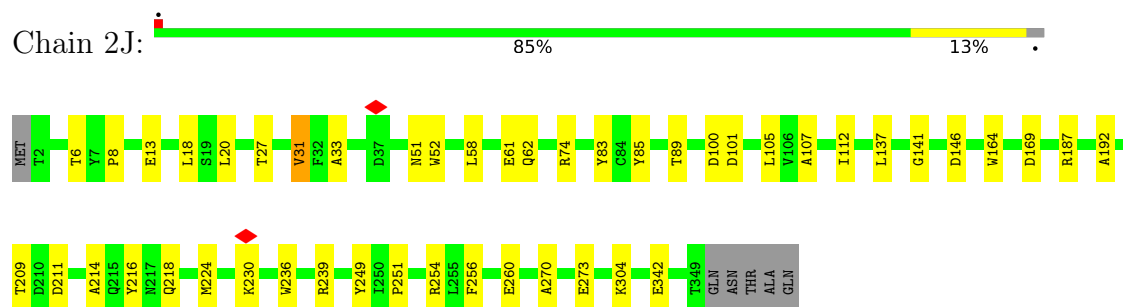
- Molecule 1: Phage tail sheath family protein



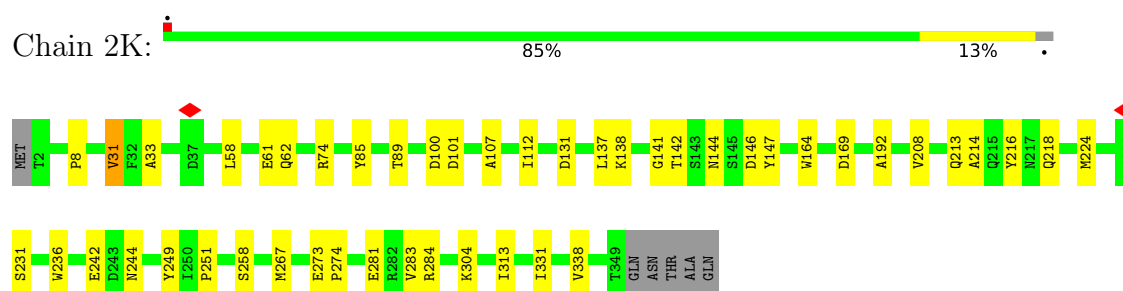
• Molecule 1: Phage tail sheath family protein



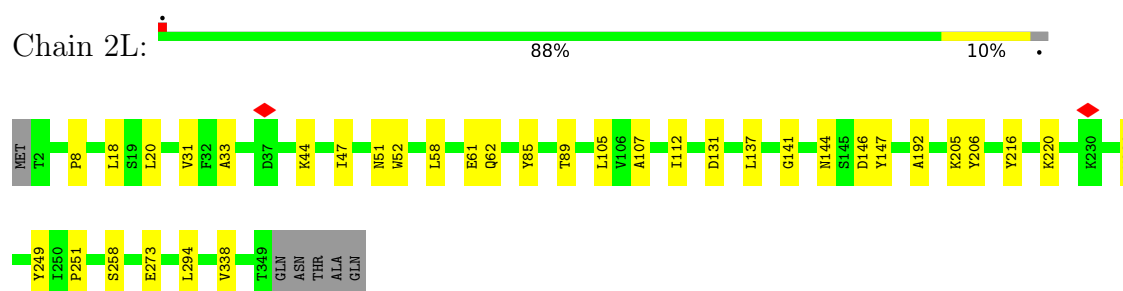
• Molecule 1: Phage tail sheath family protein



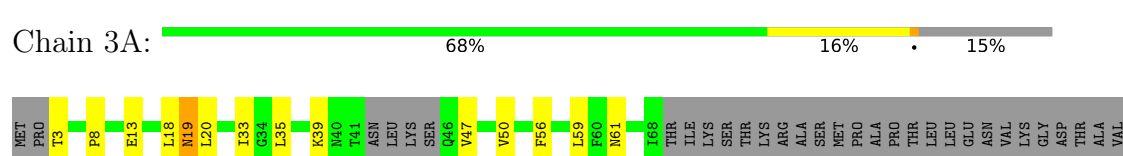
• Molecule 1: Phage tail sheath family protein

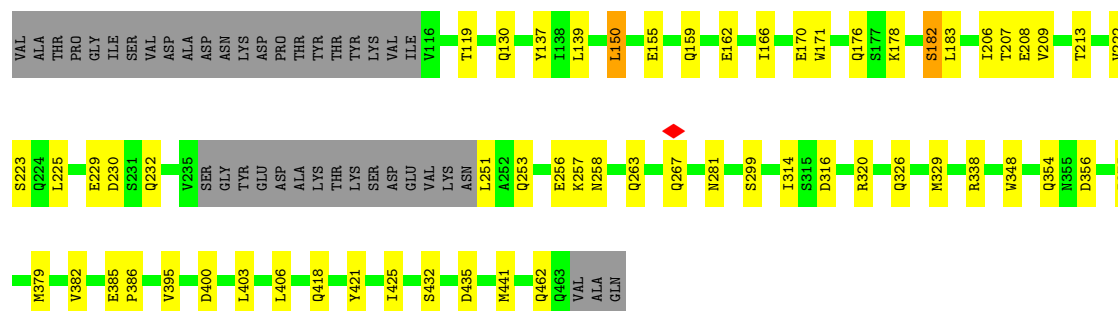


• Molecule 1: Phage tail sheath family protein



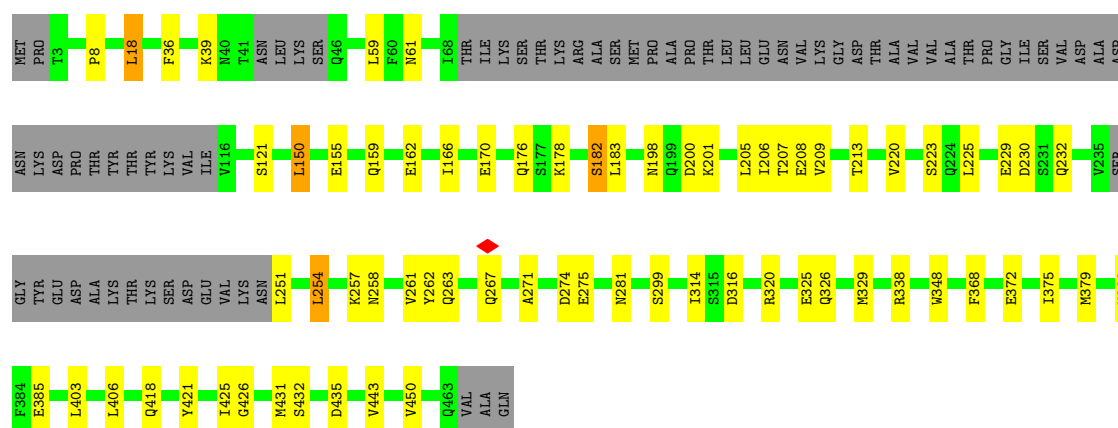
• Molecule 2: Phage tail sheath family protein





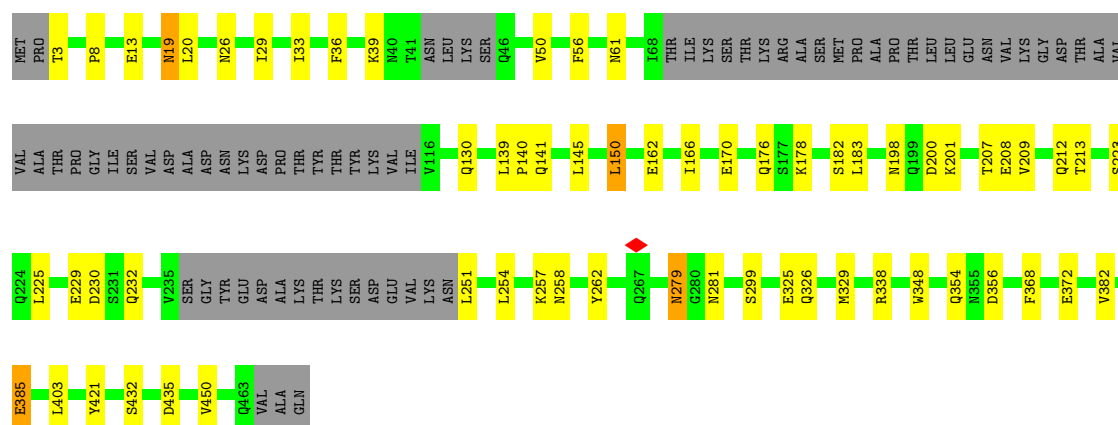
• Molecule 2: Phage tail sheath family protein

Chain 3E: 70% 14% 15%



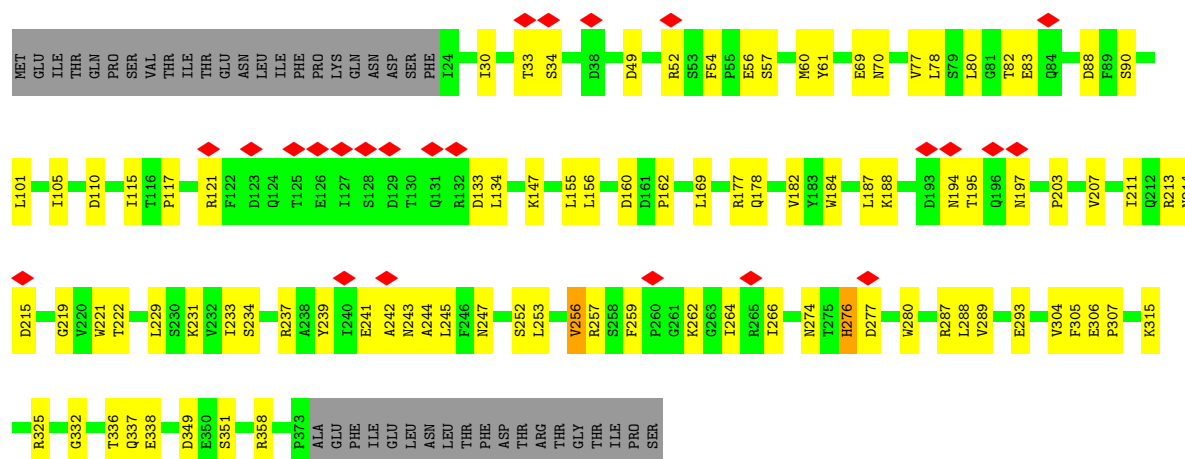
• Molecule 2: Phage tail sheath family protein

Chain 3F: 71% 13% 15%

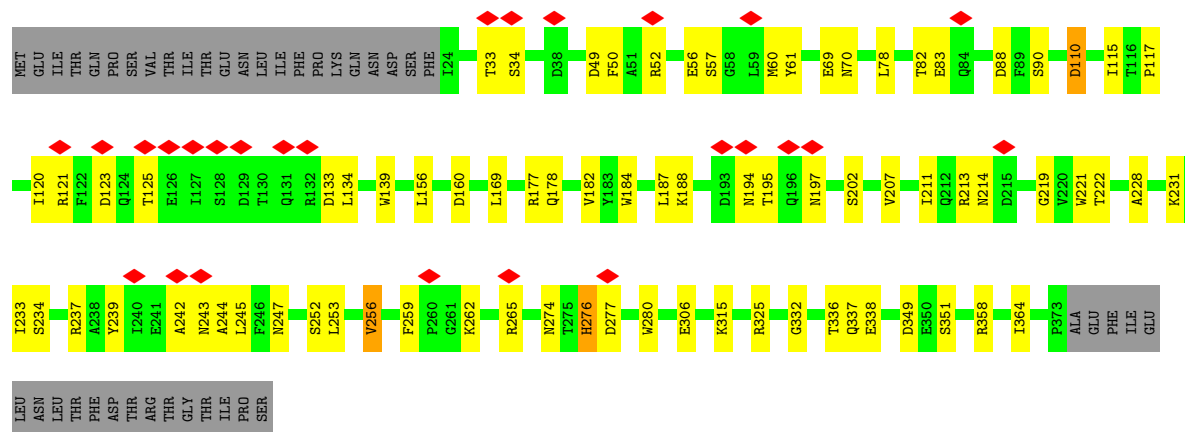


• Molecule 3: Phage tail sheath family protein

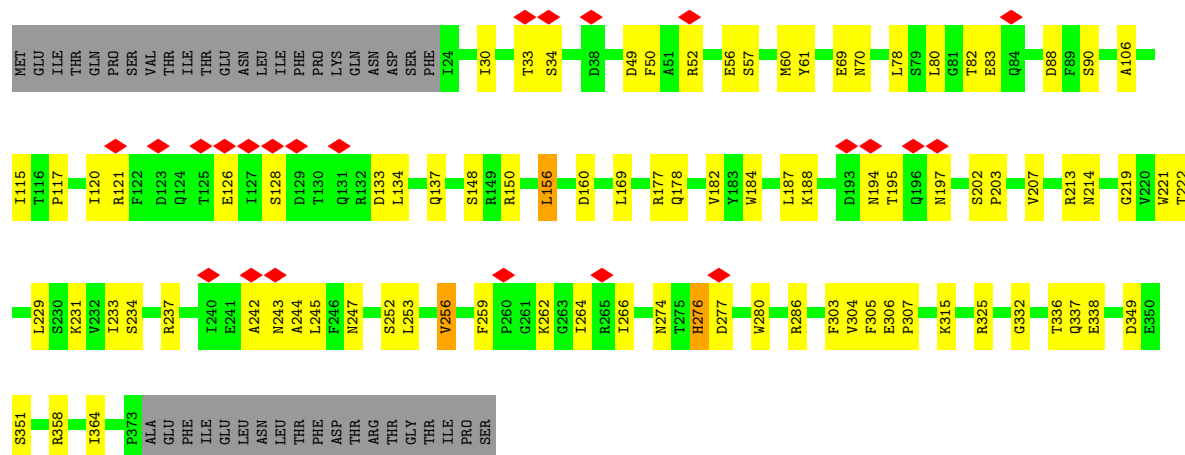
Chain 4A: 6% 66% 23% 11%



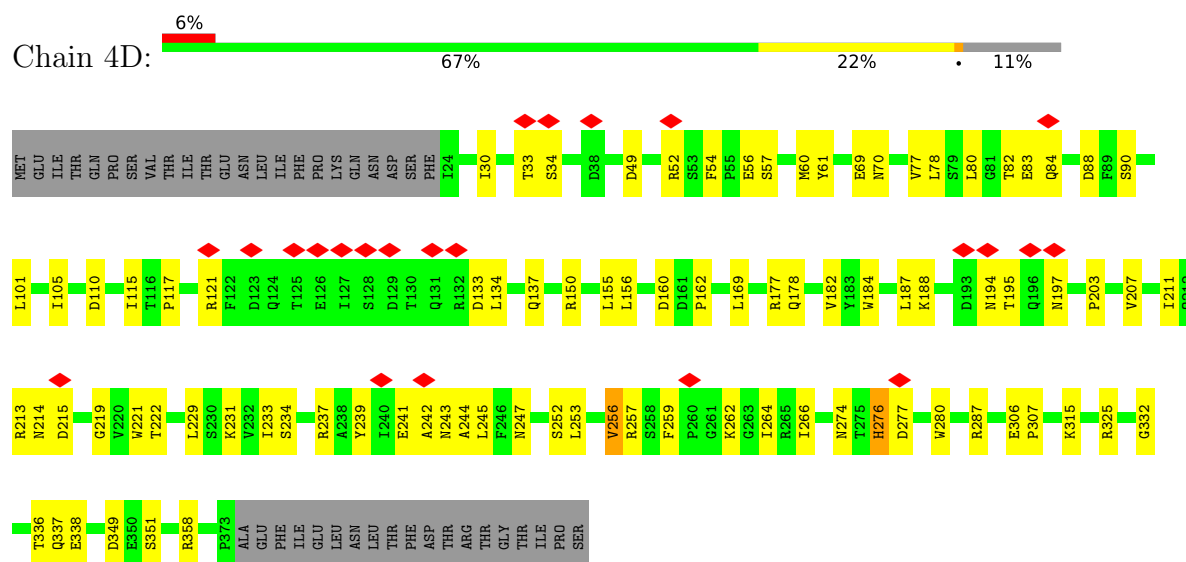
• Molecule 3: Phage tail sheath family protein



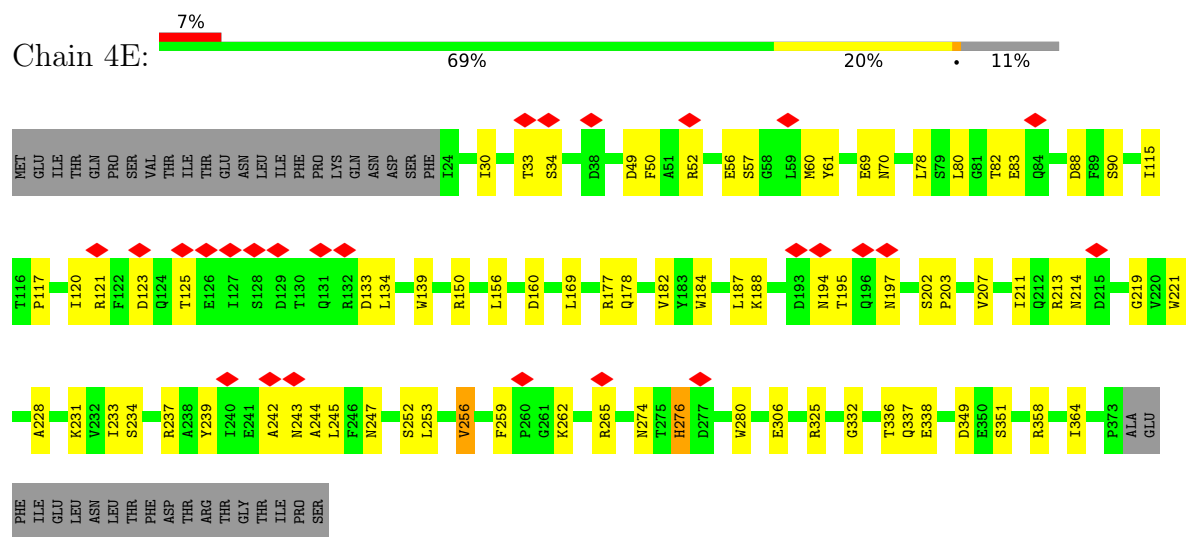
• Molecule 3: Phage tail sheath family protein



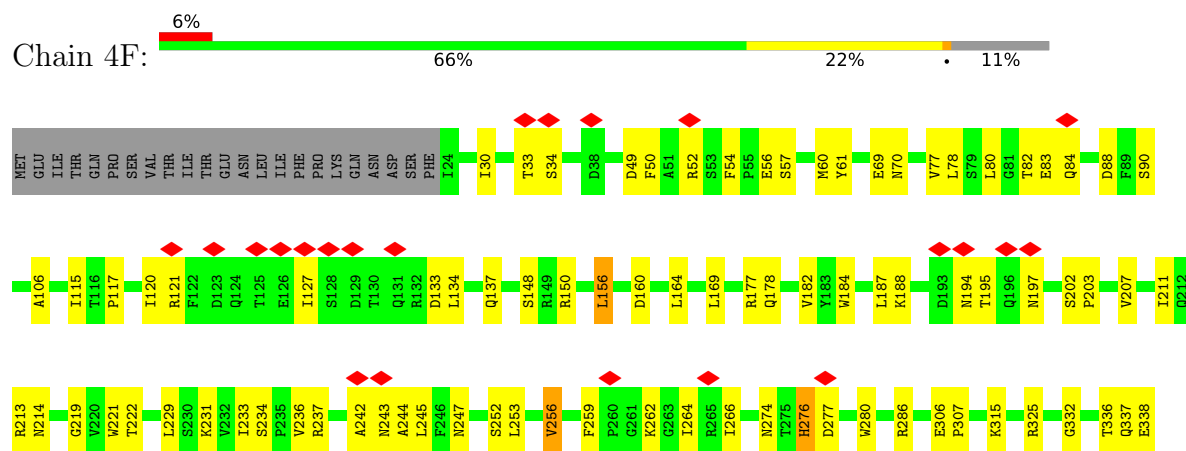
• Molecule 3: Phage tail sheath family protein



