



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 06:01 PM UTC

PDB ID : 9LWF / pdb_00009lwf
EMDB ID : EMD-63442
Title : Cryo-EM structure of dual sensor bound GATOR2 complex
Authors : Su, M.-Y.
Deposited on : 2025-02-14
Resolution : 3.41 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

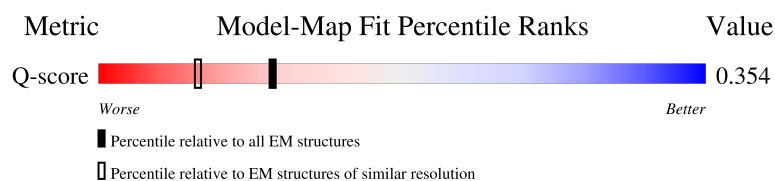
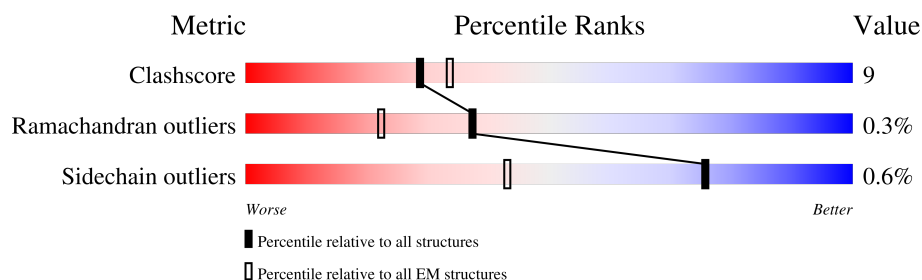
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 Å.

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



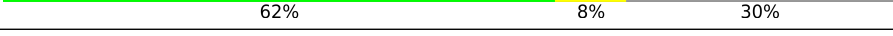
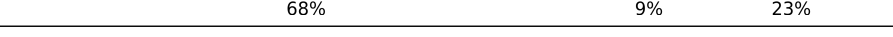
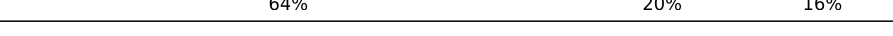
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13997 (2.91 - 3.91)

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	875	79% 7% 14%
1	B	875	67% 15% 17%
1	K	875	77% 8% 15%
1	L	875	65% 17% 17%

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Mol	Chain	Length	Quality of chain
2	C	790	
2	I	790	
3	D	974	
3	N	974	
4	E	421	
4	F	421	
4	G	421	
4	O	421	
4	P	421	
4	Q	421	
5	H	368	
5	R	368	
6	U	329	
6	V	329	
7	X	480	
7	Y	480	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 57308 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 GATOR2 complex protein MIOS.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	751	Total	C	N	O	S	0	0
			4726	2943	888	867	28		
1	B	725	Total	C	N	O	S	0	0
			5026	3242	897	856	31		
1	K	748	Total	C	N	O	S	0	0
			4666	2925	872	842	27		
1	L	727	Total	C	N	O	S	0	0
			5035	3240	900	870	25		

- Molecule 2 is a protein called GATOR2 complex protein WDR24.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	568	Total	C	N	O	S	0	0
			4152	2653	766	692	41		
2	I	573	Total	C	N	O	S	0	0
			4299	2727	787	742	43		

- Molecule 3 is a protein called GATOR2 complex protein WDR59.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	264	Total	C	N	O	S	0	0
			1885	1201	341	324	19		
3	N	264	Total	C	N	O	S	0	0
			1811	1148	336	308	19		

- Molecule 4 is a protein called Isoform B of Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	303	Total	C	N	O	S	0	0
			2235	1430	403	389	13		
4	F	302	Total	C	N	O	S	0	0
			1988	1287	359	333	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	304	Total	C	N	O	S	0	0
			2305	1464	413	412	16		
4	O	302	Total	C	N	O	S	0	0
			2186	1402	394	378	12		
4	P	295	Total	C	N	O	S	0	0
			1821	1169	336	311	5		
4	Q	302	Total	C	N	O	S	0	0
			2271	1444	412	400	15		

- Molecule 5 is a protein called Isoform 3 of Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	283	Total	C	N	O	S	0	0
			1861	1199	336	321	5		
5	R	284	Total	C	N	O	S	0	0
			1952	1255	356	336	5		

- Molecule 6 is a protein called Cytosolic arginine sensor for mTORC1 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	290	Total	C	N	O	S	0	0
			2157	1410	353	388	6		
6	V	278	Total	C	N	O	S	0	0
			2000	1321	335	337	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	304	ALA	ASP	engineered mutation	UNP Q8WTX7
V	304	ALA	ASP	engineered mutation	UNP Q8WTX7

- Molecule 7 is a protein called Sestrin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	320	Total	C	N	O	S	0	0
			2506	1636	439	419	12		
7	Y	310	Total	C	N	O	S	0	0
			2394	1578	415	388	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	375	PHE	TYR	engineered mutation	UNP P58004
Y	375	PHE	TYR	engineered mutation	UNP P58004

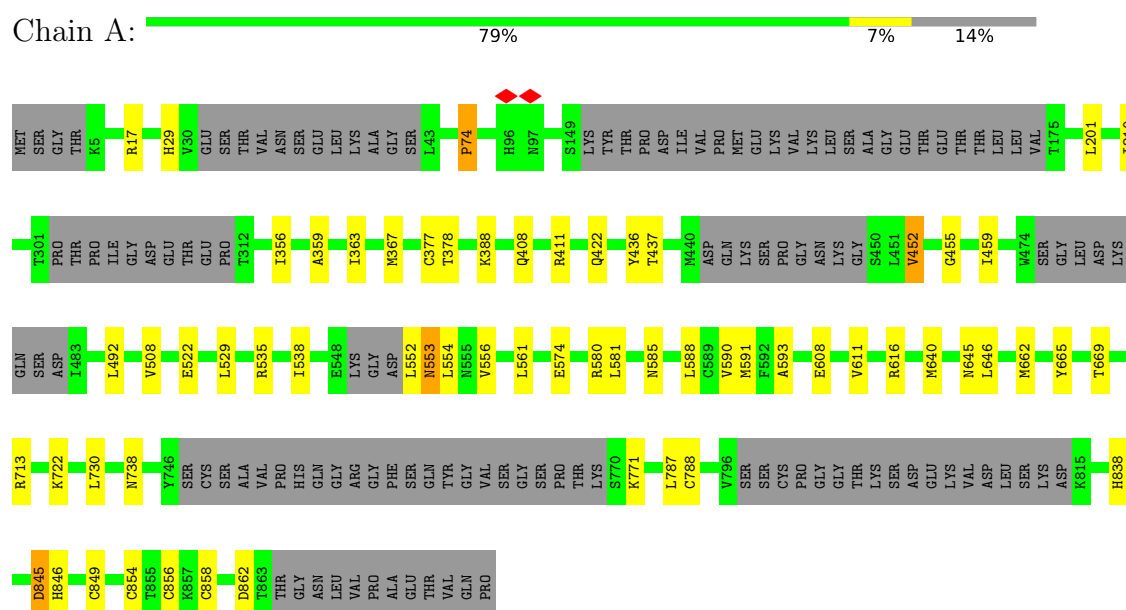
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	A	4	Total 4	Zn 4	0
8	B	4	Total 4	Zn 4	0
8	C	4	Total 4	Zn 4	0
8	D	4	Total 4	Zn 4	0
8	I	4	Total 4	Zn 4	0
8	K	4	Total 4	Zn 4	0
8	L	4	Total 4	Zn 4	0
8	N	4	Total 4	Zn 4	0

