



Full wwPDB EM Validation Report ⓘ

Feb 24, 2024 – 11:42 AM EST

PDB ID : 7KO5
EMDB ID : EMD-22965
Title : Structure of cardiac native thin filament at pCa=5.8 having upper and lower troponins in Ca²⁺ bound state
Authors : Galkin, V.E.; Risi, C.M.
Deposited on : 2020-11-06
Resolution : 7.80 Å (reported)
Based on initial model : 6KN8

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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

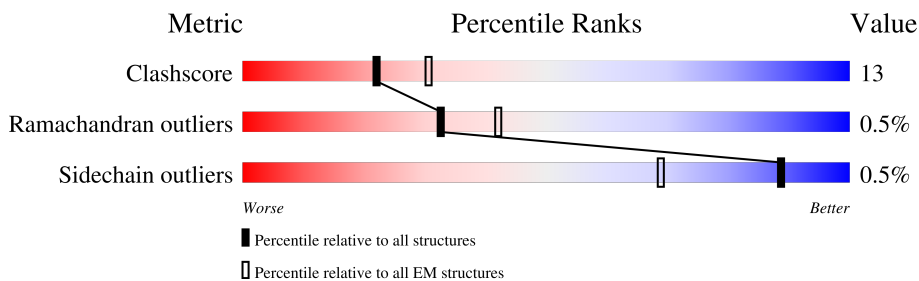
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 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.



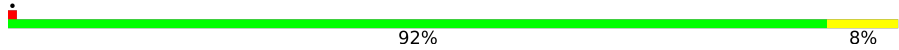
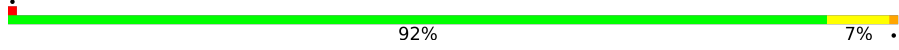
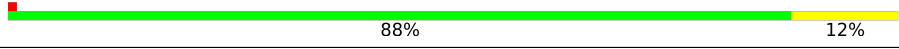
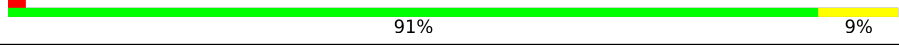
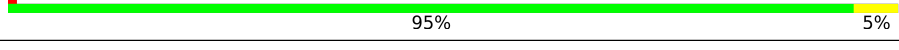
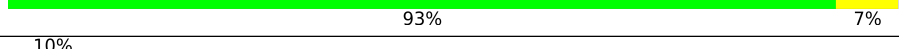
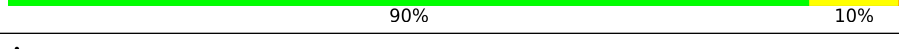
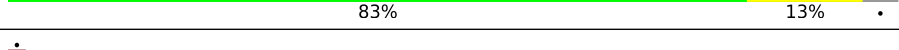
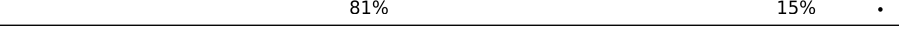
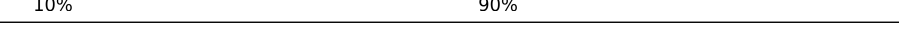

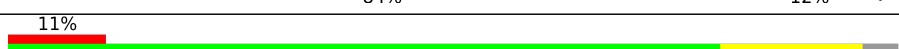


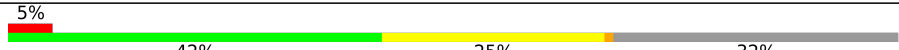

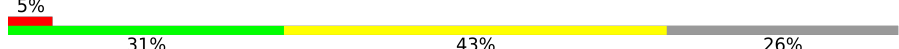


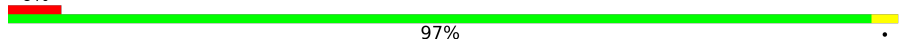

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	375	
1	B	375	
1	C	375	
1	D	375	
1	E	375	
1	F	375	
1	G	375	
1	H	375	

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Mol	Chain	Length	Quality of chain
1	I	375	 92% 8%
1	J	375	 92% 7%
1	K	375	 88% 12%
1	L	375	 91% 9%
1	M	375	 95% 5%
1	N	375	 93% 7%
1	O	375	 10% 90% 10%
2	P	286	 83% 13%
2	Q	286	 81% 15%
2	R	286	 10% 90%
2	S	286	 10% 90%
2	W	286	 7% 84% 12%
2	X	286	 11% 80% 16%
2	Y	286	 9% 90%
2	Z	286	 10% 90%
3	T	186	 5% 42% 25% 32%
3	a	186	 68% 32%
4	U	170	 5% 31% 43% 26%
4	b	170	 73% 26%
5	V	160	 8% 42% 58%
5	c	160	 6% 97%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 60511 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	375	2933	1854	493	565	21	0	0
1	B	375	2933	1854	493	565	21	0	0
1	C	375	2933	1854	493	565	21	0	0
1	D	375	2933	1854	493	565	21	0	0
1	E	375	2933	1854	493	565	21	0	0
1	F	375	2933	1854	493	565	21	0	0
1	G	375	2933	1854	493	565	21	0	0
1	H	375	2933	1854	493	565	21	0	0
1	I	375	2933	1854	493	565	21	0	0
1	J	375	2933	1854	493	565	21	0	0
1	K	375	2933	1854	493	565	21	0	0
1	L	375	2933	1854	493	565	21	0	0
1	M	375	2933	1854	493	565	21	0	0
1	N	375	2933	1854	493	565	21	0	0
1	O	375	2933	1854	493	565	21	0	0

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	Q	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	R	29	Total	C	N	O	S	0	0
			231	141	41	46	3		
2	S	29	Total	C	N	O	S	0	0
			231	141	41	46	3		
2	W	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	X	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	Y	29	Total	C	N	O	S	0	0
			231	141	41	46	3		
2	Z	29	Total	C	N	O	S	0	0
			231	141	41	46	3		

- Molecule 3 is a protein called Troponin T, cardiac muscle.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	T	126	Total	C	N	O	0	0
			1101	673	219	209		
3	a	126	Total	C	N	O	0	0
			1101	673	219	209		

- Molecule 4 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	126	Total	C	N	O	S	0	0
			1008	624	193	187	4		
4	b	126	Total	C	N	O	S	0	0
			1008	624	193	187	4		

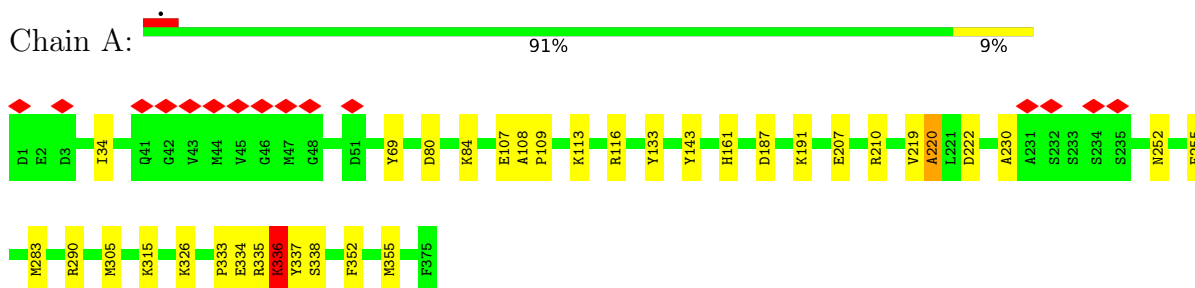
- Molecule 5 is a protein called Troponin C.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	160	Total	C	N	O	S	0	0
			1273	788	195	278	12		
5	c	160	Total	C	N	O	S	0	0
			1273	788	195	278	12		

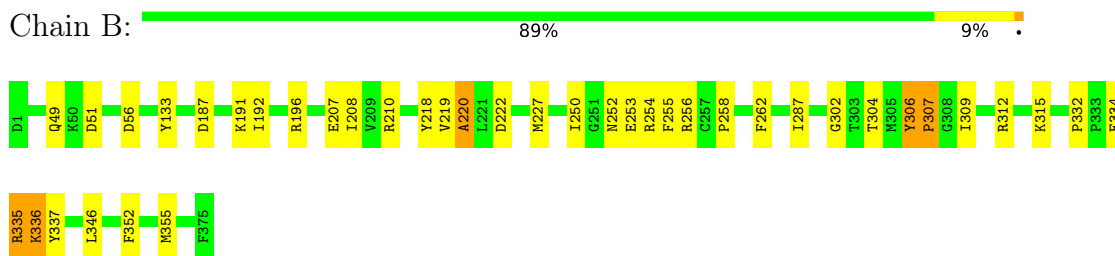
3 Residue-property plots [i](#)

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

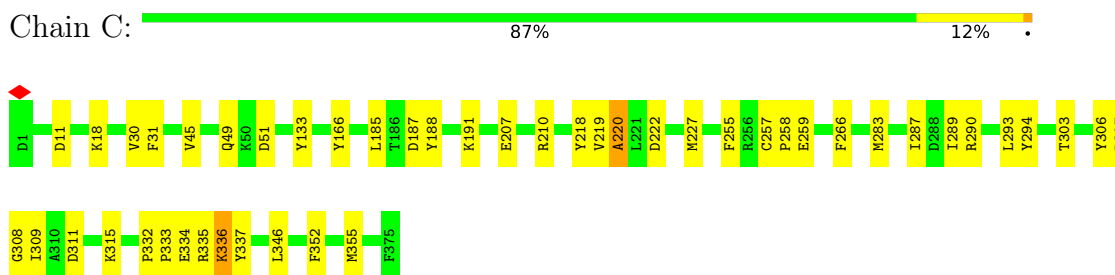
- Molecule 1: Actin, alpha skeletal muscle



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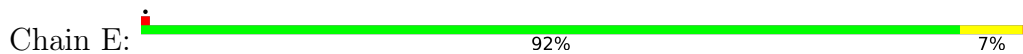


- Molecule 1: Actin, alpha skeletal muscle

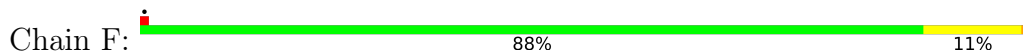




- Molecule 1: Actin, alpha skeletal muscle



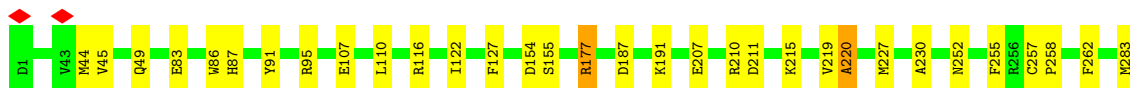
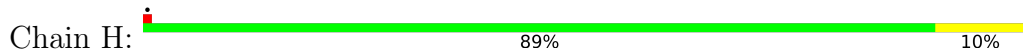
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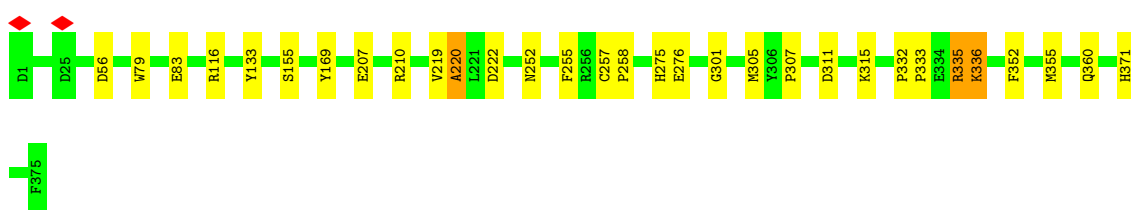
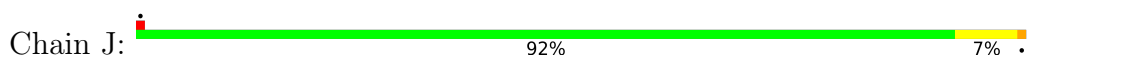
- Molecule 1: Actin, alpha skeletal muscle



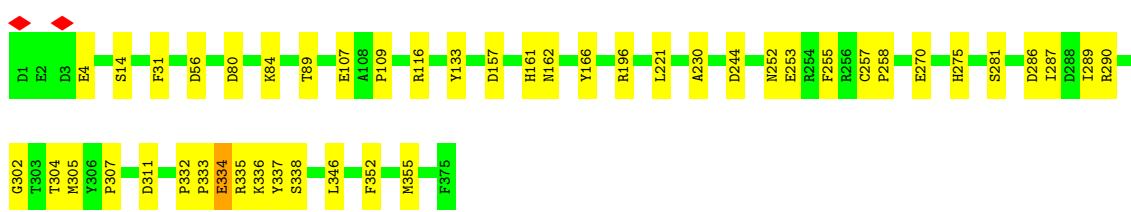
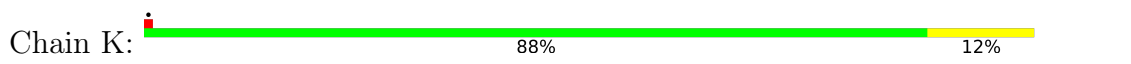
- Molecule 1: Actin, alpha skeletal muscle



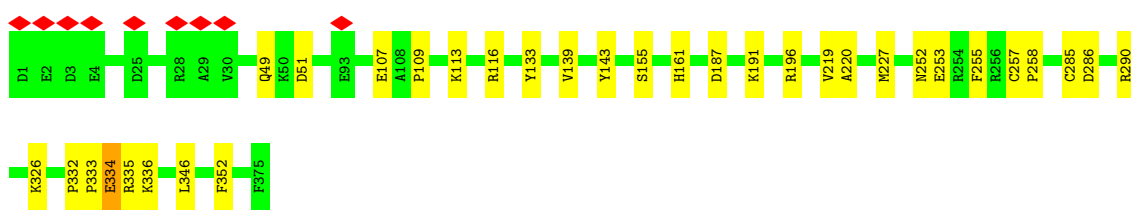
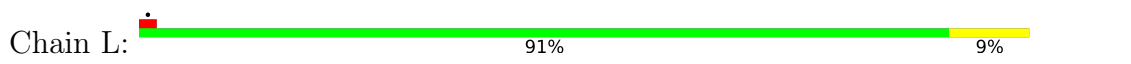
- Molecule 1: Actin, alpha skeletal muscle



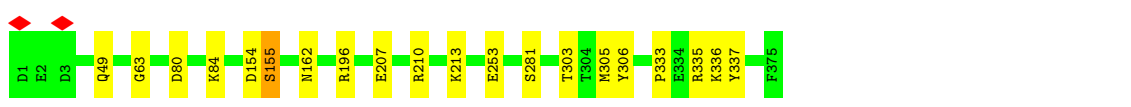
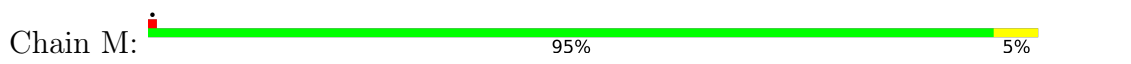
• Molecule 1: Actin, alpha skeletal muscle



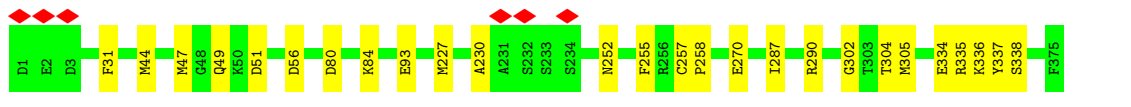
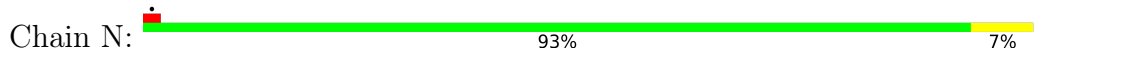
• Molecule 1: Actin, alpha skeletal muscle



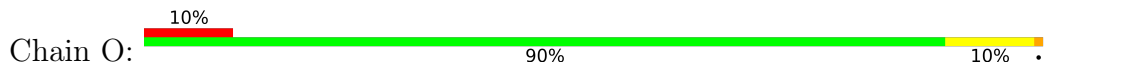
• Molecule 1: Actin, alpha skeletal muscle

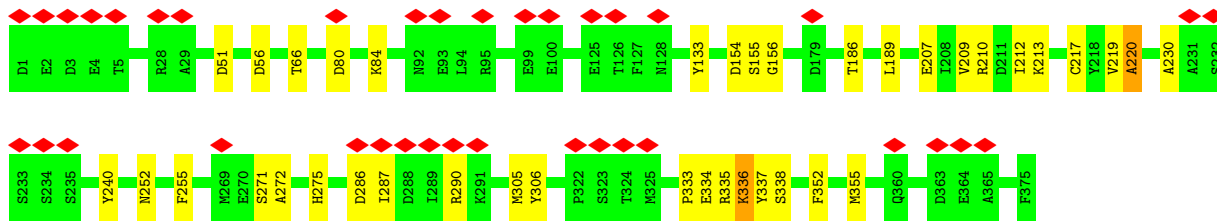


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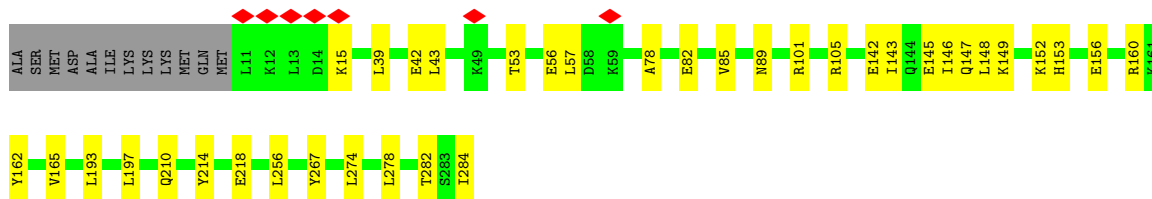
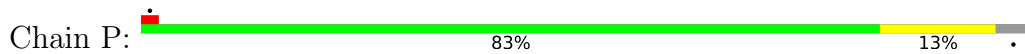


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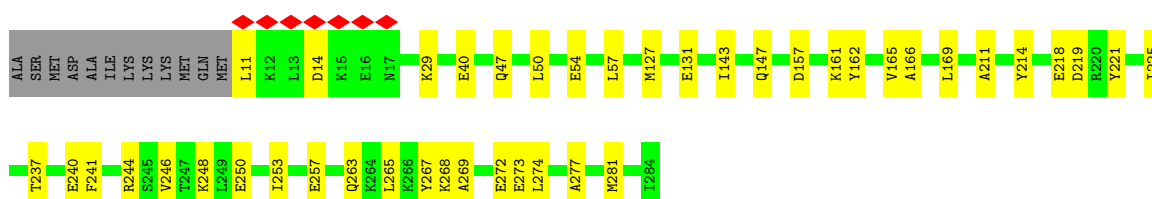
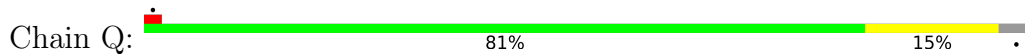




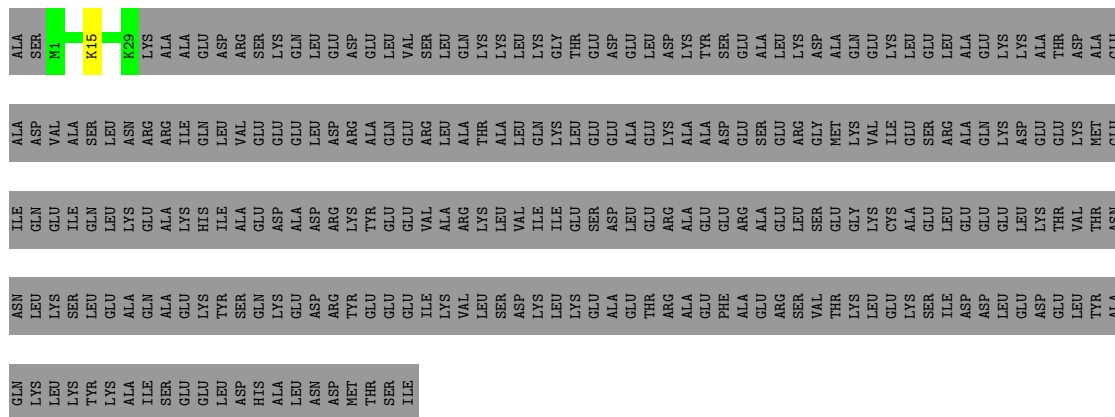
• Molecule 2: Tropomyosin alpha-1 chain



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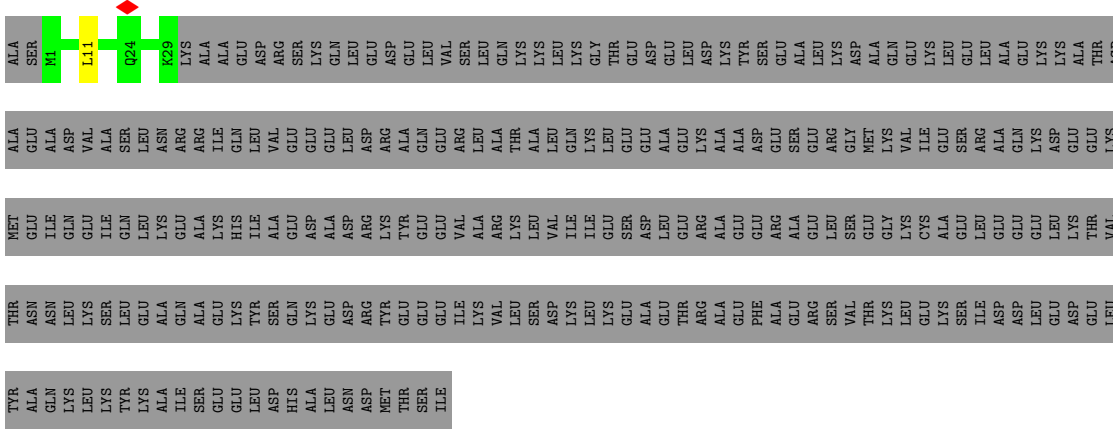