• Molecule 3: Phage tail sheath family protein



• Molecule 3: Phage tail sheath family protein



D349	E350	S351	R358	A359	G360	I364	P373	ALA	GLU	PHE	ILE	GLU	LEU	ASN	LEU	THR	PHE	ASP	THR	ARG	THR	GLY	THR	ILE	PRO	SER
------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	30862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Patch CTF Estimation in cryoSPARC, fit local CTF to micrograph, including tilted, bent, deformed samples	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.625	Depositor
Minimum map value	-0.694	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	840.00006, 840.00006, 840.00006	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2A	0.11	0/2772	0.25	0/3790
1	2B	0.11	0/2772	0.26	0/3790
1	2C	0.11	0/2772	0.26	0/3790
1	2D	0.11	0/2772	0.26	0/3790
1	2E	0.11	0/2772	0.26	0/3790
1	2F	0.11	0/2772	0.26	0/3790
1	2G	0.12	0/2772	0.29	0/3790
1	2H	0.12	0/2772	0.28	0/3790
1	2I	0.12	0/2772	0.28	0/3790
1	2J	0.12	0/2772	0.28	0/3790
1	2K	0.12	0/2772	0.28	0/3790
1	2L	0.12	0/2772	0.28	0/3790
2	3A	0.11	0/3141	0.25	0/4273
2	3B	0.12	0/3141	0.26	0/4273
2	3C	0.11	0/3141	0.24	0/4273
2	3D	0.11	0/3141	0.24	0/4273
2	3E	0.14	0/3141	0.26	0/4273
2	3F	0.11	0/3141	0.24	0/4273
3	4A	0.10	0/2839	0.29	0/3865
3	4B	0.10	0/2839	0.29	0/3865
3	4C	0.10	0/2839	0.30	0/3865
3	4D	0.10	0/2839	0.29	0/3865
3	4E	0.10	0/2839	0.29	0/3865
3	4F	0.10	0/2839	0.30	0/3865
All	All	0.11	0/69144	0.27	0/94308