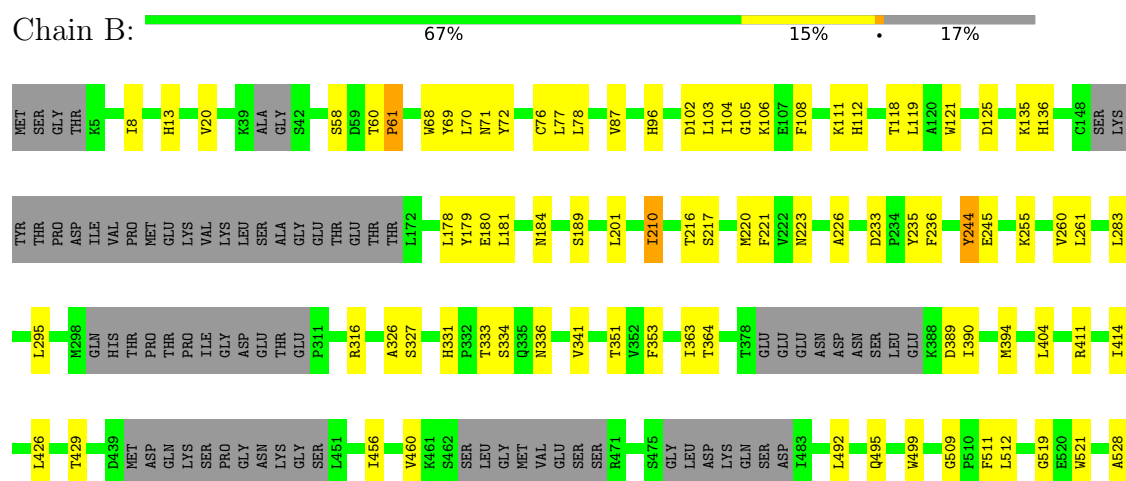
3 Residue-property plots

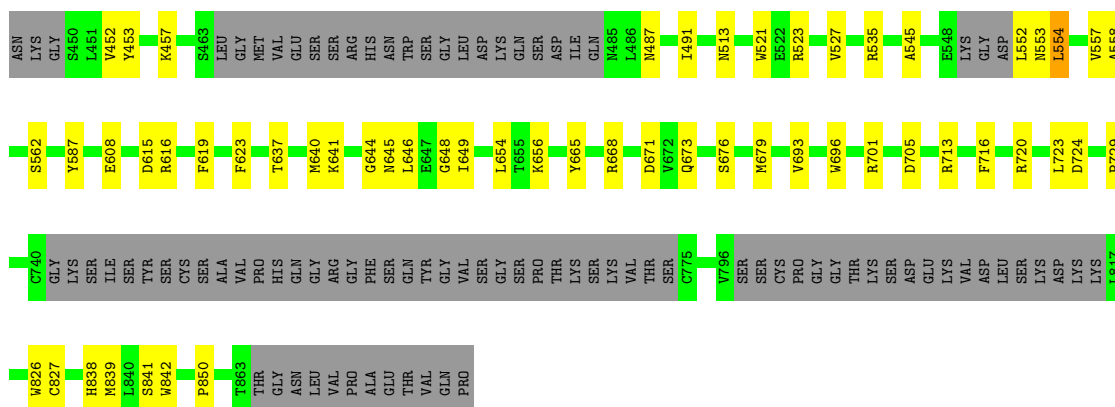
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: GATOR2 complex protein MIOS



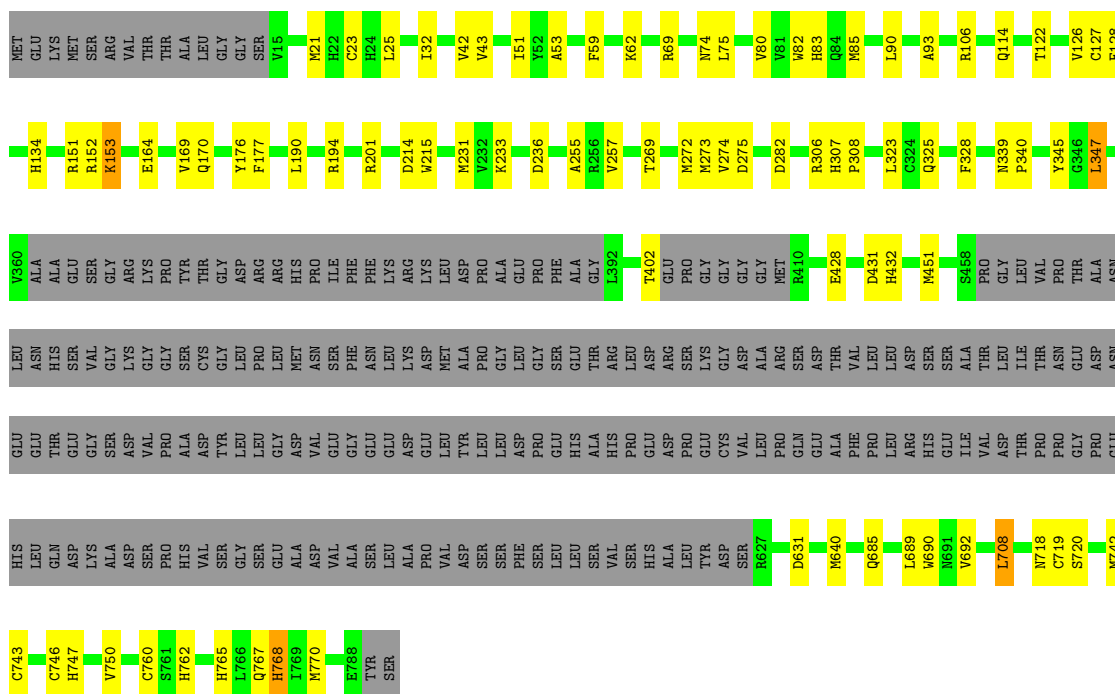
• Molecule 1: GATOR2 complex protein MIOS





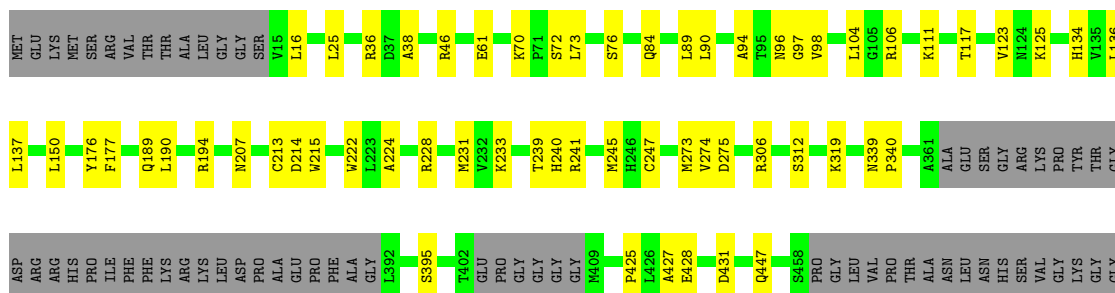
• Molecule 2: GATOR2 complex protein WDR24

