



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 06:35 PM 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

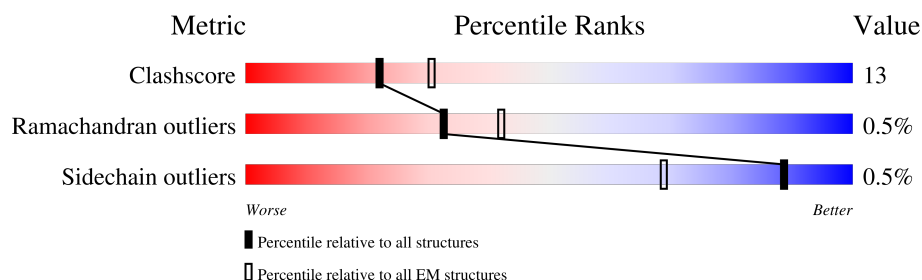
1 Overall quality at a glance

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.



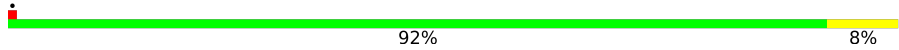
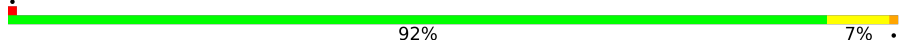
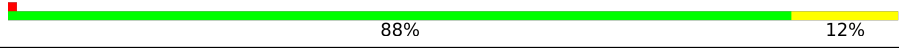
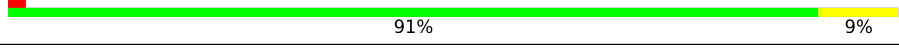
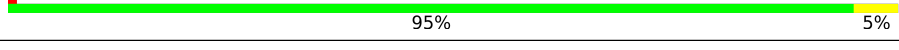
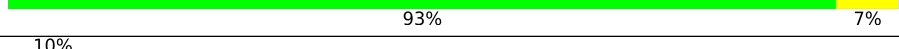
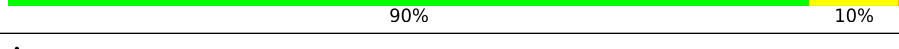
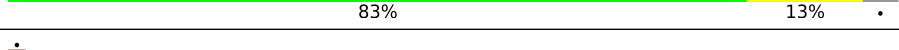
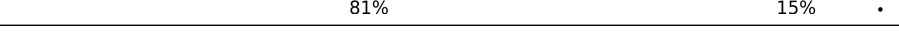
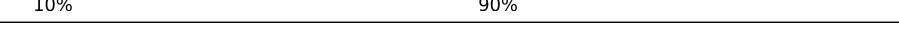

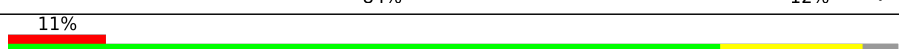


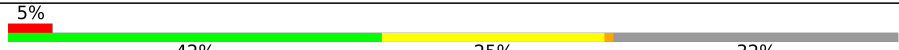

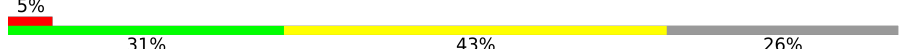


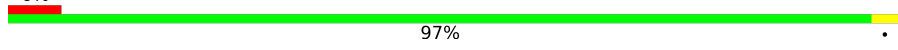

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	J	375	
1	K	375	
1	L	375	
1	M	375	
1	N	375	
1	O	375	
2	P	286	
2	Q	286	
2	R	286	
2	S	286	
2	W	286	
2	X	286	
2	Y	286	
2	Z	286	
3	T	186	
3	a	186	
4	U	170	
4	b	170	
5	V	160	
5	c	160	

2 Entry composition

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

- 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		

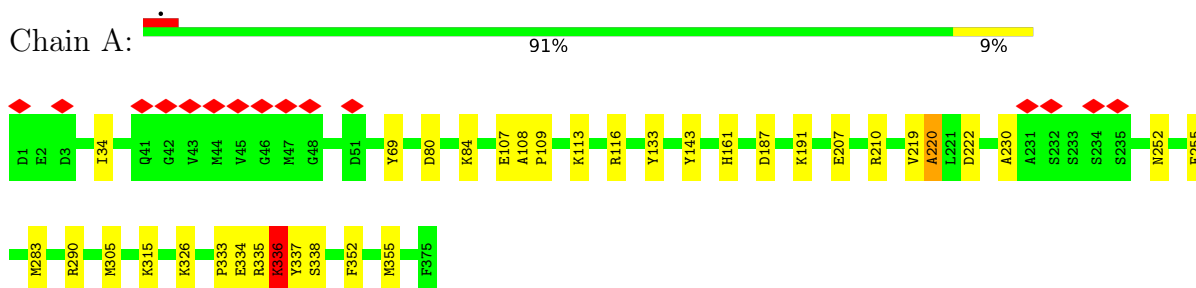
- Molecule 5 is a protein called Troponin C.

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		

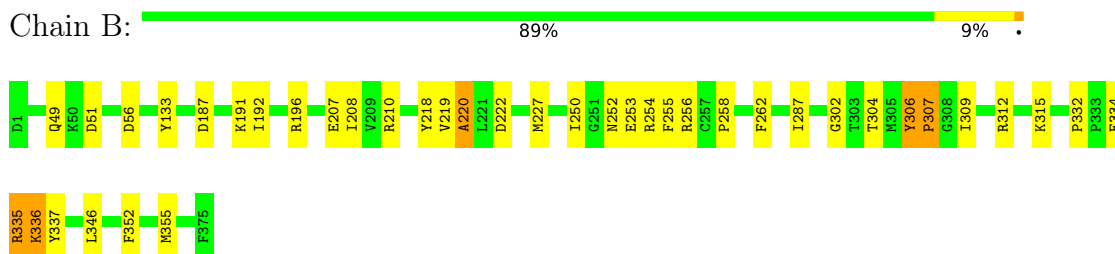
3 Residue-property plots [i](#)

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.

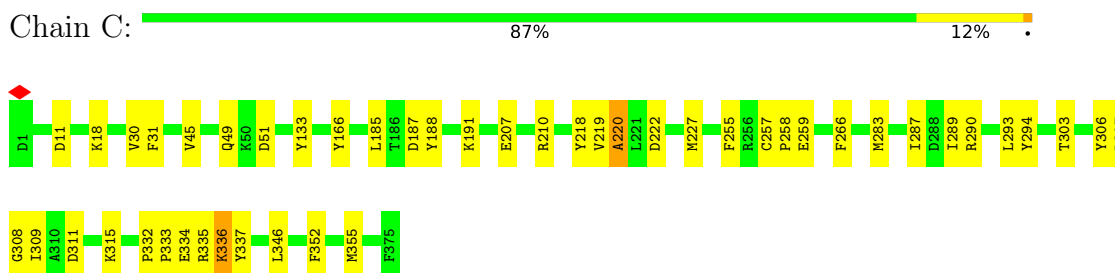
- Molecule 1: Actin, alpha skeletal muscle



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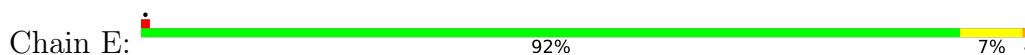