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2A	2704	0	2653	35	0
1	2B	2704	0	2653	36	0
1	2C	2704	0	2653	38	0
1	2D	2704	0	2653	37	0
1	2E	2704	0	2653	38	0
1	2F	2704	0	2653	34	0
1	2G	2704	0	2653	29	0
1	2H	2704	0	2653	31	0
1	2I	2704	0	2653	33	0
1	2J	2704	0	2653	34	0
1	2K	2704	0	2653	31	0
1	2L	2704	0	2653	22	0
2	3A	3081	0	3049	48	0
2	3B	3081	0	3049	41	0
2	3C	3081	0	3049	38	0
2	3D	3081	0	3049	47	0
2	3E	3081	0	3049	43	0
2	3F	3081	0	3049	40	0
3	4A	2774	0	2766	54	0
3	4B	2774	0	2766	50	0
3	4C	2774	0	2766	55	0
3	4D	2774	0	2766	53	0
3	4E	2774	0	2766	49	0
3	4F	2774	0	2766	56	0
All	All	67578	0	66726	898	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 (898) 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)
1:2I:144:ASN:ND2	1:2I:220:LYS:O	2.16	0.79
1:2L:144:ASN:ND2	1:2L:220:LYS:O	2.16	0.78
3:4D:60:MET:SD	3:4D:60:MET:N	2.57	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2H:144:ASN:ND2	1:2H:220:LYS:O	2.18	0.75
3:4B:60:MET:HE3	3:4B:60:MET:H	1.51	0.75
3:4A:60:MET:SD	3:4A:60:MET:N	2.56	0.74
3:4E:60:MET:HE3	3:4E:60:MET:H	1.55	0.71
3:4E:169:LEU:HD11	3:4E:253:LEU:HG	1.73	0.71
3:4D:169:LEU:HD11	3:4D:253:LEU:HG	1.74	0.69
3:4A:169:LEU:HD11	3:4A:253:LEU:HG	1.74	0.69
2:3D:18:LEU:HD13	2:3D:385:GLU:HG3	1.75	0.69
3:4B:169:LEU:HD11	3:4B:253:LEU:HG	1.73	0.69
2:3B:155:GLU:OE1	2:3B:159:GLN:NE2	2.26	0.68
2:3B:385:GLU:OE2	1:2I:187:ARG:NH1	2.28	0.67
3:4F:169:LEU:HD11	3:4F:253:LEU:HG	1.76	0.67
3:4C:169:LEU:HD11	3:4C:253:LEU:HG	1.76	0.67
2:3E:155:GLU:OE1	2:3E:159:GLN:NE2	2.27	0.67
2:3F:29:ILE:HD13	2:3F:162:GLU:HB2	1.75	0.67
1:2J:209:THR:OG1	1:2J:211:ASP:OD1	2.13	0.67
3:4E:177:ARG:NH1	3:4E:274:ASN:OD1	2.28	0.66
3:4B:177:ARG:NH1	3:4B:274:ASN:OD1	2.28	0.66
2:3F:385:GLU:OE2	1:2G:187:ARG:NH1	2.28	0.66
2:3C:385:GLU:OE2	1:2J:187:ARG:NH1	2.29	0.66
2:3E:418:GLN:OE1	2:3E:418:GLN:N	2.28	0.66
3:4D:177:ARG:NH1	3:4D:274:ASN:OD1	2.30	0.65
3:4F:177:ARG:NH1	3:4F:274:ASN:OD1	2.30	0.65
2:3D:418:GLN:OE1	2:3D:418:GLN:N	2.30	0.64
1:2H:281:GLU:OE2	1:2H:284:ARG:NH2	2.30	0.64
3:4A:177:ARG:NH1	3:4A:274:ASN:OD1	2.29	0.64
3:4C:177:ARG:NH1	3:4C:274:ASN:OD1	2.30	0.64
2:3B:418:GLN:N	2:3B:418:GLN:OE1	2.28	0.64
3:4C:306:GLU:OE1	1:2C:187:ARG:NH1	2.31	0.64
3:4D:306:GLU:OE1	1:2D:187:ARG:NH1	2.31	0.64
1:2J:13:GLU:OE2	1:2J:13:GLU:N	2.31	0.64
3:4F:306:GLU:OE1	1:2F:187:ARG:NH1	2.31	0.63
1:2C:13:GLU:OE2	1:2D:347:GLN:NE2	2.31	0.63
1:2B:306:ASP:OD1	1:2B:306:ASP:N	2.32	0.63
1:2A:306:ASP:OD1	1:2A:306:ASP:N	2.32	0.63
2:3B:208:GLU:OE1	2:3B:208:GLU:N	2.27	0.63
3:4A:239:TYR:HE1	3:4A:257:ARG:HD2	1.64	0.62
2:3B:326:GLN:HE22	2:3B:348:TRP:HB3	1.64	0.62
1:2E:13:GLU:OE1	1:2F:347:GLN:NE2	2.32	0.62
1:2B:13:GLU:OE1	1:2C:347:GLN:NE2	2.33	0.62
3:4E:150:ARG:NH2	1:2D:14:GLU:OE1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2D:13:GLU:OE2	1:2E:347:GLN:NE2	2.32	0.62
2:3E:326:GLN:HE22	2:3E:348:TRP:HB3	1.63	0.62
2:3A:418:GLN:OE1	2:3A:418:GLN:N	2.30	0.61
3:4B:60:MET:H	3:4B:60:MET:CE	2.13	0.61
1:2A:187:ARG:NH1	3:4A:306:GLU:OE1	2.32	0.61
3:4B:70:ASN:O	3:4B:213:ARG:NH1	2.34	0.61
2:3C:3:THR:N	2:3C:13:GLU:OE2	2.34	0.61
3:4C:49:ASP:OD1	3:4C:52:ARG:NH2	2.33	0.61
3:4E:60:MET:H	3:4E:60:MET:CE	2.14	0.61
1:2F:306:ASP:OD1	1:2F:306:ASP:N	2.33	0.61
3:4D:239:TYR:HE1	3:4D:257:ARG:HD2	1.65	0.61
1:2D:306:ASP:OD1	1:2D:306:ASP:N	2.33	0.61
3:4B:88:ASP:OD2	3:4B:90:SER:OG	2.17	0.60
2:3E:208:GLU:OE1	2:3E:208:GLU:N	2.27	0.60
1:2C:306:ASP:OD1	1:2C:306:ASP:N	2.33	0.60
2:3F:3:THR:N	2:3F:13:GLU:OE2	2.34	0.60
1:2E:211:ASP:OD1	1:2E:212:LEU:N	2.34	0.60
3:4C:126:GLU:HG2	3:4C:128:SER:H	1.66	0.60
3:4E:83:GLU:OE2	3:4E:121:ARG:NH2	2.34	0.60
3:4E:49:ASP:OD1	3:4E:52:ARG:NH2	2.35	0.60
3:4E:306:GLU:OE2	1:2E:187:ARG:NH1	2.35	0.60
2:3C:230:ASP:HB3	2:3C:251:LEU:HB3	1.83	0.60
3:4B:306:GLU:OE2	1:2B:187:ARG:NH1	2.35	0.60
3:4F:49:ASP:OD1	3:4F:52:ARG:NH2	2.36	0.59
3:4B:49:ASP:OD1	3:4B:52:ARG:NH2	2.35	0.59
2:3B:170:GLU:O	2:3B:176:GLN:NE2	2.33	0.59
2:3C:141:GLN:HE21	2:3C:145:LEU:HD13	1.67	0.59
2:3F:141:GLN:HE21	2:3F:145:LEU:HD13	1.67	0.59
3:4A:49:ASP:OD1	3:4A:52:ARG:NH2	2.36	0.59
2:3A:178:LYS:O	2:3A:182:SER:OG	2.21	0.59
2:3B:365:ARG:NH2	1:2H:14:GLU:OE2	2.31	0.59
1:2J:18:LEU:HD13	1:2J:273:GLU:HG3	1.84	0.59
3:4F:156:LEU:HB2	3:4F:182:VAL:HG22	1.83	0.59
2:3E:170:GLU:O	2:3E:176:GLN:NE2	2.33	0.59
1:2G:61:GLU:OE1	1:2G:61:GLU:N	2.36	0.59
3:4E:70:ASN:O	3:4E:213:ARG:NH1	2.34	0.59
2:3B:230:ASP:HB3	2:3B:251:LEU:HB3	1.84	0.59
2:3D:230:ASP:HB3	2:3D:251:LEU:HB3	1.84	0.59
3:4A:70:ASN:O	3:4A:213:ARG:NH1	2.36	0.59
3:4A:88:ASP:OD2	3:4A:90:SER:OG	2.17	0.59
1:2D:339:ARG:HH22	2:3D:462:GLN:HE21	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2J:256:PHE:O	1:2J:260:GLU:HG3	2.03	0.58
3:4C:83:GLU:OE2	3:4C:121:ARG:NH2	2.36	0.58
1:2D:267:MET:HE1	1:2D:283:VAL:HG23	1.84	0.58
2:3C:170:GLU:O	2:3C:176:GLN:NE2	2.35	0.58
3:4D:49:ASP:OD1	3:4D:52:ARG:NH2	2.36	0.58
1:2G:256:PHE:O	1:2G:260:GLU:HG3	2.03	0.58
1:2J:61:GLU:OE2	1:2J:61:GLU:N	2.36	0.58
1:2L:18:LEU:HD13	1:2L:273:GLU:HG3	1.86	0.58
1:2A:192:ALA:HA	1:2A:251:PRO:HG3	1.86	0.58
2:3A:230:ASP:HB3	2:3A:251:LEU:HB3	1.84	0.58
3:4B:83:GLU:OE2	3:4B:121:ARG:NH2	2.35	0.58
3:4B:156:LEU:HB2	3:4B:182:VAL:HG22	1.86	0.58
3:4F:70:ASN:O	3:4F:213:ARG:NH1	2.35	0.58
2:3E:230:ASP:HB3	2:3E:251:LEU:HB3	1.85	0.58
2:3F:208:GLU:OE1	2:3F:208:GLU:N	2.27	0.58
3:4F:60:MET:SD	3:4F:60:MET:N	2.73	0.58
2:3F:230:ASP:HB3	2:3F:251:LEU:HB3	1.84	0.58
2:3A:386:PRO:HB3	1:2H:338:VAL:HG11	1.86	0.58
3:4C:156:LEU:HB2	3:4C:182:VAL:HG22	1.85	0.58
1:2B:27:THR:O	1:2B:254:ARG:NH2	2.37	0.57
2:3D:386:PRO:HB3	1:2K:338:VAL:HG11	1.86	0.57
3:4A:276:HIS:ND1	3:4A:277:ASP:OD1	2.35	0.57
3:4C:150:ARG:NH2	1:2B:14:GLU:OE1	2.37	0.57
1:2E:27:THR:O	1:2E:254:ARG:NH2	2.38	0.57
2:3B:223:SER:O	2:3B:281:ASN:ND2	2.36	0.57
1:2A:347:GLN:NE2	1:2F:13:GLU:OE1	2.36	0.57
1:2E:306:ASP:OD1	1:2E:306:ASP:N	2.32	0.57
1:2I:33:ALA:HB1	1:2I:89:THR:HG22	1.86	0.57
2:3B:39:LYS:NZ	2:3B:61:ASN:OD1	2.38	0.57
2:3D:170:GLU:O	2:3D:176:GLN:NE2	2.34	0.57
2:3A:208:GLU:OE2	2:3A:208:GLU:N	2.27	0.57
2:3B:220:VAL:HB	2:3B:314:ILE:HD11	1.87	0.57
2:3C:223:SER:O	2:3C:281:ASN:ND2	2.38	0.57
2:3D:178:LYS:O	2:3D:182:SER:OG	2.22	0.57
1:2G:18:LEU:HD13	1:2G:273:GLU:HG3	1.86	0.57
1:2A:211:ASP:OD1	1:2A:212:LEU:N	2.38	0.57
2:3A:170:GLU:O	2:3A:176:GLN:NE2	2.34	0.57
1:2G:31:VAL:HG22	1:2G:85:TYR:HB2	1.87	0.57
3:4D:70:ASN:O	3:4D:213:ARG:NH1	2.36	0.56
2:3F:326:GLN:HE22	2:3F:348:TRP:HB3	1.69	0.56
2:3A:326:GLN:OE1	2:3A:338:ARG:NH1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4D:276:HIS:ND1	3:4D:277:ASP:OD1	2.34	0.56
3:4E:276:HIS:H	3:4E:276:HIS:CD2	2.23	0.56
1:2B:192:ALA:HA	1:2B:251:PRO:HG3	1.87	0.56
3:4A:187:LEU:HD11	3:4A:256:VAL:HG21	1.87	0.56
3:4D:156:LEU:HB2	3:4D:182:VAL:HG22	1.87	0.56
3:4F:88:ASP:OD2	3:4F:90:SER:OG	2.17	0.56
3:4F:229:LEU:HD11	3:4F:266:ILE:HG13	1.87	0.56
2:3D:208:GLU:OE1	2:3D:208:GLU:N	2.27	0.56
2:3D:354:GLN:NE2	2:3D:356:ASP:OD2	2.33	0.56
2:3E:220:VAL:HB	2:3E:314:ILE:HD11	1.88	0.56
1:2G:192:ALA:HA	1:2G:251:PRO:HG3	1.87	0.56
3:4E:88:ASP:OD2	3:4E:90:SER:OG	2.17	0.56
1:2E:169:ASP:OD1	1:2E:169:ASP:N	2.36	0.56
1:2I:18:LEU:HD13	1:2I:273:GLU:HG3	1.87	0.56
1:2I:131:ASP:O	1:2I:147:TYR:OH	2.22	0.56
1:2A:13:GLU:OE1	1:2B:347:GLN:NE2	2.39	0.56
1:2K:281:GLU:OE2	1:2K:284:ARG:NH2	2.36	0.56
3:4E:156:LEU:HB2	3:4E:182:VAL:HG22	1.87	0.56
1:2D:211:ASP:OD1	1:2D:212:LEU:N	2.38	0.56
1:2F:211:ASP:OD1	1:2F:212:LEU:N	2.39	0.56
3:4C:325:ARG:NE	3:4C:338:GLU:OE2	2.39	0.56
1:2J:192:ALA:HA	1:2J:251:PRO:HG3	1.88	0.56
3:4D:54:PHE:HE2	3:4D:77:VAL:HG11	1.71	0.56
2:3E:39:LYS:NZ	2:3E:61:ASN:OD1	2.38	0.56
2:3C:326:GLN:HE22	2:3C:348:TRP:HB3	1.70	0.56
1:2I:192:ALA:HA	1:2I:251:PRO:HG3	1.88	0.56
3:4B:325:ARG:NE	3:4B:338:GLU:OE2	2.38	0.56
1:2G:62:GLN:N	1:2G:62:GLN:OE1	2.39	0.56
3:4F:83:GLU:OE2	3:4F:121:ARG:NH2	2.38	0.55
1:2C:211:ASP:OD1	1:2C:212:LEU:N	2.39	0.55
3:4C:70:ASN:O	3:4C:213:ARG:NH1	2.36	0.55
1:2L:31:VAL:HG22	1:2L:85:TYR:HB2	1.89	0.55
3:4C:60:MET:H	3:4C:60:MET:CE	2.20	0.55
3:4D:83:GLU:OE2	3:4D:121:ARG:NH2	2.39	0.55
1:2C:267:MET:HE1	1:2C:283:VAL:HG23	1.89	0.55
2:3F:170:GLU:O	2:3F:176:GLN:NE2	2.35	0.55
1:2A:131:ASP:O	1:2A:147:TYR:OH	2.25	0.55
3:4A:195:THR:OG1	3:4A:197:ASN:OD1	2.22	0.55
1:2E:192:ALA:HA	1:2E:251:PRO:HG3	1.88	0.55
2:3E:223:SER:O	2:3E:281:ASN:ND2	2.38	0.55
1:2J:31:VAL:HG22	1:2J:85:TYR:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4D:187:LEU:HD11	3:4D:256:VAL:HG21	1.88	0.55
3:4F:276:HIS:ND1	3:4F:277:ASP:OD2	2.40	0.55
1:2H:192:ALA:HA	1:2H:251:PRO:HG3	1.88	0.55
2:3E:18:LEU:HD13	2:3E:385:GLU:HG3	1.89	0.55
1:2I:31:VAL:HG22	1:2I:85:TYR:HB2	1.89	0.55
1:2D:192:ALA:HA	1:2D:251:PRO:HG3	1.89	0.55
1:2J:33:ALA:HB1	1:2J:89:THR:HG22	1.88	0.55
1:2L:33:ALA:HB1	1:2L:89:THR:HG22	1.89	0.55
3:4A:83:GLU:OE2	3:4A:121:ARG:NH2	2.41	0.54
3:4C:229:LEU:HD11	3:4C:266:ILE:HG13	1.87	0.54
2:3A:39:LYS:NZ	2:3A:61:ASN:OD1	2.40	0.54
3:4D:110:ASP:OD1	3:4D:110:ASP:N	2.34	0.54
3:4B:276:HIS:H	3:4B:276:HIS:CD2	2.25	0.54
3:4B:276:HIS:ND1	3:4B:277:ASP:OD1	2.41	0.54
1:2B:211:ASP:OD2	1:2B:212:LEU:N	2.39	0.54
3:4D:229:LEU:HD11	3:4D:266:ILE:HG13	1.89	0.54
2:3D:326:GLN:HE22	2:3D:348:TRP:HB3	1.72	0.54
1:2H:33:ALA:HB1	1:2H:89:THR:HG22	1.90	0.54
2:3A:354:GLN:NE2	2:3A:356:ASP:OD2	2.33	0.54
3:4A:54:PHE:HE2	3:4A:77:VAL:HG11	1.71	0.54
1:2J:304:LYS:HB2	1:2J:304:LYS:NZ	2.23	0.54
3:4F:325:ARG:NE	3:4F:338:GLU:OE2	2.39	0.54
2:3A:326:GLN:HE22	2:3A:348:TRP:HB3	1.73	0.54
3:4A:156:LEU:HB2	3:4A:182:VAL:HG22	1.88	0.54
3:4C:276:HIS:ND1	3:4C:277:ASP:OD2	2.40	0.54
1:2C:192:ALA:HA	1:2C:251:PRO:HG3	1.90	0.54
3:4B:115:ILE:HG22	3:4B:117:PRO:HD3	1.89	0.54
1:2F:267:MET:HE1	1:2F:283:VAL:HG23	1.89	0.54
2:3B:29:ILE:HD13	2:3B:162:GLU:HB2	1.90	0.54
1:2G:304:LYS:HB2	1:2G:304:LYS:NZ	2.23	0.54
1:2K:192:ALA:HA	1:2K:251:PRO:HG3	1.89	0.54
3:4F:34:SER:N	3:4F:61:TYR:OH	2.32	0.54
1:2D:131:ASP:O	1:2D:147:TYR:OH	2.25	0.54
1:2E:141:GLY:HA2	1:2E:216:TYR:CZ	2.42	0.54
1:2F:192:ALA:HA	1:2F:251:PRO:HG3	1.90	0.54
1:2J:62:GLN:OE1	1:2J:62:GLN:N	2.39	0.54
1:2L:192:ALA:HA	1:2L:251:PRO:HG3	1.88	0.54
3:4B:34:SER:N	3:4B:61:TYR:OH	2.36	0.53
2:3C:368:PHE:O	2:3C:372:GLU:HG3	2.07	0.53
2:3F:208:GLU:HG2	2:3F:209:VAL:HG23	1.90	0.53
3:4F:243:ASN:OD1	3:4F:244:ALA:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:178:LYS:O	2:3B:182:SER:OG	2.25	0.53
1:2A:191:LYS:HD2	1:2A:192:ALA:H	1.73	0.53
3:4D:336:THR:OG1	3:4D:337:GLN:NE2	2.42	0.53
2:3C:208:GLU:HG2	2:3C:209:VAL:HG23	1.90	0.53
2:3F:200:ASP:OD1	2:3F:201:LYS:N	2.42	0.53
1:2B:141:GLY:HA2	1:2B:216:TYR:CZ	2.42	0.53
3:4A:336:THR:OG1	3:4A:337:GLN:NE2	2.41	0.53
2:3C:178:LYS:O	2:3C:182:SER:OG	2.27	0.53
2:3C:326:GLN:OE1	2:3C:338:ARG:NH1	2.35	0.53
1:2H:131:ASP:O	1:2H:147:TYR:OH	2.25	0.53
1:2I:6:THR:HB	1:2J:214:ALA:HB1	1.91	0.53
1:2K:33:ALA:HB1	1:2K:89:THR:HG22	1.90	0.53
3:4A:110:ASP:OD1	3:4A:110:ASP:N	2.33	0.53
3:4C:187:LEU:HD11	3:4C:256:VAL:HG21	1.91	0.53
3:4D:358:ARG:HA	1:2D:339:ARG:HD3	1.90	0.53
2:3B:225:LEU:HD11	2:3B:281:ASN:HB3	1.91	0.53
1:2I:304:LYS:HB2	1:2I:304:LYS:NZ	2.23	0.53
1:2L:51:ASN:OD1	1:2L:52:TRP:N	2.42	0.53
3:4F:150:ARG:NH2	1:2E:14:GLU:OE2	2.42	0.53
2:3F:178:LYS:O	2:3F:182:SER:OG	2.27	0.53
1:2G:13:GLU:N	1:2G:13:GLU:OE2	2.42	0.53
1:2L:205:LYS:HD3	1:2L:206:TYR:CZ	2.43	0.53
3:4A:229:LEU:HD11	3:4A:266:ILE:HG13	1.91	0.53
3:4D:133:ASP:OD1	3:4D:134:LEU:N	2.41	0.53
3:4A:188:LYS:HG3	3:4A:233:ILE:HB	1.91	0.53
3:4E:243:ASN:OD1	3:4E:244:ALA:N	2.42	0.53
3:4F:187:LEU:HD11	3:4F:256:VAL:HG21	1.91	0.53
2:3E:178:LYS:O	2:3E:182:SER:OG	2.26	0.53
1:2G:62:GLN:CD	1:2G:62:GLN:H	2.17	0.53
1:2K:107:ALA:HA	1:2K:112:ILE:HG12	1.91	0.53
1:2L:131:ASP:O	1:2L:147:TYR:OH	2.22	0.53
2:3C:36:PHE:HB2	2:3C:140:PRO:HB3	1.91	0.52
2:3C:229:GLU:HG2	2:3C:232:GLN:HG2	1.91	0.52
2:3F:229:GLU:HG2	2:3F:232:GLN:HG2	1.92	0.52
3:4D:325:ARG:NE	3:4D:338:GLU:OE2	2.42	0.52
3:4E:115:ILE:HG22	3:4E:117:PRO:HD3	1.91	0.52
3:4F:358:ARG:HA	1:2F:339:ARG:HD3	1.90	0.52
1:2E:131:ASP:O	1:2E:147:TYR:OH	2.27	0.52
2:3D:20:LEU:HD11	2:3D:382:VAL:HG21	1.91	0.52
1:2A:267:MET:HE1	1:2A:283:VAL:HG23	1.92	0.52
1:2I:51:ASN:OD1	1:2I:52:TRP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4B:243:ASN:OD1	3:4B:244:ALA:N	2.42	0.52
3:4C:60:MET:SD	3:4C:60:MET:N	2.77	0.52
3:4D:188:LYS:HG3	3:4D:233:ILE:HB	1.91	0.52
3:4F:54:PHE:HE2	3:4F:77:VAL:HG11	1.74	0.52
2:3C:200:ASP:OD1	2:3C:201:LYS:N	2.43	0.52
2:3F:20:LEU:HD11	2:3F:382:VAL:HG21	1.91	0.52
1:2G:137:LEU:HD21	1:2G:224:MET:HE1	1.91	0.52
1:2J:62:GLN:CD	1:2J:62:GLN:H	2.17	0.52
3:4C:336:THR:OG1	3:4C:337:GLN:NE2	2.42	0.52
1:2J:211:ASP:OD1	1:2J:211:ASP:N	2.37	0.52
2:3A:208:GLU:HG2	2:3A:209:VAL:HG23	1.92	0.52
3:4A:160:ASP:OD2	3:4A:237:ARG:NH1	2.43	0.52
3:4C:358:ARG:HA	1:2C:339:ARG:HD3	1.91	0.52
1:2D:137:LEU:HD21	1:2D:224:MET:HE1	1.92	0.52
2:3B:200:ASP:OD1	2:3B:201:LYS:N	2.42	0.52
3:4B:187:LEU:HD11	3:4B:256:VAL:HG21	1.92	0.52
3:4C:34:SER:N	3:4C:61:TYR:OH	2.34	0.52
3:4F:115:ILE:HG22	3:4F:117:PRO:HD3	1.92	0.52
3:4F:336:THR:OG1	3:4F:337:GLN:NE2	2.43	0.52
1:2H:107:ALA:HA	1:2H:112:ILE:HG12	1.91	0.52
3:4A:325:ARG:NE	3:4A:338:GLU:OE2	2.43	0.52
1:2D:339:ARG:HH22	2:3D:462:GLN:NE2	2.08	0.52
1:2I:205:LYS:HD3	1:2I:206:TYR:CZ	2.44	0.52
3:4D:115:ILE:HG22	3:4D:117:PRO:HD3	1.92	0.51
3:4D:195:THR:OG1	3:4D:197:ASN:OD1	2.22	0.51
1:2B:137:LEU:HD21	1:2B:224:MET:HE1	1.92	0.51
2:3D:257:LYS:HD3	2:3D:258:ASN:HB2	1.91	0.51
2:3D:39:LYS:NZ	2:3D:61:ASN:OD1	2.42	0.51
2:3F:36:PHE:HB2	2:3F:140:PRO:HB3	1.91	0.51
1:2K:169:ASP:OD1	1:2K:169:ASP:N	2.38	0.51
1:2E:137:LEU:HD21	1:2E:224:MET:HE1	1.92	0.51
2:3D:223:SER:O	2:3D:281:ASN:ND2	2.43	0.51
2:3A:229:GLU:HG2	2:3A:232:GLN:HG2	1.92	0.51
1:2F:131:ASP:O	1:2F:147:TYR:OH	2.28	0.51
1:2F:141:GLY:HA2	1:2F:216:TYR:CZ	2.45	0.51
3:4D:160:ASP:OD2	3:4D:237:ARG:NH1	2.43	0.51
2:3B:257:LYS:HD3	2:3B:258:ASN:HB2	1.92	0.51
3:4F:195:THR:OG1	3:4F:197:ASN:OD1	2.22	0.51
1:2C:131:ASP:O	1:2C:147:TYR:OH	2.28	0.51
1:2D:61:GLU:N	1:2D:61:GLU:OE2	2.44	0.51
2:3B:208:GLU:HG2	2:3B:209:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3C:225:LEU:HD11	2:3C:281:ASN:HB3	1.93	0.51
2:3A:257:LYS:HD3	2:3A:258:ASN:HB2	1.92	0.51
3:4A:115:ILE:HG22	3:4A:117:PRO:HD3	1.92	0.51
3:4B:188:LYS:HG3	3:4B:233:ILE:HB	1.93	0.51
3:4D:34:SER:N	3:4D:61:TYR:OH	2.33	0.51
3:4E:245:LEU:HD13	3:4E:253:LEU:HD12	1.93	0.51
2:3E:200:ASP:OD1	2:3E:201:LYS:N	2.44	0.51
1:2J:141:GLY:HA2	1:2J:216:TYR:CZ	2.46	0.51
1:2A:27:THR:O	1:2A:254:ARG:NH2	2.44	0.51
1:2A:137:LEU:HD21	1:2A:224:MET:HE1	1.92	0.51
2:3B:229:GLU:HG2	2:3B:232:GLN:HG2	1.92	0.51
2:3D:208:GLU:HG2	2:3D:209:VAL:HG23	1.92	0.51
1:2H:146:ASP:OD1	1:2H:146:ASP:N	2.43	0.51
2:3A:316:ASP:OD1	2:3A:320:ARG:NH1	2.44	0.51
1:2B:107:ALA:HA	1:2B:112:ILE:HG12	1.93	0.51
2:3B:274:ASP:OD2	2:3B:275:GLU:N	2.44	0.51
2:3D:229:GLU:HG2	2:3D:232:GLN:HG2	1.92	0.51
2:3E:257:LYS:HD3	2:3E:258:ASN:HB2	1.93	0.51
3:4B:245:LEU:HD13	3:4B:253:LEU:HD12	1.93	0.51
3:4B:336:THR:OG1	3:4B:337:GLN:NE2	2.44	0.51
3:4E:336:THR:OG1	3:4E:337:GLN:NE2	2.44	0.51
1:2C:141:GLY:HA2	1:2C:216:TYR:CZ	2.46	0.51
2:3D:316:ASP:OD1	2:3D:320:ARG:NH1	2.44	0.51
2:3A:223:SER:O	2:3A:281:ASN:ND2	2.44	0.50
3:4E:325:ARG:NE	3:4E:338:GLU:OE2	2.39	0.50
2:3C:20:LEU:HD11	2:3C:382:VAL:HG21	1.91	0.50
2:3C:208:GLU:OE1	2:3C:208:GLU:N	2.27	0.50
2:3E:326:GLN:OE1	2:3E:338:ARG:NH1	2.39	0.50
2:3F:326:GLN:OE1	2:3F:338:ARG:NH1	2.35	0.50
1:2I:61:GLU:OE2	1:2I:61:GLU:N	2.43	0.50
3:4F:133:ASP:O	3:4F:137:GLN:HG3	2.11	0.50
1:2D:141:GLY:HA2	1:2D:216:TYR:CZ	2.46	0.50
2:3D:225:LEU:HD11	2:3D:281:ASN:HB3	1.93	0.50
2:3E:229:GLU:HG2	2:3E:232:GLN:HG2	1.93	0.50
1:2I:277:GLN:NE2	1:2I:281:GLU:OE2	2.45	0.50
1:2J:146:ASP:N	1:2J:146:ASP:OD1	2.43	0.50
1:2D:27:THR:O	1:2D:254:ARG:NH2	2.44	0.50
2:3E:225:LEU:HD11	2:3E:281:ASN:HB3	1.92	0.50
1:2H:31:VAL:HG22	1:2H:85:TYR:HB2	1.94	0.50
1:2J:239:ARG:NH1	1:2J:342:GLU:OE1	2.43	0.50
3:4C:88:ASP:OD2	3:4C:90:SER:OG	2.17	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4E:120:ILE:HD11	3:4E:202:SER:HB2	1.92	0.50
3:4E:187:LEU:HD11	3:4E:256:VAL:HG21	1.92	0.50
2:3F:223:SER:O	2:3F:281:ASN:ND2	2.45	0.50
1:2A:61:GLU:OE2	1:2A:61:GLU:N	2.44	0.50
2:3A:155:GLU:OE1	2:3A:159:GLN:NE2	2.45	0.50
3:4C:133:ASP:O	3:4C:137:GLN:HG3	2.12	0.50
3:4E:188:LYS:HG3	3:4E:233:ILE:HB	1.93	0.50
1:2G:6:THR:OG1	1:2H:214:ALA:HB1	2.11	0.50
1:2F:137:LEU:HD21	1:2F:224:MET:HE1	1.94	0.50
2:3F:257:LYS:HD3	2:3F:258:ASN:HB2	1.93	0.50
1:2I:146:ASP:N	1:2I:146:ASP:OD1	2.44	0.50
3:4C:188:LYS:HG3	3:4C:233:ILE:HB	1.94	0.50
2:3C:222:VAL:O	2:3C:281:ASN:ND2	2.31	0.50
2:3E:208:GLU:HG2	2:3E:209:VAL:HG23	1.93	0.50
1:2K:31:VAL:HG22	1:2K:85:TYR:HB2	1.94	0.50
1:2A:141:GLY:HA2	1:2A:216:TYR:CZ	2.46	0.50
3:4F:188:LYS:HG3	3:4F:233:ILE:HB	1.94	0.50
1:2C:27:THR:O	1:2C:254:ARG:NH2	2.45	0.50
1:2D:31:VAL:HG22	1:2D:85:TYR:HB2	1.94	0.50
3:4C:133:ASP:OD1	3:4C:134:LEU:N	2.45	0.50
1:2D:107:ALA:HA	1:2D:112:ILE:HG12	1.94	0.50
2:3C:257:LYS:HD3	2:3C:258:ASN:HB2	1.93	0.50
2:3A:225:LEU:HD11	2:3A:281:ASN:HB3	1.94	0.49
3:4A:34:SER:N	3:4A:61:TYR:OH	2.33	0.49
3:4B:195:THR:OG1	3:4B:197:ASN:OD1	2.22	0.49
3:4C:60:MET:H	3:4C:60:MET:HE3	1.77	0.49
3:4D:221:TRP:CD1	3:4D:332:GLY:HA2	2.47	0.49
3:4E:221:TRP:CD1	3:4E:332:GLY:HA2	2.47	0.49
1:2G:74:ARG:HD3	1:2G:164:TRP:CE2	2.47	0.49
1:2I:141:GLY:HA2	1:2I:216:TYR:CZ	2.47	0.49
1:2K:61:GLU:OE1	1:2K:61:GLU:N	2.45	0.49
1:2A:339:ARG:HD3	3:4A:358:ARG:HA	1.94	0.49
1:2F:27:THR:O	1:2F:254:ARG:NH2	2.45	0.49
1:2F:107:ALA:HA	1:2F:112:ILE:HG12	1.94	0.49
2:3D:19:ASN:ND2	2:3D:19:ASN:H	2.10	0.49
1:2H:61:GLU:N	1:2H:61:GLU:OE2	2.45	0.49
3:4B:133:ASP:OD1	3:4B:134:LEU:N	2.45	0.49
1:2B:18:LEU:HD13	1:2B:273:GLU:HG3	1.94	0.49
1:2E:18:LEU:HD13	1:2E:273:GLU:HG3	1.94	0.49
2:3F:368:PHE:O	2:3F:372:GLU:HG3	2.12	0.49
2:3D:155:GLU:OE1	2:3D:159:GLN:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3E:274:ASP:OD2	2:3E:275:GLU:N	2.44	0.49
3:4F:221:TRP:CD1	3:4F:332:GLY:HA2	2.47	0.49
2:3C:39:LYS:NZ	2:3C:61:ASN:OD1	2.45	0.49
1:2J:6:THR:OG1	1:2K:214:ALA:HB1	2.12	0.49
1:2K:213:GLN:HA	1:2K:224:MET:HE2	1.94	0.49
1:2L:61:GLU:N	1:2L:61:GLU:OE1	2.45	0.49
2:3A:222:VAL:O	2:3A:281:ASN:ND2	2.34	0.49
3:4A:221:TRP:CD1	3:4A:332:GLY:HA2	2.47	0.49
3:4E:195:THR:OG1	3:4E:197:ASN:OD1	2.22	0.49
1:2C:107:ALA:HA	1:2C:112:ILE:HG12	1.94	0.49
1:2E:107:ALA:HA	1:2E:112:ILE:HG12	1.93	0.49
2:3A:18:LEU:HD13	2:3A:385:GLU:HG2	1.95	0.49
3:4B:120:ILE:HD11	3:4B:202:SER:HB2	1.95	0.49
3:4C:195:THR:OG1	3:4C:197:ASN:OD1	2.22	0.49
3:4E:160:ASP:OD2	3:4E:237:ARG:NH1	2.45	0.49
3:4F:133:ASP:OD1	3:4F:134:LEU:N	2.45	0.49
1:2B:61:GLU:N	1:2B:61:GLU:OE1	2.46	0.49
1:2H:141:GLY:HA2	1:2H:216:TYR:CZ	2.48	0.49
1:2A:31:VAL:HG22	1:2A:85:TYR:HB2	1.95	0.49
3:4C:115:ILE:HG22	3:4C:117:PRO:HD3	1.93	0.49
1:2B:131:ASP:O	1:2B:147:TYR:OH	2.27	0.49
1:2A:55:TYR:OH	1:2A:70:ASP:OD1	2.22	0.49
3:4C:33:THR:O	3:4C:82:THR:HA	2.13	0.49
3:4C:214:ASN:O	3:4C:219:GLY:N	2.46	0.49
3:4C:221:TRP:CD1	3:4C:332:GLY:HA2	2.47	0.49
1:2D:117:SER:O	1:2D:121:LYS:NZ	2.46	0.49
1:2G:33:ALA:HB1	1:2G:89:THR:HG22	1.94	0.49
1:2I:107:ALA:HA	1:2I:112:ILE:HD13	1.95	0.49
1:2K:141:GLY:HA2	1:2K:216:TYR:CZ	2.48	0.49
1:2L:141:GLY:HA2	1:2L:216:TYR:CZ	2.48	0.49
1:2C:137:LEU:HD21	1:2C:224:MET:HE1	1.95	0.49
1:2K:131:ASP:O	1:2K:147:TYR:OH	2.26	0.49
2:3A:3:THR:N	2:3A:13:GLU:OE2	2.46	0.48
3:4F:214:ASN:O	3:4F:219:GLY:N	2.45	0.48
1:2D:44:LYS:HG2	1:2D:45:PRO:HD2	1.95	0.48
1:2E:61:GLU:N	1:2E:61:GLU:OE1	2.46	0.48
2:3C:166:ILE:HG21	2:3C:183:LEU:HD21	1.94	0.48
1:2G:141:GLY:HA2	1:2G:216:TYR:CZ	2.48	0.48
1:2I:304:LYS:NZ	1:2I:307:ASP:OD2	2.45	0.48
1:2K:273:GLU:HG3	1:2K:274:PRO:HD2	1.95	0.48
1:2L:146:ASP:OD1	1:2L:146:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:107:ALA:HA	1:2A:112:ILE:HG12	1.94	0.48
3:4B:123:ASP:OD2	3:4B:125:THR:HG23	2.13	0.48
3:4C:160:ASP:OD2	3:4C:237:ARG:NH1	2.45	0.48
3:4C:184:TRP:HZ3	3:4C:242:ALA:HB2	1.78	0.48
3:4E:207:VAL:O	3:4E:211:ILE:HG13	2.13	0.48
1:2G:236:TRP:CD1	1:2L:8:PRO:HG2	2.48	0.48
1:2I:8:PRO:HG2	1:2J:236:TRP:CD1	2.48	0.48
2:3A:137:TYR:OH	2:3A:162:GLU:OE2	2.20	0.48
1:2G:146:ASP:OD1	1:2G:146:ASP:N	2.42	0.48
3:4B:207:VAL:O	3:4B:211:ILE:HG13	2.13	0.48
3:4B:221:TRP:CD1	3:4B:332:GLY:HA2	2.47	0.48
3:4E:133:ASP:OD1	3:4E:134:LEU:N	2.46	0.48
3:4F:184:TRP:HZ3	3:4F:242:ALA:HB2	1.79	0.48
1:2C:61:GLU:OE1	1:2C:61:GLU:N	2.47	0.48
2:3C:50:VAL:HG11	2:3C:56:PHE:HB2	1.95	0.48
2:3D:137:TYR:OH	2:3D:162:GLU:OE2	2.20	0.48
2:3F:39:LYS:NZ	2:3F:61:ASN:OD1	2.45	0.48
3:4E:184:TRP:HZ3	3:4E:242:ALA:HB2	1.79	0.48
3:4F:60:MET:CE	3:4F:60:MET:H	2.25	0.48
1:2B:249:TYR:HB3	1:2B:251:PRO:HD2	1.95	0.48
1:2H:213:GLN:HA	1:2H:224:MET:HE2	1.95	0.48
1:2H:273:GLU:HG3	1:2H:274:PRO:HD2	1.95	0.48
3:4B:34:SER:N	3:4B:83:GLU:HG3	2.29	0.48
1:2B:31:VAL:HG22	1:2B:85:TYR:HB2	1.96	0.48
1:2G:107:ALA:HA	1:2G:112:ILE:HD13	1.95	0.48
1:2L:107:ALA:HA	1:2L:112:ILE:HD13	1.95	0.48
1:2B:33:ALA:HB1	1:2B:89:THR:HG22	1.96	0.48
1:2E:44:LYS:HG2	1:2E:45:PRO:HD2	1.96	0.48
1:2K:101:ASP:OD2	1:2K:101:ASP:N	2.44	0.48
1:2A:191:LYS:HD2	1:2A:192:ALA:N	2.28	0.48
3:4B:184:TRP:HZ3	3:4B:242:ALA:HB2	1.78	0.48
2:3C:198:ASN:ND2	2:3C:200:ASP:O	2.47	0.48
2:3C:354:GLN:NE2	2:3C:356:ASP:OD2	2.32	0.48
1:2K:8:PRO:HG2	1:2L:236:TRP:CD1	2.49	0.48
3:4B:33:THR:O	3:4B:82:THR:HA	2.13	0.47
1:2C:55:TYR:OH	1:2C:70:ASP:OD1	2.21	0.47
1:2E:31:VAL:HG22	1:2E:85:TYR:HB2	1.96	0.47
2:3F:166:ILE:HG21	2:3F:183:LEU:HD21	1.95	0.47
2:3F:354:GLN:NE2	2:3F:356:ASP:OD2	2.32	0.47
1:2A:15:ASP:OD2	1:2A:17:SER:OG	2.28	0.47
1:2A:44:LYS:HG2	1:2A:45:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2F:44:LYS:HG2	1:2F:45:PRO:HD2	1.96	0.47
2:3F:225:LEU:HD11	2:3F:281:ASN:HB3	1.96	0.47
1:2K:146:ASP:OD1	1:2K:146:ASP:N	2.43	0.47
3:4A:133:ASP:OD1	3:4A:134:LEU:N	2.47	0.47
3:4B:160:ASP:OD2	3:4B:237:ARG:NH1	2.45	0.47
1:2E:249:TYR:HB3	1:2E:251:PRO:HD2	1.95	0.47
2:3D:3:THR:N	2:3D:13:GLU:OE2	2.46	0.47
1:2A:236:TRP:CD1	1:2F:8:PRO:HG2	2.50	0.47
3:4A:214:ASN:O	3:4A:219:GLY:N	2.47	0.47
3:4D:214:ASN:O	3:4D:219:GLY:N	2.47	0.47
3:4D:215:ASP:OD1	3:4D:287:ARG:NH2	2.43	0.47
1:2D:169:ASP:OD1	1:2D:169:ASP:N	2.35	0.47
1:2D:273:GLU:HG3	1:2D:274:PRO:HD2	1.96	0.47