Chain C: 61% 10% 28%



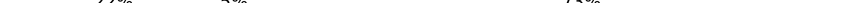
• Molecule 2: GATOR2 complex protein WDR24

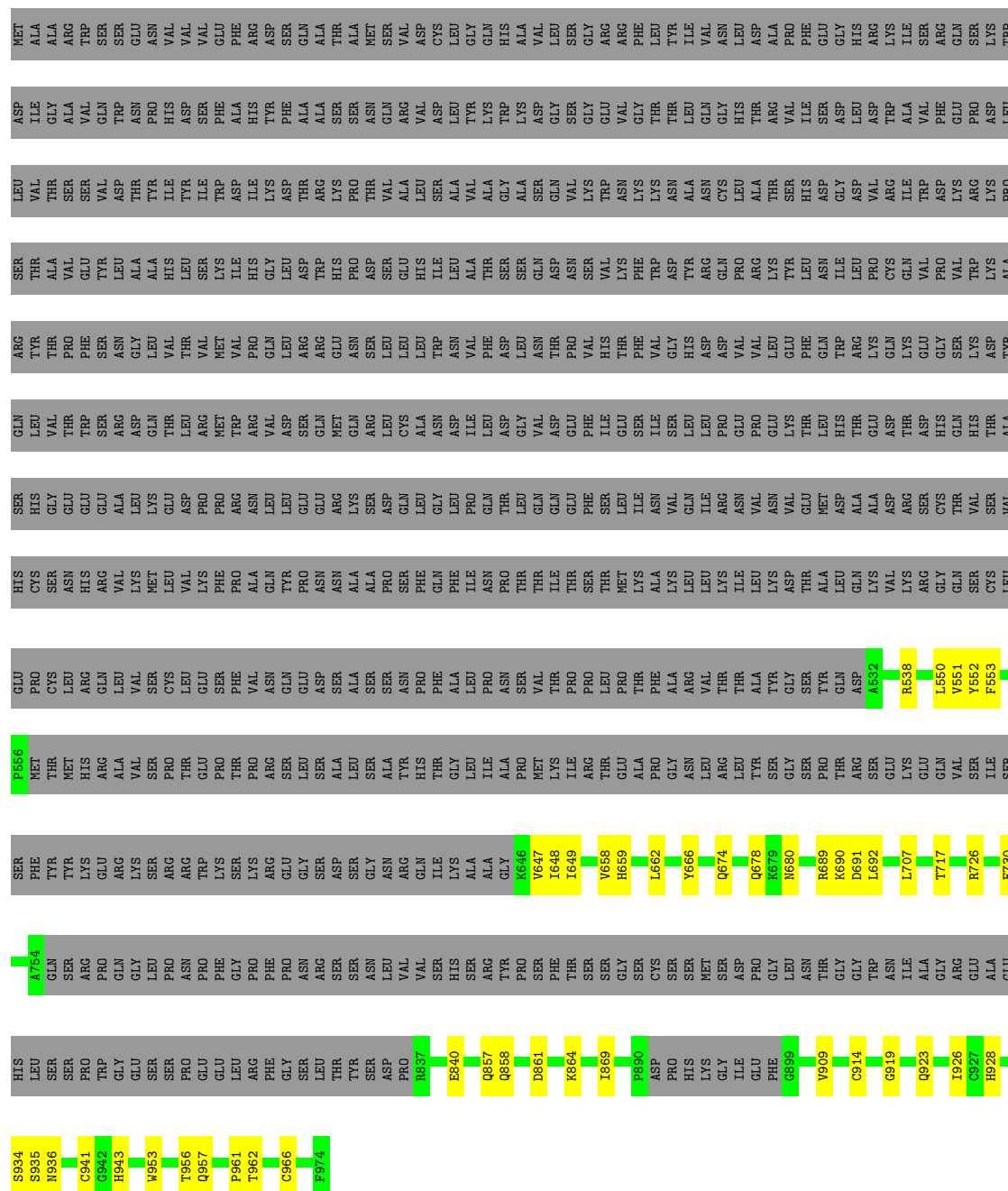
Chain I: 63% 9% 27%



HTS	VAL	SER	GLY	SER	GLU	ALA	ASP	VAL	ALA	SER	LEU	ALA	PRO	VAL	ASP	SER	SER	PHE	SER	LEU	LEU	SER	VAL	SER	HTS	ALA	ALA	LEU	TVR	ASP	S626	D631	V664	H716	C722	V732	C736	M742	V745	C746	H747	H765	L766	Q767	S776	S777	S790
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

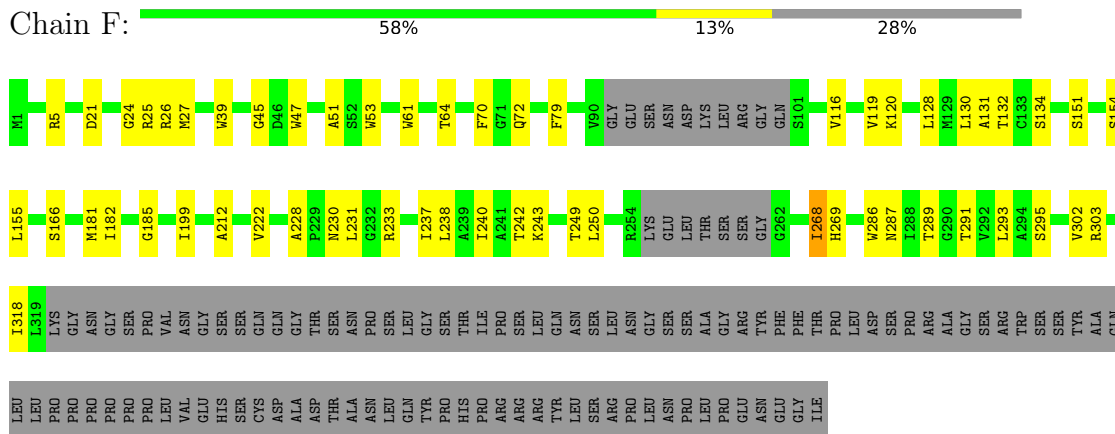
- Molecule 3: GATOR2 complex protein WDR59