• Molecule 2: Tropomyosin alpha-1 chain

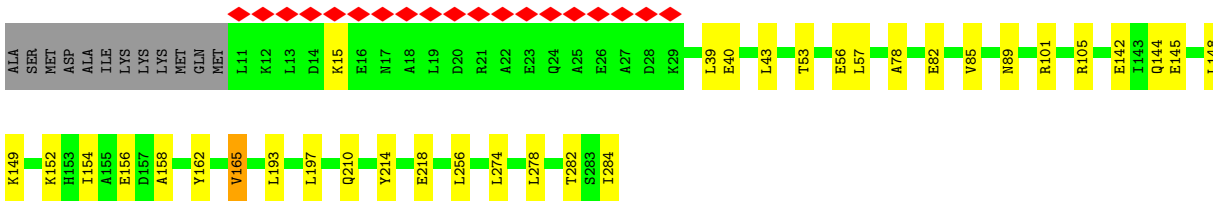
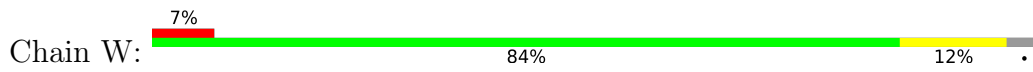


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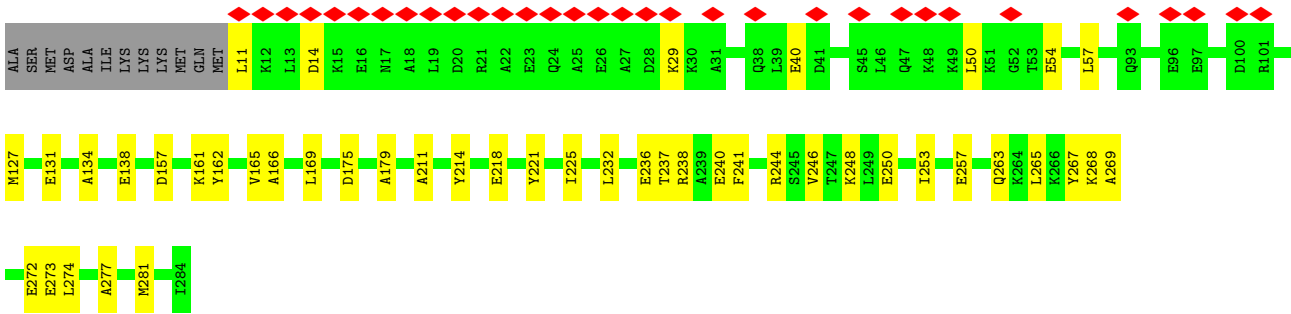
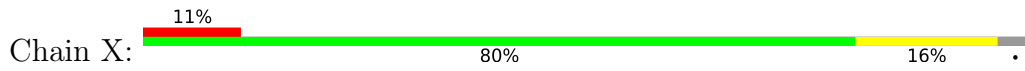




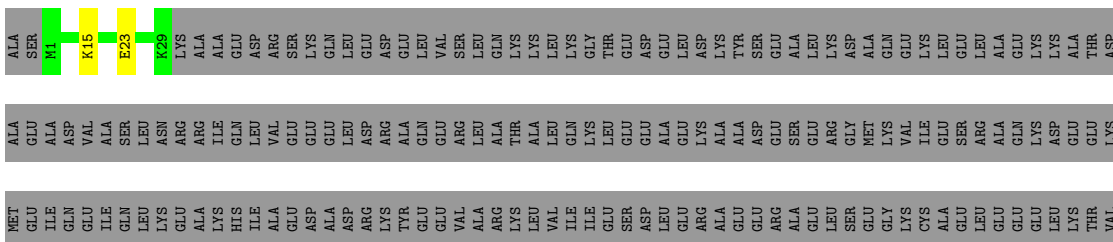
● Molecule 2: Tropomyosin alpha-1 chain

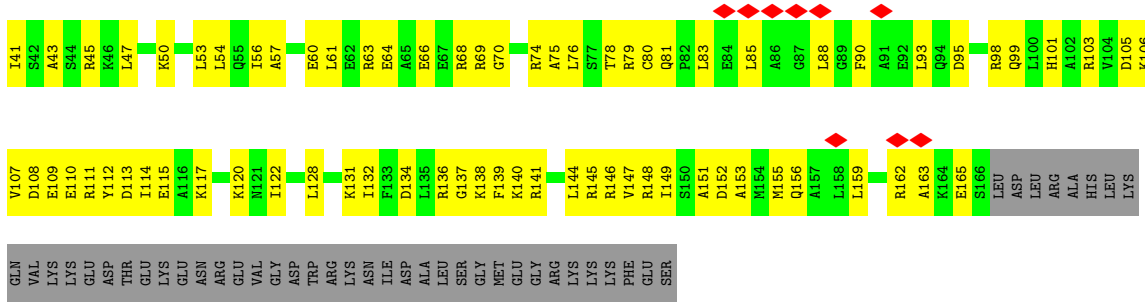


● Molecule 2: Tropomyosin alpha-1 chain

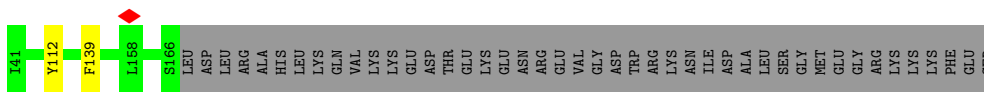
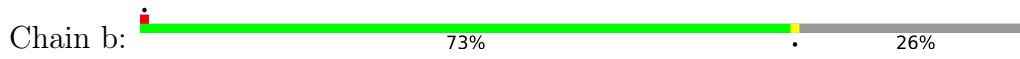


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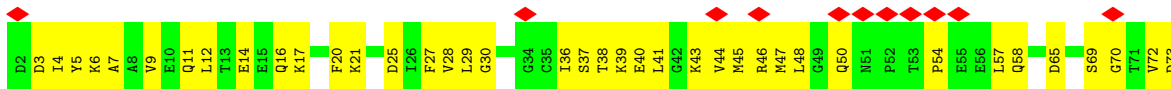




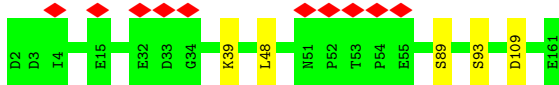
• Molecule 4: Troponin I, cardiac muscle



• Molecule 5: Troponin C



• Molecule 5: Troponin C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15569	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	439.344, 439.344, 439.344	wwPDB
Map dimensions	162, 162, 162	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.712, 2.712, 2.712	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	A	0.90	0/2996	0.89	0/4058
1	B	0.89	0/2996	0.85	0/4058
1	C	0.94	1/2996 (0.0%)	0.90	1/4058 (0.0%)
1	D	0.90	0/2996	0.89	1/4058 (0.0%)
1	E	0.90	0/2996	0.89	0/4058
1	F	0.90	0/2996	0.89	0/4058
1	G	0.93	1/2996 (0.0%)	0.89	0/4058
1	H	0.91	0/2996	0.90	0/4058
1	I	0.94	0/2996	0.91	0/4058
1	J	0.92	0/2996	0.88	0/4058
1	K	0.89	0/2996	0.88	0/4058
1	L	0.93	0/2996	0.89	0/4058
1	M	0.93	0/2996	0.89	0/4058
1	N	0.92	0/2996	0.88	0/4058
1	O	0.95	0/2996	0.92	0/4058
2	P	1.30	1/2215 (0.0%)	0.83	0/2954
2	Q	1.31	0/2215	0.89	0/2954
2	R	1.17	0/230	0.86	0/301
2	S	1.13	0/230	0.91	0/301
2	W	1.30	2/2215 (0.1%)	0.83	0/2954
2	X	1.31	0/2215	0.90	1/2954 (0.0%)
2	Y	1.17	0/230	0.86	0/301
2	Z	1.13	0/230	0.90	0/301
3	T	0.76	0/1108	0.63	0/1466
3	a	0.78	0/1108	0.66	0/1466
4	U	0.26	0/1014	0.48	0/1352
4	b	0.35	0/1014	0.51	0/1352
5	V	0.27	0/1286	0.46	0/1719
5	c	0.39	0/1286	0.54	1/1719 (0.1%)
All	All	0.95	5/61536 (0.0%)	0.86	4/82964 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	c	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	83	GLU	CD-OE1	-5.12	1.20	1.25
2	W	165	VAL	CB-CG1	-5.04	1.42	1.52
2	P	42	GLU	CD-OE2	-5.03	1.20	1.25
2	W	40	GLU	CD-OE1	-5.02	1.20	1.25
1	C	11	ASP	CB-CG	5.01	1.62	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	48	LEU	CB-CG-CD2	-5.44	101.76	111.00
1	C	31	PHE	CB-CG-CD1	-5.07	117.25	120.80
2	X	238	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	198	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	c	109	ASP	Peptide
5	c	89	SER	Peptide
5	c	93	SER	Peptide

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	A	2933	0	2894	53	0
1	B	2933	0	2894	47	0
1	C	2933	0	2894	85	0
1	D	2933	0	2894	42	0
1	E	2933	0	2894	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2933	0	2894	83	0
1	G	2933	0	2894	29	0
1	H	2933	0	2894	65	0
1	I	2933	0	2894	45	0
1	J	2933	0	2894	59	0
1	K	2933	0	2894	71	0
1	L	2933	0	2894	64	0
1	M	2933	0	2894	30	0
1	N	2933	0	2894	37	0
1	O	2933	0	2894	65	0
2	P	2207	0	2200	51	0
2	Q	2207	0	2200	56	0
2	R	231	0	245	0	0
2	S	231	0	245	1	0
2	W	2207	0	2200	72	0
2	X	2207	0	2200	59	0
2	Y	231	0	245	1	0
2	Z	231	0	245	1	0
3	T	1101	0	1120	72	0
3	a	1101	0	1120	0	0
4	U	1008	0	1064	118	0
4	b	1008	0	1064	0	0
5	V	1273	0	1201	129	0
5	c	1273	0	1201	0	0
All	All	60511	0	59960	1152	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 13.