1:2E:137:LEU:HD12	1:2E:137:LEU:HA	1.79	0.47
1:2A:249:TYR:HB3	1:2A:251:PRO:HD2	1.97	0.47
2:3A:274:ASP:OD2	2:3A:275:GLU:N	2.48	0.47
3:4B:214:ASN:O	3:4B:219:GLY:N	2.48	0.47
2:3F:19:ASN:C	2:3F:19:ASN:HD22	2.16	0.47
3:4A:33:THR:O	3:4A:82:THR:HA	2.15	0.47
3:4A:245:LEU:HD13	3:4A:253:LEU:HD12	1.95	0.47
1:2B:15:ASP:OD2	1:2B:17:SER:OG	2.30	0.47
1:2B:44:LYS:HG2	1:2B:45:PRO:HD2	1.96	0.47
1:2F:61:GLU:N	1:2F:61:GLU:OE1	2.47	0.47
2:3B:425:ILE:HD12	2:3B:443:VAL:HG22	1.96	0.47
2:3F:50:VAL:HG11	2:3F:56:PHE:HB2	1.96	0.47
1:2A:273:GLU:HG3	1:2A:274:PRO:HD2	1.96	0.47
3:4B:315:LYS:HB2	3:4B:315:LYS:HE3	1.65	0.47
3:4D:245:LEU:HD13	3:4D:253:LEU:HD12	1.96	0.47
3:4F:315:LYS:HB2	3:4F:315:LYS:HE3	1.66	0.47
2:3E:316:ASP:OD1	2:3E:320:ARG:NH1	2.48	0.47
1:2K:100:ASP:OD2	1:2K:100:ASP:N	2.46	0.47
1:2L:44:LYS:HE2	1:2L:47:ILE:HD11	1.96	0.47
2:3A:19:ASN:H	2:3A:19:ASN:ND2	2.12	0.47
3:4C:315:LYS:HB2	3:4C:315:LYS:HE3	1.66	0.47
1:2H:62:GLN:H	1:2H:62:GLN:CD	2.23	0.47
1:2J:100:ASP:OD2	1:2J:100:ASP:N	2.47	0.47
2:3A:33:ILE:HG12	2:3A:139:LEU:HD23	1.96	0.47
1:2C:313:ILE:HD12	1:2C:331:ILE:HG12	1.97	0.47
1:2F:274:PRO:HB3	2:3F:450:VAL:HG11	1.96	0.47
3:4E:123:ASP:OD2	3:4E:125:THR:HG23	2.14	0.47
2:3D:432:SER:OG	2:3D:435:ASP:OD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3E:425:ILE:HD12	2:3E:443:VAL:HG22	1.96	0.47
2:3F:198:ASN:ND2	2:3F:200:ASP:O	2.48	0.47
1:2L:62:GLN:H	1:2L:62:GLN:CD	2.22	0.47
3:4F:160:ASP:OD2	3:4F:237:ARG:NH1	2.46	0.46
1:2C:44:LYS:HG2	1:2C:45:PRO:HD2	1.97	0.46
2:3B:326:GLN:OE1	2:3B:338:ARG:NH1	2.37	0.46
2:3D:33:ILE:HG12	2:3D:139:LEU:HD23	1.96	0.46
2:3D:326:GLN:OE1	2:3D:338:ARG:NH1	2.35	0.46
1:2K:62:GLN:CD	1:2K:62:GLN:H	2.22	0.46
1:2E:15:ASP:OD1	1:2E:17:SER:OG	2.32	0.46
1:2F:313:ILE:HD12	1:2F:331:ILE:HG12	1.96	0.46
1:2I:281:GLU:OE1	1:2I:284:ARG:NH1	2.48	0.46
1:2J:249:TYR:HB3	1:2J:251:PRO:HD2	1.97	0.46
3:4B:259:PHE:HB3	3:4B:262:LYS:HB2	1.97	0.46
3:4D:33:THR:O	3:4D:82:THR:HA	2.15	0.46
3:4E:34:SER:N	3:4E:61:TYR:OH	2.36	0.46
3:4F:120:ILE:HD11	3:4F:202:SER:HB2	1.97	0.46
1:2F:55:TYR:OH	1:2F:70:ASP:OD1	2.21	0.46
1:2H:8:PRO:HG2	1:2I:236:TRP:CD1	2.51	0.46
1:2I:101:ASP:OD1	1:2I:101:ASP:N	2.47	0.46
3:4F:280:TRP:CE3	3:4F:286:ARG:HD2	2.51	0.46
1:2E:304:LYS:HE2	1:2E:304:LYS:HB2	1.64	0.46
1:2G:249:TYR:HB3	1:2G:251:PRO:HD2	1.97	0.46
3:4C:280:TRP:CE3	3:4C:286:ARG:HD2	2.51	0.46
3:4E:30:ILE:HG22	3:4E:80:LEU:HD11	1.98	0.46
2:3D:222:VAL:O	2:3D:281:ASN:ND2	2.31	0.46
3:4B:178:GLN:HE21	3:4B:280:TRP:CG	2.34	0.46
3:4D:88:ASP:OD2	3:4D:90:SER:OG	2.17	0.46
3:4D:259:PHE:HB3	3:4D:262:LYS:HB2	1.98	0.46
3:4E:33:THR:O	3:4E:82:THR:HA	2.15	0.46
1:2C:18:LEU:HD13	1:2C:273:GLU:HG3	1.98	0.46
2:3A:271:ALA:O	2:3A:275:GLU:HG2	2.16	0.46
3:4A:34:SER:N	3:4A:83:GLU:HG3	2.31	0.46
3:4D:184:TRP:HZ3	3:4D:242:ALA:HB2	1.81	0.46
1:2F:249:TYR:HB3	1:2F:251:PRO:HD2	1.98	0.46
1:2H:6:THR:OG1	1:2I:214:ALA:HB1	2.16	0.46
1:2J:51:ASN:OD1	1:2J:52:TRP:N	2.49	0.46
1:2J:74:ARG:HD3	1:2J:164:TRP:CE2	2.50	0.46
3:4D:315:LYS:HE3	3:4D:315:LYS:HB2	1.65	0.46
3:4E:34:SER:N	3:4E:83:GLU:HG3	2.31	0.46
3:4E:259:PHE:HB3	3:4E:262:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4F:33:THR:O	3:4F:82:THR:HA	2.15	0.46
2:3C:254:LEU:HD12	2:3C:262:TYR:HB2	1.98	0.46
1:2I:62:GLN:CD	1:2I:62:GLN:H	2.22	0.46
1:2K:112:ILE:HD12	1:2K:112:ILE:O	2.16	0.46
3:4C:214:ASN:ND2	3:4C:222:THR:O	2.49	0.45
3:4D:34:SER:N	3:4D:83:GLU:HG3	2.30	0.45
3:4E:178:GLN:HE21	3:4E:280:TRP:CG	2.33	0.45
1:2C:249:TYR:HB3	1:2C:251:PRO:HD2	1.98	0.45
2:3B:166:ILE:HG21	2:3B:183:LEU:HD21	1.98	0.45
2:3B:316:ASP:OD1	2:3B:320:ARG:NH1	2.49	0.45
2:3D:166:ILE:HG21	2:3D:183:LEU:HD21	1.98	0.45
1:2F:18:LEU:HD13	1:2F:273:GLU:HG3	1.97	0.45
3:4C:120:ILE:HD11	3:4C:202:SER:HB2	1.96	0.45
1:2B:214:ALA:O	1:2B:218:GLN:NE2	2.48	0.45
1:2D:249:TYR:HB3	1:2D:251:PRO:HD2	1.98	0.45
3:4A:184:TRP:HZ3	3:4A:242:ALA:HB2	1.82	0.45
3:4C:245:LEU:HD13	3:4C:253:LEU:HD12	1.99	0.45
3:4D:203:PRO:O	3:4D:207:VAL:HG22	2.16	0.45
3:4E:214:ASN:O	3:4E:219:GLY:N	2.48	0.45
3:4F:50:PHE:CZ	3:4F:61:TYR:HB3	2.50	0.45
3:4F:214:ASN:ND2	3:4F:222:THR:O	2.50	0.45
3:4F:364:ILE:HB	1:2F:346:LEU:HD23	1.98	0.45
2:3F:254:LEU:HD12	2:3F:262:TYR:HB2	1.99	0.45
1:2H:112:ILE:O	1:2H:112:ILE:HD12	2.16	0.45
1:2L:105:LEU:HD22	1:2L:112:ILE:HD12	1.97	0.45
3:4B:358:ARG:HA	1:2B:339:ARG:HD3	1.98	0.45
1:2K:144:ASN:OD1	1:2K:144:ASN:N	2.49	0.45
1:2A:33:ALA:HB1	1:2A:89:THR:HG22	1.99	0.45
2:3A:462:GLN:HE21	2:3A:462:GLN:HB2	1.57	0.45
3:4A:178:GLN:HE21	3:4A:280:TRP:CG	2.35	0.45
3:4A:259:PHE:HB3	3:4A:262:LYS:HB2	1.99	0.45
3:4A:315:LYS:HE3	3:4A:315:LYS:HB2	1.65	0.45
3:4D:247:ASN:H	3:4D:252:SER:HB3	1.81	0.45
1:2C:322:ASP:OD1	1:2C:322:ASP:N	2.50	0.45
2:3D:207:THR:HG21	2:3D:213:THR:OG1	2.17	0.45
1:2L:137:LEU:HD12	1:2L:137:LEU:HA	1.78	0.45
1:2A:313:ILE:HD12	1:2A:331:ILE:HG12	1.98	0.45
3:4B:110:ASP:OD1	3:4B:110:ASP:N	2.32	0.45
3:4D:150:ARG:NH2	1:2C:14:GLU:OE1	2.49	0.45
3:4F:56:GLU:HG3	3:4F:57:SER:N	2.31	0.45
2:3B:271:ALA:O	2:3B:275:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3A:348:TRP:CD1	2:3F:8:PRO:HG2	2.51	0.45
3:4F:50:PHE:HZ	3:4F:61:TYR:HB3	1.81	0.45
3:4F:259:PHE:HB3	3:4F:262:LYS:HB2	1.99	0.45
3:4A:247:ASN:H	3:4A:252:SER:HB3	1.80	0.45
1:2C:274:PRO:HB3	2:3C:450:VAL:HG11	1.98	0.45
1:2F:322:ASP:OD1	1:2F:322:ASP:N	2.49	0.45
3:4C:56:GLU:HG3	3:4C:57:SER:N	2.32	0.45
3:4E:194:ASN:OD1	3:4E:195:THR:N	2.49	0.45
3:4F:245:LEU:HD13	3:4F:253:LEU:HD12	1.99	0.45
1:2D:220:LYS:H	1:2D:220:LYS:HG2	1.55	0.45
1:2D:313:ILE:HD12	1:2D:331:ILE:HG12	1.98	0.45
1:2E:33:ALA:HB1	1:2E:89:THR:HG22	1.97	0.45
2:3E:271:ALA:O	2:3E:275:GLU:HG2	2.17	0.45
1:2I:105:LEU:HD22	1:2I:112:ILE:HD12	1.98	0.45
2:3A:263:GLN:O	2:3A:267:GLN:HG2	2.17	0.44
3:4C:50:PHE:HZ	3:4C:61:TYR:HB3	1.83	0.44
3:4F:307:PRO:HB3	1:2F:338:VAL:HG11	1.99	0.44
2:3D:155:GLU:O	2:3D:159:GLN:HG2	2.18	0.44
3:4C:259:PHE:HB3	3:4C:262:LYS:HB2	1.99	0.44
3:4D:178:GLN:HE21	3:4D:280:TRP:CG	2.35	0.44
1:2E:100:ASP:OD2	1:2E:100:ASP:C	2.60	0.44
1:2F:137:LEU:HD12	1:2F:137:LEU:HA	1.79	0.44
2:3C:130:GLN:HE21	2:3C:130:GLN:HB2	1.58	0.44
2:3A:207:THR:HG21	2:3A:213:THR:OG1	2.17	0.44
1:2E:8:PRO:HG2	1:2F:236:TRP:CD1	2.52	0.44
2:3D:19:ASN:H	2:3D:19:ASN:HD22	1.66	0.44
2:3E:432:SER:OG	2:3E:435:ASP:OD2	2.29	0.44
1:2G:83:TYR:H	1:2G:83:TYR:HD1	1.65	0.44
1:2G:270:ALA:HA	1:2G:273:GLU:HG2	2.00	0.44
1:2A:8:PRO:HG2	1:2B:236:TRP:CD1	2.52	0.44
2:3A:166:ILE:HG21	2:3A:183:LEU:HD21	1.99	0.44
3:4B:56:GLU:HG3	3:4B:57:SER:N	2.33	0.44
3:4B:139:TRP:CD1	3:4B:156:LEU:HD13	2.53	0.44
2:3C:8:PRO:HG2	2:3D:348:TRP:CD1	2.52	0.44
2:3E:198:ASN:ND2	2:3E:200:ASP:O	2.51	0.44
1:2J:137:LEU:HD21	1:2J:224:MET:HE1	1.99	0.44
1:2K:208:VAL:HG11	1:2K:224:MET:HE3	2.00	0.44
2:3A:20:LEU:HD11	2:3A:382:VAL:HG21	1.98	0.44
3:4B:50:PHE:CZ	3:4B:61:TYR:HB3	2.52	0.44
3:4E:364:ILE:HB	1:2E:346:LEU:HD23	1.99	0.44
1:2C:8:PRO:HG2	1:2D:236:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2C:304:LYS:HB2	1:2C:304:LYS:HE2	1.63	0.44
1:2J:83:TYR:H	1:2J:83:TYR:HD1	1.64	0.44
3:4C:307:PRO:HB3	1:2C:338:VAL:HG11	1.99	0.44
3:4F:69:GLU:O	3:4F:231:LYS:NZ	2.50	0.44
2:3B:383:VAL:HG11	1:2I:236:TRP:CH2	2.53	0.44
1:2J:270:ALA:HA	1:2J:273:GLU:HG2	2.00	0.44
1:2A:100:ASP:C	1:2A:100:ASP:OD1	2.60	0.44
1:2A:137:LEU:HD12	1:2A:137:LEU:HA	1.78	0.44
2:3A:155:GLU:O	2:3A:159:GLN:HG2	2.18	0.44
3:4C:50:PHE:CZ	3:4C:61:TYR:HB3	2.52	0.44
3:4D:194:ASN:OD1	3:4D:195:THR:N	2.50	0.44
3:4D:243:ASN:OD1	3:4D:244:ALA:N	2.51	0.44
2:3E:201:LYS:HE2	2:3E:201:LYS:HB3	1.78	0.44
1:2H:208:VAL:HG11	1:2H:224:MET:HE3	2.00	0.44
1:2I:20:LEU:HD12	1:2I:20:LEU:HA	1.85	0.44
3:4B:50:PHE:HZ	3:4B:61:TYR:HB3	1.83	0.44
3:4E:358:ARG:HA	1:2E:339:ARG:HD3	1.98	0.44
2:3E:383:VAL:HG11	1:2L:236:TRP:CH2	2.52	0.44
2:3F:325:GLU:O	2:3F:329:MET:HG3	2.17	0.44
1:2H:313:ILE:HD12	1:2H:331:ILE:HG12	2.00	0.44
2:3A:8:PRO:HG2	2:3B:348:TRP:CD1	2.52	0.44
3:4C:69:GLU:O	3:4C:231:LYS:NZ	2.50	0.44
3:4C:194:ASN:OD1	3:4C:195:THR:N	2.50	0.44
2:3B:207:THR:HG21	2:3B:213:THR:OG1	2.18	0.44
1:2G:281:GLU:OE1	1:2G:284:ARG:NH1	2.51	0.44
3:4A:349:ASP:C	3:4A:351:SER:H	2.26	0.43
3:4C:229:LEU:HD13	3:4C:264:ILE:HG22	2.00	0.43
3:4E:349:ASP:C	3:4E:351:SER:H	2.26	0.43
1:2B:313:ILE:HD12	1:2B:331:ILE:HG12	2.00	0.43
2:3B:254:LEU:HD12	2:3B:262:TYR:HB2	2.00	0.43
2:3D:8:PRO:HG2	2:3E:348:TRP:CD1	2.53	0.43
2:3F:212:GLN:HE21	2:3F:212:GLN:HB3	1.64	0.43
1:2A:214:ALA:HB1	1:2F:6:THR:HB	2.00	0.43
3:4A:203:PRO:O	3:4A:207:VAL:HG22	2.17	0.43
3:4D:229:LEU:HD13	3:4D:264:ILE:HG22	2.01	0.43
1:2B:191:LYS:HD2	1:2B:192:ALA:H	1.83	0.43
1:2D:100:ASP:OD1	1:2D:100:ASP:C	2.60	0.43
1:2F:304:LYS:HB2	1:2F:304:LYS:HE2	1.63	0.43
2:3E:207:THR:HG21	2:3E:213:THR:OG1	2.18	0.43
3:4A:56:GLU:HG3	3:4A:57:SER:N	2.33	0.43
3:4B:364:ILE:HB	1:2B:346:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4C:34:SER:N	3:4C:83:GLU:HG3	2.33	0.43
3:4C:364:ILE:HB	1:2C:346:LEU:HD23	1.99	0.43
3:4D:214:ASN:ND2	3:4D:222:THR:O	2.51	0.43
3:4E:56:GLU:HG3	3:4E:57:SER:N	2.32	0.43
3:4A:243:ASN:OD1	3:4A:244:ALA:N	2.51	0.43
3:4C:106:ALA:HB2	3:4C:148:SER:HB3	2.01	0.43
3:4D:30:ILE:HG22	3:4D:80:LEU:HD11	2.00	0.43
3:4D:69:GLU:O	3:4D:231:LYS:NZ	2.52	0.43
1:2B:100:ASP:OD2	1:2B:100:ASP:C	2.60	0.43
2:3E:166:ILE:HG21	2:3E:183:LEU:HD21	1.99	0.43
3:4A:214:ASN:ND2	3:4A:222:THR:O	2.51	0.43
3:4F:349:ASP:C	3:4F:351:SER:H	2.27	0.43
2:3B:403:LEU:HD13	2:3B:421:TYR:HB2	2.01	0.43
2:3D:263:GLN:O	2:3D:267:GLN:HG2	2.18	0.43
2:3D:406:LEU:HD23	2:3D:406:LEU:HA	1.91	0.43
1:2I:13:GLU:N	1:2I:13:GLU:OE1	2.51	0.43
3:4A:69:GLU:O	3:4A:231:LYS:NZ	2.51	0.43
3:4C:30:ILE:HG22	3:4C:80:LEU:HD11	2.00	0.43
3:4C:247:ASN:H	3:4C:252:SER:HB3	1.84	0.43
3:4D:162:PRO:HG3	3:4D:241:GLU:HB2	2.01	0.43
1:2E:101:ASP:OD1	1:2E:101:ASP:N	2.46	0.43
1:2E:313:ILE:HD12	1:2E:331:ILE:HG12	2.00	0.43
2:3E:403:LEU:HD13	2:3E:421:TYR:HB2	2.00	0.43
1:2J:8:PRO:HG2	1:2K:236:TRP:CD1	2.53	0.43
1:2J:218:GLN:H	1:2J:218:GLN:HG2	1.74	0.43
3:4D:56:GLU:HG3	3:4D:57:SER:N	2.33	0.43
3:4E:50:PHE:HZ	3:4E:61:TYR:HB3	1.84	0.43
3:4E:203:PRO:O	3:4E:207:VAL:HG22	2.18	0.43
1:2B:332:LYS:HE3	1:2B:332:LYS:HB3	1.74	0.43
1:2E:214:ALA:O	1:2E:218:GLN:NE2	2.51	0.43
2:3C:406:LEU:HD23	2:3C:406:LEU:HA	1.91	0.43
2:3D:35:LEU:HB2	2:3D:119:THR:HG21	2.01	0.43
1:2G:12:ILE:HD11	1:2H:346:LEU:HD12	2.01	0.43
1:2H:294:LEU:HD23	1:2H:294:LEU:HA	1.88	0.43
1:2A:211:ASP:OD1	1:2A:211:ASP:C	2.61	0.43
2:3A:229:GLU:CD	2:3A:229:GLU:H	2.27	0.43
3:4A:30:ILE:HG22	3:4A:80:LEU:HD11	2.00	0.43
3:4B:277:ASP:OD1	3:4B:277:ASP:N	2.51	0.43
3:4C:203:PRO:O	3:4C:207:VAL:HG22	2.19	0.43
1:2B:8:PRO:HG2	1:2C:236:TRP:CD1	2.53	0.43
1:2C:93:GLU:H	1:2C:93:GLU:HG3	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2D:8:PRO:HG2	1:2E:236:TRP:CD1	2.54	0.43
2:3C:229:GLU:H	2:3C:229:GLU:CD	2.27	0.43
2:3C:325:GLU:O	2:3C:329:MET:HG3	2.18	0.43
2:3F:207:THR:HG21	2:3F:213:THR:OG1	2.18	0.43
1:2G:8:PRO:HG2	1:2H:236:TRP:CD1	2.53	0.43
2:3A:432:SER:OG	2:3A:435:ASP:OD2	2.29	0.43
3:4C:243:ASN:OD1	3:4C:244:ALA:N	2.52	0.43
3:4D:155:LEU:C	3:4D:156:LEU:HD23	2.44	0.43
1:2D:33:ALA:HB1	1:2D:89:THR:HG22	2.00	0.43
1:2E:191:LYS:HD2	1:2E:192:ALA:H	1.83	0.43
2:3B:229:GLU:CD	2:3B:229:GLU:H	2.27	0.43
1:2G:239:ARG:NH1	1:2G:342:GLU:OE2	2.51	0.43
1:2K:304:LYS:HB2	1:2K:304:LYS:NZ	2.34	0.43
1:2L:20:LEU:HD12	1:2L:20:LEU:HA	1.83	0.43
3:4F:34:SER:N	3:4F:83:GLU:HG3	2.33	0.43
3:4F:178:GLN:HE21	3:4F:280:TRP:CG	2.37	0.43
3:4F:194:ASN:OD1	3:4F:195:THR:N	2.50	0.43
2:3E:36:PHE:CZ	2:3E:121:SER:HB2	2.54	0.43
2:3A:375:ILE:O	2:3A:379:MET:HG2	2.19	0.42
3:4A:162:PRO:HG3	3:4A:241:GLU:HB2	2.01	0.42
3:4B:69:GLU:O	3:4B:231:LYS:NZ	2.51	0.42
3:4E:50:PHE:CZ	3:4E:61:TYR:HB3	2.53	0.42
3:4F:106:ALA:HB2	3:4F:148:SER:HB3	2.01	0.42
2:3B:432:SER:OG	2:3B:435:ASP:OD2	2.30	0.42
2:3D:375:ILE:O	2:3D:379:MET:HG2	2.19	0.42
3:4B:239:TYR:C	3:4B:239:TYR:CD1	2.97	0.42
3:4C:349:ASP:C	3:4C:351:SER:H	2.27	0.42
2:3B:40:ASN:OD1	2:3B:41:THR:N	2.52	0.42
2:3B:198:ASN:ND2	2:3B:200:ASP:O	2.52	0.42
1:2H:137:LEU:HA	1:2H:137:LEU:HD12	1.75	0.42
1:2K:267:MET:HE1	1:2K:283:VAL:HG13	2.01	0.42
1:2K:313:ILE:HD12	1:2K:331:ILE:HG12	2.00	0.42
3:4A:229:LEU:HD13	3:4A:264:ILE:HG22	2.01	0.42
3:4F:229:LEU:HD13	3:4F:264:ILE:HG22	2.00	0.42
3:4F:247:ASN:H	3:4F:252:SER:HB3	1.84	0.42
2:3C:403:LEU:HD13	2:3C:421:TYR:HB2	2.02	0.42
2:3E:205:LEU:HD23	2:3E:205:LEU:HA	1.82	0.42
2:3E:254:LEU:HD12	2:3E:262:TYR:HB2	2.01	0.42
2:3A:19:ASN:HD22	2:3A:19:ASN:C	2.26	0.42
3:4E:69:GLU:O	3:4E:231:LYS:NZ	2.52	0.42
3:4E:139:TRP:CD1	3:4E:156:LEU:HD13	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4E:214:ASN:ND2	3:4E:222:THR:O	2.52	0.42
1:2C:6:THR:HB	1:2D:214:ALA:HB1	2.00	0.42
2:3C:207:THR:HG21	2:3C:213:THR:OG1	2.18	0.42
1:2J:20:LEU:HD12	1:2J:20:LEU:HA	1.82	0.42
3:4B:194:ASN:OD1	3:4B:195:THR:N	2.49	0.42
3:4F:188:LYS:HG2	3:4F:234:SER:O	2.20	0.42
2:3B:36:PHE:CZ	2:3B:121:SER:HB2	2.54	0.42
3:4B:214:ASN:ND2	3:4B:222:THR:O	2.53	0.42
3:4B:228:ALA:HB2	3:4B:265:ARG:NH1	2.35	0.42
3:4D:207:VAL:O	3:4D:211:ILE:HG13	2.19	0.42
2:3D:150:LEU:HG	2:3D:182:SER:OG	2.20	0.42
3:4D:349:ASP:C	3:4D:351:SER:H	2.26	0.42
3:4E:239:TYR:CD1	3:4E:239:TYR:C	2.97	0.42
2:3B:205:LEU:HD23	2:3B:205:LEU:HA	1.83	0.42
2:3C:33:ILE:HG12	2:3C:139:LEU:HD23	2.01	0.42
2:3E:150:LEU:HG	2:3E:182:SER:OG	2.20	0.42
1:2G:144:ASN:HD21	1:2G:222:LEU:HD13	1.85	0.42
1:2H:242:GLU:HG2	1:2H:244:ASN:OD1	2.20	0.42
1:2I:249:TYR:HB3	1:2I:251:PRO:HD2	2.02	0.42
2:3A:385:GLU:HG3	2:3A:386:PRO:HD2	2.01	0.42
3:4C:178:GLN:HE21	3:4C:280:TRP:CG	2.38	0.42
3:4D:307:PRO:HB3	1:2D:338:VAL:HG11	2.02	0.42
3:4E:247:ASN:H	3:4E:252:SER:HB3	1.85	0.42
1:2E:274:PRO:HB3	2:3E:450:VAL:HG11	2.02	0.42
2:3C:432:SER:N	2:3C:435:ASP:OD2	2.53	0.42
1:2G:73:LEU:HD13	1:2G:73:LEU:HA	1.94	0.42
2:3A:35:LEU:HB2	2:3A:119:THR:HG21	2.01	0.42
2:3A:50:VAL:HG11	2:3A:56:PHE:HB2	2.02	0.42
3:4A:155:LEU:C	3:4A:156:LEU:HD23	2.44	0.42
3:4F:203:PRO:O	3:4F:207:VAL:HG22	2.19	0.42
1:2C:15:ASP:OD1	1:2C:17:SER:OG	2.32	0.42
2:3E:368:PHE:O	2:3E:372:GLU:HB2	2.20	0.42
1:2K:137:LEU:HD12	1:2K:137:LEU:HA	1.75	0.42
1:2K:249:TYR:HB3	1:2K:251:PRO:HD2	2.01	0.42
1:2A:36:GLY:HA2	1:2A:88:GLN:NE2	2.35	0.42
3:4A:207:VAL:O	3:4A:211:ILE:HG13	2.20	0.42
3:4A:215:ASP:OD1	3:4A:287:ARG:NH2	2.44	0.42
3:4A:289:VAL:O	3:4A:293:GLU:HG2	2.20	0.42
3:4E:228:ALA:HB2	3:4E:265:ARG:NH1	2.35	0.42
2:3F:130:GLN:HE21	2:3F:130:GLN:HB2	1.58	0.42
2:3F:229:GLU:CD	2:3F:229:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2J:304:LYS:HB2	1:2J:304:LYS:HZ3	1.85	0.42
1:2H:249:TYR:HB3	1:2H:251:PRO:HD2	2.00	0.41
1:2L:249:TYR:HB3	1:2L:251:PRO:HD2	2.02	0.41
1:2E:140:ASP:OD1	1:2E:142:THR:HG22	2.20	0.41
1:2F:4:ILE:HG21	2:3F:26:ASN:HD21	1.84	0.41
2:3E:406:LEU:HD23	2:3E:406:LEU:HA	1.89	0.41
1:2I:100:ASP:OD1	1:2I:100:ASP:N	2.45	0.41
1:2J:27:THR:O	1:2J:254:ARG:NH2	2.53	0.41
2:3A:251:LEU:HD12	2:3A:251:LEU:HA	1.87	0.41
3:4A:101:LEU:O	3:4A:105:ILE:HG13	2.20	0.41
3:4A:194:ASN:OD1	3:4A:195:THR:N	2.50	0.41
3:4E:188:LYS:HG2	3:4E:234:SER:O	2.20	0.41
2:3D:403:LEU:HD13	2:3D:421:TYR:HB2	2.02	0.41
2:3E:375:ILE:O	2:3E:379:MET:HG2	2.21	0.41
1:2K:62:GLN:OE1	1:2K:62:GLN:N	2.47	0.41
3:4B:349:ASP:C	3:4B:351:SER:H	2.28	0.41
3:4F:30:ILE:HG22	3:4F:80:LEU:HD11	2.03	0.41
1:2B:140:ASP:OD1	1:2B:142:THR:HG22	2.20	0.41
2:3D:50:VAL:HG11	2:3D:56:PHE:HB2	2.02	0.41
1:2J:230:LYS:HA	1:2J:230:LYS:HD2	1.88	0.41
1:2K:138:LYS:NZ	1:2K:142:THR:OG1	2.50	0.41
1:2L:62:GLN:OE1	1:2L:62:GLN:N	2.47	0.41
1:2B:67:ASN:HB3	1:2B:70:ASP:OD2	2.21	0.41
1:2F:169:ASP:OD1	1:2F:169:ASP:N	2.35	0.41
2:3D:19:ASN:HD22	2:3D:19:ASN:C	2.28	0.41
2:3D:395:VAL:HG21	2:3D:441:MET:HE1	2.03	0.41
2:3F:432:SER:N	2:3F:435:ASP:OD2	2.51	0.41
3:4A:239:TYR:CE1	3:4A:257:ARG:HD2	2.50	0.41
3:4B:188:LYS:HG2	3:4B:234:SER:O	2.20	0.41
3:4C:188:LYS:HG2	3:4C:234:SER:O	2.19	0.41
1:2C:71:ILE:H	1:2C:71:ILE:HG12	1.69	0.41
1:2E:332:LYS:HB3	1:2E:332:LYS:HE3	1.74	0.41
2:3F:33:ILE:HG12	2:3F:139:LEU:HD23	2.02	0.41
2:3F:403:LEU:HD13	2:3F:421:TYR:HB2	2.02	0.41
1:2G:92:LEU:HD23	1:2G:92:LEU:HA	1.85	0.41
1:2H:74:ARG:HD3	1:2H:164:TRP:CE2	2.55	0.41
1:2H:100:ASP:OD2	1:2H:100:ASP:N	2.46	0.41
1:2A:338:VAL:HG11	3:4A:307:PRO:HB3	2.03	0.41
3:4A:188:LYS:HG2	3:4A:234:SER:O	2.21	0.41
1:2B:168:ILE:HD13	1:2B:168:ILE:HA	1.90	0.41
1:2B:294:LEU:HD23	1:2B:294:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3E:229:GLU:CD	2:3E:229:GLU:H	2.27	0.41
1:2I:218:GLN:H	1:2I:218:GLN:HG2	1.78	0.41
1:2J:107:ALA:HA	1:2J:112:ILE:HD13	2.02	0.41
2:3A:19:ASN:H	2:3A:19:ASN:HD22	1.68	0.41
2:3A:150:LEU:HG	2:3A:182:SER:OG	2.21	0.41
2:3A:207:THR:HG22	2:3A:209:VAL:H	1.86	0.41
3:4F:207:VAL:O	3:4F:211:ILE:HG13	2.21	0.41
2:3D:130:GLN:HE21	2:3D:130:GLN:HB2	1.60	0.41
2:3D:207:THR:HG22	2:3D:209:VAL:H	1.86	0.41
2:3E:426:GLY:O	2:3E:431:MET:HE3	2.21	0.41
1:2H:101:ASP:OD2	1:2H:101:ASP:N	2.44	0.41
1:2I:280:TRP:CD1	1:2I:329:MET:HE2	2.56	0.41
1:2J:101:ASP:OD1	1:2J:101:ASP:N	2.45	0.41
2:3A:253:GLN:O	2:3A:256:GLU:HG3	2.21	0.41
3:4D:133:ASP:O	3:4D:137:GLN:HG3	2.21	0.41
1:2D:67:ASN:HB3	1:2D:70:ASP:OD2	2.21	0.41
1:2E:319:MET:SD	1:2E:329:MET:HA	2.61	0.41
1:2F:33:ALA:HB1	1:2F:89:THR:HG22	2.02	0.41
2:3B:426:GLY:O	2:3B:431:MET:HE3	2.21	0.41
2:3E:325:GLU:O	2:3E:329:MET:HG3	2.21	0.41
2:3F:150:LEU:HG	2:3F:182:SER:OG	2.21	0.41
1:2I:58:LEU:HD13	1:2I:58:LEU:HA	1.95	0.41
1:2I:137:LEU:HA	1:2I:137:LEU:HD12	1.78	0.41
3:4B:247:ASN:H	3:4B:252:SER:HB3	1.86	0.41
3:4D:101:LEU:O	3:4D:105:ILE:HG13	2.20	0.41
2:3C:20:LEU:HD23	2:3C:20:LEU:HA	1.94	0.41
1:2K:242:GLU:HG2	1:2K:244:ASN:OD1	2.20	0.41
3:4A:221:TRP:HB3	3:4A:288:LEU:HD13	2.02	0.40
3:4D:188:LYS:HG2	3:4D:234:SER:O	2.21	0.40
1:2B:7:TYR:HB3	1:2C:214:ALA:HB2	2.03	0.40
1:2D:69:LEU:HD12	1:2D:73:LEU:HD23	2.03	0.40
2:3B:150:LEU:HG	2:3B:182:SER:OG	2.20	0.40
2:3D:253:GLN:O	2:3D:256:GLU:HG3	2.21	0.40
1:2G:20:LEU:HD12	1:2G:20:LEU:HA	1.81	0.40
1:2A:169:ASP:OD1	1:2A:169:ASP:N	2.35	0.40
2:3A:200:ASP:OD1	2:3A:201:LYS:N	2.54	0.40
2:3A:368:PHE:O	2:3A:372:GLU:HG3	2.20	0.40
3:4C:303:PHE:O	1:2C:344:ILE:HD11	2.21	0.40
1:2B:124:LYS:HA	1:2B:124:LYS:HD2	1.88	0.40
1:2B:274:PRO:HB3	2:3B:450:VAL:HG11	2.02	0.40
1:2C:211:ASP:OD1	1:2C:211:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2D:318:THR:HG22	1:2D:332:LYS:HD3	2.03	0.40
1:2E:7:TYR:HB3	1:2F:214:ALA:HB2	2.02	0.40
2:3B:130:GLN:HE21	2:3B:130:GLN:HB2	1.70	0.40
2:3B:375:ILE:O	2:3B:379:MET:HG2	2.21	0.40
2:3D:251:LEU:HD12	2:3D:251:LEU:HA	1.87	0.40
2:3E:8:PRO:HG2	2:3F:348:TRP:CD1	2.56	0.40
1:2A:71:ILE:H	1:2A:71:ILE:HG12	1.72	0.40
1:2A:140:ASP:OD1	1:2A:142:THR:HG23	2.22	0.40
3:4F:360:GLY:O	1:2F:342:GLU:N	2.55	0.40
1:2C:4:ILE:HG21	2:3C:26:ASN:HD21	1.86	0.40
1:2D:4:ILE:HD13	1:2D:4:ILE:HA	1.89	0.40
1:2D:211:ASP:OD1	1:2D:211:ASP:C	2.64	0.40
2:3B:406:LEU:HD23	2:3B:406:LEU:HA	1.89	0.40
2:3F:279:ASN:OD1	2:3F:279:ASN:N	2.54	0.40
3:4A:304:VAL:HG12	3:4A:305:PHE:CD2	2.57	0.40
3:4C:304:VAL:HG12	3:4C:305:PHE:CD2	2.57	0.40
3:4D:105:ILE:HG13	3:4D:105:ILE:H	1.67	0.40
1:2E:20:LEU:HD12	1:2E:20:LEU:HA	1.89	0.40
2:3C:254:LEU:HD11	2:3C:261:VAL:HG23	2.04	0.40
2:3D:229:GLU:H	2:3D:229:GLU:CD	2.27	0.40
2:3E:263:GLN:O	2:3E:267:GLN:HG2	2.21	0.40
1:2K:74:ARG:HD3	1:2K:164:TRP:CE2	2.56	0.40
2:3A:403:LEU:HD13	2:3A:421:TYR:HB2	2.03	0.40
3:4F:127:ILE:HG23	3:4F:164:LEU:HB2	2.03	0.40
3:4F:236:VAL:HG13	3:4F:237:ARG:HG3	2.03	0.40
1:2B:137:LEU:HD22	1:2B:157:TYR:CE1	2.57	0.40
1:2C:67:ASN:HB3	1:2C:70:ASP:OD2	2.21	0.40
1:2C:69:LEU:HD12	1:2C:73:LEU:HD23	2.03	0.40
1:2C:303:ASN:OD1	1:2C:303:ASN:N	2.54	0.40
1:2D:36:GLY:HA2	1:2D:88:GLN:NE2	2.35	0.40
1:2E:67:ASN:HB3	1:2E:70:ASP:OD2	2.21	0.40
1:2F:69:LEU:HD12	1:2F:73:LEU:HD23	2.03	0.40
2:3E:254:LEU:HD11	2:3E:261:VAL:HG23	2.03	0.40
1:2H:304:LYS:NZ	1:2H:304:LYS:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2A	346/354 (98%)	339 (98%)	7 (2%)	0	100	100
1	2B	346/354 (98%)	338 (98%)	8 (2%)	0	100	100
1	2C	346/354 (98%)	337 (97%)	9 (3%)	0	100	100
1	2D	346/354 (98%)	339 (98%)	7 (2%)	0	100	100
1	2E	346/354 (98%)	338 (98%)	8 (2%)	0	100	100
1	2F	346/354 (98%)	337 (97%)	9 (3%)	0	100	100
1	2G	346/354 (98%)	341 (99%)	5 (1%)	0	100	100
1	2H	346/354 (98%)	338 (98%)	8 (2%)	0	100	100
1	2I	346/354 (98%)	340 (98%)	6 (2%)	0	100	100
1	2J	346/354 (98%)	339 (98%)	7 (2%)	0	100	100
1	2K	346/354 (98%)	339 (98%)	7 (2%)	0	100	100
1	2L	346/354 (98%)	340 (98%)	6 (2%)	0	100	100
2	3A	387/466 (83%)	378 (98%)	9 (2%)	0	100	100
2	3B	387/466 (83%)	380 (98%)	7 (2%)	0	100	100
2	3C	387/466 (83%)	379 (98%)	8 (2%)	0	100	100
2	3D	387/466 (83%)	377 (97%)	10 (3%)	0	100	100
2	3E	387/466 (83%)	380 (98%)	7 (2%)	0	100	100
2	3F	387/466 (83%)	380 (98%)	7 (2%)	0	100	100
3	4A	348/392 (89%)	338 (97%)	10 (3%)	0	100	100
3	4B	348/392 (89%)	339 (97%)	9 (3%)	0	100	100
3	4C	348/392 (89%)	339 (97%)	9 (3%)	0	100	100
3	4D	348/392 (89%)	338 (97%)	10 (3%)	0	100	100
3	4E	348/392 (89%)	338 (97%)	10 (3%)	0	100	100
3	4F	348/392 (89%)	339 (97%)	9 (3%)	0	100	100
All	All	8562/9396 (91%)	8370 (98%)	192 (2%)	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	2A	293/298 (98%)	284 (97%)	9 (3%)	35	63
1	2B	293/298 (98%)	286 (98%)	7 (2%)	44	70
1	2C	293/298 (98%)	285 (97%)	8 (3%)	40	67
1	2D	293/298 (98%)	285 (97%)	8 (3%)	40	67
1	2E	293/298 (98%)	286 (98%)	7 (2%)	44	70
1	2F	293/298 (98%)	284 (97%)	9 (3%)	35	63
1	2G	293/298 (98%)	290 (99%)	3 (1%)	73	86
1	2H	293/298 (98%)	287 (98%)	6 (2%)	50	74
1	2I	293/298 (98%)	290 (99%)	3 (1%)	73	86
1	2J	293/298 (98%)	289 (99%)	4 (1%)	62	81
1	2K	293/298 (98%)	288 (98%)	5 (2%)	56	78
1	2L	293/298 (98%)	289 (99%)	4 (1%)	62	81
2	3A	334/395 (85%)	319 (96%)	15 (4%)	23	53
2	3B	334/395 (85%)	325 (97%)	9 (3%)	40	67
2	3C	334/395 (85%)	329 (98%)	5 (2%)	60	80
2	3D	334/395 (85%)	322 (96%)	12 (4%)	30	60
2	3E	334/395 (85%)	326 (98%)	8 (2%)	44	70
2	3F	334/395 (85%)	329 (98%)	5 (2%)	60	80
3	4A	297/337 (88%)	293 (99%)	4 (1%)	65	82
3	4B	297/337 (88%)	293 (99%)	4 (1%)	65	82
3	4C	297/337 (88%)	293 (99%)	4 (1%)	65	82
3	4D	297/337 (88%)	293 (99%)	4 (1%)	65	82
3	4E	297/337 (88%)	294 (99%)	3 (1%)	73	86
3	4F	297/337 (88%)	292 (98%)	5 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7302/7968 (92%)	7151 (98%)	151 (2%)	49 72