- Molecule 1: Actin, alpha skeletal muscle

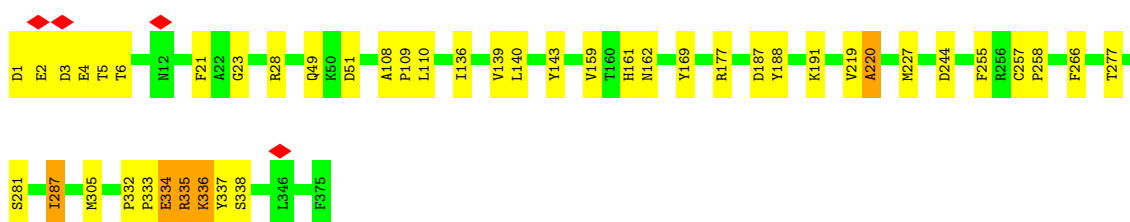
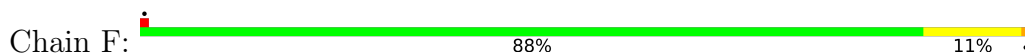




- Molecule 1: Actin, alpha skeletal muscle



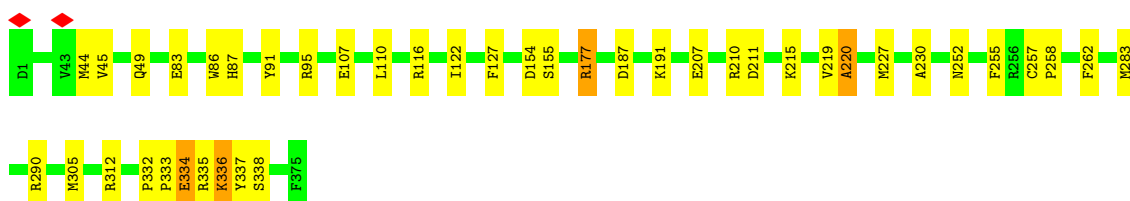
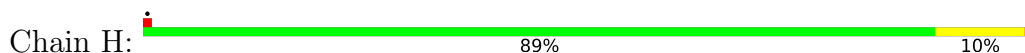
- Molecule 1: Actin, alpha skeletal muscle



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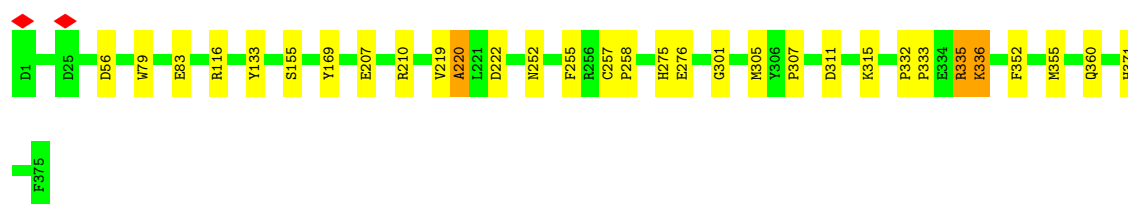


- Molecule 1: Actin, alpha skeletal muscle




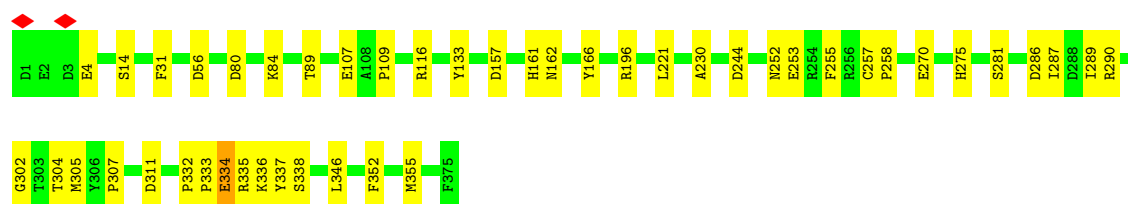
- Molecule 1: Actin, alpha skeletal muscle

Chain J:  92% 7%




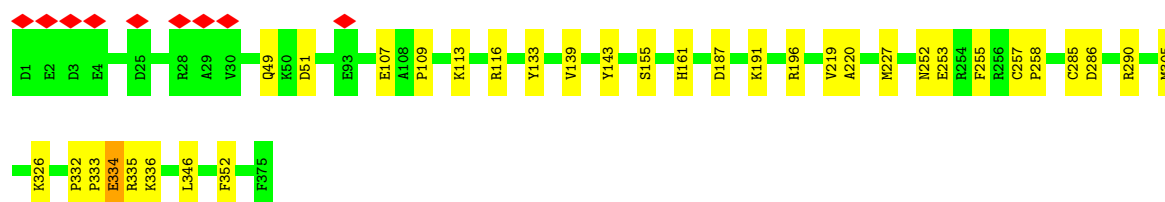
- Molecule 1: Actin, alpha skeletal muscle

Chain K:  88% 12%



- Molecule 1: Actin, alpha skeletal muscle

Chain L:  91% 9%



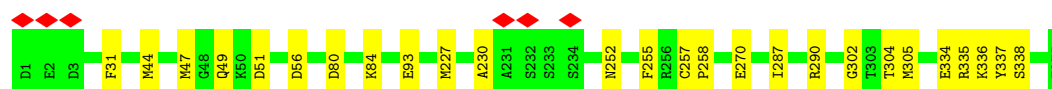
- Molecule 1: Actin, alpha skeletal muscle

Chain M:  95% 5%



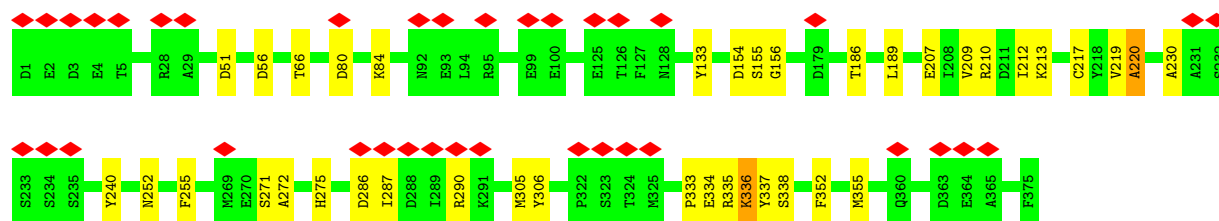
- Molecule 1: Actin, alpha skeletal muscle

Chain N:  93% 7%

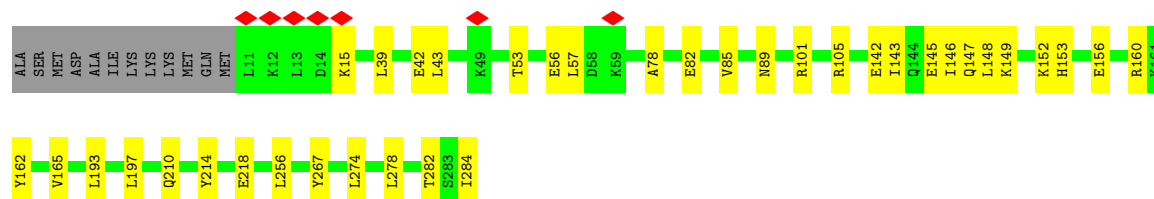
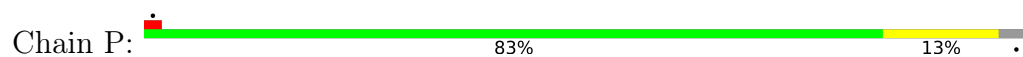