All (1152) 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:F:1:ASP:HB3	4:U:149:ILE:CD1	1.25	1.57
1:F:305:MET:CE	1:F:335:ARG:HB2	1.35	1.55
1:M:305:MET:CE	1:M:335:ARG:HG3	1.33	1.53
5:V:38:THR:CB	2:W:149:LYS:HE2	1.53	1.37
1:J:311:ASP:OD1	2:X:248:LYS:HD2	1.24	1.37
1:B:252:ASN:HA	1:B:255:PHE:CE2	1.59	1.36
5:V:38:THR:HB	2:W:149:LYS:CE	1.56	1.36
1:F:1:ASP:CB	4:U:149:ILE:CD1	2.08	1.32
1:O:252:ASN:HA	1:O:255:PHE:CE2	1.65	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:39:LYS:HG2	2:W:149:LYS:NZ	1.46	1.29
1:L:143:TYR:CE2	1:N:44:MET:HE2	1.68	1.29
1:H:87:HIS:HD2	1:H:127:PHE:CE2	1.50	1.27
1:L:133:TYR:CD2	1:L:352:PHE:HZ	1.54	1.25
5:V:39:LYS:H	2:W:149:LYS:NZ	1.31	1.25
1:D:252:ASN:HA	1:D:255:PHE:CE2	1.70	1.24
1:I:332:PRO:O	1:I:335:ARG:HG3	1.38	1.24
1:A:252:ASN:HA	1:A:255:PHE:CE2	1.73	1.23
1:I:133:TYR:CD2	1:I:352:PHE:HZ	1.58	1.21
1:K:252:ASN:HA	1:K:255:PHE:CE2	1.75	1.19
1:L:133:TYR:CE2	1:L:352:PHE:CE1	2.30	1.19
1:C:133:TYR:CD2	1:C:352:PHE:HZ	1.62	1.17
1:K:332:PRO:O	1:K:335:ARG:HG3	1.45	1.17
1:F:332:PRO:O	1:F:335:ARG:HG2	1.44	1.16
1:L:133:TYR:CD2	1:L:352:PHE:CZ	2.33	1.16
1:A:133:TYR:CD2	1:A:352:PHE:HZ	1.63	1.15
1:E:109:PRO:HD2	1:E:161:HIS:NE2	1.59	1.15
1:D:332:PRO:O	1:D:335:ARG:HG3	1.45	1.15
1:H:87:HIS:CD2	1:H:127:PHE:CE2	2.33	1.15
1:J:311:ASP:OD2	2:X:248:LYS:HD3	1.47	1.15
1:O:217:CYS:HB2	1:O:306:TYR:CE2	1.82	1.15
1:F:136:ILE:O	1:F:139:VAL:HG22	1.45	1.15
1:H:87:HIS:CD2	1:H:127:PHE:CZ	2.35	1.14
1:J:311:ASP:CG	2:X:248:LYS:CD	2.16	1.13
1:L:143:TYR:HE2	1:N:47:MET:HE1	1.00	1.13
1:C:18:LYS:HD2	1:C:337:TYR:CD1	1.84	1.12
1:J:311:ASP:CG	2:X:248:LYS:HD2	1.69	1.12
1:C:332:PRO:O	1:C:335:ARG:HG3	1.49	1.12
1:J:252:ASN:HA	1:J:255:PHE:CE2	1.84	1.12
1:L:332:PRO:O	1:L:335:ARG:HG3	1.50	1.11
1:N:252:ASN:HA	1:N:255:PHE:CE2	1.83	1.11
1:C:290:ARG:HD3	1:E:244:ASP:CB	1.79	1.11
1:K:133:TYR:CD2	1:K:352:PHE:HZ	1.66	1.11
1:I:133:TYR:CD2	1:I:352:PHE:CZ	2.38	1.11
1:M:213:LYS:HG2	1:M:306:TYR:OH	1.48	1.10
1:M:305:MET:CE	1:M:335:ARG:CG	2.29	1.10
1:C:18:LYS:HD2	1:C:337:TYR:HD1	1.04	1.09
1:K:289:ILE:HD11	1:M:63:GLY:O	1.52	1.09
1:M:305:MET:HE2	1:M:335:ARG:HG3	1.19	1.09
1:I:133:TYR:CE2	1:I:352:PHE:CE1	2.39	1.09
1:C:133:TYR:CE2	1:C:352:PHE:CE1	2.41	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:ASP:HB3	4:U:149:ILE:HD12	1.13	1.09
1:L:143:TYR:CE2	1:N:47:MET:HE1	1.85	1.09
5:V:58:GLN:HG2	2:W:156:GLU:OE2	1.53	1.09
1:H:83:GLU:HG2	1:H:122:ILE:HD11	1.23	1.09
1:H:332:PRO:O	1:H:335:ARG:HG3	1.51	1.09
1:J:332:PRO:O	1:J:335:ARG:HG2	1.51	1.09
1:L:143:TYR:OH	1:N:44:MET:HB3	1.51	1.09
1:L:133:TYR:CZ	1:L:352:PHE:HE1	1.71	1.08
1:F:305:MET:HE2	1:F:335:ARG:HB2	1.15	1.08
1:F:305:MET:CE	1:F:335:ARG:CB	2.31	1.07
1:F:1:ASP:HB3	4:U:149:ILE:HD11	1.07	1.07
1:C:133:TYR:CD2	1:C:352:PHE:CZ	2.43	1.06
1:J:311:ASP:OD2	2:X:248:LYS:CD	2.04	1.06
1:C:133:TYR:CZ	1:C:352:PHE:HE1	1.72	1.06
1:F:305:MET:HE1	1:F:335:ARG:HB2	1.15	1.06
1:H:252:ASN:HA	1:H:255:PHE:CE2	1.91	1.06
1:N:252:ASN:HA	1:N:255:PHE:CZ	1.91	1.05
1:F:143:TYR:CE1	1:H:44:MET:HE2	1.90	1.05
1:I:86:TRP:CE3	1:I:122:ILE:HD13	1.92	1.04
5:V:39:LYS:N	2:W:149:LYS:NZ	2.05	1.04
1:C:18:LYS:CD	1:C:337:TYR:HD1	1.70	1.04
1:G:26:ALA:HB1	1:G:27:PRO:HD2	1.07	1.04
1:F:1:ASP:H1	4:U:149:ILE:HD13	1.16	1.03
5:V:39:LYS:N	2:W:149:LYS:HZ3	1.55	1.03
1:I:133:TYR:CZ	1:I:352:PHE:HE1	1.76	1.03
1:M:305:MET:HE1	1:M:335:ARG:HG3	1.10	1.03
1:M:305:MET:HE1	1:M:335:ARG:CG	1.86	1.02
1:I:87:HIS:CD2	1:I:91:TYR:CE2	2.47	1.02
1:E:252:ASN:HA	1:E:255:PHE:CZ	1.94	1.02
1:F:1:ASP:CB	4:U:149:ILE:HD12	1.76	1.01
1:J:311:ASP:OD1	2:X:248:LYS:CD	2.08	1.01
1:G:26:ALA:HB1	1:G:27:PRO:CD	1.90	1.01
1:C:290:ARG:HD3	1:E:244:ASP:HB3	1.40	1.01
1:O:217:CYS:CB	1:O:306:TYR:CE2	2.44	1.01
1:O:252:ASN:HB2	1:O:255:PHE:CZ	1.95	1.01
2:W:142:GLU:HG2	2:W:145:GLU:OE2	1.60	1.01
2:P:142:GLU:HG2	2:P:145:GLU:OE2	1.61	1.00
5:V:39:LYS:CG	2:W:149:LYS:NZ	2.24	1.00
1:J:305:MET:SD	1:J:335:ARG:HB2	2.00	1.00
1:L:143:TYR:CZ	1:N:44:MET:HE2	1.96	1.00
5:V:39:LYS:CB	2:W:149:LYS:HZ1	1.75	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:GLU:HG2	1:I:119:MET:HE1	1.39	1.00
5:V:39:LYS:CG	2:W:149:LYS:HZ1	1.73	1.00
1:C:18:LYS:CD	1:C:337:TYR:CD1	2.42	0.99
1:D:305:MET:HE1	1:D:335:ARG:HB2	1.45	0.99
1:K:133:TYR:CZ	1:K:352:PHE:HE1	1.81	0.99
1:K:252:ASN:HB2	1:K:255:PHE:CZ	1.97	0.99
1:A:326:LYS:HE3	2:Q:47:GLN:HE21	1.22	0.99
1:E:252:ASN:HA	1:E:255:PHE:CE2	1.96	0.99
1:A:326:LYS:HE3	2:Q:47:GLN:NE2	1.76	0.98
1:E:109:PRO:CD	1:E:161:HIS:NE2	2.25	0.98
1:O:217:CYS:CB	1:O:306:TYR:HE2	1.75	0.98
1:A:133:TYR:CD2	1:A:352:PHE:CZ	2.52	0.97
1:F:143:TYR:CE1	1:H:44:MET:CE	2.47	0.97
1:L:133:TYR:CE2	1:L:352:PHE:HE1	1.70	0.97
1:H:87:HIS:HD2	1:H:127:PHE:HE2	1.10	0.96
1:M:213:LYS:HG2	1:M:306:TYR:HH	1.30	0.96
1:K:166:TYR:CD1	1:K:289:ILE:HG23	2.01	0.96
1:K:133:TYR:CD2	1:K:352:PHE:CZ	2.52	0.96
1:F:1:ASP:N	4:U:149:ILE:HD13	1.78	0.96
1:K:31:PHE:CZ	1:K:89:THR:HA	2.01	0.96
1:C:188:TYR:CE1	1:C:266:PHE:HB3	2.02	0.95
1:B:252:ASN:CA	1:B:255:PHE:CE2	2.48	0.95
1:H:87:HIS:HD2	1:H:127:PHE:CZ	1.79	0.95
1:D:252:ASN:HA	1:D:255:PHE:CZ	2.02	0.94
1:D:305:MET:CE	1:D:335:ARG:HB2	1.97	0.94
1:F:2:GLU:OE1	1:F:21:PHE:CE2	2.20	0.94
1:L:133:TYR:CE2	1:L:352:PHE:CZ	2.55	0.94
1:O:217:CYS:HB2	1:O:306:TYR:HE2	1.22	0.94
1:I:133:TYR:CE2	1:I:352:PHE:HE1	1.81	0.94
1:K:133:TYR:CE2	1:K:352:PHE:CE1	2.56	0.93
1:M:305:MET:SD	1:M:335:ARG:NE	2.41	0.93
1:G:26:ALA:CB	1:G:27:PRO:HD2	1.99	0.93
1:C:290:ARG:CD	1:E:244:ASP:CB	2.47	0.93
1:A:252:ASN:HA	1:A:255:PHE:CZ	2.03	0.92
1:B:252:ASN:HA	1:B:255:PHE:HE2	1.31	0.92
1:A:133:TYR:CE2	1:A:352:PHE:CZ	2.57	0.92
5:V:58:GLN:CG	2:W:156:GLU:OE2	2.15	0.92
1:B:252:ASN:HA	1:B:255:PHE:CZ	2.05	0.92
1:C:218:TYR:HA	1:C:307:PRO:HD2	1.52	0.92
1:A:133:TYR:CE2	1:A:352:PHE:CE1	2.57	0.91
1:O:186:THR:OG1	1:O:213:LYS:HE2	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:142:GLU:HA	2:W:145:GLU:HG2	1.51	0.91
1:L:143:TYR:HE2	1:N:47:MET:CE	1.83	0.91
1:F:305:MET:HE1	1:F:335:ARG:CB	1.95	0.91
1:C:133:TYR:CZ	1:C:352:PHE:CE1	2.58	0.91
1:L:143:TYR:CE2	1:N:44:MET:CE	2.52	0.91
1:O:252:ASN:CA	1:O:255:PHE:CE2	2.53	0.90
1:C:133:TYR:CE2	1:C:352:PHE:CZ	2.59	0.90
1:H:83:GLU:HG2	1:H:122:ILE:CD1	2.02	0.90
2:X:161:LYS:O	2:X:165:VAL:HG22	1.72	0.89
1:E:109:PRO:HD2	1:E:161:HIS:CD2	2.06	0.89
1:F:109:PRO:HD2	1:F:161:HIS:CD2	2.06	0.89
1:C:133:TYR:CE2	1:C:352:PHE:HE1	1.82	0.89
1:G:305:MET:SD	1:G:335:ARG:HG3	2.12	0.89
1:C:290:ARG:CD	1:E:244:ASP:HB2	2.03	0.89
1:O:252:ASN:HA	1:O:255:PHE:HE2	1.38	0.89
1:O:186:THR:HA	1:O:213:LYS:HD3	1.54	0.88
2:P:142:GLU:HA	2:P:145:GLU:HG2	1.51	0.88
1:D:133:TYR:CD2	1:D:352:PHE:HZ	1.91	0.88
1:K:305:MET:HE1	1:K:335:ARG:HB2	1.56	0.88
1:B:252:ASN:CB	1:B:255:PHE:CZ	2.56	0.88
1:M:213:LYS:CG	1:M:306:TYR:OH	2.22	0.88
2:Q:161:LYS:O	2:Q:165:VAL:HG22	1.72	0.87
1:K:252:ASN:CB	1:K:255:PHE:CZ	2.56	0.87
1:J:252:ASN:HB2	1:J:255:PHE:CZ	2.09	0.87
1:B:252:ASN:HB2	1:B:255:PHE:CZ	2.09	0.87
5:V:39:LYS:HG2	2:W:149:LYS:HZ2	1.32	0.86
1:K:133:TYR:CZ	1:K:352:PHE:CE1	2.63	0.86
1:D:133:TYR:CD2	1:D:352:PHE:CZ	2.63	0.86
1:D:133:TYR:CE2	1:D:352:PHE:HE1	1.94	0.86
1:F:305:MET:HE2	1:F:335:ARG:CB	1.98	0.85
1:I:133:TYR:CE2	1:I:352:PHE:CZ	2.59	0.85
1:K:133:TYR:CE2	1:K:352:PHE:CZ	2.63	0.85
1:A:252:ASN:CB	1:A:255:PHE:CZ	2.60	0.85
1:D:133:TYR:CE2	1:D:352:PHE:CE1	2.65	0.85
1:O:252:ASN:CB	1:O:255:PHE:CZ	2.59	0.85
5:V:39:LYS:HG2	2:W:149:LYS:HZ1	1.25	0.85
1:B:250:ILE:O	1:B:254:ARG:HD2	1.77	0.85
1:F:332:PRO:O	1:F:335:ARG:CG	2.24	0.84
1:O:189:LEU:CD2	1:O:213:LYS:HG2	2.06	0.84
1:B:133:TYR:CE2	1:B:352:PHE:HE1	1.96	0.83
1:J:305:MET:SD	1:J:335:ARG:CB	2.66	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:HB2	1:A:255:PHE:CZ	2.13	0.83
5:V:111:TYR:HB3	5:V:147:ARG:HB2	1.60	0.83
1:D:230:ALA:HB3	1:D:255:PHE:HZ	1.44	0.83
2:X:253:ILE:O	2:X:257:GLU:HG2	1.79	0.83
1:N:252:ASN:CA	1:N:255:PHE:CZ	2.62	0.82
1:I:196:ARG:HD2	1:I:253:GLU:OE2	1.78	0.82
1:K:252:ASN:CA	1:K:255:PHE:CE2	2.62	0.82
3:T:212:LEU:HD22	4:U:109:GLU:HG2	1.61	0.82
1:D:116:ARG:HG3	1:D:134:VAL:HG11	1.60	0.82
1:B:252:ASN:CA	1:B:255:PHE:CZ	2.61	0.82
1:J:252:ASN:CB	1:J:255:PHE:CZ	2.63	0.82
2:W:142:GLU:HA	2:W:145:GLU:CG	2.09	0.82
1:B:133:TYR:CD2	1:B:352:PHE:CZ	2.68	0.82
2:P:142:GLU:HA	2:P:145:GLU:CG	2.09	0.82
1:I:133:TYR:CZ	1:I:352:PHE:CE1	2.63	0.82
1:L:133:TYR:CZ	1:L:352:PHE:CE1	2.58	0.82
2:W:53:THR:HA	2:X:57:LEU:HD11	1.62	0.81
2:W:148:LEU:HG	2:W:152:LYS:HE2	1.62	0.81
1:B:133:TYR:CD2	1:B:352:PHE:HZ	1.98	0.81
2:P:148:LEU:HG	2:P:152:LYS:HE2	1.62	0.81
1:J:133:TYR:CE2	1:J:352:PHE:HE1	1.99	0.81
2:W:142:GLU:HA	2:W:145:GLU:OE2	1.81	0.80
1:N:305:MET:HG2	1:N:335:ARG:HD2	1.62	0.80
2:P:142:GLU:HA	2:P:145:GLU:OE2	1.81	0.80
2:P:53:THR:HA	2:Q:57:LEU:HD11	1.62	0.80
1:K:305:MET:CE	1:K:335:ARG:HB2	2.11	0.80
2:Q:253:ILE:O	2:Q:257:GLU:HG2	1.79	0.80
1:F:1:ASP:CA	4:U:149:ILE:CD1	2.60	0.80
1:I:196:ARG:HD2	1:I:253:GLU:CD	2.02	0.80
1:A:109:PRO:HD2	1:A:161:HIS:NE2	1.97	0.79
1:K:196:ARG:HD2	1:K:253:GLU:CD	2.03	0.79
5:V:38:THR:HB	2:W:149:LYS:CD	2.13	0.79
1:E:109:PRO:CG	1:E:161:HIS:NE2	2.46	0.79
1:A:326:LYS:CE	2:Q:47:GLN:NE2	2.44	0.79
1:B:133:TYR:CE2	1:B:352:PHE:CE1	2.70	0.79
1:C:290:ARG:NE	1:E:244:ASP:HB2	1.98	0.79
1:I:86:TRP:CZ3	1:I:122:ILE:HD13	2.17	0.79
1:K:31:PHE:CE1	1:K:89:THR:HG23	2.17	0.79
1:E:109:PRO:HD2	1:E:161:HIS:CE1	2.15	0.79
2:W:148:LEU:CG	2:W:152:LYS:HE2	2.12	0.79
1:K:196:ARG:HD2	1:K:253:GLU:OE2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:332:PRO:O	1:J:335:ARG:CG	2.31	0.78
2:P:148:LEU:CG	2:P:152:LYS:HE2	2.12	0.78
1:O:217:CYS:HB2	1:O:306:TYR:CZ	2.19	0.78
1:N:252:ASN:CB	1:N:255:PHE:CZ	2.67	0.78
1:G:305:MET:SD	1:G:335:ARG:CG	2.72	0.78
5:V:40:GLU:HA	5:V:43:LYS:HE2	1.66	0.78
1:I:107:GLU:CG	1:I:119:MET:HE1	2.14	0.78
1:A:133:TYR:CZ	1:A:352:PHE:HE1	2.01	0.77
1:A:334:GLU:O	1:A:338:SER:HB3	1.84	0.77
1:D:116:ARG:HG2	1:D:370:VAL:HG21	1.65	0.77
1:L:133:TYR:CG	1:L:352:PHE:HZ	2.02	0.77
1:H:252:ASN:HB2	1:H:255:PHE:CZ	2.19	0.77
1:L:143:TYR:CE2	1:N:47:MET:CE	2.64	0.77
1:F:1:ASP:CA	4:U:149:ILE:HD13	2.13	0.77
1:N:227:MET:HB3	1:N:255:PHE:HE1	1.48	0.77
1:H:207:GLU:HA	1:H:210:ARG:HG2	1.67	0.77
1:J:311:ASP:OD2	2:X:248:LYS:NZ	2.18	0.77
1:L:252:ASN:HB2	1:L:255:PHE:CE2	2.20	0.77
5:V:130:GLU:HA	5:V:133:ILE:HD12	1.65	0.77
1:J:311:ASP:CG	2:X:248:LYS:HD3	1.92	0.77
3:T:244:GLU:HB3	4:U:79:ARG:HD3	1.67	0.77
1:A:207:GLU:HA	1:A:210:ARG:HG2	1.66	0.77
1:M:305:MET:HE2	1:M:335:ARG:CG	2.06	0.77
1:B:250:ILE:HG22	1:B:254:ARG:HG3	1.67	0.76
1:K:311:ASP:OD2	2:Q:248:LYS:HD3	1.84	0.76
1:C:18:LYS:HD3	1:C:337:TYR:CD1	2.19	0.76
1:L:196:ARG:HD2	1:L:253:GLU:CD	2.06	0.76
1:F:1:ASP:CB	4:U:149:ILE:HD11	1.96	0.76
1:I:107:GLU:HG2	1:I:119:MET:CE	2.15	0.76
1:E:230:ALA:HB3	1:E:255:PHE:HZ	1.50	0.76
1:L:252:ASN:HB2	1:L:255:PHE:CZ	2.21	0.76
1:O:189:LEU:HD22	1:O:213:LYS:HG2	1.67	0.76
4:U:159:LEU:HB3	4:U:163:ALA:HB2	1.67	0.76
1:D:252:ASN:CB	1:D:255:PHE:CZ	2.69	0.75
1:H:95:ARG:HH22	3:T:265:ARG:HD3	1.50	0.75
2:P:142:GLU:CA	2:P:145:GLU:HG2	2.16	0.75
1:L:143:TYR:CZ	1:N:44:MET:CE	2.70	0.75
1:A:252:ASN:CA	1:A:255:PHE:CZ	2.69	0.75
1:D:252:ASN:CA	1:D:255:PHE:CZ	2.69	0.75
1:C:289:ILE:HD11	1:E:63:GLY:O	1.85	0.75
1:E:252:ASN:CA	1:E:255:PHE:CZ	2.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:133:TYR:CE2	1:J:352:PHE:CE1	2.74	0.75
1:J:252:ASN:HA	1:J:255:PHE:CZ	2.22	0.75
1:F:6:THR:HG21	4:U:146:ARG:HH12	1.52	0.74
2:P:142:GLU:HA	2:P:145:GLU:CD	2.07	0.74
3:T:224:LEU:HB3	3:T:228:GLN:HB2	1.67	0.74
2:W:142:GLU:CA	2:W:145:GLU:HG2	2.16	0.74
1:C:207:GLU:HA	1:C:210:ARG:HG2	1.68	0.74
5:V:38:THR:HB	2:W:149:LYS:HE2	0.77	0.74
1:F:169:TYR:OH	1:H:49:GLN:HB3	1.88	0.74
1:O:252:ASN:HA	1:O:255:PHE:CZ	2.20	0.74
1:D:252:ASN:HB2	1:D:255:PHE:CZ	2.23	0.74
5:V:36:ILE:HB	5:V:72:VAL:HB	1.67	0.74
1:F:139:VAL:HG23	1:F:140:LEU:N	2.01	0.74
1:C:227:MET:HB3	1:C:255:PHE:CZ	2.23	0.74
1:F:21:PHE:HD1	1:F:28:ARG:HE	1.35	0.74
1:H:87:HIS:CD2	1:H:127:PHE:HZ	2.01	0.73
2:W:142:GLU:HA	2:W:145:GLU:CD	2.07	0.73
1:I:334:GLU:O	1:I:338:SER:HB3	1.88	0.73
1:B:219:VAL:HG23	1:B:306:TYR:HB3	1.70	0.73
1:D:252:ASN:CA	1:D:255:PHE:CE2	2.64	0.73
1:K:133:TYR:CE2	1:K:352:PHE:HE1	2.02	0.73
3:T:237:TRP:NE1	4:U:81:GLN:O	2.21	0.73
5:V:38:THR:HA	5:V:57:LEU:HD21	1.71	0.73
1:C:290:ARG:CD	1:E:244:ASP:HB3	2.14	0.73
1:H:87:HIS:O	1:H:91:TYR:HD2	1.71	0.73
2:P:148:LEU:CD2	2:P:152:LYS:HE2	2.19	0.72
3:T:263:VAL:HG22	5:V:110:GLY:HA2	1.69	0.72
1:J:133:TYR:CZ	1:J:352:PHE:HE1	2.06	0.72
2:W:148:LEU:CD2	2:W:152:LYS:HE2	2.19	0.72
1:D:230:ALA:HB3	1:D:255:PHE:CZ	2.24	0.72
1:F:1:ASP:CG	4:U:149:ILE:HD12	2.08	0.72
5:V:38:THR:CG2	2:W:149:LYS:HE2	2.17	0.72
1:O:217:CYS:O	1:O:306:TYR:CD2	2.42	0.72
1:B:252:ASN:CB	1:B:255:PHE:HZ	2.03	0.71
1:C:227:MET:HB3	1:C:255:PHE:HZ	1.54	0.71
1:E:169:TYR:OH	1:G:49:GLN:HG3	1.90	0.71
1:I:326:LYS:NZ	2:Q:219:ASP:OD1	2.22	0.71
1:C:188:TYR:CZ	1:C:266:PHE:HB3	2.25	0.71