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2A	58	LEU
1	2A	112	ILE
1	2A	169	ASP
1	2A	218	GLN
1	2A	220	LYS
1	2A	242	GLU
1	2A	258	SER
1	2A	303	ASN
1	2A	306	ASP
2	3A	19	ASN
2	3A	47	VAL
2	3A	59	LEU
2	3A	126	LYS
2	3A	150	LEU
2	3A	171	TRP
2	3A	182	SER
2	3A	206	ILE
2	3A	299	SER
2	3A	314	ILE
2	3A	329	MET
2	3A	385	GLU
2	3A	400	ASP
2	3A	425	ILE
2	3A	462	GLN
3	4A	78	LEU
3	4A	147	LYS
3	4A	256	VAL
3	4A	276	HIS
3	4B	78	LEU
3	4B	110	ASP
3	4B	256	VAL
3	4B	276	HIS
3	4C	78	LEU
3	4C	156	LEU
3	4C	256	VAL
3	4C	276	HIS
3	4D	78	LEU

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Mol	Chain	Res	Type
3	4D	84	GLN
3	4D	256	VAL
3	4D	276	HIS
3	4E	78	LEU
3	4E	256	VAL
3	4E	276	HIS
3	4F	78	LEU
3	4F	84	GLN
3	4F	156	LEU
3	4F	256	VAL
3	4F	276	HIS
1	2B	44	LYS
1	2B	58	LEU
1	2B	105	LEU
1	2B	112	ILE
1	2B	258	SER
1	2B	303	ASN
1	2B	306	ASP
1	2C	58	LEU
1	2C	112	ILE
1	2C	169	ASP
1	2C	218	GLN
1	2C	220	LYS
1	2C	258	SER
1	2C	303	ASN
1	2C	306	ASP
1	2D	58	LEU
1	2D	112	ILE
1	2D	169	ASP
1	2D	218	GLN
1	2D	220	LYS
1	2D	258	SER
1	2D	306	ASP
1	2D	335	MET
1	2E	44	LYS
1	2E	58	LEU
1	2E	105	LEU
1	2E	112	ILE
1	2E	258	SER
1	2E	303	ASN
1	2E	306	ASP
1	2F	58	LEU