Chain D:  22% 5% 73%

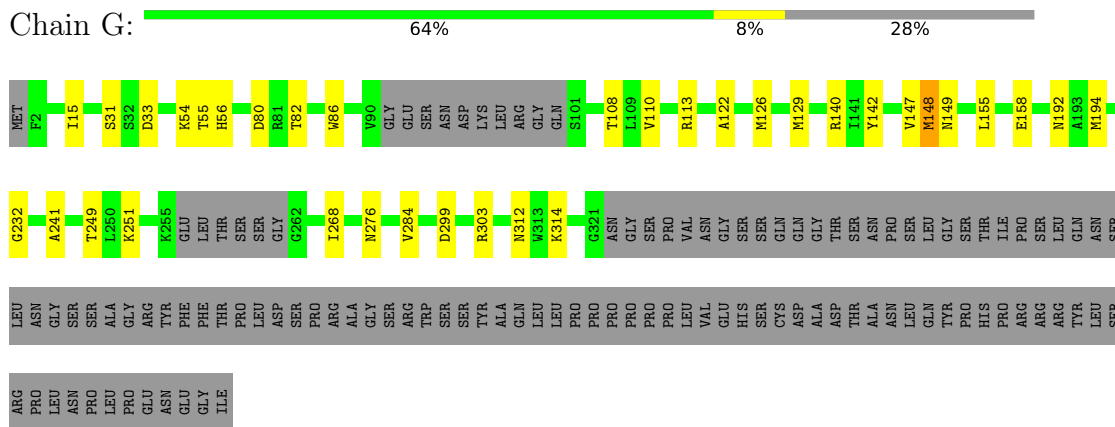


ASN	SER	LEU	ARG	PRO	LEU	ASN	PRO	LEU	PRO	GLY	ASN	GLY	ILE
SER	LEU	ARG	PRO	LEU	ASN	PRO	LEU	PRO	GLY	ASN	GLY	ILE	

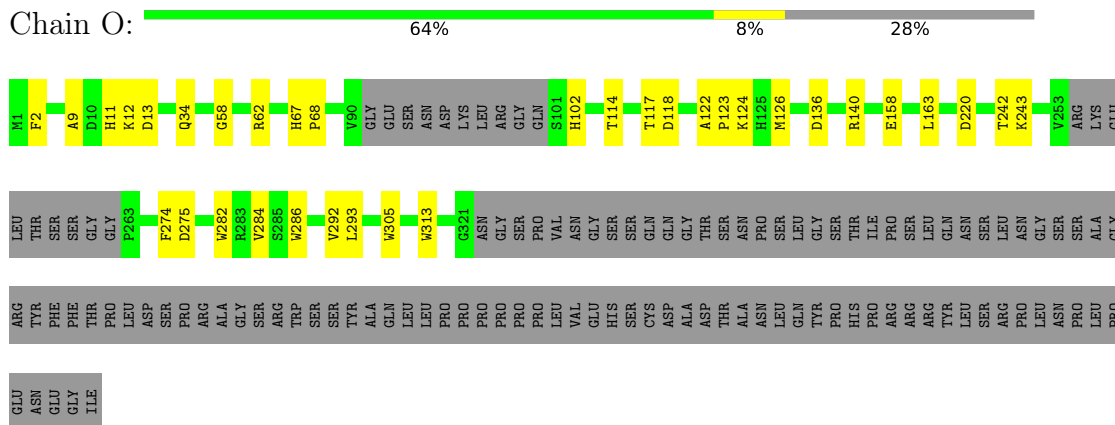
- Molecule 4: Isoform B of Nucleoporin SEH1



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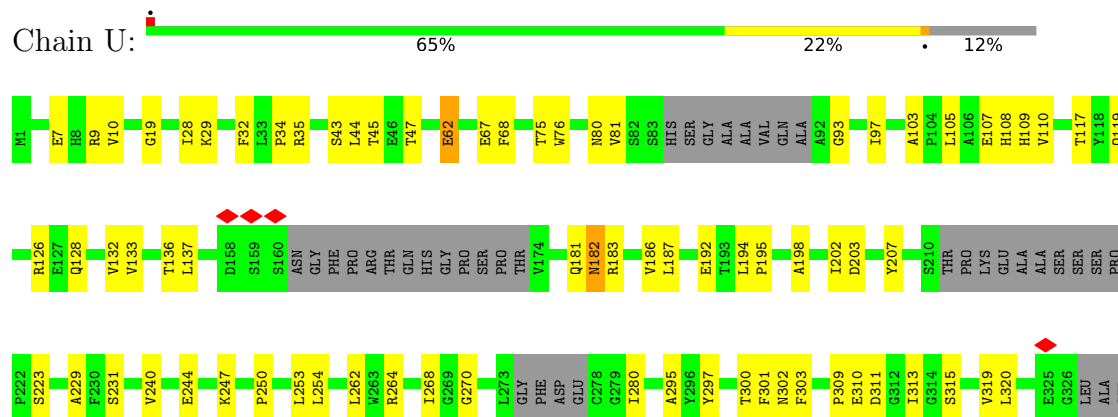


- Molecule 4: Isoform B of Nucleoporin SEH1

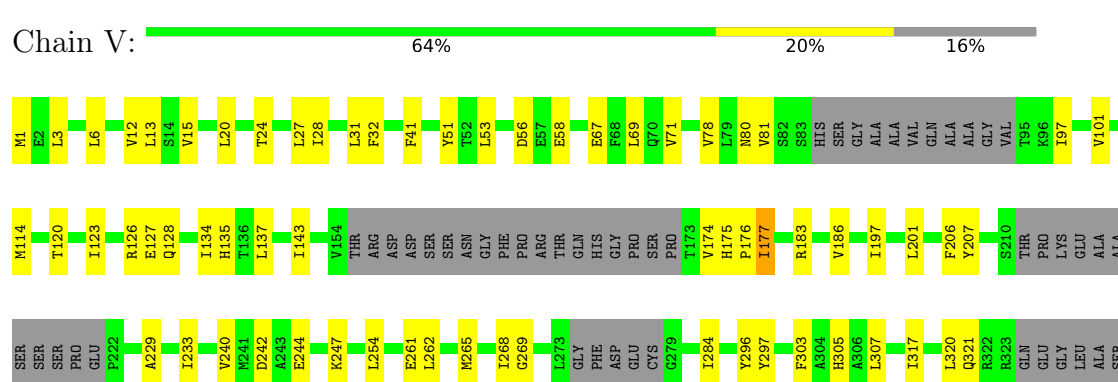




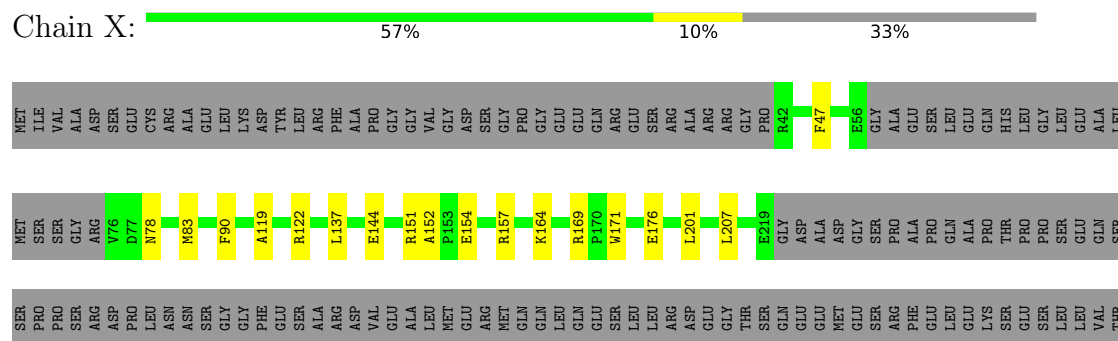
- Molecule 6: Cytosolic arginine sensor for mTORC1 subunit 1