- Molecule 1: Actin, alpha skeletal muscle

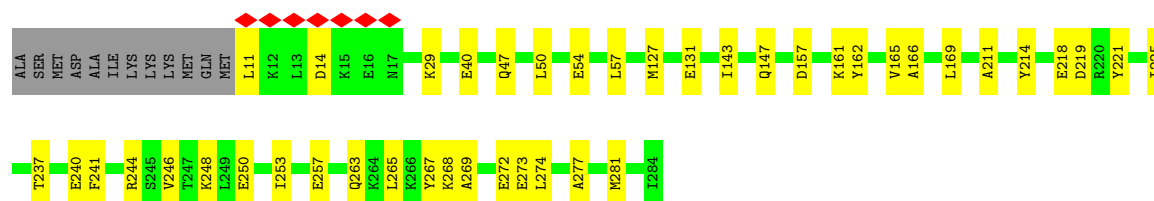
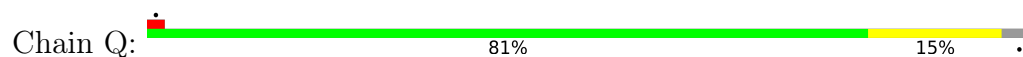
Chain O:  10% 90% 10%



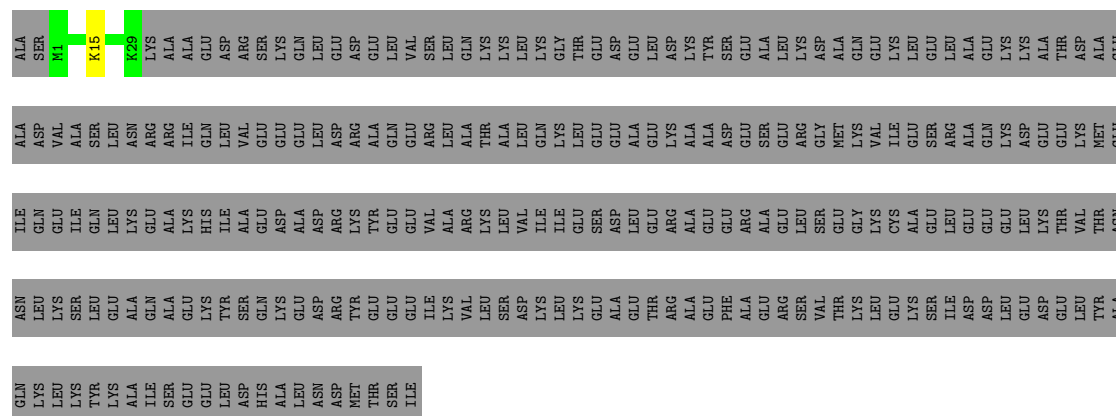
• Molecule 2: Tropomyosin alpha-1 chain



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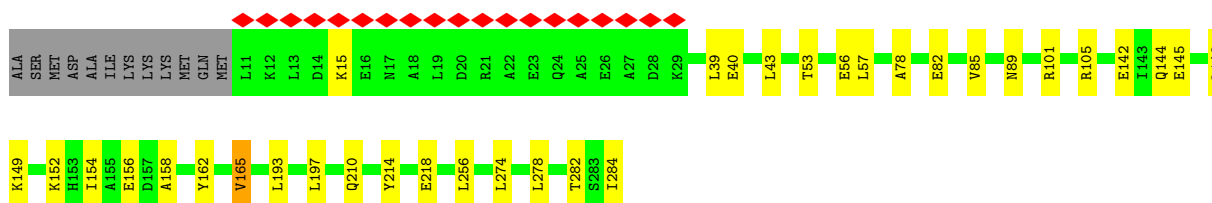
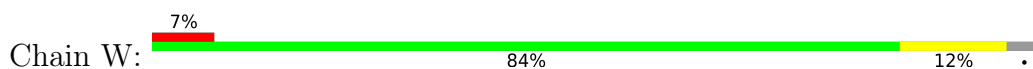


• Molecule 2: Tropomyosin alpha-1 chain

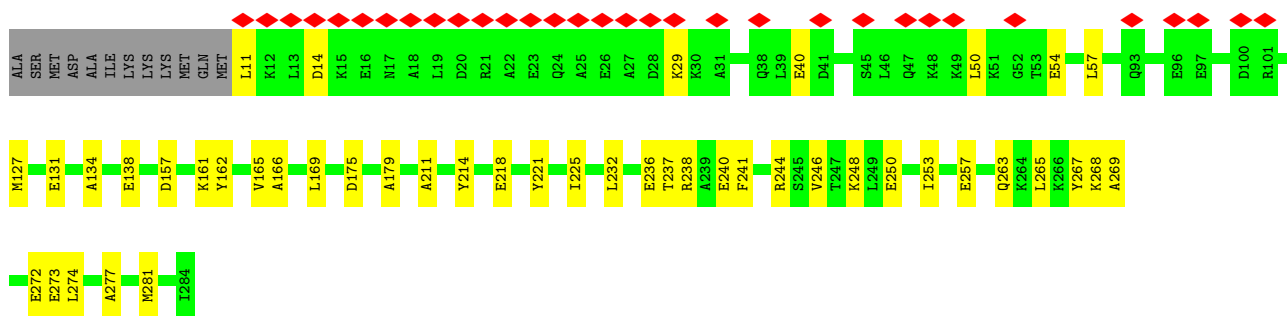
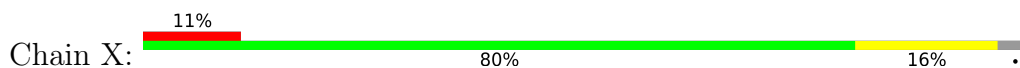




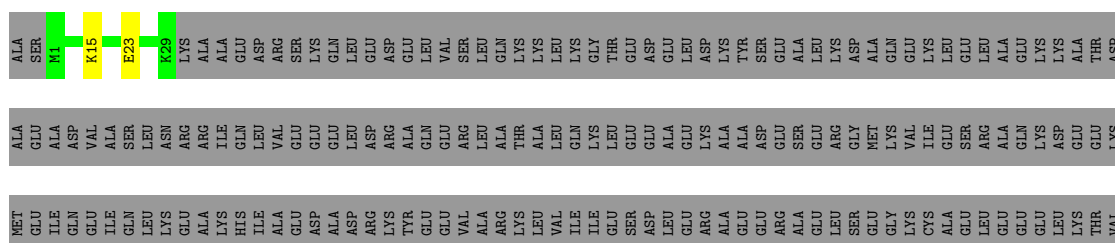
- Molecule 2: Tropomyosin alpha-1 chain



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- Molecule 2: Tropomyosin alpha-1 chain



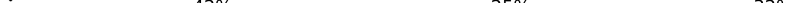
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Thr	Asn	Asn	Lys	Leu	Ser	Leu	Glu	Lys	Tyr	Gln	Lys	Gly	Glu	Arg	Asp	Ser	Ser	Asp	Leu

- Molecule 2: Tropomyosin alpha-1 chain

Chain Z: 10% 90%

[illegible]

- Molecule 3: Troponin T, cardiac muscle

Chain T: 