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Mol	Chain	Res	Type
1	2F	112	ILE
1	2F	169	ASP
1	2F	191	LYS
1	2F	220	LYS
1	2F	258	SER
1	2F	303	ASN
1	2F	306	ASP
1	2F	319	MET
2	3B	59	LEU
2	3B	150	LEU
2	3B	182	SER
2	3B	201	LYS
2	3B	206	ILE
2	3B	254	LEU
2	3B	299	SER
2	3B	314	ILE
2	3B	385	GLU
2	3C	150	LEU
2	3C	162	GLU
2	3C	299	SER
2	3C	385	GLU
2	3C	393	GLU
2	3D	19	ASN
2	3D	47	VAL
2	3D	59	LEU
2	3D	150	LEU
2	3D	171	TRP
2	3D	182	SER
2	3D	206	ILE
2	3D	299	SER
2	3D	314	ILE
2	3D	329	MET
2	3D	400	ASP
2	3D	425	ILE
2	3E	18	LEU
2	3E	59	LEU
2	3E	150	LEU
2	3E	162	GLU
2	3E	182	SER
2	3E	206	ILE
2	3E	254	LEU
2	3E	299	SER

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Mol	Chain	Res	Type
2	3F	19	ASN
2	3F	150	LEU
2	3F	279	ASN
2	3F	299	SER
2	3F	385	GLU
1	2G	31	VAL
1	2G	73	LEU
1	2G	169	ASP
1	2H	31	VAL
1	2H	49	ILE
1	2H	58	LEU
1	2H	218	GLN
1	2H	231	SER
1	2H	258	SER
1	2I	258	SER
1	2I	294	LEU
1	2I	338	VAL
1	2J	31	VAL
1	2J	58	LEU
1	2J	105	LEU
1	2J	169	ASP
1	2K	31	VAL
1	2K	58	LEU
1	2K	218	GLN
1	2K	231	SER
1	2K	258	SER
1	2L	58	LEU
1	2L	258	SER
1	2L	294	LEU
1	2L	338	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	2A	144	ASN
2	3A	23	ASN
2	3A	199	GLN
3	4A	73	GLN
3	4A	84	GLN
3	4A	140	GLN
3	4A	196	GLN
3	4A	214	ASN

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Mol	Chain	Res	Type
3	4B	73	GLN
3	4C	73	GLN
3	4C	196	GLN
3	4D	73	GLN
3	4D	140	GLN
3	4E	73	GLN
3	4F	73	GLN
1	2D	88	GLN
1	2D	144	ASN
1	2D	246	ASN
1	2F	296	GLN
2	3B	23	ASN
2	3B	199	GLN
2	3B	330	ASN
2	3B	408	GLN
2	3B	409	GLN
2	3C	19	ASN
2	3C	23	ASN
2	3C	141	GLN
2	3C	199	GLN
2	3C	212	GLN
2	3C	330	ASN
2	3C	369	ASN
2	3C	408	GLN
2	3C	409	GLN
2	3D	23	ASN
2	3D	408	GLN
2	3D	462	GLN
2	3E	23	ASN
2	3E	199	GLN
2	3E	330	ASN
2	3E	408	GLN
2	3E	409	GLN
2	3F	23	ASN
2	3F	141	GLN
2	3F	199	GLN
2	3F	212	GLN
2	3F	330	ASN
2	3F	369	ASN
2	3F	408	GLN
2	3F	409	GLN
1	2G	195	ASN

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Mol	Chain	Res	Type
1	2G	257	ASN
1	2H	195	ASN
1	2H	213	GLN
1	2H	257	ASN
1	2I	195	ASN
1	2I	257	ASN
1	2I	277	GLN
1	2J	195	ASN
1	2J	213	GLN
1	2J	257	ASN
1	2K	195	ASN
1	2K	213	GLN
1	2K	257	ASN
1	2L	195	ASN
1	2L	257	ASN

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.

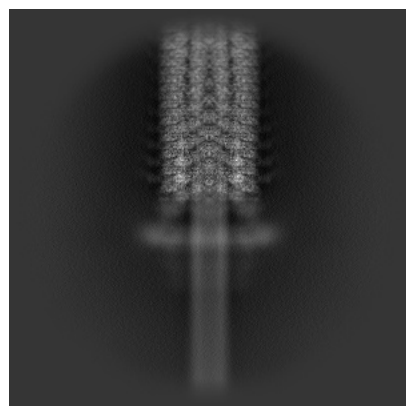
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53141. These allow visual inspection of the internal detail of the map and identification of artifacts.

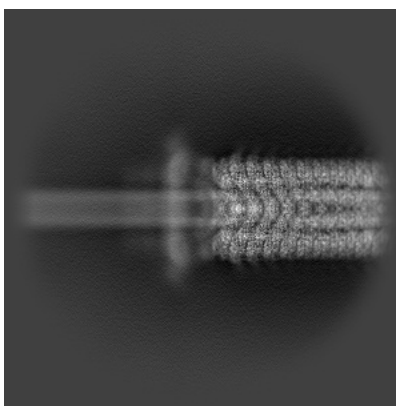
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

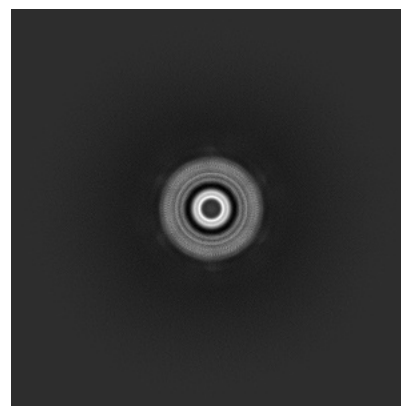
6.1.1 Primary map



X

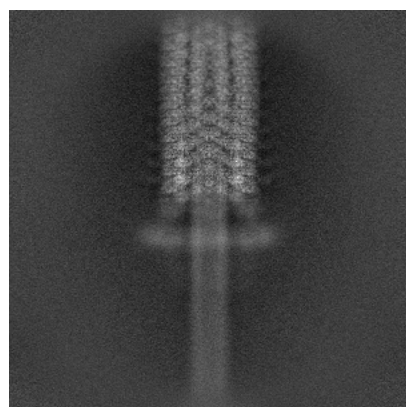


Y

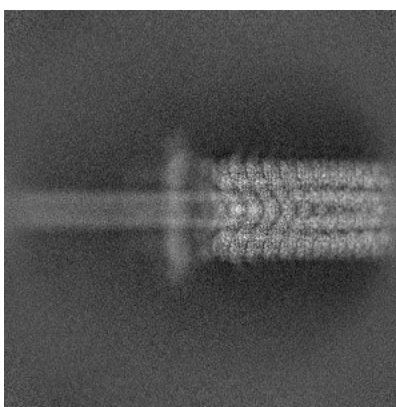


Z

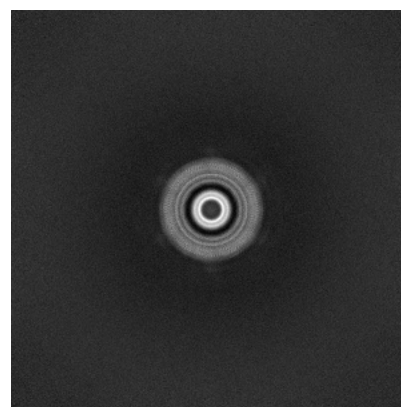
6.1.2 Raw map



X



Y

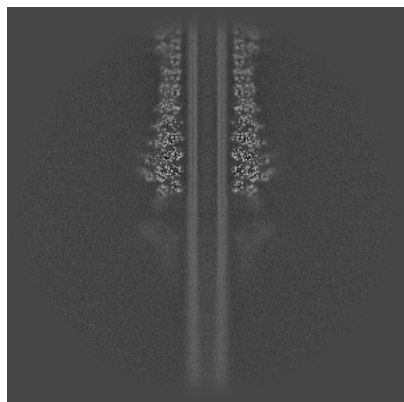


Z

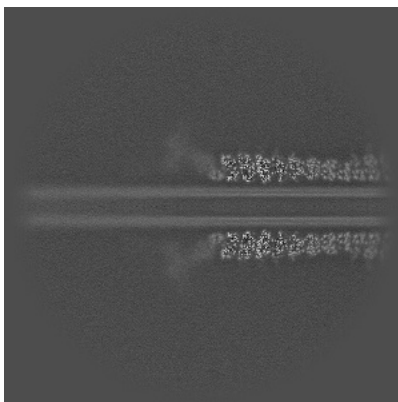
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