1:A:133:TYR:CZ	1:A:352:PHE:CE1	2.76	0.71
1:B:258:PRO:HB3	1:B:306:TYR:CE1	2.26	0.71
1:I:107:GLU:CG	1:I:119:MET:CE	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:230:ALA:HB3	1:N:255:PHE:HZ	1.56	0.70
1:C:188:TYR:CE2	1:C:266:PHE:CD2	2.79	0.70
1:H:305:MET:SD	1:H:335:ARG:NE	2.63	0.70
1:J:169:TYR:OH	1:L:49:GLN:HB3	1.90	0.70
5:V:14:GLU:HA	5:V:17:LYS:HD2	1.71	0.70
1:J:133:TYR:CD2	1:J:352:PHE:CZ	2.79	0.70
1:L:252:ASN:HA	1:L:255:PHE:CE2	2.27	0.70
5:V:102:ARG:O	5:V:102:ARG:NH1	2.24	0.70
1:C:18:LYS:CD	1:C:337:TYR:CE1	2.75	0.70
1:L:252:ASN:CB	1:L:255:PHE:CE2	2.73	0.70
2:P:149:LYS:HE3	2:P:153:HIS:NE2	2.06	0.70
1:C:258:PRO:HG3	1:C:306:TYR:CE2	2.27	0.70
4:U:47:LEU:HD22	5:V:4:ILE:HA	1.72	0.70
4:U:56:ILE:HG13	5:V:124:THR:HA	1.72	0.70
1:F:139:VAL:CG2	1:F:140:LEU:N	2.54	0.70
2:W:57:LEU:HA	2:X:57:LEU:HD23	1.74	0.70
1:O:207:GLU:HA	1:O:210:ARG:HG2	1.72	0.70
2:P:57:LEU:HA	2:Q:57:LEU:HD23	1.74	0.70
1:C:133:TYR:CG	1:C:352:PHE:HZ	2.09	0.70
1:O:252:ASN:CA	1:O:255:PHE:CZ	2.75	0.69
1:I:87:HIS:CD2	1:I:91:TYR:CD2	2.79	0.69
5:V:102:ARG:NH1	5:V:105:ASP:O	2.25	0.69
1:O:189:LEU:HD23	1:O:213:LYS:CG	2.22	0.69
2:P:57:LEU:N	2:Q:57:LEU:HD21	2.08	0.69
1:O:252:ASN:HB2	1:O:255:PHE:HZ	1.56	0.69
1:A:109:PRO:HD2	1:A:161:HIS:CE1	2.28	0.68
1:K:289:ILE:HD11	1:M:63:GLY:C	2.13	0.68
1:N:252:ASN:HB2	1:N:255:PHE:CZ	2.28	0.68
1:K:252:ASN:HA	1:K:255:PHE:CZ	2.27	0.68
1:B:133:TYR:CZ	1:B:352:PHE:HE1	2.11	0.68
3:T:244:GLU:O	4:U:79:ARG:NH1	2.26	0.68
1:F:188:TYR:CE1	1:F:266:PHE:HB3	2.28	0.68
1:F:143:TYR:CE1	1:H:44:MET:HE3	2.28	0.67
2:W:57:LEU:N	2:X:57:LEU:HD21	2.08	0.67
1:F:143:TYR:OH	1:H:45:VAL:N	2.27	0.67
1:J:307:PRO:HG2	2:X:244:ARG:HH12	1.59	0.67
1:A:109:PRO:HD2	1:A:161:HIS:CD2	2.30	0.67
1:K:133:TYR:CG	1:K:352:PHE:HZ	2.11	0.67
1:E:169:TYR:OH	1:G:49:GLN:HB3	1.95	0.67
5:V:39:LYS:H	2:W:149:LYS:HZ3	0.70	0.67
1:H:207:GLU:O	1:H:210:ARG:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:352:PHE:CE1	1:O:355:MET:CB	2.78	0.66
4:U:78:THR:O	4:U:81:GLN:NE2	2.28	0.66
1:O:209:VAL:O	1:O:213:LYS:HG3	1.94	0.66
1:L:109:PRO:HD2	1:L:161:HIS:NE2	2.11	0.66
1:O:334:GLU:O	1:O:338:SER:HB3	1.96	0.66
1:D:133:TYR:CZ	1:D:352:PHE:HE1	2.12	0.66
1:F:143:TYR:OH	1:H:44:MET:HB3	1.96	0.66
5:V:21:LYS:NZ	5:V:25:ASP:OD1	2.27	0.66
1:E:252:ASN:CB	1:E:255:PHE:CZ	2.79	0.66
1:O:217:CYS:C	1:O:306:TYR:CE2	2.69	0.66
1:D:116:ARG:HG2	1:D:370:VAL:CG2	2.25	0.66
1:O:352:PHE:CD1	1:O:355:MET:HG3	2.30	0.66
2:P:142:GLU:CG	2:P:145:GLU:OE2	2.42	0.66
2:W:148:LEU:HD21	2:W:152:LYS:HE2	1.77	0.66
1:E:169:TYR:OH	1:G:49:GLN:CG	2.43	0.66
4:U:165:GLU:OE1	5:V:16:GLN:NE2	2.28	0.66
1:C:218:TYR:CA	1:C:307:PRO:HD2	2.24	0.65
1:H:252:ASN:CB	1:H:255:PHE:CZ	2.79	0.65
1:L:133:TYR:HE2	1:L:346:LEU:HD21	1.59	0.65
1:I:107:GLU:HG3	1:I:119:MET:HE2	1.78	0.65
1:I:133:TYR:CG	1:I:352:PHE:HZ	2.10	0.65
1:O:217:CYS:O	1:O:306:TYR:HD2	1.79	0.65
1:A:133:TYR:CE2	1:A:352:PHE:HE1	2.05	0.65
2:P:148:LEU:HD21	2:P:152:LYS:HE2	1.77	0.65
3:T:267:ARG:HD2	5:V:150:TYR:HB3	1.78	0.65
1:M:207:GLU:HA	1:M:210:ARG:HG2	1.78	0.65
2:P:156:GLU:HG2	2:P:160:ARG:NH2	2.10	0.65
1:K:252:ASN:CA	1:K:255:PHE:CZ	2.80	0.65
1:J:307:PRO:CG	2:X:244:ARG:HH12	2.10	0.65
1:I:87:HIS:CG	1:I:91:TYR:CD2	2.85	0.65
2:W:142:GLU:CG	2:W:145:GLU:OE2	2.41	0.65
3:T:267:ARG:O	3:T:271:ASN:N	2.30	0.65
1:C:30:VAL:HG21	1:C:337:TYR:OH	1.95	0.64
1:O:189:LEU:HD23	1:O:213:LYS:HG2	1.78	0.64
1:A:305:MET:SD	1:A:336:LYS:HB3	2.37	0.64
1:O:217:CYS:CA	1:O:306:TYR:HE2	2.09	0.64
1:H:333:PRO:C	1:H:335:ARG:H	2.01	0.64
4:U:108:ASP:OD1	4:U:111:ARG:NH2	2.27	0.64
5:V:39:LYS:CB	2:W:149:LYS:NZ	2.57	0.64
1:C:188:TYR:CZ	1:C:266:PHE:CD2	2.84	0.64
1:E:305:MET:SD	1:E:336:LYS:HD2	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:352:PHE:CE1	1:O:355:MET:HB2	2.33	0.64
1:F:1:ASP:N	4:U:149:ILE:CD1	2.57	0.63
1:F:143:TYR:HE1	1:H:44:MET:HE2	1.55	0.63
1:F:333:PRO:C	1:F:335:ARG:H	2.02	0.63
1:K:333:PRO:C	1:K:335:ARG:H	2.02	0.63
1:I:86:TRP:CE3	1:I:122:ILE:CD1	2.77	0.63
1:K:252:ASN:HA	1:K:255:PHE:HE2	1.55	0.63
1:L:143:TYR:CZ	1:N:44:MET:HB3	2.33	0.63
5:V:48:LEU:HB3	5:V:50:GLN:HE22	1.64	0.63
1:F:139:VAL:CG2	1:F:140:LEU:HG	2.29	0.63
1:I:87:HIS:O	1:I:91:TYR:HD2	1.82	0.62
4:U:165:GLU:HB3	5:V:16:GLN:HE21	1.63	0.62
2:X:272:GLU:OE1	2:X:272:GLU:HA	1.99	0.62
1:C:18:LYS:HD3	1:C:337:TYR:CE1	2.33	0.62
1:M:207:GLU:O	1:M:210:ARG:CG	2.48	0.62
1:J:169:TYR:OH	1:L:49:GLN:CG	2.47	0.61
1:J:252:ASN:CA	1:J:255:PHE:CZ	2.82	0.61
4:U:75:ALA:O	4:U:79:ARG:HB2	2.01	0.61
1:K:287:ILE:HA	1:K:290:ARG:HD2	1.82	0.61
1:K:307:PRO:HB3	2:Q:244:ARG:HH12	1.64	0.61
1:L:333:PRO:C	1:L:335:ARG:H	2.04	0.61
1:E:169:TYR:OH	1:G:49:GLN:CB	2.48	0.61
1:L:252:ASN:CA	1:L:255:PHE:CE2	2.82	0.61
1:I:106:THR:O	1:I:107:GLU:HG2	2.00	0.61
1:C:333:PRO:C	1:C:335:ARG:H	2.03	0.61
1:G:334:GLU:O	1:G:338:SER:HB3	2.00	0.61
2:Q:272:GLU:OE1	2:Q:272:GLU:HA	1.99	0.61
1:E:230:ALA:CB	1:E:255:PHE:HZ	2.13	0.60
1:F:143:TYR:CD1	1:H:44:MET:CE	2.84	0.60
1:C:290:ARG:O	1:C:294:TYR:CD1	2.54	0.60
1:F:159:VAL:HG21	1:F:177:ARG:HE	1.67	0.60
4:U:45:ARG:NH1	5:V:127:THR:OG1	2.34	0.60
5:V:121:LEU:HD11	5:V:136:LEU:HD12	1.82	0.60
5:V:76:GLU:O	5:V:80:MET:HG2	2.01	0.60
2:X:269:ALA:O	2:X:273:GLU:HB2	2.01	0.60
1:J:207:GLU:HA	1:J:210:ARG:HG2	1.82	0.60
1:K:286:ASP:O	1:K:290:ARG:HG3	2.01	0.60
1:H:87:HIS:NE2	1:H:127:PHE:CZ	2.70	0.60
3:T:250:LEU:HD22	4:U:115:GLU:HA	1.83	0.60
1:I:332:PRO:O	1:I:335:ARG:CG	2.31	0.60
1:K:31:PHE:CE2	1:K:89:THR:HA	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:207:GLU:O	1:M:210:ARG:HG2	2.02	0.60
2:Q:269:ALA:O	2:Q:273:GLU:HB2	2.01	0.60
1:E:334:GLU:O	1:E:338:SER:HB3	2.02	0.60
3:T:208:LYS:O	3:T:212:LEU:HG	2.02	0.60
4:U:134:ASP:O	4:U:138:LYS:NZ	2.32	0.60
5:V:39:LYS:N	2:W:149:LYS:CE	2.65	0.60
5:V:154:LEU:O	5:V:158:LYS:N	2.35	0.60
1:C:290:ARG:O	1:C:294:TYR:HD1	1.85	0.59
1:N:335:ARG:C	1:N:337:TYR:H	2.05	0.59
1:N:252:ASN:HB2	1:N:255:PHE:CE1	2.37	0.59
3:T:263:VAL:HG11	5:V:150:TYR:HB2	1.83	0.59
4:U:159:LEU:HD11	4:U:162:ARG:HE	1.66	0.59
1:G:26:ALA:CB	1:G:27:PRO:CD	2.65	0.59
1:H:252:ASN:HA	1:H:255:PHE:CZ	2.36	0.59
1:E:109:PRO:HG2	1:E:161:HIS:NE2	2.17	0.59
3:T:237:TRP:HA	3:T:240:ILE:HD12	1.85	0.59
5:V:37:SER:OG	5:V:40:GLU:OE1	2.10	0.59
1:D:207:GLU:HA	1:D:210:ARG:HG2	1.85	0.59
1:J:257:CYS:HB3	1:J:258:PRO:HD3	1.85	0.59
4:U:137:GLY:HA3	4:U:141:ARG:HH22	1.67	0.59
1:J:133:TYR:CD2	1:J:352:PHE:HZ	2.17	0.59
1:D:230:ALA:CB	1:D:255:PHE:CZ	2.85	0.59
3:T:256:GLN:HE22	5:V:102:ARG:HB2	1.68	0.59
5:V:39:LYS:HB3	2:W:149:LYS:HZ1	1.60	0.59
4:U:103:ARG:O	4:U:107:VAL:HG12	2.02	0.59
1:F:143:TYR:HH	1:H:45:VAL:N	2.01	0.59
1:H:252:ASN:CA	1:H:255:PHE:CE2	2.79	0.59
1:J:311:ASP:OD2	2:X:248:LYS:CE	2.51	0.58
2:P:142:GLU:O	2:P:145:GLU:HG2	2.03	0.58
1:L:305:MET:SD	1:L:335:ARG:CB	2.92	0.58
2:P:142:GLU:C	2:P:145:GLU:HG2	2.24	0.58
4:U:140:LYS:NZ	5:V:155:GLU:OE2	2.36	0.58
1:E:108:ALA:HB1	1:E:161:HIS:ND1	2.19	0.58
1:O:217:CYS:HB2	1:O:306:TYR:OH	2.03	0.58
1:A:305:MET:SD	1:A:336:LYS:HD2	2.44	0.58
1:J:169:TYR:OH	1:L:49:GLN:CB	2.51	0.58
1:G:26:ALA:HA	1:G:340:TRP:CZ3	2.39	0.58
1:J:169:TYR:OH	1:L:49:GLN:HG3	2.03	0.58
2:W:142:GLU:O	2:W:145:GLU:HG2	2.03	0.58
1:C:218:TYR:CB	1:C:307:PRO:HD2	2.34	0.58
1:E:109:PRO:CD	1:E:161:HIS:CE1	2.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:TYR:HB2	1:C:309:ILE:HB	1.84	0.57
1:L:305:MET:SD	1:L:335:ARG:HB2	2.43	0.57
5:V:7:ALA:O	5:V:11:GLN:N	2.37	0.57
5:V:112:ILE:HD12	5:V:148:ILE:HB	1.85	0.57
1:D:305:MET:HE2	1:D:335:ARG:HB2	1.85	0.57
1:E:252:ASN:HB2	1:E:255:PHE:CZ	2.39	0.57
1:K:166:TYR:CG	1:K:289:ILE:HG23	2.38	0.57
1:K:270:GLU:O	1:K:270:GLU:HG2	2.04	0.57
3:T:243:LEU:HB2	4:U:107:VAL:HG13	1.86	0.57
1:A:222:ASP:OD1	1:A:315:LYS:NZ	2.38	0.57
1:I:257:CYS:HB3	1:I:258:PRO:HD3	1.85	0.57
2:Q:157:ASP:OD2	2:Q:161:LYS:NZ	2.37	0.57
3:T:244:GLU:OE1	3:T:247:LYS:NZ	2.31	0.57
5:V:20:PHE:HB3	5:V:77:PHE:HE2	1.70	0.57
1:L:139:VAL:CG1	1:L:143:TYR:CE1	2.88	0.57
2:X:157:ASP:OD2	2:X:161:LYS:NZ	2.37	0.57
2:P:162:TYR:CE1	2:Q:165:VAL:HG11	2.40	0.57
2:W:142:GLU:C	2:W:145:GLU:HG2	2.24	0.57
2:W:162:TYR:CE1	2:X:165:VAL:HG11	2.40	0.57
4:U:132:ILE:O	4:U:136:ARG:N	2.21	0.57
1:A:333:PRO:C	1:A:335:ARG:H	2.07	0.57
1:E:230:ALA:CB	1:E:255:PHE:CZ	2.87	0.57
1:J:133:TYR:CD2	1:J:352:PHE:CE1	2.93	0.57
1:K:157:ASP:OD1	1:K:157:ASP:N	2.38	0.57
1:K:289:ILE:CD1	1:M:63:GLY:O	2.38	0.57
3:T:268:ILE:HG12	4:U:131:LYS:HZ2	1.69	0.57
5:V:154:LEU:HB3	5:V:158:LYS:HE3	1.87	0.57
1:C:207:GLU:O	1:C:210:ARG:HG3	2.05	0.57
1:C:283:MET:CE	1:C:290:ARG:NH2	2.68	0.57
1:C:289:ILE:HD11	1:E:63:GLY:C	2.25	0.57
1:C:257:CYS:HB3	1:C:258:PRO:HD3	1.87	0.56
4:U:64:GLU:OE2	4:U:68:ARG:NH2	2.38	0.56
1:B:133:TYR:CD2	1:B:352:PHE:CE1	2.93	0.56
1:E:326:LYS:HE3	2:Q:131:GLU:OE2	2.05	0.56
1:K:133:TYR:HE2	1:K:346:LEU:HD21	1.71	0.56
1:K:335:ARG:C	1:K:337:TYR:H	2.08	0.56
1:L:196:ARG:HD2	1:L:253:GLU:OE2	2.04	0.56
2:P:278:LEU:O	2:P:282:THR:N	2.38	0.56
3:T:225:ASN:HA	4:U:90:PHE:HE1	1.69	0.56
4:U:165:GLU:HB3	5:V:16:GLN:HG2	1.88	0.56
1:C:283:MET:CE	1:C:290:ARG:HH22	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:247:LYS:HG3	4:U:114:ILE:HG13	1.87	0.56
1:A:207:GLU:O	1:A:210:ARG:HG2	2.06	0.56
1:B:250:ILE:O	1:B:254:ARG:CD	2.52	0.56
1:H:335:ARG:C	1:H:337:TYR:H	2.09	0.56
4:U:88:LEU:HD23	4:U:93:LEU:HD23	1.85	0.56
2:W:278:LEU:O	2:W:282:THR:N	2.38	0.56
1:A:187:ASP:OD2	1:A:191:LYS:NZ	2.39	0.56
1:J:252:ASN:CA	1:J:255:PHE:CE2	2.75	0.56
1:C:335:ARG:C	1:C:337:TYR:H	2.09	0.56
1:L:332:PRO:O	1:L:335:ARG:CG	2.40	0.56
5:V:29:LEU:HD23	5:V:43:LYS:HE3	1.86	0.56
1:K:252:ASN:CB	1:K:255:PHE:HZ	2.17	0.56
4:U:117:LYS:HA	4:U:120:LYS:HD2	1.87	0.56
5:V:96:GLU:O	5:V:100:LEU:HG	2.06	0.56
1:B:187:ASP:OD2	1:B:191:LYS:NZ	2.39	0.56
1:C:188:TYR:CE2	1:C:266:PHE:HD2	2.22	0.56
5:V:83:ARG:NH1	5:V:84:CYS:SG	2.77	0.56
1:J:333:PRO:C	1:J:335:ARG:H	2.08	0.56
1:F:2:GLU:HG3	1:F:2:GLU:O	2.06	0.55
1:O:217:CYS:HB3	1:O:306:TYR:CE2	2.39	0.55
3:T:259:TYR:O	3:T:263:VAL:HG23	2.06	0.55
1:A:207:GLU:O	1:A:210:ARG:CG	2.54	0.55
1:C:207:GLU:O	1:C:210:ARG:CG	2.55	0.55
1:C:332:PRO:O	1:C:335:ARG:CG	2.38	0.55
1:G:187:ASP:OD2	1:G:191:LYS:NZ	2.40	0.55
1:J:307:PRO:CB	2:X:244:ARG:NH1	2.70	0.55
5:V:72:VAL:HG13	5:V:76:GLU:HB2	1.88	0.55
5:V:105:ASP:OD2	5:V:110:GLY:N	2.29	0.55
1:F:305:MET:HE1	1:F:335:ARG:CG	2.36	0.55
1:L:51:ASP:N	1:L:51:ASP:OD1	2.39	0.55
2:P:214:TYR:CD2	2:Q:211:ALA:HB1	2.42	0.55
5:V:54:PRO:CB	2:W:152:LYS:NZ	2.69	0.55
1:H:211:ASP:OD1	1:H:215:LYS:NZ	2.39	0.55
2:W:214:TYR:CD2	2:X:211:ALA:HB1	2.42	0.55
1:A:109:PRO:CD	1:A:161:HIS:NE2	2.67	0.55
1:A:335:ARG:C	1:A:337:TYR:H	2.10	0.55
1:E:252:ASN:HB2	1:E:255:PHE:CE1	2.42	0.55
1:K:221:LEU:HD21	1:K:311:ASP:OD2	2.06	0.55
1:C:283:MET:HE1	1:C:290:ARG:HH22	1.72	0.55
1:F:108:ALA:HB1	1:F:161:HIS:CE1	2.42	0.55
1:D:334:GLU:O	1:D:338:SER:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:54:PRO:HB3	2:W:152:LYS:HE3	1.87	0.55
5:V:104:PHE:O	5:V:116:GLU:HB3	2.07	0.55
1:O:189:LEU:HD23	1:O:213:LYS:HG3	1.87	0.55
1:C:289:ILE:O	1:C:289:ILE:HG22	2.07	0.55
1:H:83:GLU:CG	1:H:122:ILE:CD1	2.82	0.55
1:K:289:ILE:HG22	1:K:289:ILE:O	2.06	0.55
1:B:51:ASP:N	1:B:51:ASP:OD1	2.40	0.54
1:C:51:ASP:OD1	1:C:51:ASP:N	2.38	0.54
1:I:107:GLU:HG3	1:I:119:MET:CE	2.35	0.54
1:O:133:TYR:CG	1:O:352:PHE:HZ	2.24	0.54
3:T:216:ARG:HA	4:U:105:ASP:OD1	2.07	0.54
1:C:283:MET:SD	1:C:290:ARG:NH2	2.80	0.54
1:D:133:TYR:CD2	1:D:352:PHE:CE1	2.92	0.54
1:H:257:CYS:HB3	1:H:258:PRO:HD3	1.89	0.54
1:I:133:TYR:HE2	1:I:346:LEU:HD21	1.72	0.54
1:O:287:ILE:HA	1:O:290:ARG:CD	2.37	0.54
3:T:262:ASN:OD1	3:T:265:ARG:NH1	2.36	0.54
1:B:332:PRO:C	1:B:334:GLU:H	2.10	0.54
1:G:305:MET:SD	1:G:335:ARG:HB2	2.47	0.54
5:V:118:LYS:HA	5:V:133:ILE:HG12	1.88	0.54
1:A:252:ASN:CA	1:A:255:PHE:CE2	2.67	0.54
1:C:187:ASP:OD2	1:C:191:LYS:NZ	2.41	0.54
1:K:311:ASP:HB3	2:Q:248:LYS:HZ3	1.72	0.54
1:F:108:ALA:HB1	1:F:161:HIS:ND1	2.21	0.54
1:A:113:LYS:O	1:A:116:ARG:HG2	2.07	0.54
1:L:143:TYR:CD2	1:N:44:MET:CE	2.91	0.54
1:O:133:TYR:CD2	1:O:352:PHE:HZ	2.25	0.54
4:U:50:LYS:NZ	5:V:156:PHE:O	2.36	0.54
5:V:75:ASP:O	5:V:79:VAL:HG23	2.08	0.54
2:X:268:LYS:O	2:X:272:GLU:HB2	2.08	0.54
1:B:222:ASP:OD1	1:B:315:LYS:NZ	2.41	0.54
1:H:87:HIS:O	1:H:91:TYR:CD2	2.58	0.54
1:O:217:CYS:C	1:O:306:TYR:CD2	2.81	0.54
1:I:187:ASP:OD2	1:I:191:LYS:NZ	2.41	0.54
5:V:43:LYS:HA	5:V:46:ARG:HG3	1.88	0.54
1:K:257:CYS:HB3	1:K:258:PRO:HD3	1.90	0.54
1:L:227:MET:HB3	1:L:255:PHE:CZ	2.43	0.54
3:T:251:GLN:HG3	4:U:114:ILE:HG21	1.90	0.54
5:V:58:GLN:HG3	2:W:156:GLU:OE2	2.01	0.54
1:G:257:CYS:HB2	1:G:258:PRO:HD3	1.90	0.53
1:L:133:TYR:CG	1:L:352:PHE:CZ	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:MET:HA	1:E:255:PHE:CE1	2.43	0.53
1:I:333:PRO:C	1:I:335:ARG:H	2.11	0.53
1:C:166:TYR:CD1	1:C:289:ILE:HG23	2.43	0.53
1:G:51:ASP:OD1	1:G:51:ASP:N	2.40	0.53
1:O:217:CYS:O	1:O:306:TYR:CE2	2.61	0.53
5:V:137:MET:O	5:V:141:ASP:N	2.41	0.53
1:C:133:TYR:CG	1:C:352:PHE:CZ	2.92	0.53