E280	E286	E288	E290	E292	E294	E296	E298	E300	E302	E304	E306	E308	E310	E312	E314	E316	E318	E320	E322	E324	E326	E328	E330	E332	E334	E336	E338	E340	E342	E344	E346	E348	E350	E352	E354	E356	E358	E360	E362	E364	E366	E368	E370	E372	E374	E376	E378	E380	E382	E384	E386	E388	E390	E392	E394	E396	E398	E400	E402	E404	E406	E408	E410	E412	E414	E416	E418	E420	E422	E424	E426	E428	E430	E432	E434	E436	E438	E440	E442	E444	E446	E448	E450	E452	E454	E456	E458	E460	E462	E464	E466	E468	E470	E472	E474	E476	E478	E480	E482	E484	E486	E488	E490	E492	E494	E496	E498	E500	E502	E504	E506	E508	E510	E512	E514	E516	E518	E520	E522	E524	E526	E528	E530	E532	E534	E536	E538	E540	E542	E544	E546	E548	E550	E552	E554	E556	E558	E560	E562	E564	E566	E568	E570	E572	E574	E576	E578	E580	E582	E584	E586	E588	E590	E592	E594	E596	E598	E600	E602	E604	E606	E608	E610	E612	E614	E616	E618	E620	E622	E624	E626	E628	E630	E632	E634	E636	E638	E640	E642	E644	E646	E648	E650	E652	E654	E656	E658	E660	E662	E664	E666	E668	E670	E672	E674	E676	E678	E680	E682	E684	E686	E688	E690	E692	E694	E696	E698	E700	E702	E704	E706	E708	E710	E712	E714	E716	E718	E720	E722	E724	E726	E728	E730	E732	E734	E736	E738	E740	E742	E744	E746	E748	E750	E752	E754	E756	E758	E760	E762	E764	E766	E768	E770	E772	E774	E776	E778	E780	E782	E784	E786	E788	E790	E792	E794	E796	E798	E800	E802	E804	E806	E808	E810	E812	E814	E816	E818	E820	E822	E824	E826	E828	E830	E832	E834	E836	E838	E840	E842	E844	E846	E848	E850	E852	E854	E856	E858	E860	E862	E864	E866	E868	E870	E872	E874	E876	E878	E880	E882	E884	E886	E888	E890	E892	E894	E896	E898	E900	E902	E904	E906	E908	E910	E912	E914	E916	E918	E920	E922	E924	E926	E928	E930	E932	E934	E936	E938	E940	E942	E944	E946	E948	E950	E952	E954	E956	E958	E960	E962	E964	E966	E968	E970	E972	E974	E976	E978	E980	E982	E984	E986	E988	E990	E992	E994	E996	E998	E1000	E1002	E1004	E1006	E1008	E1010	E1012	E1014	E1016	E1018	E1020	E1022	E1024	E1026	E1028	E1030	E1032	E1034	E1036	E1038	E1040	E1042	E1044	E1046	E1048	E1050	E1052	E1054	E1056	E1058	E1060	E1062	E1064	E1066	E1068	E1070	E1072	E1074	E1076	E1078	E1080	E1082	E1084	E1086	E1088	E1090	E1092	E1094	E1096	E1098	E1100	E1102	E1104	E1106	E1108	E1110	E1112	E1114	E1116	E1118	E1120	E1122	E1124	E1126	E1128	E1130	E1132	E1134	E1136	E1138	E1140	E1142	E1144	E1146	E1148	E1150	E1152	E1154	E1156	E1158	E1160	E1162	E1164	E1166	E1168	E1170	E1172	E1174	E1176	E1178	E1180	E1182	E1184	E1186	E1188	E1190	E1192	E1194	E1196	E1198	E1200	E1202	E1204	E1206	E1208	E1210	E1212	E1214	E1216	E1218	E1220	E1222	E1224	E1226	E1228	E1230	E1232	E1234	E1236	E1238	E1240	E1242	E1244	E1246	E1248	E1250	E1252	E1254	E1256	E1258	E1260	E1262	E1264	E1266	E1268	E1270
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- Molecule 3: Troponin T, cardiac muscle

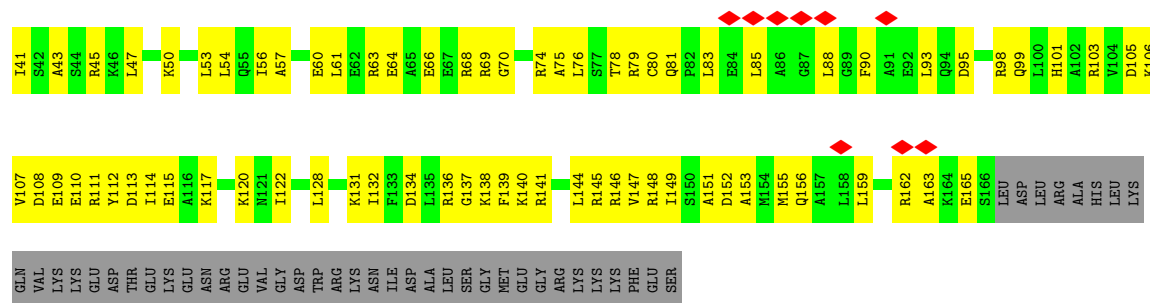
Chain a:  68% 32%

PHE ASP ASP ILE HIS ARG LYS ARG MET GLU LYS ASP
L99 A135 Q138 R139 N142 N150
ARG LEU ALA GLU GLU ARG ALA ARG ARG GLU GLU GLU ASN ARG ARG LYS ALA ASP GLU ALA ARG LYS LYS LYS LEU SER ASN MET MET HIS PHE GLY TYR

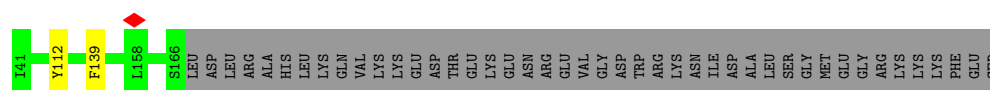
GLN LYS GLN ALA GLN THR GLU ARG LYS SER
G199 D222 H223 Q272

- Molecule 4: Troponin I, cardiac muscle

Chain U: 



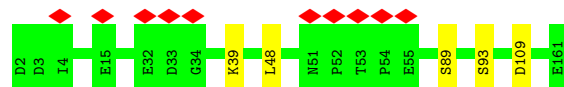
- Molecule 4: Troponin I, cardiac muscle



- 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 (\AA)	439.344, 439.344, 439.344	wwPDB
Map dimensions	162, 162, 162	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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

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 ⓘ

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	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 ⓘ

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.

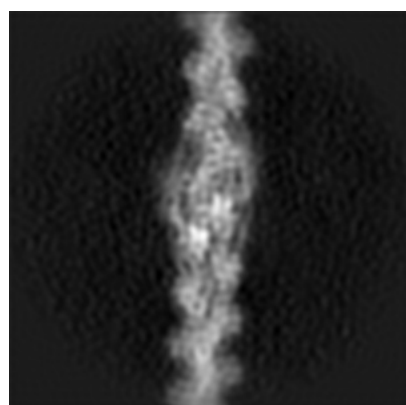
6 Map visualisation [i](#)

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.