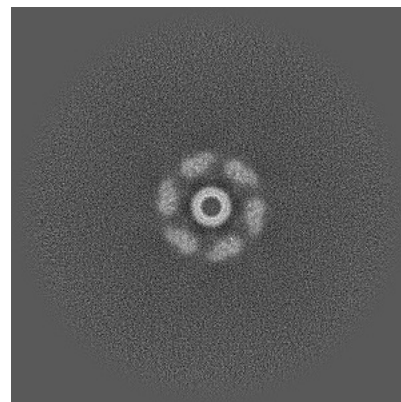
6.2.1 Primary map



X Index: 350



Y Index: 350

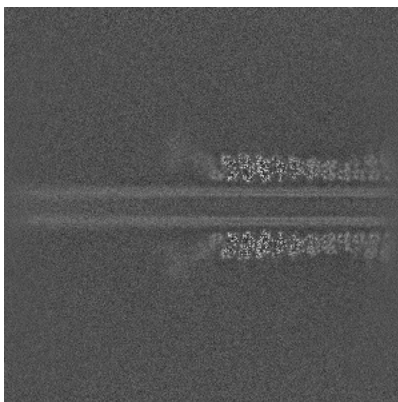


Z Index: 350

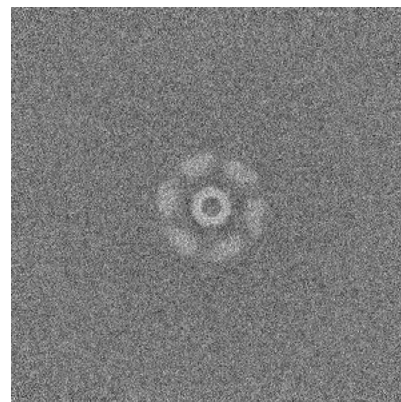
6.2.2 Raw map



X Index: 350



Y Index: 350

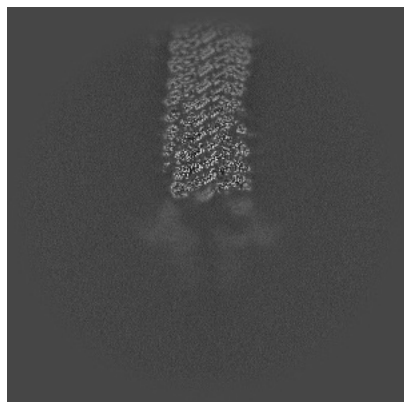


Z Index: 350

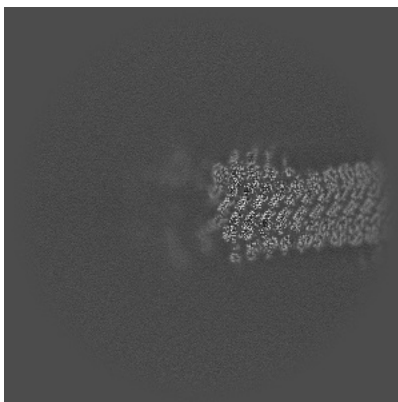
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

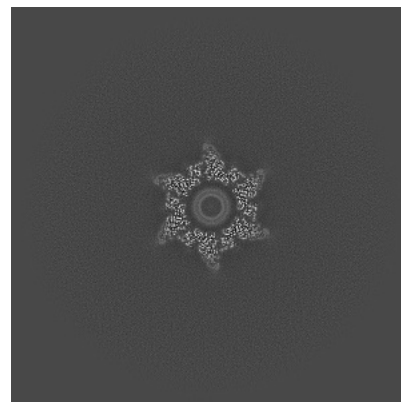
6.3.1 Primary map



X Index: 400

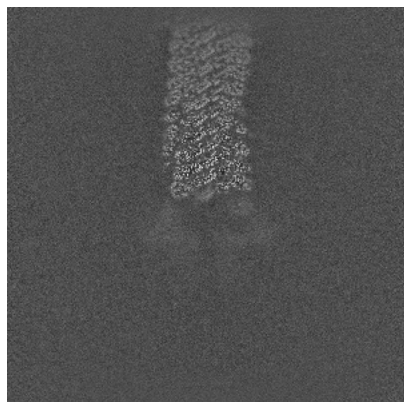


Y Index: 301

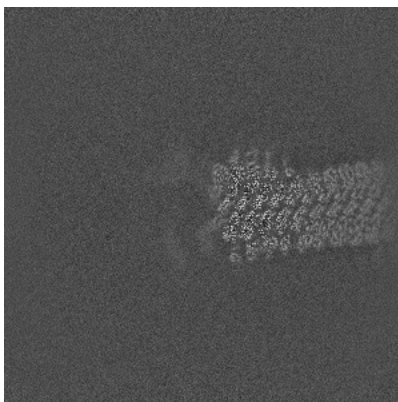


Z Index: 435

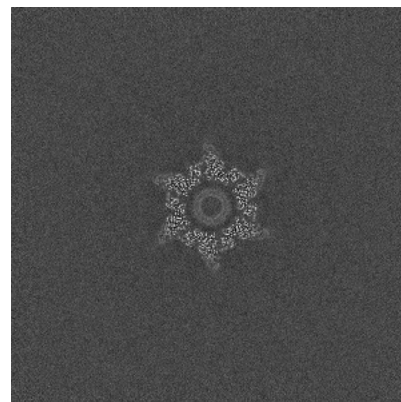
6.3.2 Raw map



X Index: 400



Y Index: 301

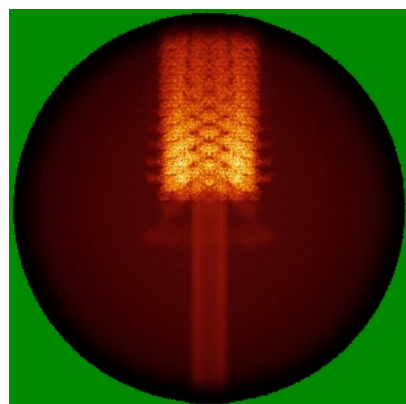


Z Index: 435

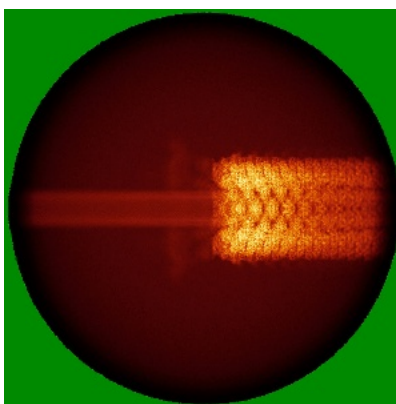
The images above show the largest variance slices of the map in three orthogonal directions.

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

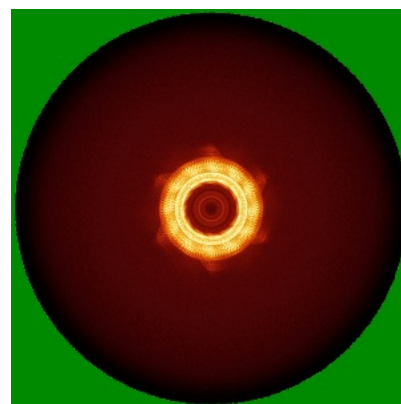
6.4.1 Primary map



X

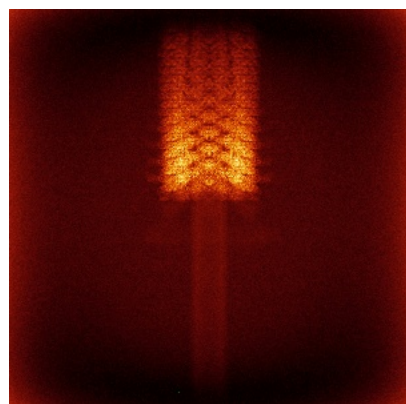


Y

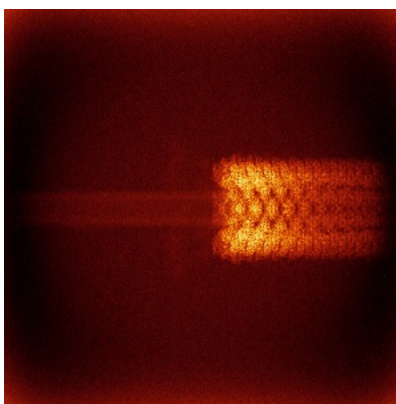


Z

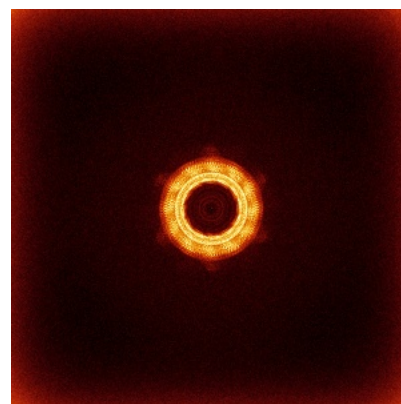
6.4.2 Raw map



X



Y

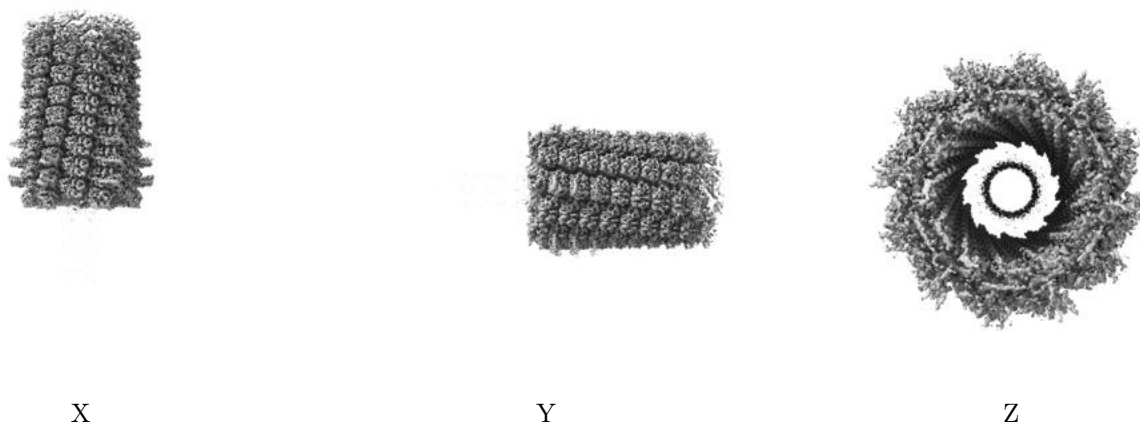


Z

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.

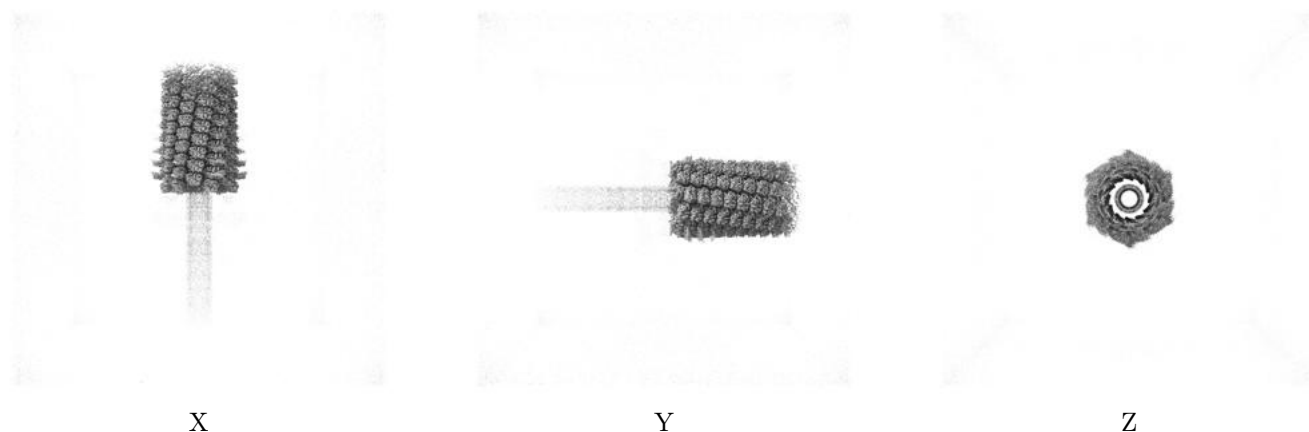
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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



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.

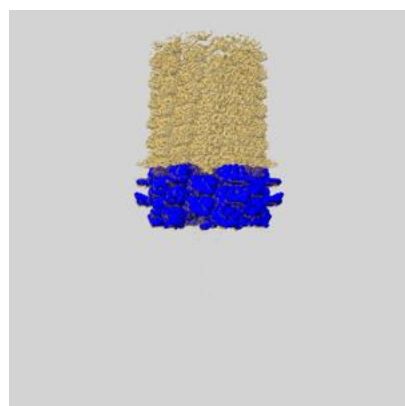
6.6 Mask visualisation [i](#)

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

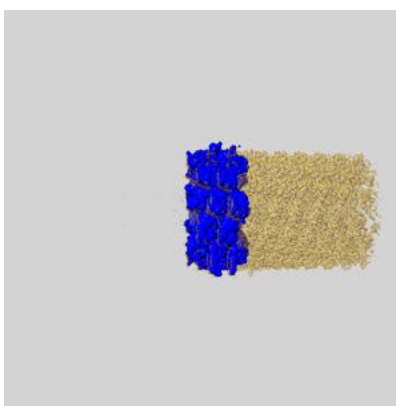
A mask typically either:

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

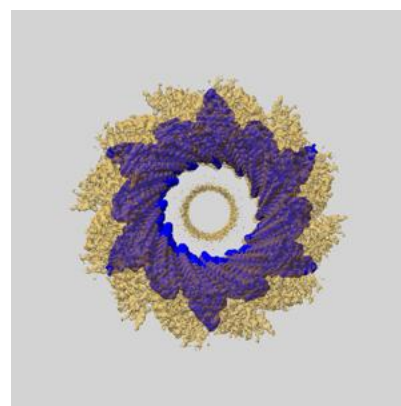
6.6.1 emd_53141_msk_1.map [i](#)



X



Y

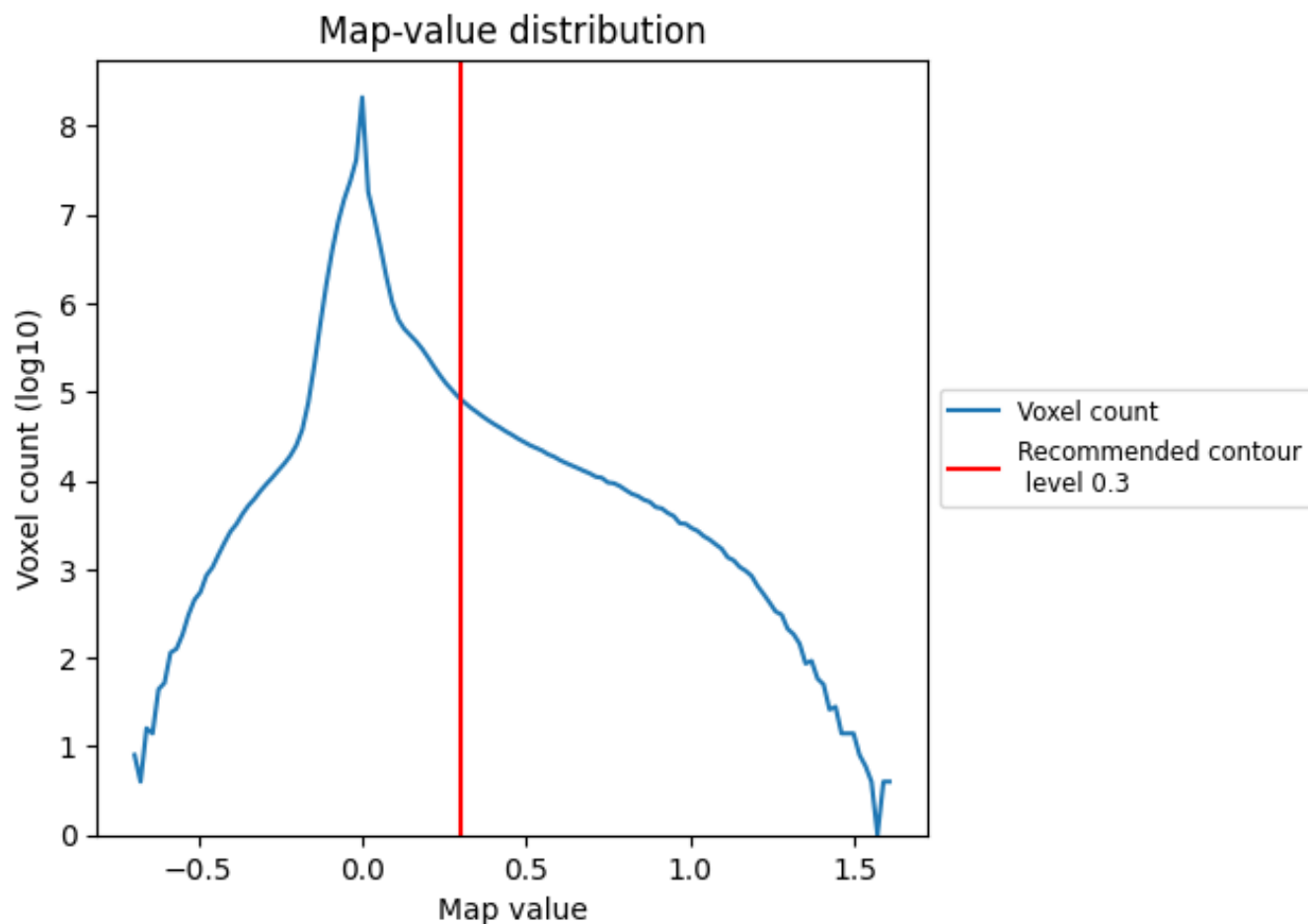


Z

7 Map analysis [i](#)

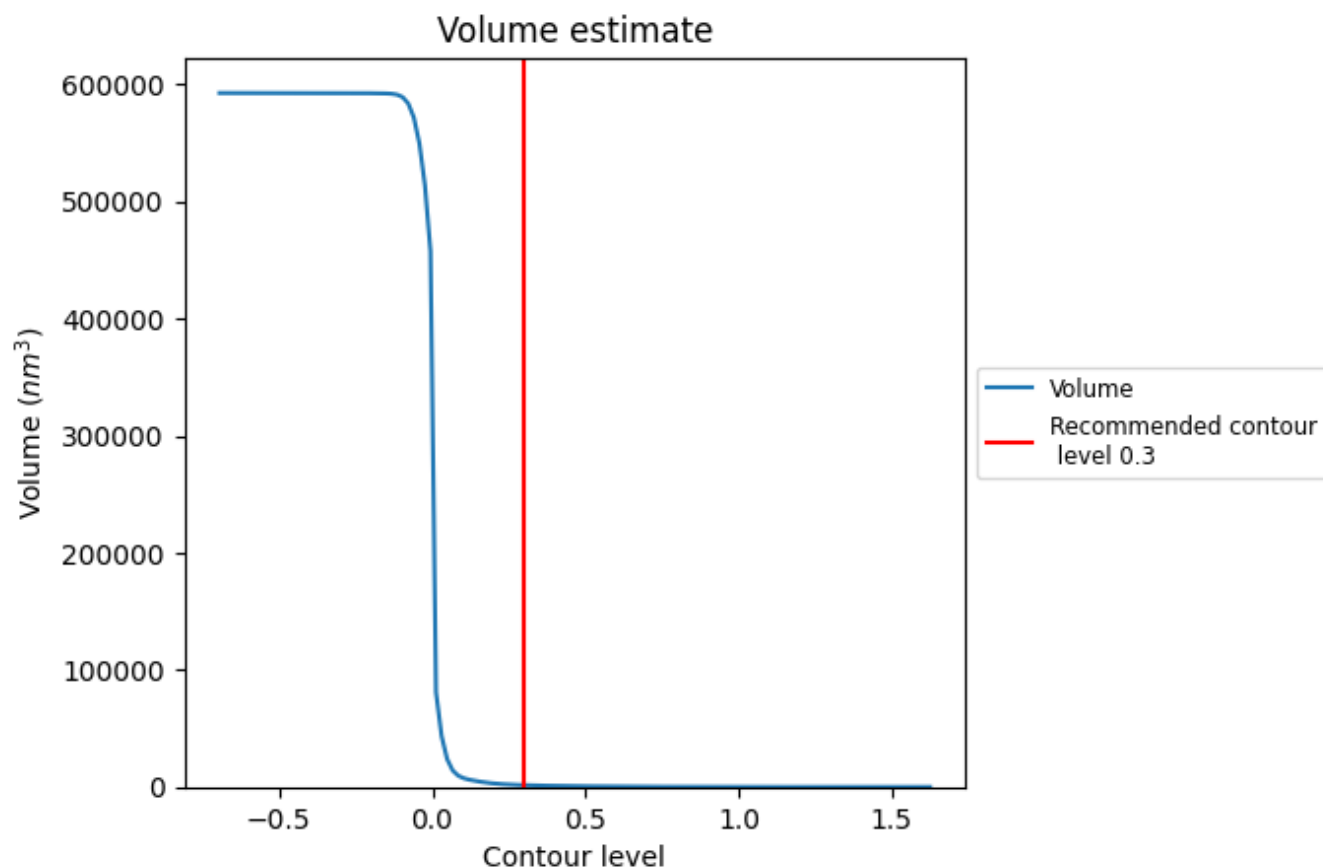
This section contains the results of statistical analysis of the map.