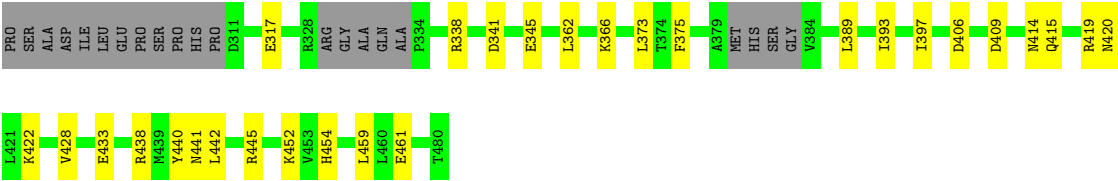


- Molecule 6: Cytosolic arginine sensor for mTORC1 subunit 1

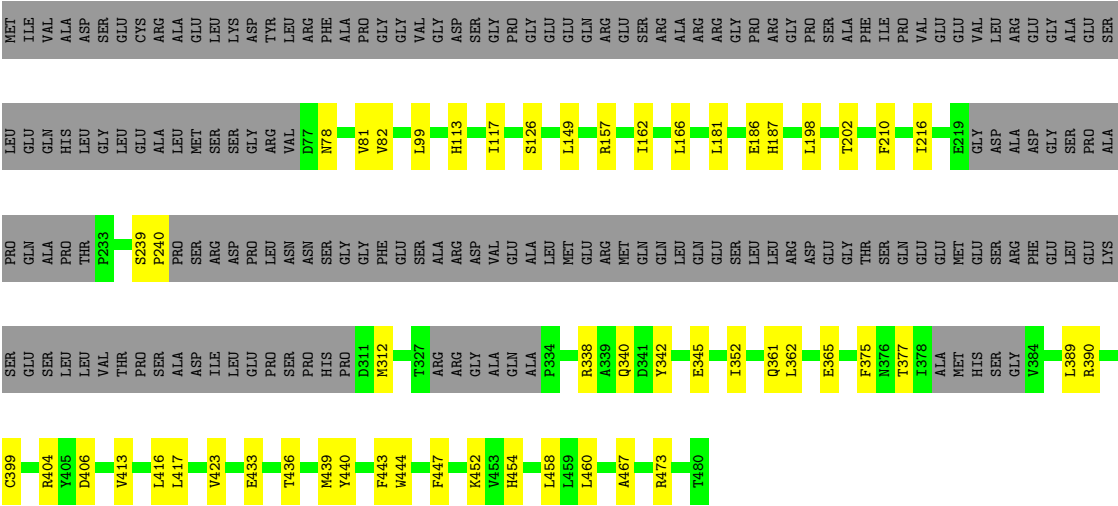


- Molecule 7: Sestrin-2





• Molecule 7: Sestrin-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	586448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.87	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.933	Depositor
Minimum map value	-0.189	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.103	Depositor
Map size ($\text{\AA}$)	578.0, 578.0, 578.0	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.22	0/4790	0.47	1/6570 (0.0%)
1	B	0.31	2/5146 (0.0%)	0.63	9/7070 (0.1%)
1	K	0.24	1/4733 (0.0%)	0.41	1/6503 (0.0%)
1	L	0.30	2/5150 (0.0%)	0.56	4/7075 (0.1%)
2	C	0.24	0/4263	0.52	1/5823 (0.0%)
2	I	0.23	0/4411	0.46	1/6009 (0.0%)
3	D	0.27	0/1929	0.44	0/2631
3	N	0.23	0/1847	0.40	0/2519
4	E	0.23	0/2296	0.46	1/3142 (0.0%)
4	F	0.21	0/2044	0.52	0/2826
4	G	0.21	0/2367	0.41	0/3228
4	O	0.26	0/2248	0.41	0/3080
4	P	0.22	0/1867	0.48	1/2583 (0.0%)
4	Q	0.21	0/2332	0.36	0/3185
5	H	0.19	0/1915	0.42	0/2654
5	R	0.20	0/2010	0.44	0/2774
6	U	0.23	0/2206	0.49	2/3018 (0.1%)
6	V	0.33	1/2047 (0.0%)	0.51	1/2811 (0.0%)
7	X	0.23	0/2577	0.44	0/3504
7	Y	0.27	0/2467	0.47	0/3362
All	All	0.25	6/58645 (0.0%)	0.48	22/80367 (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
2	C	0	1
6	V	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	355	ARG	CZ-NH2	-8.25	1.22	1.33
1	B	60	THR	C-N	7.66	1.51	1.33
1	B	61	PRO	N-CD	6.62	1.57	1.47
1	L	351	THR	N-CA	5.09	1.52	1.46
1	L	331	HIS	CG-ND1	-5.06	1.32	1.38
6	V	177	ILE	C-O	-5.03	1.18	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	352	VAL	N-CA-C	9.75	129.63	109.34
1	A	74	PRO	CA-N-CD	-8.92	99.01	111.50
1	K	74	PRO	CA-N-CD	-8.82	99.15	111.50
1	B	61	PRO	CA-N-CD	-8.81	99.67	112.00
1	B	60	THR	CA-C-N	-8.78	108.86	119.84
1	B	60	THR	C-N-CA	-8.78	108.86	119.84
1	B	780	LYS	CA-C-N	7.35	129.02	119.84
1	B	780	LYS	C-N-CA	7.35	129.02	119.84
1	L	10	TRP	CE3-CZ3-CH2	6.82	129.96	121.10
4	P	31	SER	N-CA-C	5.96	116.28	107.88
2	I	664	VAL	N-CA-C	-5.91	107.52	113.20
6	U	270	GLY	CA-C-N	5.82	129.53	120.68
6	U	270	GLY	C-N-CA	5.82	129.53	120.68
1	B	672	VAL	N-CA-C	-5.71	107.93	113.53
4	E	275	ASP	CB-CA-C	5.47	118.61	109.80
2	C	768	HIS	N-CA-C	-5.46	107.28	114.04
1	B	789	LEU	N-CA-CB	-5.36	108.06	114.17
1	B	61	PRO	N-CA-CB	-5.36	97.63	103.25
1	B	60	THR	C-N-CD	5.31	146.78	125.00
1	L	350	PHE	CA-C-N	5.28	131.63	121.54
1	L	350	PHE	C-N-CA	5.28	131.63	121.54
6	V	135	HIS	N-CA-C	-5.26	106.19	113.18

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	347	LEU	Peptide
6	V	134	ILE	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	4726	0	3529	65	0
1	B	5026	0	4301	112	0
1	K	4666	0	3455	87	0
1	L	5035	0	4324	180	0
2	C	4152	0	3756	64	0
2	I	4299	0	3983	59	0
3	D	1885	0	1698	49	0
3	N	1811	0	1586	33	0
4	E	2235	0	2075	35	0
4	F	1988	0	1576	35	0
4	G	2305	0	2180	26	0
4	O	2186	0	1952	51	0
4	P	1821	0	1261	25	0
4	Q	2271	0	2114	25	0
5	H	1861	0	1442	26	0
5	R	1952	0	1642	42	0
6	U	2157	0	2108	53	0
6	V	2000	0	1905	57	0
7	X	2506	0	2377	36	0
7	Y	2394	0	2248	45	0
8	A	4	0	0	0	0
8	B	4	0	0	0	0
8	C	4	0	0	0	0
8	D	4	0	0	0	0
8	I	4	0	0	0	0
8	K	4	0	0	0	0
8	L	4	0	0	0	0
8	N	4	0	0	0	0
All	All	57308	0	49512	1008	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 9.