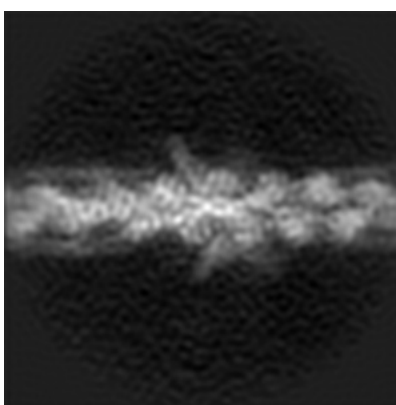
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

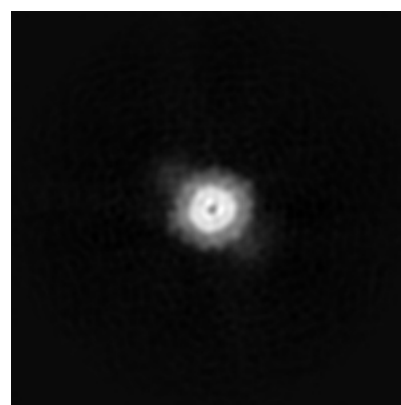
6.1.1 Primary map



X



Y



Z

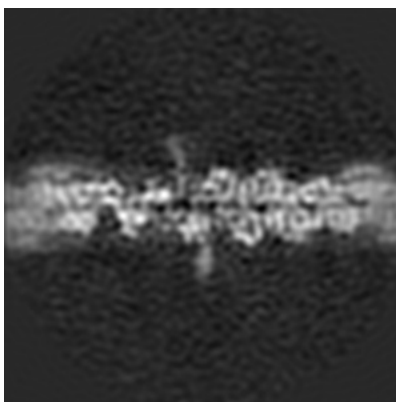
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

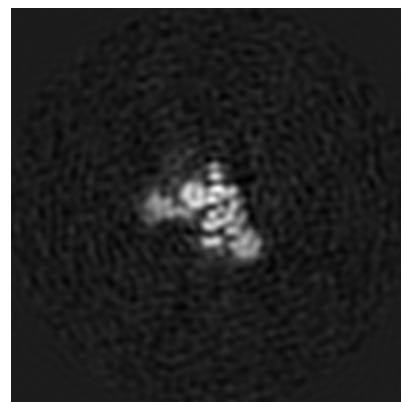
6.2.1 Primary map



X Index: 81



Y Index: 81

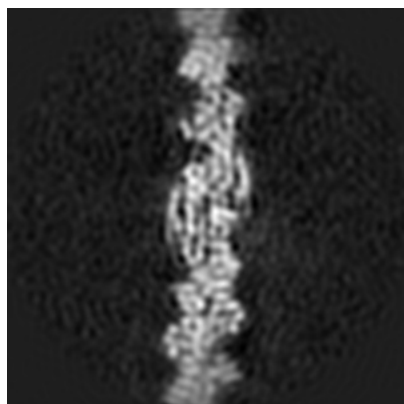


Z Index: 81

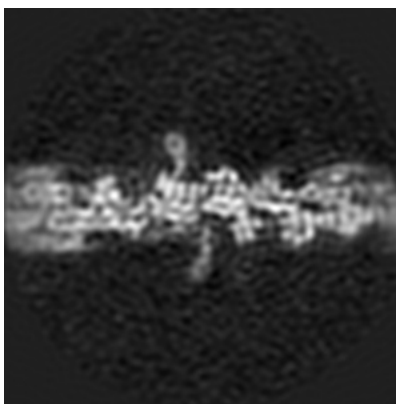
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

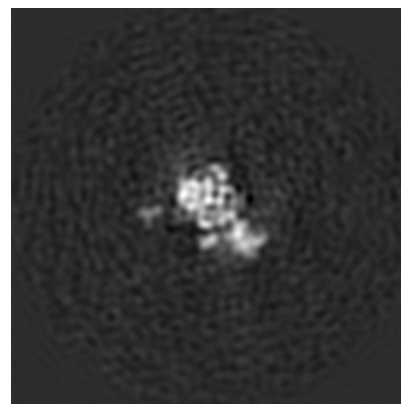
6.3.1 Primary map



X Index: 79



Y Index: 78



Z Index: 77

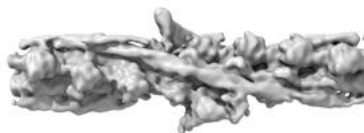
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