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.

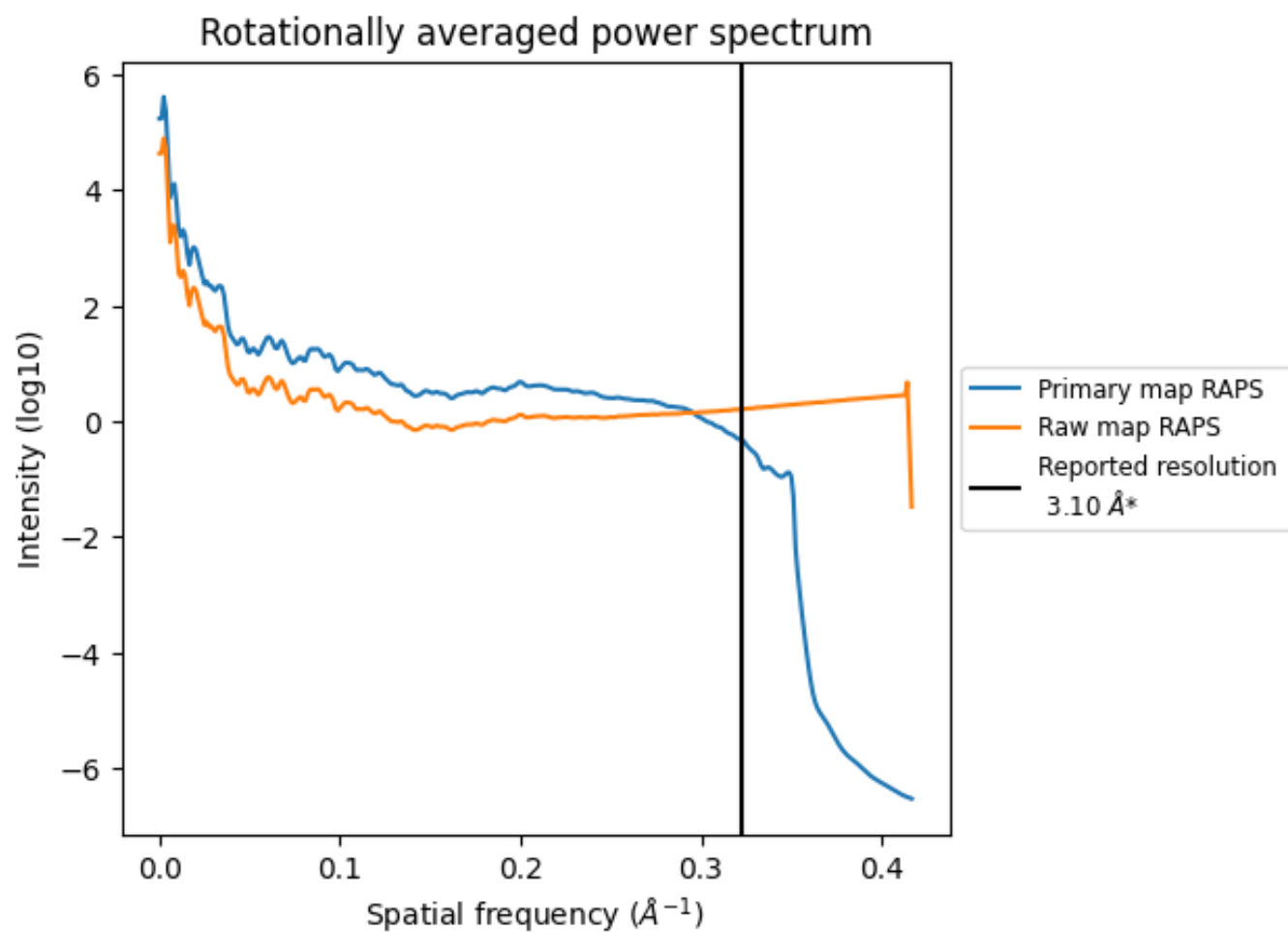
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1525 nm³; this corresponds to an approximate mass of 1378 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

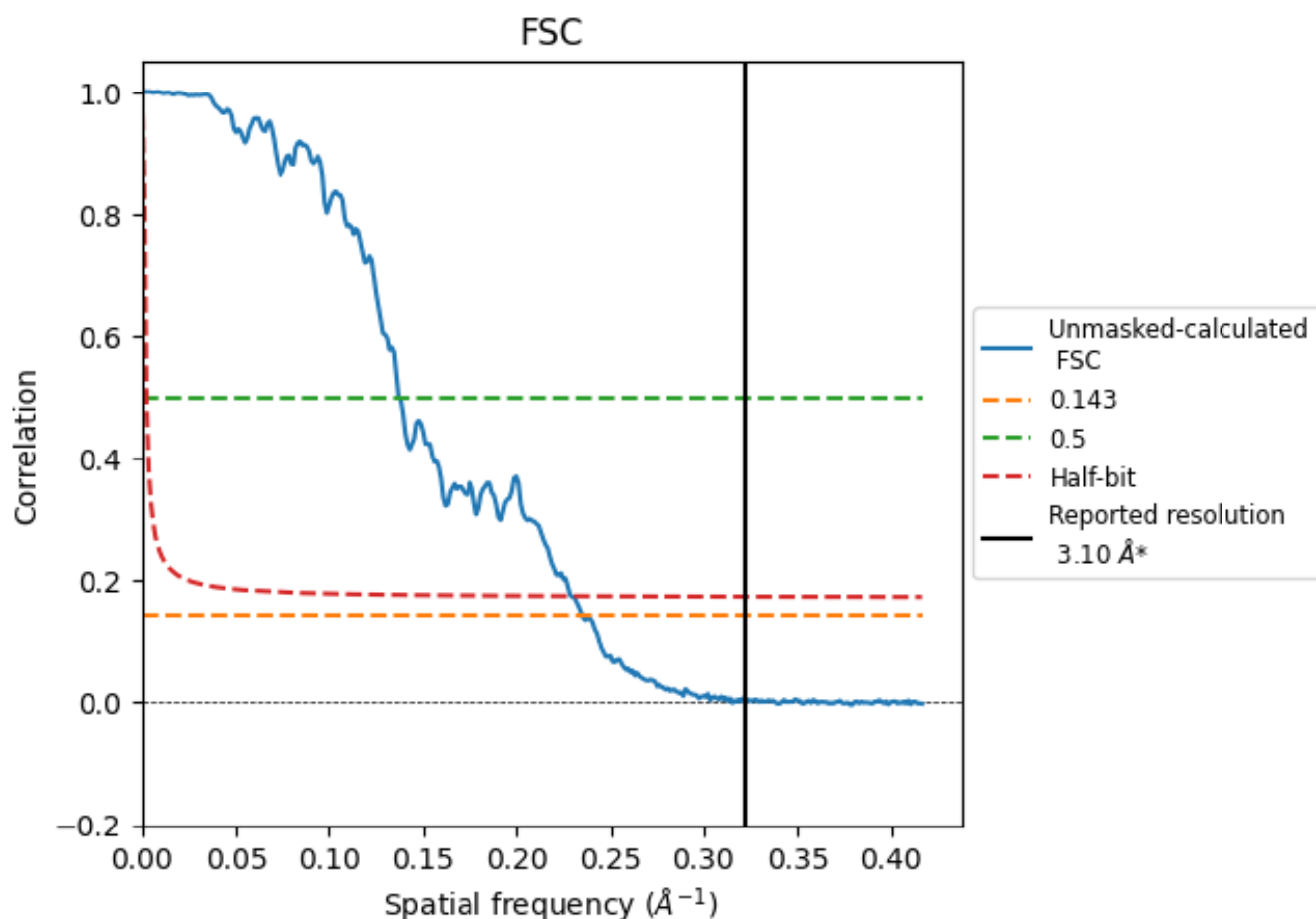


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

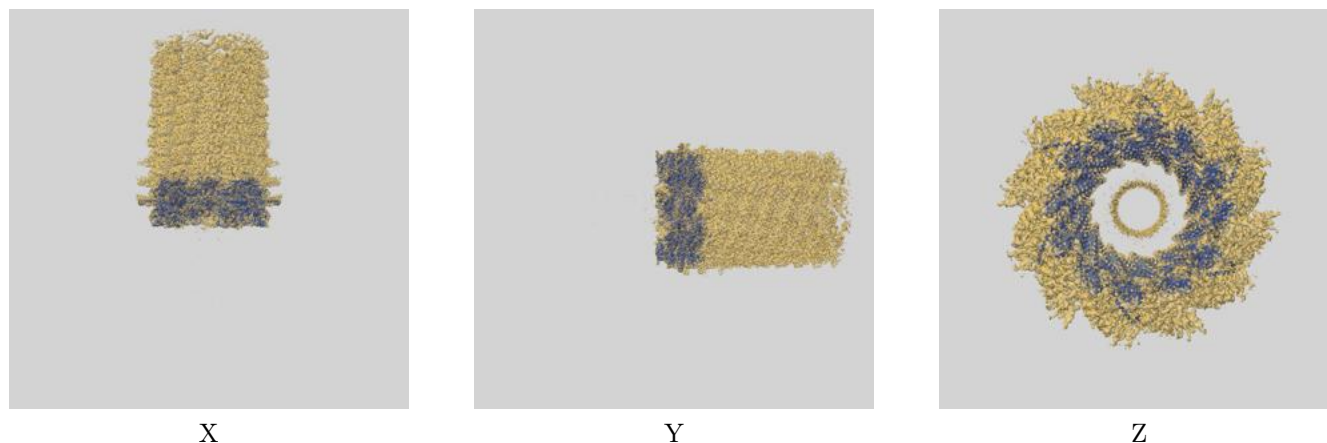
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.25	7.30	4.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.25 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

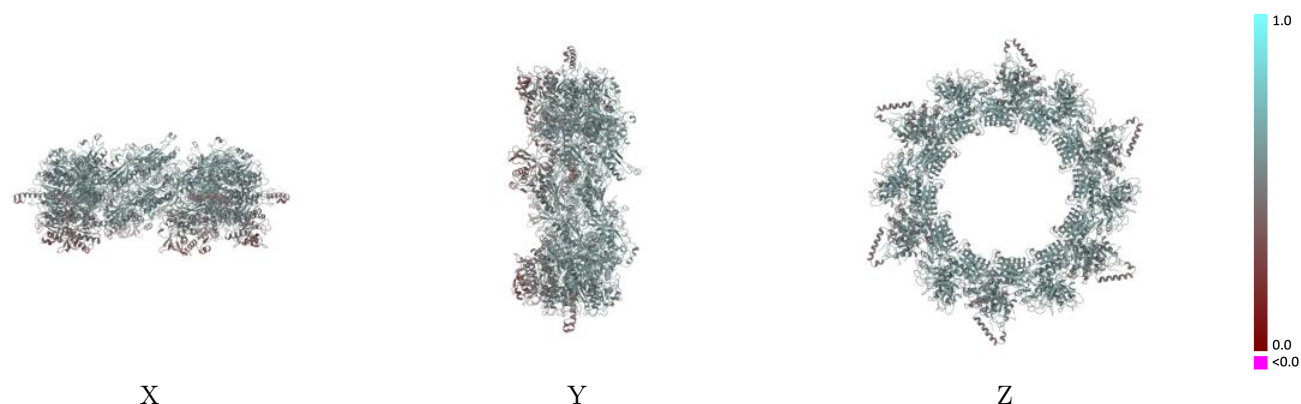
This section contains information regarding the fit between EMDB map EMD-53141 and PDB model 9QGP. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



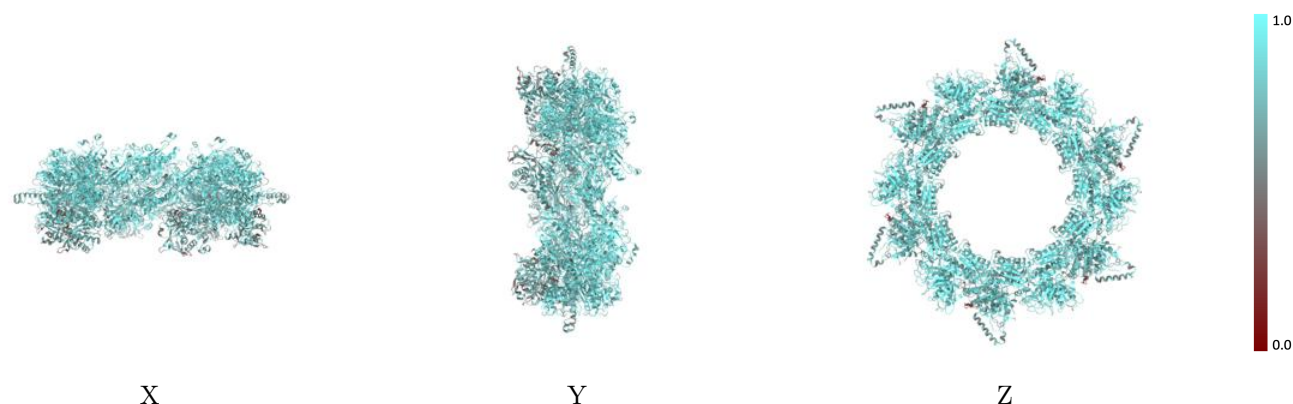
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



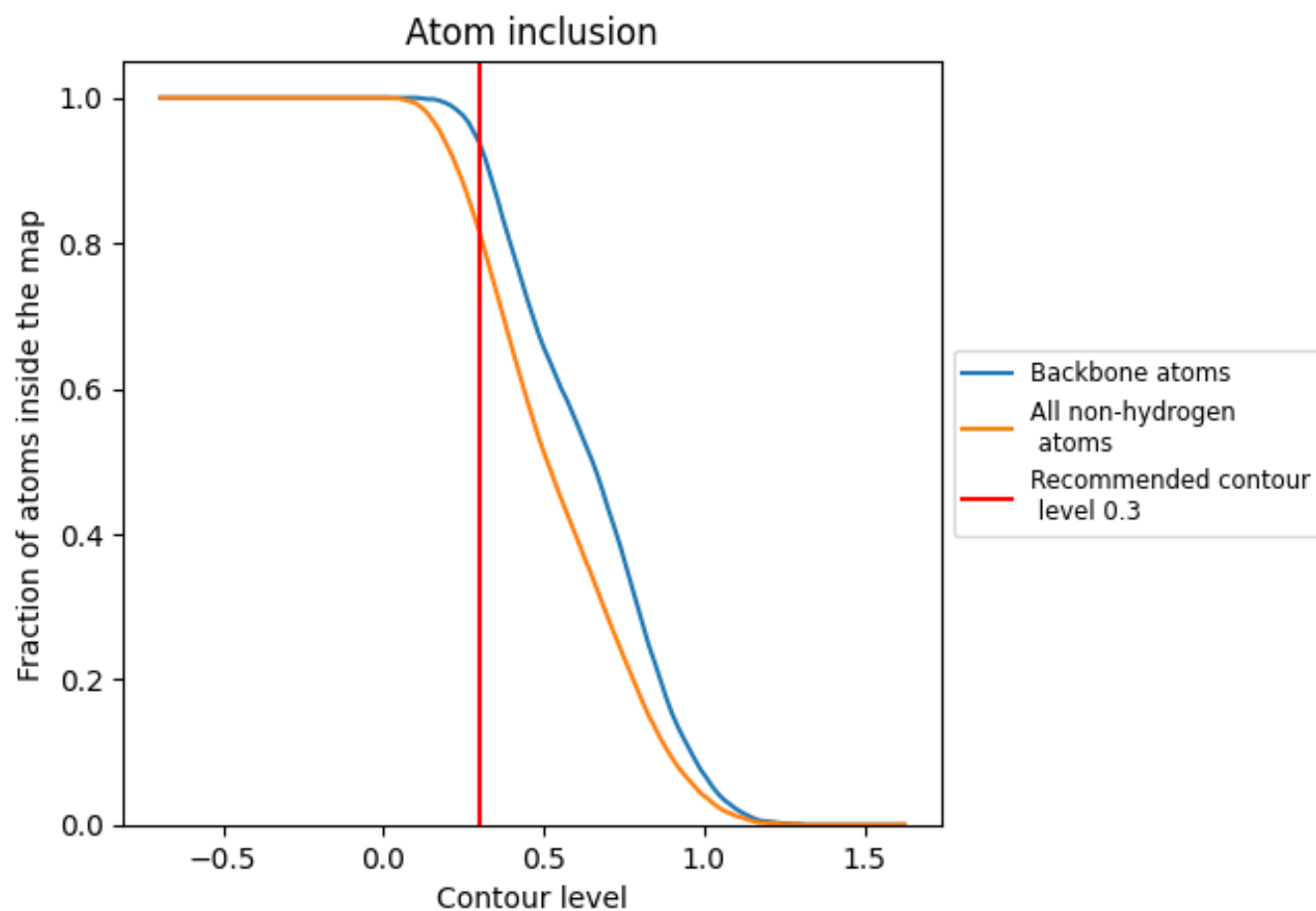
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8150	 0.5320
2A	 0.8440	 0.5440
2B	 0.8410	 0.5460
2C	 0.8430	 0.5460
2D	 0.8460	 0.5450
2E	 0.8410	 0.5460
2F	 0.8440	 0.5470
2G	 0.8800	 0.5600
2H	 0.8830	 0.5600
2I	 0.8840	 0.5600
2J	 0.8800	 0.5590
2K	 0.8840	 0.5600
2L	 0.8850	 0.5600
3A	 0.8380	 0.5510
3B	 0.8410	 0.5500
3C	 0.8380	 0.5510
3D	 0.8380	 0.5520
3E	 0.8410	 0.5500
3F	 0.8390	 0.5500
4A	 0.6920	 0.4720
4B	 0.6920	 0.4720
4C	 0.6950	 0.4730
4D	 0.6930	 0.4740
4E	 0.6920	 0.4710
4F	 0.6960	 0.4710