All (1008) 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)
7:Y:444:TRP:HE3	7:Y:447:PHE:CD2	1.17	1.62
7:Y:444:TRP:CE3	7:Y:447:PHE:CE2	1.93	1.53
1:L:10:TRP:CZ3	1:L:331:HIS:HB2	1.51	1.44
3:N:923:GLN:HE22	3:N:928:HIS:C	1.30	1.36
7:Y:444:TRP:CE3	7:Y:447:PHE:CD2	2.10	1.34
7:Y:444:TRP:HE3	7:Y:447:PHE:CE2	1.32	1.34
4:O:62:ARG:NH1	4:O:118:ASP:OD1	1.58	1.33
1:L:10:TRP:HZ3	1:L:331:HIS:CD2	1.46	1.33
1:L:10:TRP:CZ3	1:L:331:HIS:CB	2.11	1.31
1:L:10:TRP:HZ3	1:L:331:HIS:CG	1.52	1.28
1:K:355:ARG:NH2	4:O:282:TRP:CD2	2.01	1.26
1:L:10:TRP:CH2	1:L:331:HIS:HB2	1.70	1.25
1:L:10:TRP:CZ3	1:L:331:HIS:CD2	2.24	1.25
1:L:10:TRP:CZ3	1:L:331:HIS:CG	2.26	1.21
1:L:8:ILE:CD1	1:L:339:ILE:HD12	1.71	1.19
1:K:355:ARG:NH2	4:O:282:TRP:CG	2.12	1.18
4:P:30:CYS:CB	4:P:36:VAL:HG23	1.73	1.17
1:K:355:ARG:NH2	4:O:282:TRP:CE2	2.15	1.15
1:L:8:ILE:HD11	1:L:339:ILE:CD1	1.76	1.14
7:Y:338:ARG:NH2	7:Y:406:ASP:OD2	1.80	1.14
1:L:135:LYS:HZ1	6:V:120:THR:HG23	0.99	1.13
7:X:419:ARG:NH2	7:X:420:ASN:OD1	1.81	1.13
1:K:408:GLN:HE22	1:K:410:TRP:CD1	1.68	1.12
1:K:372:ARG:HH22	4:O:12:LYS:C	1.57	1.11
1:B:521:TRP:CZ3	1:B:544:GLY:HA3	1.88	1.09
1:L:640:MET:HE1	1:L:645:ASN:HB3	1.31	1.08
7:X:154:GLU:OE1	7:X:154:GLU:O	1.70	1.08
1:L:135:LYS:NZ	6:V:120:THR:HG23	1.71	1.06
1:B:61:PRO:HD2	1:B:61:PRO:O	1.54	1.04
1:K:372:ARG:HH22	4:O:12:LYS:CA	1.71	1.02
1:K:408:GLN:HB3	1:K:411:ARG:HH22	1.16	1.02
3:N:923:GLN:NE2	3:N:928:HIS:C	2.16	1.02
1:L:336:ASN:O	1:L:351:THR:OG1	1.79	0.99
7:X:144:GLU:OE2	7:X:151:ARG:NH2	1.97	0.98
1:K:355:ARG:NH2	4:O:282:TRP:CD1	2.31	0.98
1:A:574:GLU:OE1	1:B:535:ARG:NH2	1.97	0.97
1:K:355:ARG:HH22	4:O:282:TRP:CD1	1.82	0.97
2:C:134:HIS:CE1	2:C:151:ARG:NH2	2.32	0.96
7:Y:433:GLU:OE1	7:Y:433:GLU:N	1.97	0.96
1:K:372:ARG:HH12	4:O:13:ASP:CA	1.77	0.96
1:L:135:LYS:NZ	6:V:120:THR:CG2	2.28	0.96
1:L:135:LYS:HZ1	6:V:120:THR:CG2	1.77	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:408:GLN:HE22	1:K:410:TRP:HD1	0.97	0.96
1:B:521:TRP:CZ3	1:B:544:GLY:CA	2.49	0.95
7:Y:444:TRP:CE3	7:Y:447:PHE:HE2	1.52	0.93
4:O:62:ARG:NH1	4:O:118:ASP:HA	1.85	0.92
1:K:408:GLN:HB3	1:K:411:ARG:NH2	1.85	0.92
1:K:408:GLN:NE2	1:K:410:TRP:CD1	2.36	0.92
1:L:228:GLN:HE22	1:L:244:TYR:HD1	1.09	0.92
1:K:372:ARG:HH12	4:O:13:ASP:C	1.79	0.90
1:L:11:ALA:HA	1:L:68:TRP:CZ3	2.07	0.89
7:Y:444:TRP:CZ3	7:Y:447:PHE:CE2	2.61	0.89
1:L:44:ARG:NH1	1:L:47:GLU:HA	1.88	0.88
1:L:44:ARG:HH12	1:L:47:GLU:HA	1.38	0.88
1:L:10:TRP:CZ3	1:L:331:HIS:HD2	1.88	0.88
1:B:789:LEU:HD23	5:R:115:MET:HE1	1.54	0.87
4:O:102:HIS:O	4:O:102:HIS:ND1	2.06	0.87
3:N:923:GLN:NE2	3:N:928:HIS:O	2.05	0.87
1:L:640:MET:CE	1:L:645:ASN:HB3	2.05	0.87
1:L:552:LEU:HB3	1:L:554:LEU:HD22	1.56	0.86
3:D:941:CYS:SG	3:D:966:CYS:HB3	2.16	0.86
1:B:521:TRP:CH2	1:B:544:GLY:HA2	2.10	0.86
1:K:372:ARG:NH2	4:O:12:LYS:C	2.33	0.86
4:Q:123:PRO:HD2	4:Q:126:MET:HE3	1.58	0.86
7:Y:162:ILE:HD12	7:Y:181:LEU:HD11	1.57	0.85
1:K:372:ARG:NH1	4:O:13:ASP:C	2.34	0.84
1:L:10:TRP:HE1	1:L:339:ILE:HG12	1.42	0.84
2:C:106:ARG:NH1	2:C:106:ARG:HB2	1.94	0.83
1:B:680:LEU:HD11	1:B:720:ARG:HG3	1.61	0.82
1:A:580:ARG:HH12	1:A:593:ALA:HB2	1.43	0.82
6:V:265:MET:HE1	6:V:305:HIS:HB3	1.62	0.82
1:K:408:GLN:NE2	1:K:410:TRP:HD1	1.74	0.81
7:X:366:LYS:NZ	7:X:461:GLU:OE1	2.13	0.81
1:L:10:TRP:CE3	1:L:331:HIS:CD2	2.69	0.81
7:X:433:GLU:OE2	7:X:433:GLU:N	2.13	0.81
1:L:422:GLN:NE2	1:L:645:ASN:OD1	2.14	0.81
1:L:103:LEU:HA	1:L:106:LYS:HZ3	1.46	0.80
2:C:134:HIS:CE1	2:C:151:ARG:HH21	1.96	0.80
1:L:433:MET:HE2	1:L:452:VAL:O	1.82	0.80
7:X:176:GLU:OE2	7:X:176:GLU:N	2.15	0.80
2:C:32:ILE:HG22	2:C:43:VAL:HG22	1.63	0.79
7:Y:433:GLU:H	7:Y:433:GLU:CD	1.89	0.79
4:O:62:ARG:CZ	4:O:118:ASP:OD1	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:MET:HA	1:A:640:MET:HE3	1.64	0.78