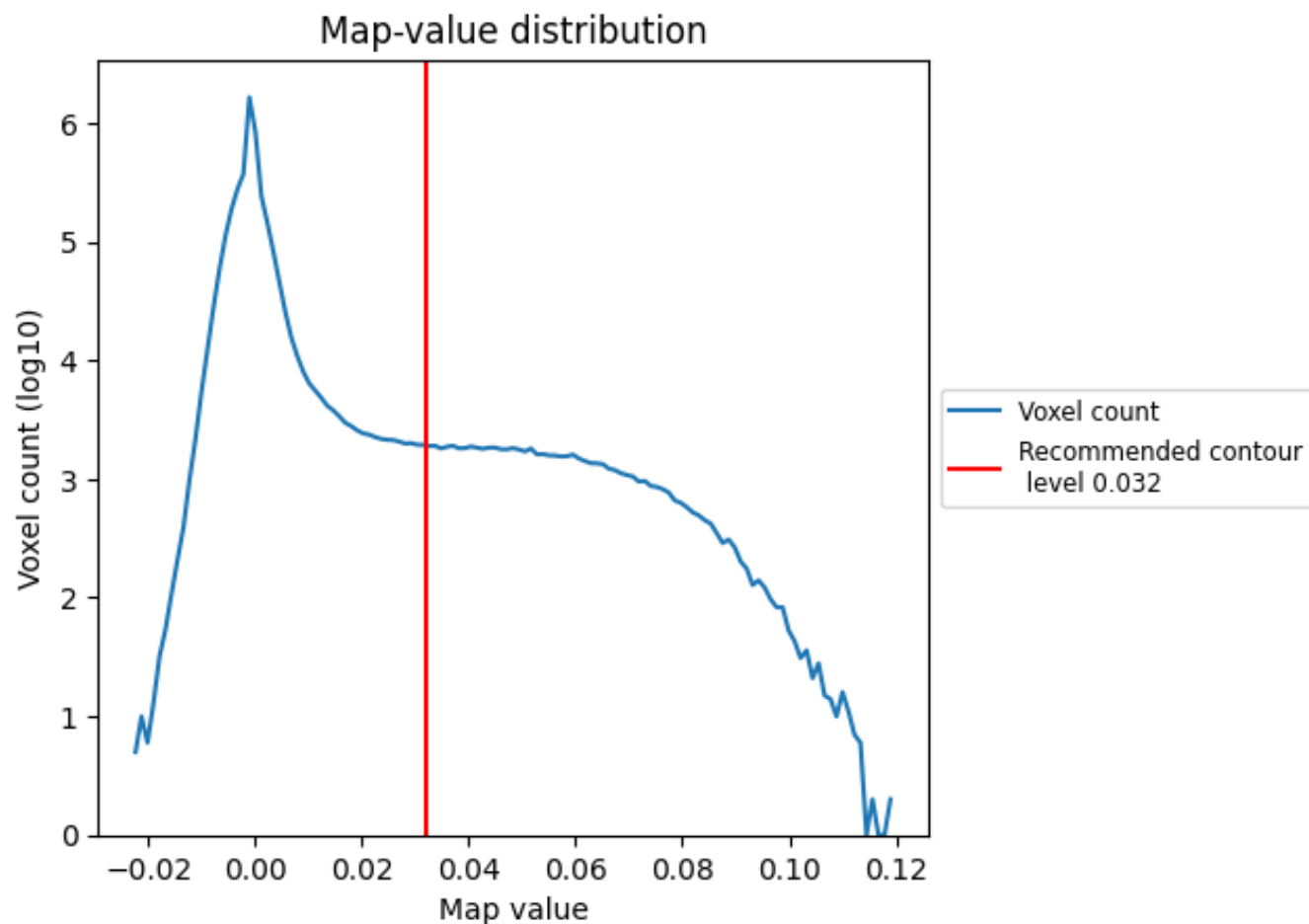
6.5 Mask visualisation

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

7 Map analysis [i](#)

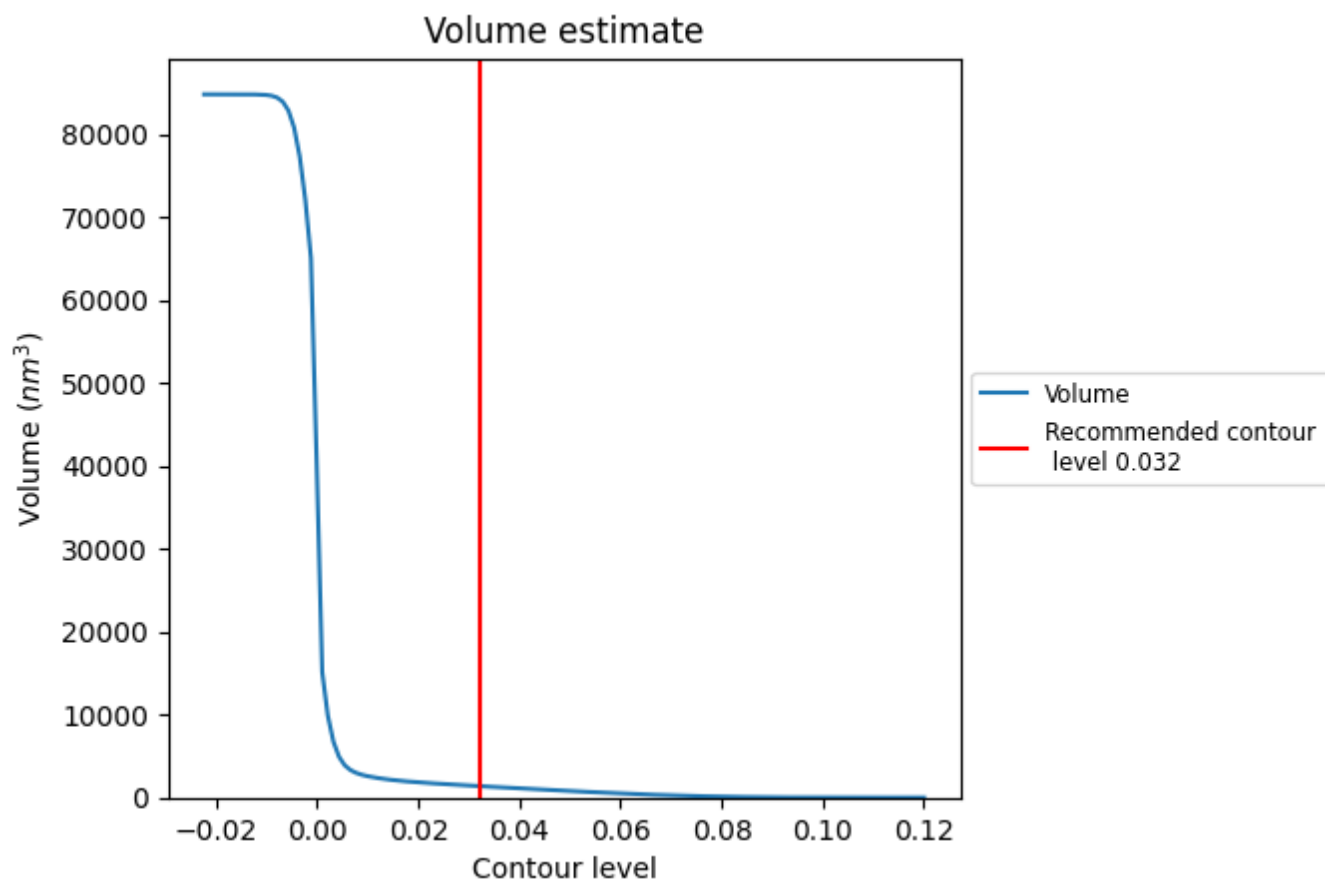
This section contains the results of statistical analysis of the map.

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.

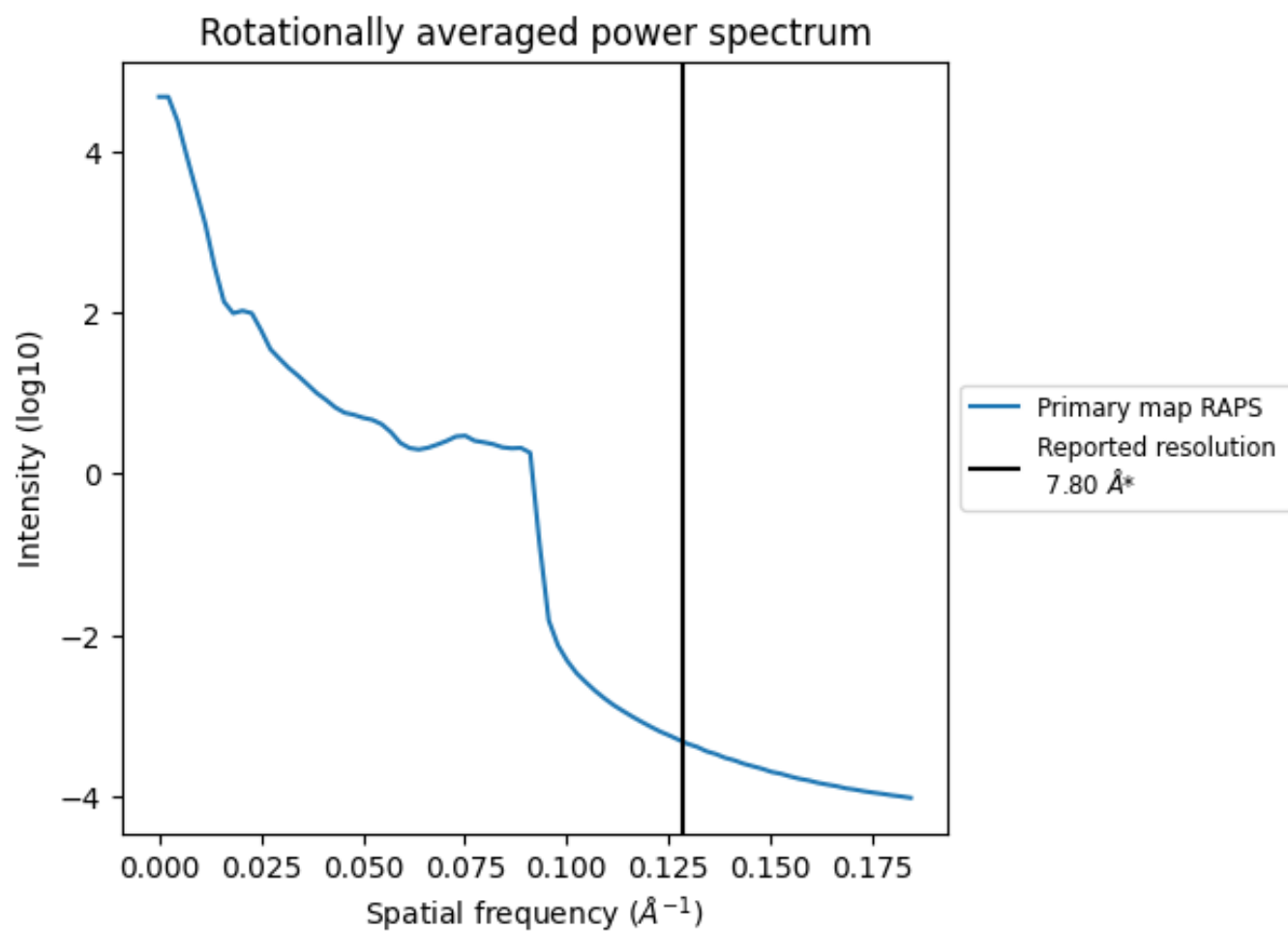
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1379 nm³; 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 ⓘ