1:H:187:ASP:OD2	1:H:191:LYS:NZ	2.42	0.53
1:O:217:CYS:C	1:O:306:TYR:HE2	2.09	0.53
2:P:146:ILE:HG23	2:P:147:GLN:N	2.24	0.53
1:A:252:ASN:HB2	1:A:255:PHE:CE1	2.43	0.53
3:T:236:LEU:HD22	4:U:101:HIS:HA	1.91	0.53
1:F:110:LEU:H	1:F:161:HIS:CE1	2.26	0.53
1:I:86:TRP:HE3	1:I:122:ILE:HD13	1.68	0.53
1:I:335:ARG:C	1:I:337:TYR:H	2.12	0.53
1:N:287:ILE:HA	1:N:290:ARG:HD3	1.90	0.53
1:O:252:ASN:CB	1:O:255:PHE:HZ	2.14	0.53
2:P:149:LYS:HG2	2:P:153:HIS:CD2	2.43	0.53
2:P:256:LEU:HD11	2:Q:257:GLU:OE2	2.09	0.53
2:Q:165:VAL:O	2:Q:169:LEU:N	2.42	0.53
2:Q:268:LYS:O	2:Q:272:GLU:HB2	2.08	0.53
1:C:133:TYR:HE2	1:C:346:LEU:HD21	1.73	0.53
1:B:253:GLU:HA	1:B:256:ARG:HB2	1.91	0.52
1:O:51:ASP:OD1	1:O:51:ASP:N	2.38	0.52
4:U:60:GLU:O	4:U:63:ARG:HG3	2.08	0.52
2:W:56:GLU:C	2:X:57:LEU:HD21	2.30	0.52
1:H:87:HIS:CD2	1:H:127:PHE:HE2	1.97	0.52
1:F:227:MET:HB3	1:F:255:PHE:HZ	1.75	0.52
1:L:334:GLU:N	1:L:334:GLU:OE1	2.40	0.52
1:A:252:ASN:CB	1:A:255:PHE:HZ	2.22	0.52
1:E:51:ASP:OD1	1:E:51:ASP:N	2.42	0.52
3:T:247:LYS:HB3	4:U:79:ARG:HH12	1.73	0.52
5:V:140:GLY:HA2	5:V:156:PHE:HB2	1.91	0.52
2:W:256:LEU:HD11	2:X:257:GLU:OE2	2.09	0.52
1:C:133:TYR:CE1	1:C:355:MET:HB3	2.44	0.52
1:F:169:TYR:HH	1:H:49:GLN:HB3	1.73	0.52
3:T:225:ASN:N	3:T:228:GLN:OE1	2.43	0.52
3:T:268:ILE:HD11	4:U:128:LEU:HD22	1.91	0.52
1:D:51:ASP:OD1	1:D:51:ASP:N	2.43	0.52
1:D:207:GLU:O	1:D:210:ARG:CG	2.58	0.52
1:K:230:ALA:HB3	1:K:255:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:243:LEU:HA	3:T:246:GLU:OE1	2.10	0.52
1:B:250:ILE:HB	1:B:254:ARG:HG2	1.92	0.52
1:M:196:ARG:HD2	1:M:253:GLU:CD	2.30	0.52
1:H:110:LEU:HB3	1:H:177:ARG:HG3	1.92	0.52
1:L:139:VAL:HG13	1:L:143:TYR:CE1	2.44	0.52
2:P:56:GLU:C	2:Q:57:LEU:HD21	2.30	0.52
3:T:268:ILE:O	3:T:272:GLN:N	2.42	0.52
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.91	0.52
1:F:51:ASP:OD1	1:F:51:ASP:N	2.42	0.52
1:J:169:TYR:HH	1:L:49:GLN:HB3	1.71	0.52
1:J:257:CYS:CB	1:J:258:PRO:HD3	2.40	0.52
1:N:227:MET:CB	1:N:255:PHE:HE1	2.19	0.52
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.91	0.51
1:E:257:CYS:HB3	1:E:258:PRO:HD3	1.93	0.51
1:O:186:THR:HG1	1:O:213:LYS:HE2	1.70	0.51
2:X:165:VAL:O	2:X:169:LEU:N	2.42	0.51
3:T:217:LYS:O	4:U:101:HIS:NE2	2.43	0.51
2:X:240:GLU:O	2:X:244:ARG:HG3	2.11	0.51
1:L:286:ASP:O	1:L:290:ARG:HG3	2.11	0.51
2:Q:240:GLU:O	2:Q:244:ARG:HG3	2.11	0.51
3:T:257:GLN:NE2	4:U:122:ILE:HG13	2.25	0.51
5:V:73:ASP:HB3	5:V:75:ASP:OD1	2.11	0.51
1:O:352:PHE:CD1	1:O:355:MET:CG	2.93	0.51
5:V:94:GLU:HA	5:V:154:LEU:HD22	1.91	0.51
5:V:54:PRO:HB2	2:W:152:LYS:HZ2	1.75	0.51
1:H:252:ASN:CA	1:H:255:PHE:CZ	2.94	0.51
1:J:222:ASP:OD1	1:J:315:LYS:NZ	2.43	0.51
1:K:166:TYR:CE1	1:K:289:ILE:HG23	2.45	0.51
1:M:207:GLU:O	1:M:210:ARG:HG3	2.10	0.51
1:E:110:LEU:H	1:E:161:HIS:HE1	1.57	0.51
1:J:79:TRP:HZ3	1:J:83:GLU:OE1	1.94	0.51
1:K:311:ASP:OD2	2:Q:248:LYS:CD	2.58	0.51
1:K:311:ASP:HB3	2:Q:248:LYS:NZ	2.25	0.51
5:V:150:TYR:CZ	5:V:154:LEU:HD21	2.46	0.51
2:W:53:THR:CA	2:X:57:LEU:HD11	2.39	0.51
1:C:222:ASP:OD1	1:C:315:LYS:NZ	2.43	0.51
2:P:57:LEU:N	2:Q:57:LEU:CD2	2.74	0.51
2:X:221:TYR:O	2:X:225:ILE:N	2.38	0.51
1:L:305:MET:SD	1:L:335:ARG:HB3	2.51	0.50
4:U:41:ILE:HD12	4:U:45:ARG:HE	1.76	0.50
5:V:12:LEU:HD13	5:V:20:PHE:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:94:GLU:O	5:V:150:TYR:OH	2.28	0.50
2:W:57:LEU:N	2:X:57:LEU:CD2	2.74	0.50
1:D:333:PRO:C	1:D:335:ARG:H	2.13	0.50
1:F:136:ILE:HB	1:F:139:VAL:HG13	1.93	0.50
1:O:210:ARG:HA	1:O:213:LYS:HE3	1.92	0.50
2:Q:221:TYR:O	2:Q:225:ILE:N	2.38	0.50
5:V:104:PHE:HB3	5:V:112:ILE:HG12	1.93	0.50
1:B:335:ARG:C	1:B:337:TYR:H	2.14	0.50
1:F:109:PRO:HD2	1:F:161:HIS:NE2	2.27	0.50
1:K:107:GLU:OE2	1:K:116:ARG:NE	2.45	0.50
1:L:227:MET:HB3	1:L:255:PHE:HZ	1.76	0.50
3:T:261:ILE:HA	3:T:264:LEU:HD12	1.93	0.50
1:A:207:GLU:CA	1:A:210:ARG:HG2	2.36	0.50
1:J:307:PRO:HB3	2:X:244:ARG:NH1	2.27	0.50
2:X:246:VAL:O	2:X:250:GLU:N	2.45	0.50
1:I:106:THR:O	1:I:107:GLU:CG	2.59	0.50
3:T:243:LEU:HD22	4:U:111:ARG:HE	1.77	0.50
1:A:80:ASP:OD2	1:A:84:LYS:NZ	2.45	0.50
1:A:109:PRO:CG	1:A:161:HIS:NE2	2.75	0.50
1:I:257:CYS:CB	1:I:258:PRO:HD3	2.42	0.50
1:K:230:ALA:HB3	1:K:255:PHE:HZ	1.76	0.50
3:T:265:ARG:HA	3:T:268:ILE:HD12	1.93	0.50
4:U:103:ARG:CZ	4:U:107:VAL:HB	2.42	0.50
1:C:188:TYR:CZ	1:C:266:PHE:CG	3.00	0.50
1:D:252:ASN:HA	1:D:255:PHE:HE2	1.61	0.50
1:K:221:LEU:HD11	2:Q:248:LYS:HZ3	1.77	0.50
4:U:137:GLY:C	4:U:139:PHE:H	2.15	0.50
1:C:207:GLU:CA	1:C:210:ARG:HG2	2.41	0.49
1:E:332:PRO:O	1:E:335:ARG:HB3	2.12	0.49
3:T:263:VAL:HG11	5:V:101:PHE:CE2	2.47	0.49
1:D:332:PRO:O	1:D:335:ARG:CG	2.38	0.49
1:H:207:GLU:O	1:H:210:ARG:CG	2.60	0.49
3:T:230:ARG:HG2	4:U:85:LEU:HB3	1.94	0.49
1:D:207:GLU:O	1:D:210:ARG:HG3	2.11	0.49
1:D:305:MET:HE2	1:D:335:ARG:CB	2.42	0.49
1:F:187:ASP:OD2	1:F:191:LYS:NZ	2.44	0.49
1:N:230:ALA:HB3	1:N:255:PHE:CZ	2.41	0.49
1:C:257:CYS:CB	1:C:258:PRO:HD3	2.42	0.49
1:L:187:ASP:OD2	1:L:191:LYS:NZ	2.46	0.49
3:T:263:VAL:CG1	5:V:150:TYR:HB2	2.43	0.49
4:U:61:LEU:N	5:V:103:MET:HG3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:HD2	1:B:253:GLU:CD	2.33	0.49
3:T:243:LEU:HD22	4:U:108:ASP:HA	1.95	0.49
4:U:155:MET:HG3	4:U:163:ALA:HB1	1.94	0.49
2:P:162:TYR:HE1	2:Q:165:VAL:HG11	1.78	0.49
1:E:167:GLU:O	1:E:169:TYR:CD1	2.65	0.49
1:G:305:MET:SD	1:G:335:ARG:CD	3.01	0.49
1:K:14:SER:N	1:K:157:ASP:OD2	2.46	0.49
1:O:352:PHE:CD1	1:O:355:MET:HB2	2.48	0.49
5:V:39:LYS:CA	2:W:149:LYS:HZ1	2.26	0.49
1:N:230:ALA:CB	1:N:255:PHE:CZ	2.96	0.49
1:O:207:GLU:O	1:O:210:ARG:HG2	2.12	0.49
1:F:188:TYR:CZ	1:F:266:PHE:CD2	3.00	0.48
1:I:133:TYR:CG	1:I:352:PHE:CZ	2.92	0.48
1:J:252:ASN:HB2	1:J:255:PHE:CE1	2.46	0.48
1:K:80:ASP:OD2	1:K:84:LYS:NZ	2.45	0.48
4:U:110:GLU:O	4:U:114:ILE:HG12	2.13	0.48
1:C:30:VAL:HG21	1:C:337:TYR:CZ	2.48	0.48
2:W:39:LEU:O	2:W:43:LEU:N	2.46	0.48
1:A:335:ARG:O	1:A:337:TYR:N	2.44	0.48
1:L:139:VAL:CG1	1:L:143:TYR:HE1	2.26	0.48
1:J:207:GLU:O	1:J:210:ARG:CG	2.62	0.48
2:Q:246:VAL:O	2:Q:250:GLU:N	2.45	0.48
3:T:254:PHE:CE1	4:U:117:LYS:HB3	2.48	0.48
5:V:137:MET:SD	5:V:148:ILE:HG13	2.54	0.48
5:V:143:ASN:ND2	5:V:152:GLU:OE2	2.47	0.48
1:L:109:PRO:HD2	1:L:161:HIS:CE1	2.48	0.48
1:L:143:TYR:OH	1:N:47:MET:HE3	2.13	0.48
2:P:39:LEU:O	2:P:43:LEU:N	2.46	0.48
1:F:6:THR:CG2	4:U:146:ARG:HH12	2.22	0.48
2:Q:11:LEU:N	2:Q:14:ASP:OD2	2.47	0.48
4:U:61:LEU:HD22	5:V:99:ASP:HB3	1.94	0.48
2:X:11:LEU:N	2:X:14:ASP:OD2	2.47	0.48
1:B:133:TYR:CE1	1:B:355:MET:HB3	2.49	0.48
1:F:305:MET:HE1	1:F:335:ARG:HG3	1.96	0.48
5:V:9:VAL:HA	5:V:12:LEU:HG	1.96	0.48
5:V:39:LYS:N	2:W:149:LYS:HZ1	2.02	0.48
5:V:142:LYS:HG2	5:V:152:GLU:HG2	1.95	0.48
1:J:305:MET:SD	1:J:335:ARG:HB3	2.52	0.48
1:O:80:ASP:OD2	1:O:84:LYS:NZ	2.47	0.48
1:B:133:TYR:CG	1:B:352:PHE:HZ	2.31	0.48
1:H:207:GLU:HA	1:H:210:ARG:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:287:ILE:HA	1:N:290:ARG:CD	2.44	0.48
3:T:243:LEU:HD13	4:U:108:ASP:HB2	1.95	0.48
5:V:27:PHE:CG	5:V:44:VAL:HG21	2.48	0.48
1:B:250:ILE:CG2	1:B:254:ARG:HG3	2.40	0.48
1:F:335:ARG:C	1:F:337:TYR:H	2.17	0.48
1:K:289:ILE:HG12	1:M:63:GLY:HA3	1.96	0.48
1:C:290:ARG:CG	1:E:244:ASP:HB3	2.43	0.47
1:H:262:PHE:CZ	1:H:312:ARG:HG2	2.48	0.47
1:H:305:MET:SD	1:H:335:ARG:HB2	2.54	0.47
1:L:257:CYS:HB3	1:L:258:PRO:HD3	1.96	0.47
3:T:268:ILE:HG13	4:U:132:ILE:HD11	1.96	0.47
1:B:335:ARG:H	1:B:335:ARG:HG2	1.44	0.47
1:G:252:ASN:HB2	1:G:255:PHE:CE2	2.49	0.47
1:G:335:ARG:C	1:G:337:TYR:H	2.17	0.47
1:H:257:CYS:CB	1:H:258:PRO:HD3	2.44	0.47
1:J:133:TYR:CG	1:J:352:PHE:HZ	2.32	0.47
1:K:334:GLU:O	1:K:338:SER:HB3	2.14	0.47
3:T:227:ASP:OD1	3:T:227:ASP:N	2.47	0.47
5:V:28:VAL:HG12	5:V:40:GLU:HG2	1.96	0.47
2:X:127:MET:O	2:X:131:GLU:N	2.45	0.47
1:A:133:TYR:CG	1:A:352:PHE:HZ	2.25	0.47
1:A:326:LYS:CE	2:Q:47:GLN:HE22	2.24	0.47
1:F:139:VAL:HG23	1:F:140:LEU:HG	1.95	0.47
1:H:207:GLU:CA	1:H:210:ARG:HG2	2.42	0.47
1:C:219:VAL:HG23	1:C:306:TYR:HB3	1.96	0.47
1:I:87:HIS:CE1	1:I:91:TYR:CD2	3.02	0.47
3:T:241:TYR:CD1	4:U:80:CYS:HB3	2.49	0.47
3:T:244:GLU:HG2	4:U:107:VAL:HG21	1.95	0.47
1:A:109:PRO:HG2	1:A:161:HIS:NE2	2.29	0.47
1:D:116:ARG:NH1	1:D:375:PHE:CE1	2.82	0.47
1:E:108:ALA:HB1	1:E:161:HIS:CE1	2.49	0.47
1:J:133:TYR:CE1	1:J:355:MET:HB3	2.50	0.47
1:M:335:ARG:C	1:M:337:TYR:H	2.17	0.47
1:B:56:ASP:OD1	1:B:56:ASP:N	2.46	0.47
1:G:80:ASP:OD2	1:G:84:LYS:NZ	2.48	0.47
4:U:60:GLU:HA	4:U:63:ARG:HG3	1.97	0.47
5:V:30:GLY:O	5:V:39:LYS:NZ	2.37	0.47
2:W:78:ALA:O	2:W:82:GLU:N	2.47	0.47
1:F:4:GLU:O	1:F:6:THR:N	2.46	0.47
1:F:336:LYS:HG2	1:F:337:TYR:CD1	2.49	0.47
1:B:133:TYR:HE2	1:B:346:LEU:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:MET:CE	1:D:335:ARG:CB	2.81	0.47
1:C:303:THR:O	1:C:306:TYR:CD1	2.68	0.46
1:D:335:ARG:C	1:D:337:TYR:H	2.17	0.46
1:C:18:LYS:HG2	1:C:337:TYR:HE1	1.80	0.46
1:E:305:MET:SD	1:E:336:LYS:CD	3.03	0.46
1:J:252:ASN:CB	1:J:255:PHE:HZ	2.27	0.46
1:K:133:TYR:CG	1:K:352:PHE:CZ	2.95	0.46
1:M:196:ARG:HD2	1:M:253:GLU:OE2	2.15	0.46
1:G:333:PRO:C	1:G:335:ARG:H	2.18	0.46
1:J:307:PRO:CG	2:X:244:ARG:NH1	2.77	0.46
1:H:305:MET:SD	1:H:335:ARG:CB	3.03	0.46
1:O:352:PHE:HD1	1:O:355:MET:HG3	1.80	0.46
2:P:78:ALA:O	2:P:82:GLU:N	2.47	0.46
2:P:85:VAL:O	2:P:89:ASN:N	2.45	0.46
5:V:116:GLU:N	5:V:116:GLU:OE1	2.49	0.46
5:V:137:MET:HA	5:V:148:ILE:HD11	1.97	0.46
1:O:352:PHE:CE1	1:O:355:MET:HG3	2.50	0.46
2:P:53:THR:CA	2:Q:57:LEU:HD11	2.39	0.46
3:T:200:LYS:O	3:T:204:GLU:HG2	2.15	0.46
3:T:232:LYS:O	3:T:235:GLU:HG3	2.15	0.46
1:A:230:ALA:HB3	1:A:255:PHE:HZ	1.81	0.46
1:C:219:VAL:HG23	1:C:306:TYR:CB	2.45	0.46
1:K:230:ALA:CB	1:K:255:PHE:CE2	2.98	0.46
2:P:284:ILE:HD12	2:S:11:LEU:HB2	1.98	0.46
2:Q:265:LEU:O	2:Q:269:ALA:HB3	2.15	0.46
2:W:154:ILE:O	2:W:158:ALA:N	2.42	0.46
1:A:143:TYR:OH	1:C:45:VAL:N	2.47	0.46
1:F:108:ALA:HB1	1:F:161:HIS:CG	2.51	0.46
1:L:252:ASN:CB	1:L:255:PHE:HE2	2.27	0.46
2:P:149:LYS:HG2	2:P:153:HIS:NE2	2.30	0.46
2:X:265:LEU:O	2:X:269:ALA:HB3	2.16	0.46
1:J:332:PRO:O	1:J:335:ARG:CD	2.63	0.46
2:X:40:GLU:OE1	2:X:40:GLU:HA	2.16	0.46
1:C:219:VAL:O	1:C:220:ALA:HB3	2.16	0.46
1:H:334:GLU:O	1:H:338:SER:HB3	2.16	0.46
1:O:286:ASP:O	1:O:290:ARG:HG2	2.15	0.46
4:U:41:ILE:HD12	4:U:45:ARG:NE	2.30	0.46
2:W:274:LEU:HD13	2:X:274:LEU:HB3	1.98	0.46
1:F:257:CYS:CB	1:F:258:PRO:HD3	2.46	0.46
1:F:333:PRO:C	1:F:335:ARG:N	2.69	0.46
4:U:138:LYS:H	4:U:141:ARG:HH12	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:4:ILE:HG13	5:V:5:TYR:H	1.80	0.46
1:C:255:PHE:CE1	1:C:259:GLU:OE1	2.70	0.45
1:F:143:TYR:OH	1:H:44:MET:CB	2.64	0.45
1:F:169:TYR:OH	1:H:49:GLN:CB	2.62	0.45
1:H:154:ASP:O	1:H:155:SER:C	2.54	0.45
2:Q:214:TYR:O	2:Q:218:GLU:HG3	2.16	0.45
2:W:162:TYR:HE1	2:X:165:VAL:HG11	1.77	0.45
2:W:193:LEU:O	2:W:197:LEU:N	2.45	0.45
1:H:230:ALA:HB3	1:H:255:PHE:CZ	2.51	0.45
2:P:148:LEU:HD21	2:P:152:LYS:CE	2.46	0.45
1:H:283:MET:O	1:H:290:ARG:NH2	2.47	0.45
2:P:193:LEU:O	2:P:197:LEU:N	2.45	0.45
1:G:305:MET:SD	1:G:335:ARG:CB	3.05	0.45
2:Q:40:GLU:OE1	2:Q:40:GLU:HA	2.16	0.45
4:U:54:LEU:HD13	5:V:92:LYS:HD3	1.99	0.45
1:H:230:ALA:HB3	1:H:255:PHE:HZ	1.82	0.45
1:O:230:ALA:HB3	1:O:255:PHE:CZ	2.52	0.45
2:P:142:GLU:CA	2:P:145:GLU:OE2	2.58	0.45
3:T:226:GLU:HB3	3:T:230:ARG:NH1	2.32	0.45
4:U:148:ARG:HG2	5:V:83:ARG:NH2	2.32	0.45
5:V:134:GLU:OE2	5:V:138:LYS:NZ	2.34	0.45
1:A:230:ALA:HB3	1:A:255:PHE:CZ	2.52	0.45
1:E:154:ASP:N	1:E:154:ASP:OD1	2.45	0.45
1:H:110:LEU:CB	1:H:177:ARG:HG3	2.47	0.45
1:M:213:LYS:CD	1:M:306:TYR:OH	2.64	0.45
2:Q:127:MET:O	2:Q:131:GLU:N	2.45	0.45
5:V:27:PHE:CE2	5:V:40:GLU:HB3	2.52	0.45
5:V:38:THR:CA	2:W:149:LYS:HE2	2.37	0.45
2:W:284:ILE:HD12	2:Z:11:LEU:HB2	1.97	0.45
1:E:169:TYR:CZ	1:G:49:GLN:HG3	2.52	0.45
1:O:333:PRO:C	1:O:335:ARG:H	2.19	0.45
3:T:204:GLU:HA	3:T:207:LYS:HB2	1.99	0.45
3:T:262:ASN:HA	3:T:265:ARG:NH1	2.32	0.45
5:V:9:VAL:HG13	5:V:82:VAL:HG21	1.99	0.45
2:W:85:VAL:O	2:W:89:ASN:N	2.45	0.45
2:W:142:GLU:CA	2:W:145:GLU:OE2	2.58	0.45
1:C:218:TYR:HB3	1:C:307:PRO:HG2	1.98	0.45
1:E:333:PRO:C	1:E:335:ARG:H	2.20	0.45
1:H:333:PRO:C	1:H:335:ARG:N	2.69	0.45
1:J:219:VAL:O	1:J:220:ALA:HB3	2.17	0.45
2:P:101:ARG:O	2:P:105:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:207:GLU:O	1:J:210:ARG:HG2	2.17	0.45
1:J:301:GLY:C	1:J:336:LYS:HA	2.37	0.45
1:K:335:ARG:C	1:K:337:TYR:N	2.71	0.45
1:N:257:CYS:HB3	1:N:258:PRO:HD3	1.99	0.45
2:P:162:TYR:HE1	2:Q:165:VAL:CG1	2.30	0.45
5:V:65:ASP:OD2	5:V:70:GLY:N	2.27	0.45
2:X:214:TYR:O	2:X:218:GLU:HG3	2.16	0.45
2:X:246:VAL:O	2:X:250:GLU:HG3	2.16	0.45
1:B:227:MET:HB2	1:B:255:PHE:HE1	1.82	0.45
5:V:54:PRO:HB3	2:W:152:LYS:CE	2.46	0.45
5:V:141:ASP:N	5:V:148:ILE:HG12	2.32	0.45
5:V:153:PHE:HA	5:V:156:PHE:HB3	1.99	0.45
1:C:290:ARG:NH1	1:E:244:ASP:OD2	2.50	0.44
1:D:257:CYS:CB	1:D:258:PRO:HD3	2.47	0.44
1:H:262:PHE:CE2	1:H:312:ARG:HG2	2.52	0.44
3:T:252:GLU:HA	3:T:255:LYS:HE3	1.98	0.44
1:C:188:TYR:CZ	1:C:266:PHE:CB	2.99	0.44
1:C:308:GLY:HA2	1:C:311:ASP:OD2	2.18	0.44