2:C:347:LEU:HD11	4:Q:287:ASN:HB2	1.64	0.78
1:L:68:TRP:CD1	1:L:69:TYR:H	2.02	0.78
1:B:644:GLY:O	1:B:668:ARG:NH1	2.17	0.78
1:L:842:TRP:CD1	1:L:850:PRO:HG3	2.19	0.77
1:L:422:GLN:HE22	1:L:645:ASN:HA	1.48	0.77
4:E:148:MET:CE	2:I:732:VAL:HB	2.14	0.77
1:L:637:THR:HA	1:L:640:MET:HB2	1.64	0.77
4:G:126:MET:HE3	4:G:129:MET:SD	2.24	0.77
5:H:259:ASP:O	5:H:260:TRP:CD1	2.38	0.77
1:K:355:ARG:NH2	4:O:282:TRP:NE1	2.32	0.77
1:B:135:LYS:NZ	1:B:184:ASN:OD1	2.16	0.77
1:K:372:ARG:HH12	4:O:13:ASP:N	1.82	0.76
1:A:640:MET:HE1	1:A:645:ASN:HB2	1.68	0.76
1:B:61:PRO:O	1:B:61:PRO:CD	2.32	0.76
1:L:228:GLN:NE2	1:L:244:TYR:HD1	1.81	0.76
7:Y:444:TRP:CE3	7:Y:447:PHE:HD2	1.86	0.76
1:B:331:HIS:HD2	1:B:334:SER:H	1.32	0.75
4:O:34:GLN:HE22	4:O:58:GLY:C	1.95	0.75
1:A:856:CYS:HB3	1:A:858:CYS:SG	2.26	0.75
3:D:648:ILE:HG22	5:H:53:THR:HA	1.67	0.75
6:U:29:LYS:NZ	6:U:62:GLU:OE1	2.18	0.74
2:I:231:MET:HE3	2:I:233:LYS:HE3	1.69	0.74
2:C:746:CYS:SG	2:C:765:HIS:ND1	2.60	0.74
6:U:244:GLU:O	6:U:247:LYS:NZ	2.20	0.74
1:L:28:TYR:CE1	1:L:53:LEU:HD22	2.23	0.74
1:A:552:LEU:O	1:A:554:LEU:N	2.21	0.73
1:K:372:ARG:NH2	4:O:12:LYS:CA	2.49	0.73
1:L:10:TRP:HE1	1:L:339:ILE:CG1	2.01	0.73
1:B:785:CYS:HB3	1:B:789:LEU:H	1.54	0.73
1:L:69:TYR:CZ	1:L:71:ASN:HB2	2.24	0.73
3:D:923:GLN:CD	3:D:928:HIS:HA	2.13	0.73
6:V:177:ILE:HD13	6:V:320:LEU:HB2	1.71	0.73
2:I:631:ASP:OD1	2:I:631:ASP:O	2.06	0.72
2:C:106:ARG:CB	2:C:106:ARG:HH11	2.02	0.72
3:D:857:GLN:O	3:D:861:ASP:OD1	2.08	0.72
1:L:10:TRP:CE3	1:L:331:HIS:CG	2.77	0.72
6:U:117:THR:HG22	6:U:119:GLN:H	1.54	0.72
1:B:519:GLY:O	1:B:521:TRP:HD1	1.73	0.71
5:H:345:CYS:SG	5:H:346:ILE:N	2.63	0.71
1:K:372:ARG:NH1	4:O:13:ASP:CA	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:ILE:HD11	1:L:339:ILE:HD12	0.82	0.71
6:V:1:MET:H1	6:V:1:MET:HE2	1.56	0.71
1:B:519:GLY:O	1:B:521:TRP:CD1	2.43	0.71
6:V:269:GLY:HA2	6:V:303:PHE:CE1	2.26	0.71
3:D:941:CYS:SG	3:D:966:CYS:CB	2.77	0.71
1:L:368:TRP:HE1	1:L:375:TYR:HB2	1.55	0.71
5:R:66:GLN:HE22	5:R:110:ALA:HA	1.56	0.71
1:B:87:VAL:HG22	1:B:108:PHE:HB2	1.72	0.70
4:F:287:ASN:HD21	4:F:289:THR:HG22	1.56	0.70
1:L:178:LEU:H	1:L:178:LEU:HD12	1.55	0.70
1:K:372:ARG:HH22	4:O:12:LYS:HA	1.56	0.70
1:A:611:VAL:O	1:A:616:ARG:NH1	2.24	0.70
1:B:789:LEU:HD23	5:R:115:MET:CE	2.21	0.70
2:C:106:ARG:HB2	2:C:106:ARG:HH11	1.56	0.70
4:O:122:ALA:HB1	4:O:126:MET:CE	2.22	0.70
7:Y:443:PHE:HD1	7:Y:444:TRP:HD1	1.38	0.70
1:K:116:CYS:HA	1:K:133:LEU:HA	1.72	0.70
1:L:103:LEU:O	1:L:105:GLY:N	2.25	0.70
1:A:640:MET:CE	1:A:645:ASN:HB2	2.21	0.69
1:B:316:ARG:NH2	1:B:353:PHE:O	2.24	0.69
2:C:53:ALA:HB2	2:C:62:LYS:HZ2	1.55	0.69
2:I:176:TYR:CD1	2:I:177:PHE:CE2	2.80	0.69
1:B:521:TRP:CE3	1:B:544:GLY:HA3	2.28	0.69
1:A:608:GLU:O	1:A:616:ARG:NH1	2.25	0.69
3:D:551:VAL:HG22	3:D:649:ILE:HD12	1.75	0.69
1:K:513:ASN:O	1:K:517:GLN:NE2	2.25	0.69
4:F:268:ILE:O	4:F:269:HIS:ND1	2.21	0.68
1:B:521:TRP:CH2	1:B:544:GLY:CA	2.75	0.68
6:U:229:ALA:HB3	6:U:240:VAL:HB	1.74	0.68
4:F:116:VAL:HA	4:F:134:SER:HA	1.74	0.68
1:L:223:ASN:OD1	1:L:223:ASN:O	2.12	0.68
4:F:154:SER:O	4:F:155:LEU:HD22	1.94	0.68
1:K:372:ARG:NH2	4:O:12:LYS:HA	2.08	0.68
1:L:720:ARG:O	1:L:720:ARG:NH1	2.27	0.68
4:O:122:ALA:HB1	4:O:126:MET:HE3	1.76	0.68
1:K:408:GLN:OE1	1:K:410:TRP:CD1	2.46	0.67
6:U:187:LEU:HD22	6:U:254:LEU:HB3	1.74	0.67
6:V:1:MET:HE2	6:V:1:MET:N	2.08	0.67
7:Y:454:HIS:O	7:Y:454:HIS:ND1	2.27	0.67
1:L:619:PHE:HE1	1:L:623:PHE:HD2	1.41	0.67
2:C:746:CYS:SG	2:C:768:HIS:ND1	2.67	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:858:GLN:HA	3:D:861:ASP:OD1	1.93	0.66
6:V:67:GLU:OE1	6:V:67:GLU:O	2.14	0.66
1:L:552:LEU:CD2	1:L:553:ASN:H	2.08	0.66
1:L:644:GLY:O	1:L:668:ARG:NH1	2.27	0.66
2:I:73:LEU:HB3	2:I:96:ASN:HD21	1.59	0.66
1:A:377:CYS:HA	4:E:5:ARG:NH2	2.10	0.66
4:E:119:VAL:HG23	4:E:132:THR:HG22	1.76	0.66