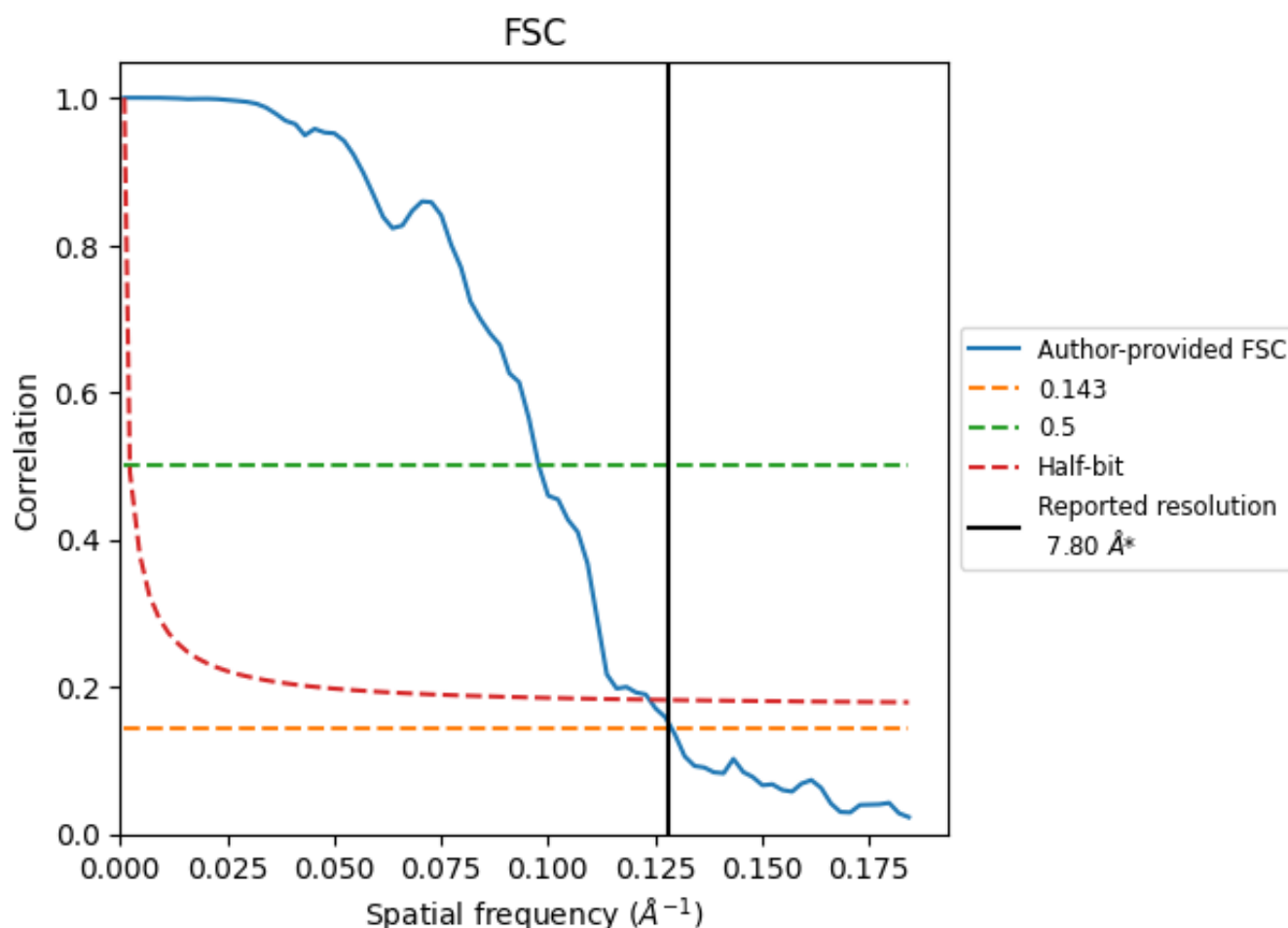


*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

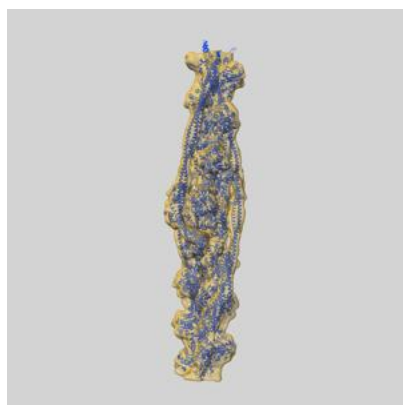
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	7.75	10.21	8.08
Unmasked-calculated*	-	-	-

*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.

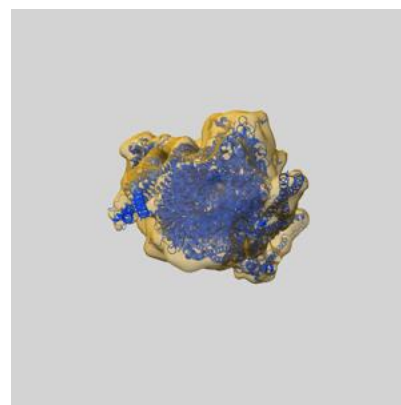
9.1 Map-model overlay [i](#)