1:K:4:GLU:OE2	1:K:4:GLU:HA	2.17	0.44
1:O:207:GLU:CA	1:O:210:ARG:HG2	2.43	0.44
2:Q:143:ILE:O	2:Q:147:GLN:HG3	2.18	0.44
2:Q:246:VAL:O	2:Q:250:GLU:HG3	2.16	0.44
2:W:101:ARG:O	2:W:105:ARG:HG3	2.16	0.44
2:W:162:TYR:HE1	2:X:165:VAL:CG1	2.30	0.44
1:D:207:GLU:O	1:D:210:ARG:HG2	2.18	0.44
1:D:227:MET:HA	1:D:255:PHE:CE1	2.53	0.44
1:N:335:ARG:C	1:N:337:TYR:N	2.70	0.44
4:U:152:ASP:OD1	4:U:153:ALA:N	2.51	0.44
2:W:210:GLN:O	2:W:214:TYR:CG	2.71	0.44
1:C:188:TYR:CD1	1:C:266:PHE:HB3	2.51	0.44
1:K:56:ASP:OD1	1:K:56:ASP:N	2.50	0.44
1:K:333:PRO:C	1:K:335:ARG:N	2.69	0.44
2:P:143:ILE:O	2:P:146:ILE:HG22	2.17	0.44
2:P:210:GLN:O	2:P:214:TYR:CG	2.70	0.44
4:U:106:LYS:NZ	4:U:110:GLU:HG3	2.32	0.44
4:U:113:ASP:O	4:U:117:LYS:HG3	2.16	0.44
1:M:207:GLU:CA	1:M:210:ARG:HG2	2.45	0.44
4:U:132:ILE:HG22	4:U:136:ARG:HH11	1.82	0.44
4:U:147:VAL:HG23	5:V:83:ARG:HH22	1.81	0.44
5:V:21:LYS:HD2	5:V:21:LYS:HA	1.80	0.44
2:W:214:TYR:HB3	2:X:214:TYR:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ILE:CD1	1:B:256:ARG:HD3	2.47	0.44
2:Q:237:THR:O	2:Q:241:PHE:N	2.46	0.44
2:Q:257:GLU:HA	2:Q:257:GLU:OE1	2.18	0.44
5:V:90:LYS:NZ	5:V:92:LYS:HB3	2.33	0.44
1:O:352:PHE:CG	1:O:352:PHE:O	2.71	0.44
1:F:227:MET:CB	1:F:255:PHE:HZ	2.30	0.44
2:P:218:GLU:OE1	2:Q:214:TYR:CE1	2.71	0.44
2:P:274:LEU:HD13	2:Q:274:LEU:HB3	1.98	0.44
1:B:133:TYR:CG	1:B:352:PHE:CZ	3.06	0.44
1:C:287:ILE:O	1:C:290:ARG:HG2	2.18	0.44
1:H:227:MET:HA	1:H:255:PHE:CE1	2.53	0.44
1:K:305:MET:HE2	1:K:335:ARG:CB	2.48	0.44
1:M:80:ASP:OD2	1:M:84:LYS:NZ	2.51	0.44
4:U:54:LEU:HD22	5:V:92:LYS:HE2	2.00	0.44
2:W:218:GLU:OE1	2:X:214:TYR:CE1	2.71	0.44
1:A:133:TYR:CE1	1:A:355:MET:HB3	2.53	0.43
1:A:207:GLU:O	1:A:210:ARG:HG3	2.17	0.43
1:F:244:ASP:N	1:F:244:ASP:OD1	2.51	0.43
1:J:332:PRO:O	1:J:335:ARG:HD3	2.17	0.43
1:B:207:GLU:O	1:B:210:ARG:HB3	2.18	0.43
1:F:139:VAL:HG23	1:F:140:LEU:HD23	2.00	0.43
1:H:87:HIS:C	1:H:91:TYR:HD2	2.21	0.43
2:P:214:TYR:HB3	2:Q:214:TYR:CB	2.48	0.43
3:T:257:GLN:HE22	4:U:122:ILE:HG13	1.83	0.43
5:V:40:GLU:HG3	5:V:43:LYS:HE2	2.00	0.43
5:V:150:TYR:O	5:V:154:LEU:HG	2.19	0.43
2:W:53:THR:HG22	2:X:57:LEU:HD12	2.01	0.43
1:C:258:PRO:CG	1:C:306:TYR:CE2	2.98	0.43
1:O:305:MET:SD	1:O:336:LYS:HD2	2.57	0.43
3:T:212:LEU:HD23	3:T:215:ARG:HH21	1.83	0.43
4:U:108:ASP:O	4:U:111:ARG:HG3	2.18	0.43
4:U:151:ALA:O	4:U:155:MET:HB2	2.18	0.43
1:B:208:ILE:HD13	1:B:208:ILE:HA	1.79	0.43
1:N:80:ASP:OD2	1:N:84:LYS:NZ	2.51	0.43
2:P:214:TYR:HB3	2:Q:214:TYR:HB2	2.00	0.43
3:T:241:TYR:CE2	4:U:76:LEU:HB3	2.53	0.43
4:U:66:GLU:HA	4:U:69:ARG:HG3	2.00	0.43
5:V:136:LEU:HD22	5:V:156:PHE:HE1	1.83	0.43
1:G:335:ARG:O	1:G:337:TYR:N	2.47	0.43
1:K:162:ASN:ND2	1:K:281:SER:OG	2.51	0.43
1:K:257:CYS:CB	1:K:258:PRO:HD3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:229:LEU:HB3	4:U:93:LEU:HB3	2.01	0.43
4:U:63:ARG:HA	4:U:66:GLU:OE1	2.18	0.43
1:C:290:ARG:CG	1:E:244:ASP:CB	2.95	0.43
1:L:333:PRO:C	1:L:335:ARG:N	2.70	0.43
4:U:145:ARG:H	4:U:148:ARG:NH2	2.17	0.43
5:V:126:GLU:HG2	5:V:127:THR:H	1.82	0.43
2:X:257:GLU:HA	2:X:257:GLU:OE1	2.18	0.43
1:B:302:GLY:C	1:B:304:THR:H	2.21	0.43
1:H:83:GLU:O	1:H:87:HIS:CG	2.72	0.43
1:H:335:ARG:C	1:H:337:TYR:N	2.72	0.43
1:I:336:LYS:HG2	1:I:337:TYR:CD1	2.53	0.43
1:K:230:ALA:CB	1:K:255:PHE:CZ	3.02	0.43
1:N:31:PHE:CZ	1:N:93:GLU:HG2	2.54	0.43
3:T:247:LYS:HB2	4:U:111:ARG:HB3	2.01	0.43
4:U:165:GLU:HB3	5:V:16:GLN:NE2	2.31	0.43
2:W:214:TYR:HB3	2:X:214:TYR:HB2	2.00	0.43
1:B:262:PHE:CE2	1:B:312:ARG:HG2	2.54	0.43
1:K:109:PRO:HD2	1:K:161:HIS:CD2	2.54	0.43
3:T:100:ASN:OD1	3:T:100:ASN:N	2.52	0.43
3:T:264:LEU:HD22	4:U:128:LEU:HB2	2.00	0.43
1:H:219:VAL:O	1:H:220:ALA:HB3	2.17	0.43
1:I:87:HIS:O	1:I:91:TYR:CD2	2.69	0.43
1:L:219:VAL:O	1:L:220:ALA:HB3	2.18	0.43
2:P:53:THR:HG22	2:Q:57:LEU:HD12	2.00	0.43
3:T:240:ILE:O	3:T:244:GLU:HG2	2.19	0.43
5:V:72:VAL:HA	5:V:76:GLU:OE1	2.18	0.43
2:X:232:LEU:O	2:X:236:GLU:N	2.47	0.43
1:D:56:ASP:OD1	1:D:56:ASP:N	2.50	0.43
1:N:334:GLU:O	1:N:338:SER:HB3	2.18	0.43
4:U:152:ASP:O	4:U:156:GLN:HG2	2.19	0.43
1:F:334:GLU:OE1	1:F:334:GLU:N	2.49	0.42
1:J:133:TYR:CG	1:J:352:PHE:CZ	3.06	0.42
1:N:270:GLU:OE2	1:O:66:THR:HA	2.19	0.42
1:O:335:ARG:C	1:O:337:TYR:H	2.22	0.42
2:X:237:THR:O	2:X:241:PHE:N	2.46	0.42
2:X:263:GLN:O	2:X:267:TYR:N	2.45	0.42
1:F:334:GLU:O	1:F:338:SER:HB3	2.19	0.42
1:M:333:PRO:C	1:M:335:ARG:H	2.21	0.42
3:T:219:LEU:HB2	4:U:101:HIS:ND1	2.34	0.42
1:C:255:PHE:CD1	1:C:255:PHE:C	2.92	0.42
1:H:86:TRP:CZ3	1:H:122:ILE:HD13	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:275:HIS:ND1	1:O:275:HIS:N	2.66	0.42
2:P:146:ILE:CG2	2:P:147:GLN:N	2.82	0.42
3:T:221:ILE:HG22	3:T:224:LEU:HD12	2.01	0.42
3:T:256:GLN:HB2	4:U:68:ARG:HH12	1.83	0.42
4:U:74:ARG:O	4:U:78:THR:HG23	2.20	0.42
1:L:285:CYS:O	1:L:290:ARG:NE	2.52	0.42
1:O:219:VAL:O	1:O:220:ALA:HB3	2.20	0.42
5:V:41:LEU:O	5:V:45:MET:HG2	2.19	0.42
5:V:65:ASP:OD2	5:V:69:SER:N	2.52	0.42
2:X:54:GLU:O	2:X:57:LEU:HB2	2.20	0.42
1:G:26:ALA:CA	1:G:340:TRP:CZ3	3.02	0.42
3:T:219:LEU:HD23	4:U:98:ARG:CZ	2.49	0.42
3:T:219:LEU:HD23	4:U:98:ARG:NE	2.34	0.42
5:V:121:LEU:O	5:V:128:ILE:HG13	2.19	0.42
1:E:196:ARG:HD2	1:E:253:GLU:CD	2.39	0.42
1:F:23:GLY:O	4:U:144:LEU:O	2.38	0.42
4:U:138:LYS:H	4:U:141:ARG:HH22	1.67	0.42
2:W:144:GLN:O	2:W:148:LEU:N	2.53	0.42
2:X:162:TYR:O	2:X:166:ALA:N	2.52	0.42
1:F:3:ASP:OD1	1:F:3:ASP:N	2.41	0.42
1:L:227:MET:CB	1:L:255:PHE:HZ	2.33	0.42
2:Q:50:LEU:O	2:Q:54:GLU:N	2.52	0.42
3:T:225:ASN:O	3:T:229:LEU:HG	2.20	0.42
3:T:234:LYS:HE2	4:U:83:LEU:HB2	2.01	0.42
1:A:108:ALA:HB1	1:A:161:HIS:ND1	2.35	0.42
1:B:258:PRO:HB3	1:B:306:TYR:CZ	2.54	0.42
1:B:306:TYR:HB2	1:B:309:ILE:HB	2.02	0.42
1:F:6:THR:HG21	4:U:146:ARG:NH1	2.28	0.42
2:P:156:GLU:CG	2:P:160:ARG:NH2	2.81	0.42
4:U:43:ALA:HB3	5:V:6:LYS:CG	2.49	0.42
4:U:159:LEU:HG	4:U:162:ARG:HB2	2.02	0.42
5:V:126:GLU:O	5:V:128:ILE:HG12	2.20	0.42
1:E:169:TYR:HH	1:G:49:GLN:HB3	1.81	0.42
2:Q:277:ALA:O	2:Q:281:MET:N	2.40	0.42
5:V:54:PRO:HB2	2:W:152:LYS:NZ	2.34	0.42
2:W:56:GLU:C	2:X:57:LEU:CD2	2.89	0.42
1:A:335:ARG:H	1:A:335:ARG:HG2	1.60	0.42
1:C:333:PRO:C	1:C:335:ARG:N	2.70	0.42
1:J:169:TYR:CZ	1:L:49:GLN:HG3	2.55	0.42
1:L:107:GLU:OE1	1:L:116:ARG:HB3	2.20	0.42
1:M:154:ASP:O	1:M:155:SER:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:162:TYR:O	2:Q:166:ALA:N	2.52	0.42
1:A:335:ARG:C	1:A:337:TYR:N	2.73	0.41
1:B:219:VAL:O	1:B:220:ALA:HB3	2.19	0.41
1:F:139:VAL:CG2	1:F:140:LEU:H	2.29	0.41
1:F:219:VAL:O	1:F:220:ALA:HB3	2.19	0.41
1:N:302:GLY:C	1:N:304:THR:H	2.23	0.41
1:O:154:ASP:O	1:O:156:GLY:N	2.51	0.41
1:O:212:ILE:HG12	1:O:240:TYR:CD2	2.55	0.41
2:Q:54:GLU:O	2:Q:57:LEU:HB2	2.20	0.41
4:U:56:ILE:HA	4:U:56:ILE:HD13	1.86	0.41
5:V:113:ASP:HB3	5:V:116:GLU:OE1	2.20	0.41
1:D:207:GLU:OE1	1:D:210:ARG:HD3	2.20	0.41
1:L:143:TYR:OH	1:N:44:MET:CB	2.43	0.41
1:M:305:MET:SD	1:M:335:ARG:CD	3.07	0.41
1:N:56:ASP:OD1	1:N:56:ASP:N	2.51	0.41
2:P:56:GLU:C	2:Q:57:LEU:CD2	2.89	0.41
4:U:43:ALA:HB3	5:V:6:LYS:HG3	2.01	0.41
4:U:53:LEU:HD22	5:V:104:PHE:HZ	1.85	0.41
5:V:122:GLN:HA	5:V:128:ILE:HG21	2.02	0.41
1:A:34:ILE:HD11	1:A:69:TYR:OH	2.20	0.41
1:J:207:GLU:O	1:J:210:ARG:HG3	2.20	0.41
1:K:302:GLY:C	1:K:304:THR:H	2.23	0.41
1:O:287:ILE:HA	1:O:290:ARG:HD3	2.02	0.41
3:T:234:LYS:NZ	4:U:83:LEU:H	2.19	0.41
4:U:63:ARG:HD2	4:U:64:GLU:N	2.36	0.41
1:B:250:ILE:CG2	1:B:254:ARG:CG	2.98	0.41
1:C:227:MET:HB3	1:C:255:PHE:CE2	2.55	0.41
1:E:56:ASP:OD1	1:E:56:ASP:N	2.53	0.41
1:F:143:TYR:OH	1:H:44:MET:CA	2.68	0.41
1:M:162:ASN:ND2	1:M:281:SER:OG	2.53	0.41
2:P:142:GLU:O	2:P:146:ILE:HG22	2.19	0.41
2:P:267:TYR:HB2	2:Q:267:TYR:HB3	2.02	0.41
4:U:57:ALA:HB3	5:V:100:LEU:HD22	2.02	0.41
4:U:137:GLY:HA3	4:U:141:ARG:NH2	2.33	0.41
5:V:106:LYS:HB2	5:V:116:GLU:HG3	2.02	0.41
2:W:148:LEU:HD21	2:W:152:LYS:CE	2.46	0.41
2:X:50:LEU:O	2:X:54:GLU:N	2.52	0.41
1:F:162:ASN:ND2	1:F:277:THR:OG1	2.54	0.41
1:I:275:HIS:ND1	1:I:275:HIS:N	2.67	0.41
1:J:116:ARG:HD2	1:J:371:HIS:CE1	2.56	0.41
1:L:113:LYS:O	1:L:116:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:326:LYS:HE2	2:Y:23:GLU:OE2	2.21	0.41
1:O:271:SER:OG	1:O:272:ALA:N	2.52	0.41
1:B:192:ILE:HD11	1:B:256:ARG:HD3	2.01	0.41
1:D:275:HIS:ND1	1:D:275:HIS:N	2.63	0.41
1:H:107:GLU:OE1	1:H:116:ARG:HB3	2.20	0.41
1:L:109:PRO:CD	1:L:161:HIS:NE2	2.80	0.41
4:U:95:ASP:OD1	4:U:99:GLN:NE2	2.54	0.41
5:V:121:LEU:HB3	5:V:128:ILE:HD12	2.03	0.41
1:F:2:GLU:OE1	1:F:21:PHE:CD2	2.71	0.41
1:I:87:HIS:NE2	1:I:91:TYR:CE2	2.85	0.41
1:I:219:VAL:O	1:I:220:ALA:HB3	2.21	0.41
1:J:275:HIS:CG	1:J:276:GLU:N	2.88	0.41
1:O:207:GLU:OE1	1:O:210:ARG:HD3	2.21	0.41
5:V:97:LEU:HD23	5:V:100:LEU:HD12	2.01	0.41
2:X:277:ALA:O	2:X:281:MET:N	2.40	0.41
1:F:159:VAL:HG21	1:F:177:ARG:NE	2.34	0.41
1:F:305:MET:HE2	1:F:335:ARG:C	2.41	0.41
1:K:221:LEU:HD21	1:K:311:ASP:CG	2.41	0.41
1:K:244:ASP:N	1:K:244:ASP:OD1	2.52	0.41
1:O:56:ASP:OD1	1:O:56:ASP:N	2.48	0.41
2:Q:263:GLN:O	2:Q:267:TYR:HB2	2.21	0.41
2:Q:263:GLN:O	2:Q:267:TYR:N	2.45	0.41
3:T:240:ILE:HG12	4:U:103:ARG:HG3	2.03	0.41
3:T:241:TYR:CZ	4:U:76:LEU:HB3	2.55	0.41
5:V:3:ASP:OD1	5:V:4:ILE:N	2.53	0.41
5:V:128:ILE:HA	5:V:128:ILE:HD13	1.85	0.41
1:C:207:GLU:O	1:C:210:ARG:HG2	2.19	0.41
1:F:227:MET:HB3	1:F:255:PHE:CZ	2.56	0.41
1:G:219:VAL:O	1:G:220:ALA:HB3	2.20	0.41
1:I:86:TRP:HE3	1:I:122:ILE:CD1	2.28	0.41
1:K:275:HIS:ND1	1:K:275:HIS:N	2.64	0.41
1:N:51:ASP:OD1	1:N:51:ASP:N	2.49	0.41
3:T:240:ILE:HA	4:U:107:VAL:HG11	2.03	0.41
3:T:264:LEU:HA	3:T:267:ARG:HD3	2.01	0.41
4:U:50:LYS:O	4:U:54:LEU:HG	2.21	0.41
4:U:53:LEU:HD13	5:V:157:MET:HE1	2.02	0.41
5:V:141:ASP:OD2	5:V:145:ASP:N	2.54	0.41
1:B:250:ILE:HG22	1:B:254:ARG:CG	2.44	0.41
1:J:56:ASP:OD1	1:J:56:ASP:N	2.52	0.41
1:K:305:MET:HE2	1:K:335:ARG:HB2	1.95	0.41
3:T:203:THR:HG22	3:T:207:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:175:ASP:O	2:X:179:ALA:N	2.47	0.41
2:X:263:GLN:O	2:X:267:TYR:HB2	2.21	0.41
1:A:283:MET:O	1:A:290:ARG:NE	2.54	0.40
1:G:263:GLN:N	1:G:264:PRO:HD3	2.36	0.40
1:O:335:ARG:H	1:O:335:ARG:HG2	1.69	0.40
3:T:215:ARG:HH12	4:U:112:TYR:HB2	1.86	0.40
4:U:53:LEU:HD21	5:V:121:LEU:HG	2.02	0.40
5:V:44:VAL:HG22	5:V:47:MET:HE3	2.03	0.40
1:A:107:GLU:OE2	1:A:116:ARG:NE	2.48	0.40
1:F:287:ILE:H	1:F:287:ILE:HD13	1.85	0.40
1:K:305:MET:CE	1:K:335:ARG:CB	2.92	0.40
1:M:155:SER:OG	1:M:303:THR:OG1	2.34	0.40
4:U:70:GLY:O	4:U:74:ARG:HG3	2.21	0.40
2:W:165:VAL:HG13	2:X:165:VAL:HG23	2.03	0.40
1:B:218:TYR:HB2	1:B:307:PRO:HB2	2.03	0.40
1:C:289:ILE:O	1:C:293:LEU:HG	2.21	0.40
1:D:176:MET:HB2	1:D:277:THR:OG1	2.21	0.40
1:E:109:PRO:CB	1:E:161:HIS:NE2	2.84	0.40
1:E:257:CYS:CB	1:E:258:PRO:HD3	2.49	0.40
1:G:6:THR:OG1	1:G:7:ALA:N	2.54	0.40
1:J:333:PRO:C	1:J:335:ARG:N	2.74	0.40
1:K:133:TYR:CE1	1:K:355:MET:HB3	2.57	0.40
1:L:107:GLU:OE2	1:L:116:ARG:NE	2.46	0.40
1:M:207:GLU:C	1:M:210:ARG:HG2	2.41	0.40
4:U:56:ILE:O	4:U:60:GLU:HG2	2.21	0.40
1:C:185:LEU:HD13	1:C:306:TYR:OH	2.21	0.40
1:C:303:THR:O	1:C:306:TYR:HD1	2.04	0.40
1:F:162:ASN:ND2	1:F:281:SER:OG	2.54	0.40
2:P:165:VAL:HG13	2:Q:165:VAL:HG23	2.03	0.40
2:X:134:ALA:O	2:X:138:GLU:N	2.49	0.40
1:A:219:VAL:O	1:A:220:ALA:HB3	2.22	0.40
1:A:333:PRO:C	1:A:335:ARG:N	2.74	0.40
1:F:21:PHE:CE1	1:F:28:ARG:NE	2.86	0.40
1:I:87:HIS:NE2	1:I:91:TYR:CD2	2.89	0.40
4:U:53:LEU:HD22	5:V:104:PHE:CZ	2.56	0.40
5:V:152:GLU:O	5:V:156:PHE:HB2	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	A	373/375 (100%)	361 (97%)	10 (3%)	2 (0%)	29	69
1	B	373/375 (100%)	360 (96%)	9 (2%)	4 (1%)	14	52
1	C	373/375 (100%)	362 (97%)	7 (2%)	4 (1%)	14	52
1	D	373/375 (100%)	361 (97%)	10 (3%)	2 (0%)	29	69
1	E	373/375 (100%)	363 (97%)	7 (2%)	3 (1%)	19	60
1	F	373/375 (100%)	361 (97%)	7 (2%)	5 (1%)	12	48
1	G	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	29	69
1	H	373/375 (100%)	362 (97%)	8 (2%)	3 (1%)	19	60
1	I	373/375 (100%)	361 (97%)	9 (2%)	3 (1%)	19	60
1	J	373/375 (100%)	357 (96%)	13 (4%)	3 (1%)	19	60
1	K	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	29	69
1	L	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	29	69
1	M	373/375 (100%)	362 (97%)	9 (2%)	2 (0%)	29	69
1	N	373/375 (100%)	363 (97%)	8 (2%)	2 (0%)	29	69
1	O	373/375 (100%)	359 (96%)	12 (3%)	2 (0%)	29	69
2	P	272/286 (95%)	272 (100%)	0	0	100	100
2	Q	272/286 (95%)	272 (100%)	0	0	100	100
2	R	27/286 (9%)	27 (100%)	0	0	100	100
2	S	27/286 (9%)	27 (100%)	0	0	100	100
2	W	272/286 (95%)	272 (100%)	0	0	100	100
2	X	272/286 (95%)	272 (100%)	0	0	100	100
2	Y	27/286 (9%)	27 (100%)	0	0	100	100
2	Z	27/286 (9%)	27 (100%)	0	0	100	100
3	T	122/186 (66%)	121 (99%)	1 (1%)	0	100	100
3	a	122/186 (66%)	120 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	U	124/170 (73%)	120 (97%)	4 (3%)	0	100	100
4	b	124/170 (73%)	115 (93%)	9 (7%)	0	100	100
5	V	158/160 (99%)	149 (94%)	9 (6%)	0	100	100
5	c	158/160 (99%)	139 (88%)	19 (12%)	0	100	100
All	All	7599/8945 (85%)	7368 (97%)	190 (2%)	41 (0%)	32	69

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	155	SER
1	J	155	SER
1	L	155	SER
1	M	155	SER
1	O	155	SER
1	D	360	GLN
1	E	360	GLN
1	I	360	GLN
1	J	360	GLN
1	D	155	SER
1	L	334	GLU
1	A	220	ALA
1	A	336	LYS
1	B	49	GLN
1	C	334	GLU
1	C	336	LYS
1	F	220	ALA
1	F	334	GLU
1	F	336	LYS
1	H	220	ALA
1	H	334	GLU
1	H	336	LYS
1	K	336	LYS
1	N	336	LYS
1	B	336	LYS
1	C	220	ALA
1	F	5	THR
1	I	49	GLN
1	I	336	LYS
1	J	220	ALA
1	K	334	GLU
1	O	220	ALA

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Mol	Chain	Res	Type
1	B	220	ALA
1	B	307	PRO
1	C	49	GLN
1	E	49	GLN
1	F	49	GLN
1	G	49	GLN
1	M	49	GLN
1	N	49	GLN
1	G	26	ALA

5.3.2 Protein sidechains [i](#)

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	A	318/318 (100%)	317 (100%)	1 (0%)	92	95
1	B	318/318 (100%)	314 (99%)	4 (1%)	69	81
1	C	318/318 (100%)	317 (100%)	1 (0%)	92	95
1	D	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	E	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	F	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	G	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	H	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	I	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	J	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	K	318/318 (100%)	318 (100%)	0	100	100
1	L	318/318 (100%)	317 (100%)	1 (0%)	92	95
1	M	318/318 (100%)	317 (100%)	1 (0%)	92	95
1	N	318/318 (100%)	318 (100%)	0	100	100
1	O	318/318 (100%)	317 (100%)	1 (0%)	92	95
2	P	236/246 (96%)	235 (100%)	1 (0%)	91	94
2	Q	236/246 (96%)	235 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	24/246 (10%)	23 (96%)	1 (4%)	30	54
2	S	24/246 (10%)	24 (100%)	0	100	100
2	W	236/246 (96%)	235 (100%)	1 (0%)	91	94
2	X	236/246 (96%)	235 (100%)	1 (0%)	91	94
2	Y	24/246 (10%)	23 (96%)	1 (4%)	30	54
2	Z	24/246 (10%)	24 (100%)	0	100	100
3	T	117/169 (69%)	116 (99%)	1 (1%)	78	87
3	a	117/169 (69%)	117 (100%)	0	100	100
4	U	106/145 (73%)	106 (100%)	0	100	100
4	b	106/145 (73%)	104 (98%)	2 (2%)	57	75
5	V	141/141 (100%)	140 (99%)	1 (1%)	84	90
5	c	141/141 (100%)	140 (99%)	1 (1%)	84	90
All	All	6538/7648 (86%)	6504 (100%)	34 (0%)	89	93

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	LYS
1	B	287	ILE
1	B	306	TYR
1	B	335	ARG
1	B	336	LYS
1	C	336	LYS
1	D	116	ARG
1	D	336	LYS
1	E	335	ARG
1	E	336	LYS
1	F	287	ILE
1	F	335	ARG
1	G	335	ARG
1	G	336	LYS
1	H	177	ARG
1	H	336	LYS
1	I	287	ILE
1	I	336	LYS
1	J	335	ARG
1	J	336	LYS
1	L	336	LYS

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Mol	Chain	Res	Type
1	M	336	LYS
1	O	336	LYS
2	P	15	LYS
2	Q	29	LYS
2	R	15	LYS
3	T	215	ARG
5	V	90	LYS
2	W	15	LYS
2	X	29	LYS
2	Y	15	LYS
4	b	112	TYR
4	b	139	PHE
5	c	39	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	162	ASN
1	H	87	HIS
1	I	87	HIS
1	K	162	ASN
1	N	162	ASN
1	O	162	ASN
2	Q	47	GLN
3	T	202	GLN
3	T	238	GLN
4	U	48	GLN
4	U	55	GLN
4	U	156	GLN
5	V	107	ASN
5	V	143	ASN
3	a	225	ASN
3	a	228	GLN
3	a	266	ASN
3	a	269	ASN
3	a	271	ASN
4	b	94	GLN
4	b	121	ASN
4	b	130	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 monosaccharides 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.

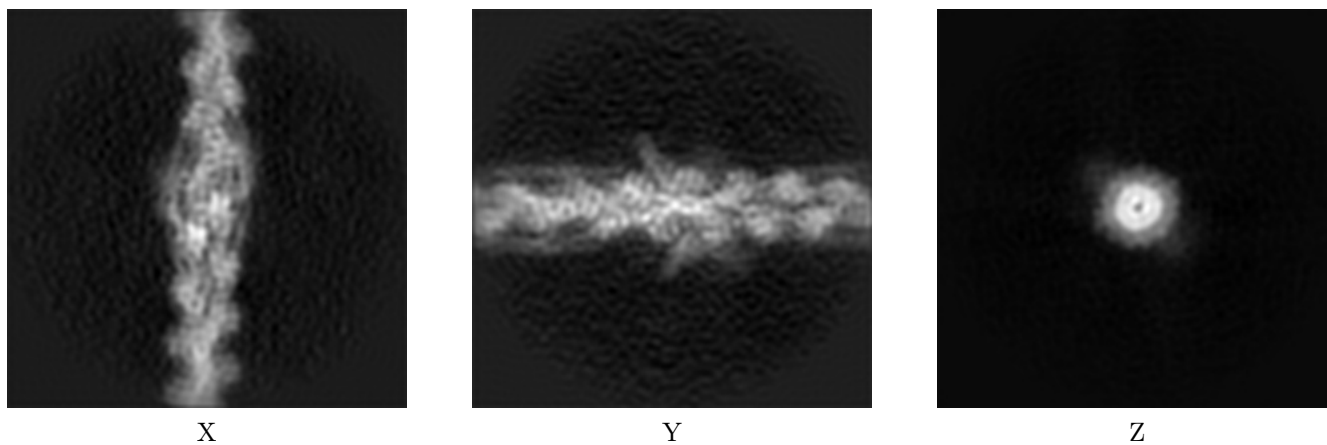
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22965. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

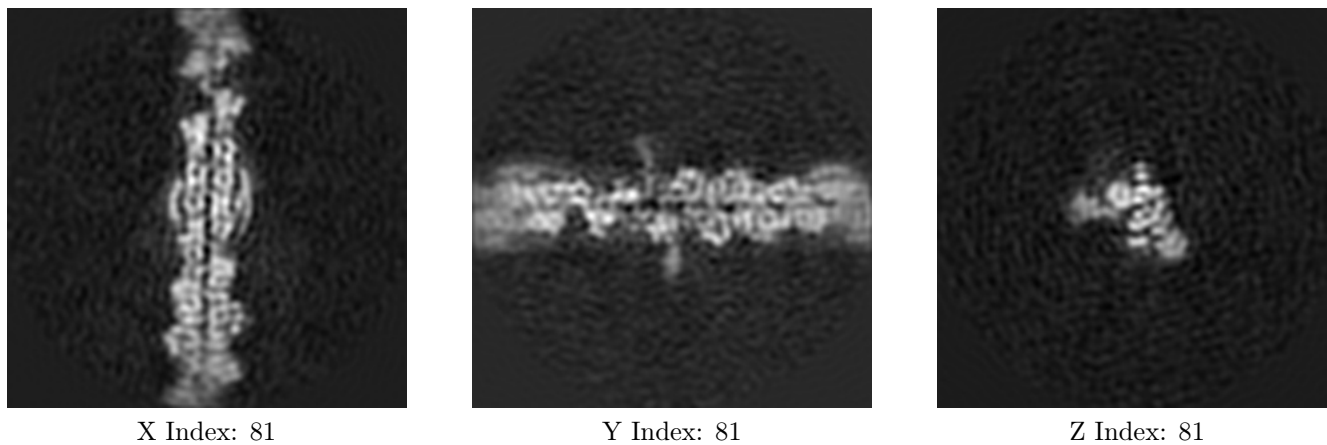
6.1.1 Primary map



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

6.2 Central slices [i](#)

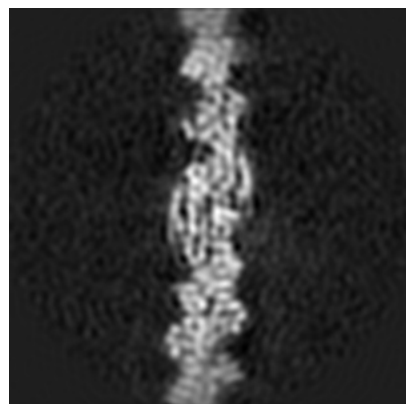
6.2.1 Primary map



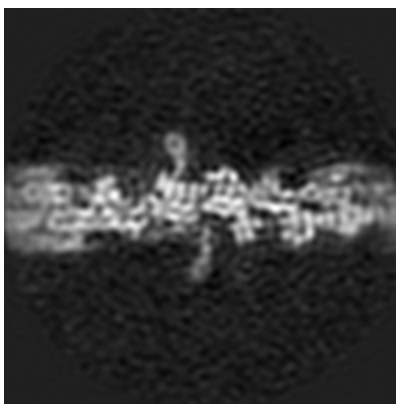
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

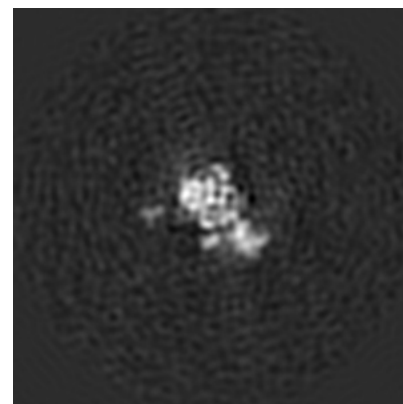
6.3.1 Primary map



X Index: 79



Y Index: 78

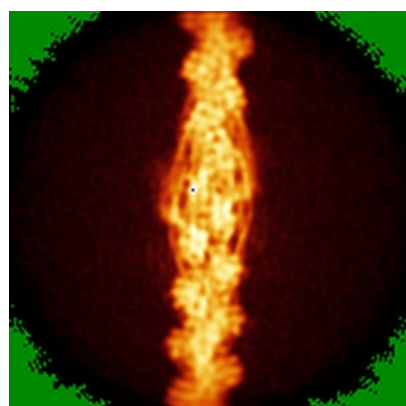


Z Index: 77

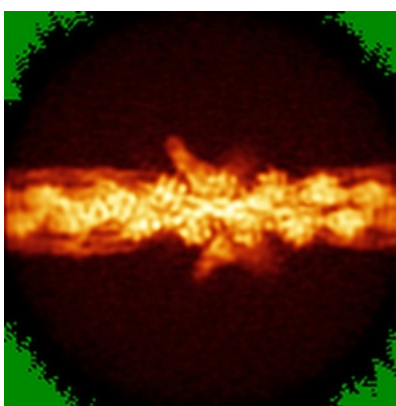
The images above show the largest variance slices of the map in three orthogonal directions.

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

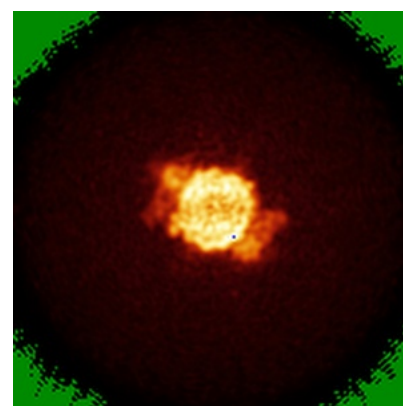
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

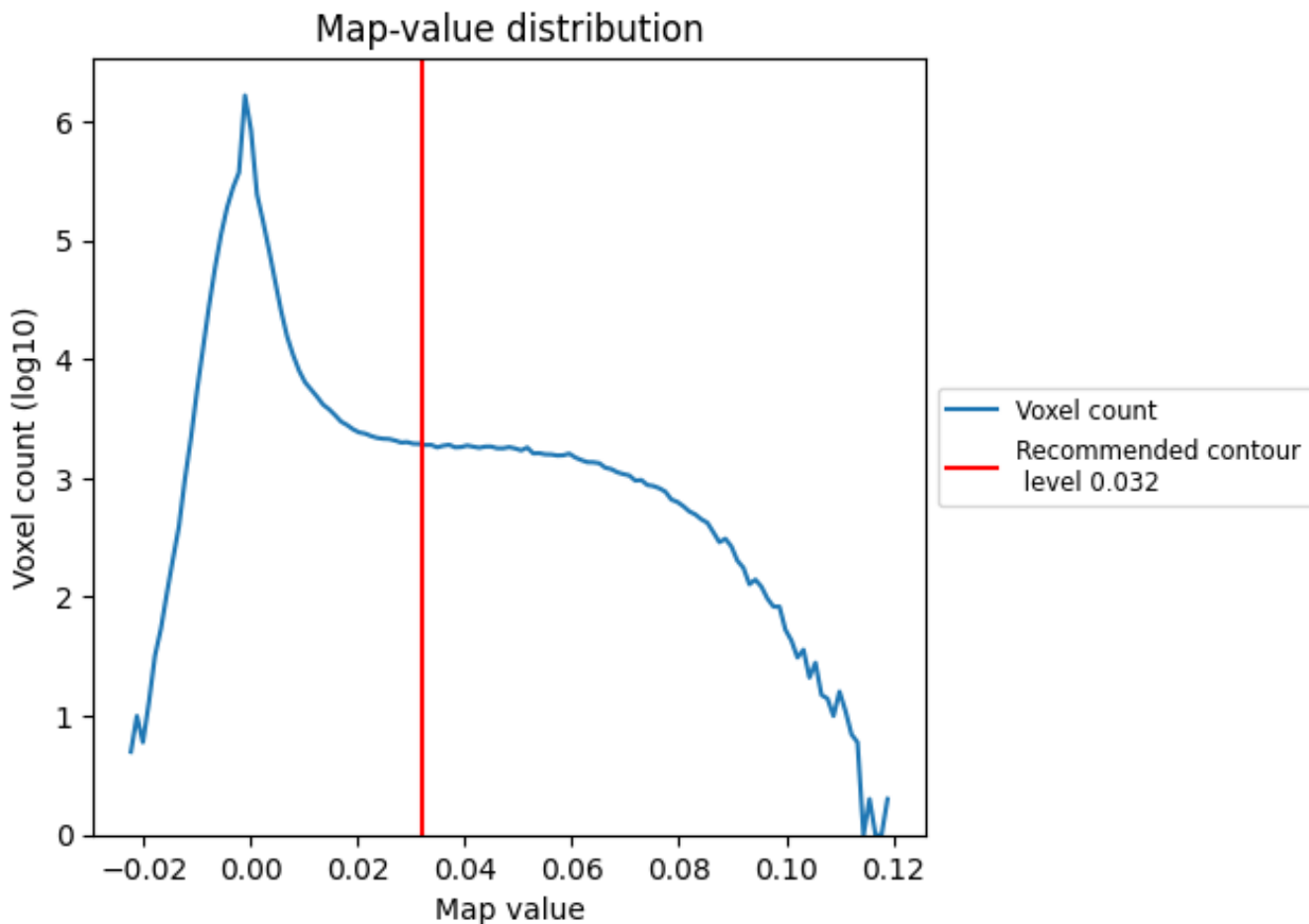
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