X



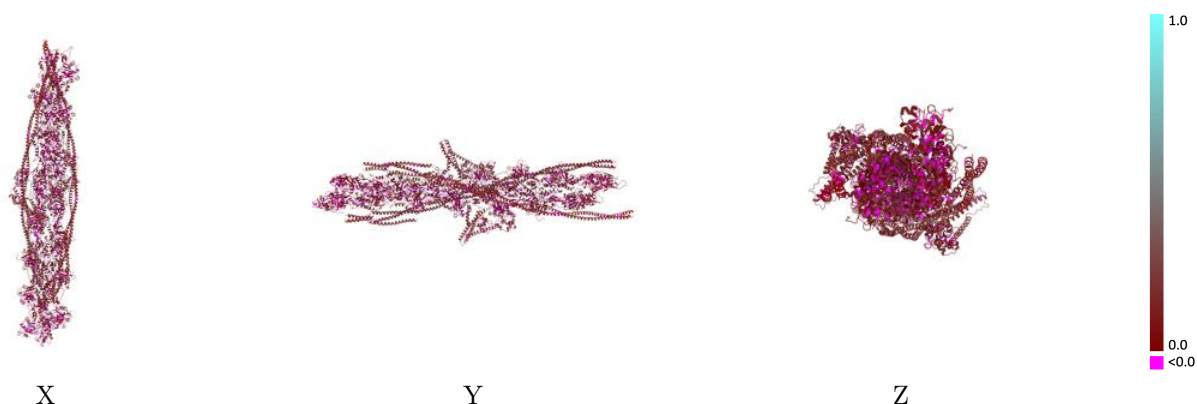
Y



Z

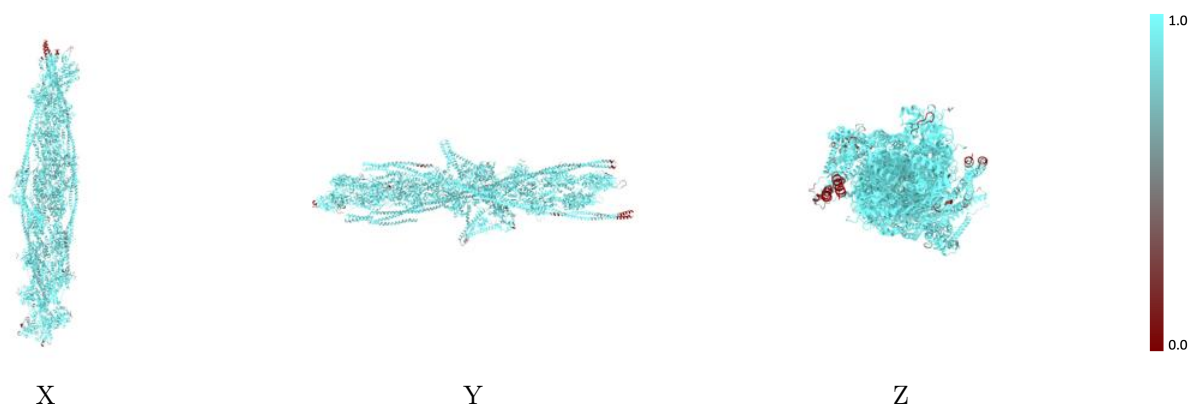
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



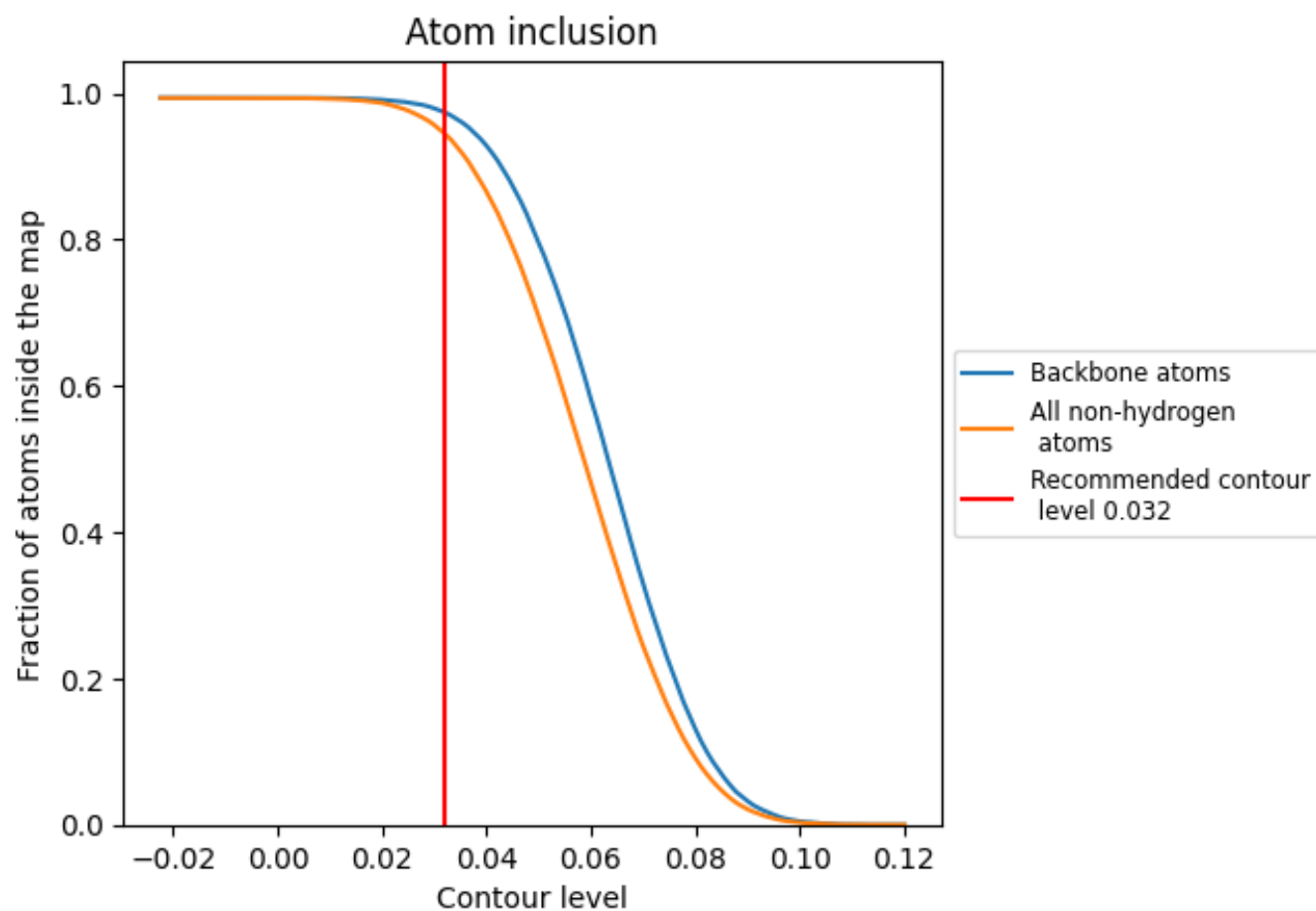
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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





























































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	 0.9448	 0.1130
A	 0.9465	 0.0860
B	 0.9913	 0.1020
C	 0.9892	 0.1040
D	 0.9788	 0.1010
E	 0.9712	 0.1040
F	 0.9649	 0.1080
G	 0.9673	 0.1140
H	 0.9760	 0.1020
I	 0.9753	 0.1030
J	 0.9795	 0.1010
K	 0.9812	 0.1070
L	 0.9621	 0.1030
M	 0.9844	 0.0950
N	 0.9677	 0.0930
O	 0.8801	 0.0600
P	 0.8968	 0.1560
Q	 0.9019	 0.1530
R	 0.9869	 0.1600
S	 0.8646	 0.1060
T	 0.8374	 0.1640
U	 0.8782	 0.1490
V	 0.9041	 0.1260
W	 0.8614	 0.1530
X	 0.8208	 0.1250
Y	 0.9389	 0.1790
Z	 0.9607	 0.1660
a	 0.8477	 0.1560
b	 0.9867	 0.1780
c	 0.9120	 0.1470