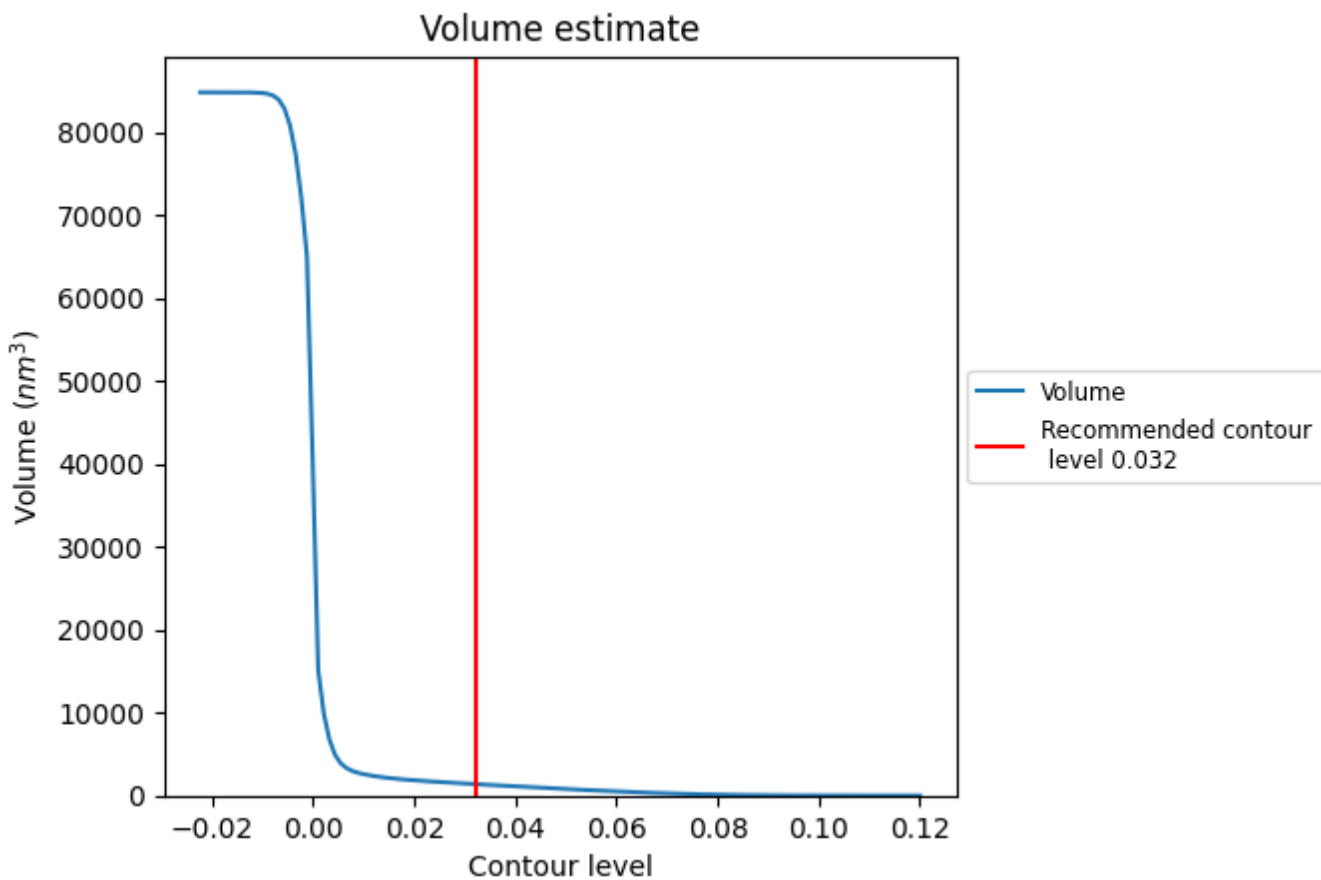
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

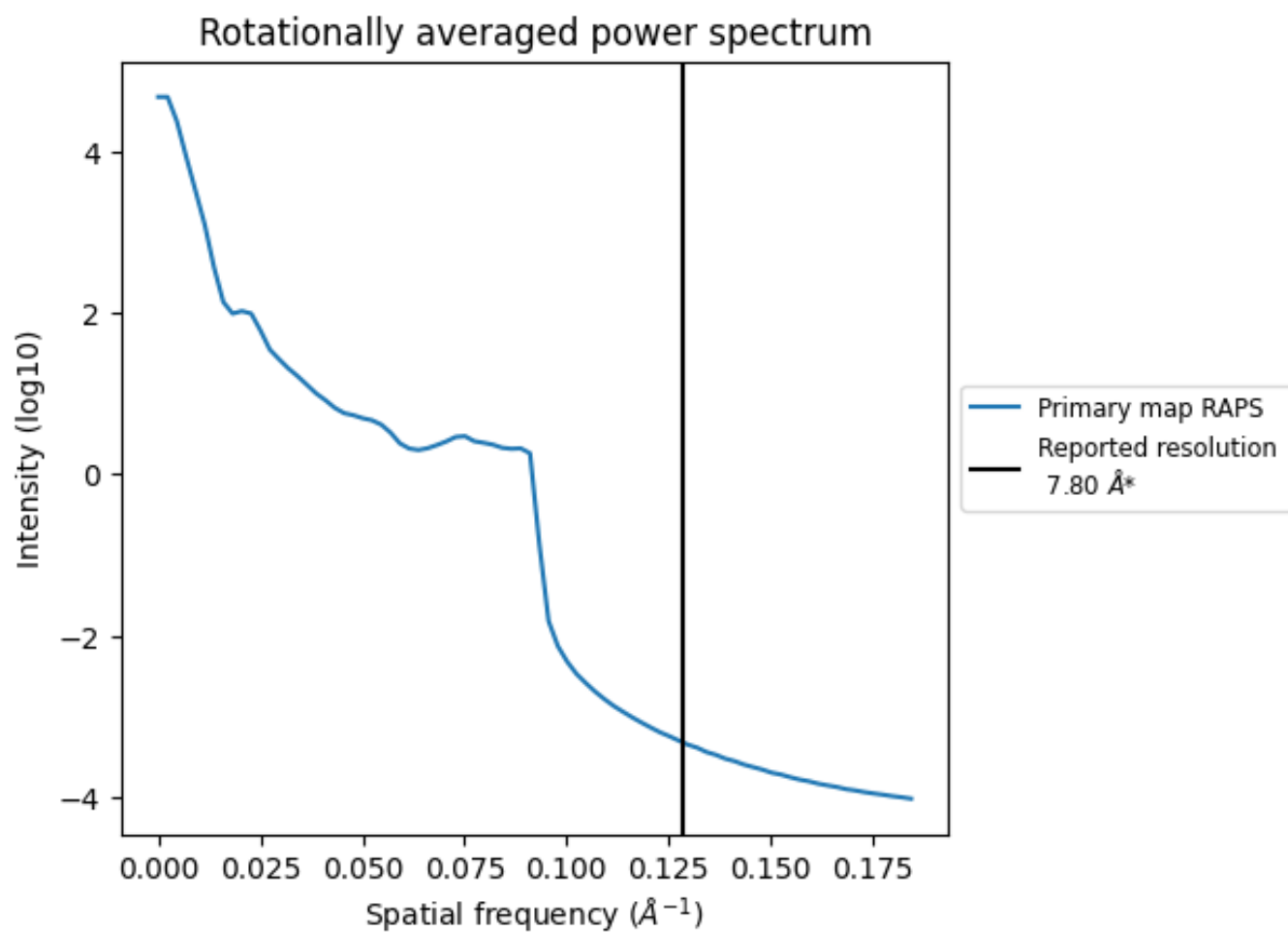
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1379 nm^3 ; this corresponds to an approximate mass of 1246 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 [i](#)

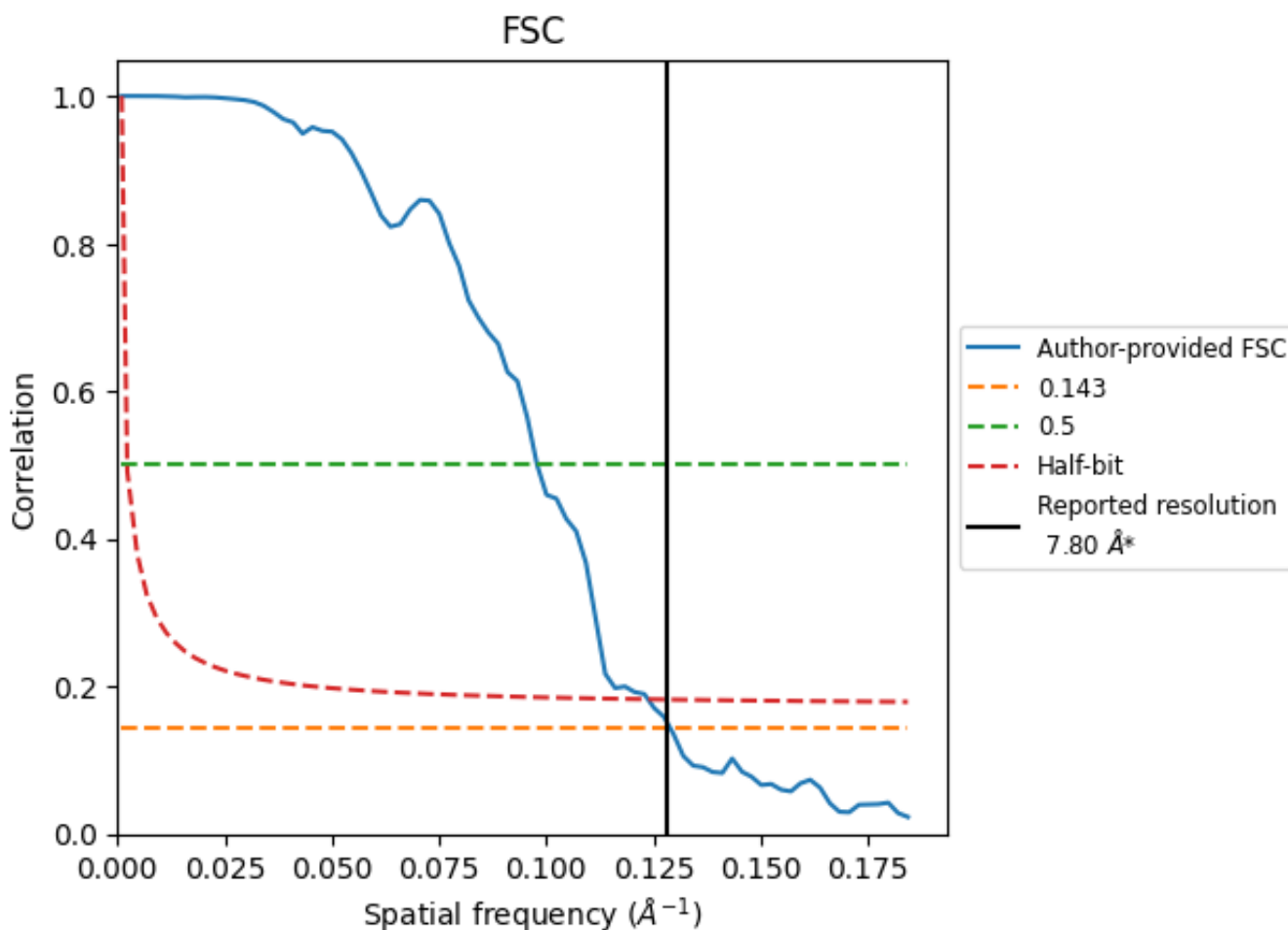


*Reported resolution corresponds to spatial frequency of 0.128\AA^{-1}

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 0.128 Å⁻¹

8.2 Resolution estimates [i](#)

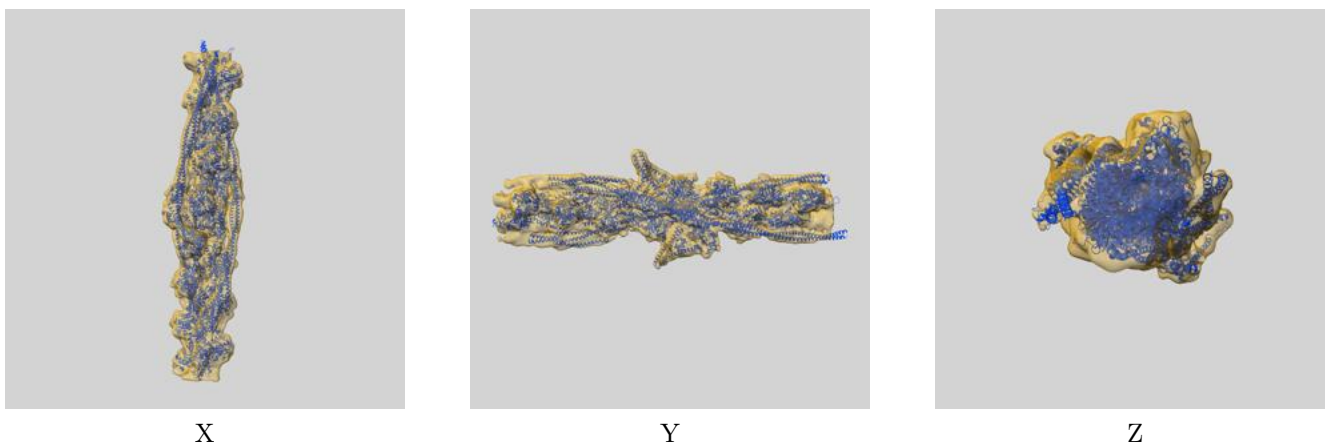
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	7.75	10.21	8.08
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

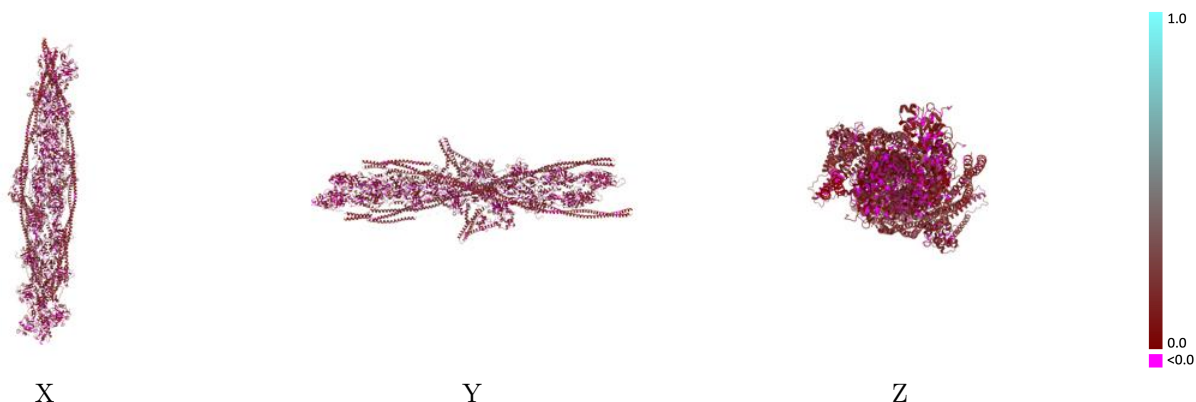
This section contains information regarding the fit between EMDB map EMD-22965 and PDB model 7KO5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



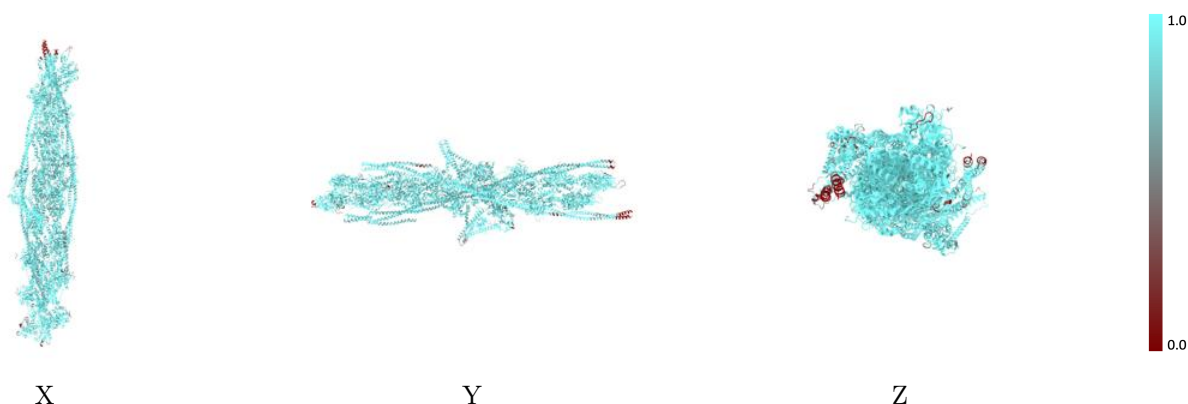
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



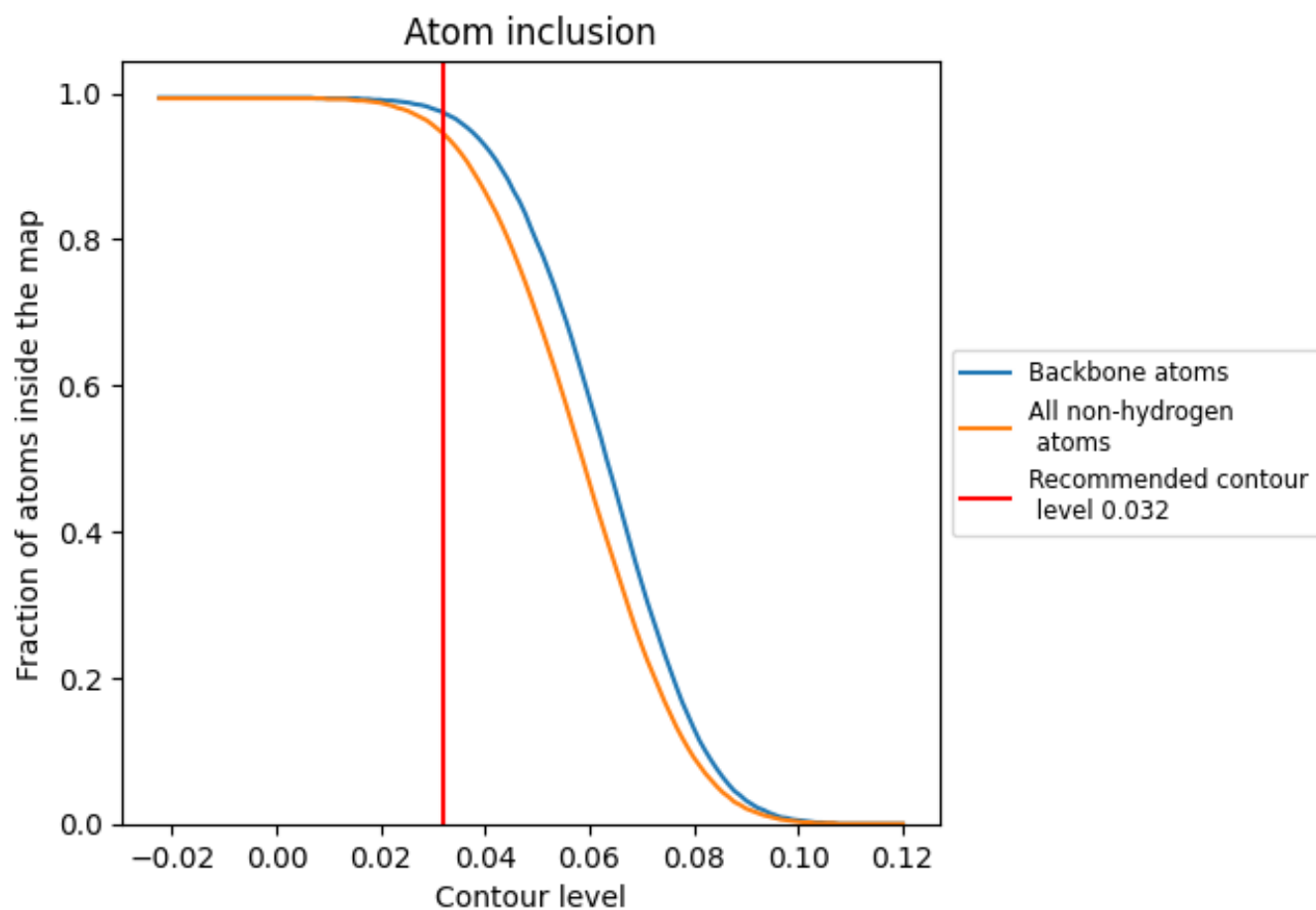
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.1130
A	 0.9470	 0.0870
B	 0.9910	 0.1020
C	 0.9890	 0.1040
D	 0.9790	 0.1010
E	 0.9710	 0.1040
F	 0.9650	 0.1080
G	 0.9670	 0.1140
H	 0.9760	 0.1020
I	 0.9750	 0.1030
J	 0.9800	 0.1010
K	 0.9810	 0.1070
L	 0.9620	 0.1030
M	 0.9840	 0.0950
N	 0.9680	 0.0930
O	 0.8800	 0.0600
P	 0.8970	 0.1560
Q	 0.9020	 0.1530
R	 0.9870	 0.1600
S	 0.8650	 0.1060
T	 0.8370	 0.1640
U	 0.8780	 0.1490
V	 0.9040	 0.1260
W	 0.8610	 0.1530
X	 0.8210	 0.1250
Y	 0.9390	 0.1790
Z	 0.9610	 0.1660
a	 0.8480	 0.1560
b	 0.9870	 0.1780
c	 0.9120	 0.1470