2:I:176:TYR:HD1	2:I:177:PHE:CD2	2.13	0.66
4:O:114:THR:OG1	4:O:136:ASP:OD2	2.14	0.66
4:G:80:ASP:OD1	4:G:82:THR:OG1	2.13	0.65
1:L:228:GLN:CD	1:L:244:TYR:HA	2.21	0.65
1:K:408:GLN:CD	1:K:410:TRP:CD1	2.74	0.65
6:V:13:LEU:HD22	6:V:71:VAL:HG22	1.77	0.65
6:V:183:ARG:HH11	6:V:262:LEU:HD12	1.61	0.65
5:R:198:GLY:HA3	5:R:233:CYS:H	1.62	0.65
4:E:148:MET:HE2	2:I:732:VAL:HB	1.79	0.65
4:Q:207:ARG:HG3	4:Q:207:ARG:HH11	1.61	0.65
1:A:580:ARG:NH1	1:A:593:ALA:HB2	2.11	0.65
3:D:956:THR:HG23	3:D:957:GLN:HG3	1.79	0.65
3:N:876:ARG:HH12	3:N:879:ARG:HD3	1.60	0.65
2:I:176:TYR:HD1	2:I:177:PHE:CE2	2.16	0.64
1:L:103:LEU:HA	1:L:106:LYS:NZ	2.11	0.64
4:Q:205:ASN:O	4:Q:207:ARG:NH1	2.25	0.64
7:Y:82:VAL:HG11	7:Y:216:ILE:HD11	1.78	0.64
1:A:377:CYS:CA	4:E:5:ARG:NH2	2.60	0.64
3:D:690:LYS:NZ	2:I:626:SER:C	2.55	0.64
1:K:778:CYS:HB3	1:K:780:LYS:CG	2.28	0.64
1:L:86:ARG:NH1	1:L:86:ARG:HB2	2.13	0.64
1:B:226:ALA:HA	1:B:244:TYR:HB3	1.78	0.64
3:N:536:PHE:O	5:R:262:ARG:NH2	2.26	0.64
7:Y:399:CYS:SG	7:Y:404:ARG:NH1	2.71	0.63
5:H:259:ASP:O	5:H:260:TRP:HD1	1.81	0.63
4:F:45:GLY:O	4:F:47:TRP:CZ3	2.50	0.63
1:L:701:ARG:HH21	1:L:713:ARG:HH21	1.45	0.63
1:B:326:ALA:HB3	1:B:341:VAL:HG13	1.80	0.63
1:L:8:ILE:HG22	1:L:327:SER:OG	1.99	0.63
4:P:67:HIS:HB3	4:P:124:LYS:HZ2	1.64	0.63
1:K:372:ARG:NH2	4:O:11:HIS:O	2.32	0.63
1:L:587:TYR:OH	1:L:615:ASP:OD2	2.16	0.63
6:V:101:VAL:HG23	6:V:137:LEU:HD11	1.80	0.63
6:V:183:ARG:NH1	6:V:262:LEU:HD12	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:255:ALA:HB2	2:C:272:MET:HB2	1.80	0.63
1:A:553:ASN:O	1:A:556:VAL:N	2.29	0.63
5:R:345:CYS:SG	5:R:346:ILE:N	2.72	0.63
1:A:377:CYS:CA	4:E:5:ARG:HH22	2.12	0.62
1:L:10:TRP:CE3	1:L:331:HIS:HA	2.34	0.62
1:B:785:CYS:HB3	1:B:789:LEU:N	2.14	0.62
2:C:347:LEU:HD12	4:Q:288:ILE:H	1.64	0.62
3:D:928:HIS:CD2	1:L:713:ARG:HH12	2.18	0.62
3:N:849:ARG:HH21	3:N:853:PRO:HG3	1.63	0.62
5:R:66:GLN:NE2	5:R:110:ALA:HA	2.13	0.62
1:A:713:ARG:NH2	2:I:745:VAL:O	2.32	0.62
1:L:228:GLN:OE1	1:L:244:TYR:HB2	1.99	0.62
4:F:119:VAL:HG13	4:F:130:LEU:HD21	1.81	0.62
2:I:239:THR:OG1	2:I:240:HIS:N	2.32	0.62
1:L:10:TRP:CE3	1:L:331:HIS:CB	2.81	0.62
1:K:67:ALA:HB3	1:K:79:ALA:HB3	1.81	0.62
1:L:673:GLN:O	1:L:676:SER:OG	2.14	0.62
6:V:27:LEU:HD21	6:V:53:LEU:HD11	1.81	0.62
7:X:338:ARG:NH2	7:X:406:ASP:OD1	2.25	0.62
2:C:631:ASP:OD1	2:C:631:ASP:O	2.18	0.61
7:Y:210:PHE:HB2	7:Y:460:LEU:HD11	1.82	0.61
1:L:331:HIS:CE1	1:L:334:SER:H	2.18	0.61
1:L:368:TRP:NE1	1:L:375:TYR:HB2	2.15	0.61
2:I:136:LEU:HD12	2:I:150:LEU:HD21	1.81	0.61
2:I:425:PRO:HD2	2:I:428:GLU:OE1	2.00	0.61
5:R:333:THR:OG1	5:R:335:TRP:NE1	2.33	0.61
1:B:260:VAL:HG22	1:B:261:LEU:HD12	1.82	0.61
1:L:86:ARG:HG3	1:L:108:PHE:O	2.00	0.61
6:V:20:LEU:HD21	6:V:206:PHE:HD1	1.66	0.61
2:I:722:CYS:HB3	2:I:736:CYS:SG	2.41	0.61
1:L:426:LEU:HD12	1:L:649:ILE:HG21	1.82	0.61
4:E:244:ASP:OD2	4:E:273:GLN:NE2	2.30	0.61
6:V:229:ALA:HB3	6:V:240:VAL:HB	1.83	0.61
1:L:53:LEU:CD1	1:L:56:ILE:HD11	2.31	0.61
1:L:433:MET:CE	1:L:452:VAL:O	2.48	0.61
3:D:691:ASP:OD2	3:D:692:LEU:N	2.33	0.60
6:U:19:GLY:HA3	6:U:68:PHE:CD2	2.36	0.60
1:B:456:ILE:O	1:B:460:VAL:HG22	2.01	0.60
1:B:785:CYS:O	1:B:789:LEU:HA	2.01	0.60
3:D:909:VAL:HG11	3:D:914:CYS:HA	1.83	0.60
4:G:126:MET:CE	4:G:129:MET:SD	2.89	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:411:ARG:HG3	1:K:411:ARG:HH11	1.65	0.60
1:K:529:LEU:HD23	1:K:591:MET:HG3	1.82	0.60
1:K:608:GLU:O	1:K:616:ARG:NH1	2.34	0.60
3:N:926:ILE:HD12	3:N:949:HIS:HB3	1.83	0.60
2:I:228:ARG:NH1	7:X:345:GLU:OE1	2.34	0.60
1:K:389:ASP:OD1	4:O:292:VAL:HG23	2.01	0.60
1:A:580:ARG:HG3	1:A:581:LEU:N	2.16	0.60
1:B:178:LEU:HB3	1:B:179:TYR:HD1	1.67	0.60
4:O:123:PRO:HG2	4:O:126:MET:HE2	1.83	0.60
2:C:190:LEU:HD13	2:C:201:ARG:HB3	1.83	0.60
1:A:580:ARG:HH12	1:A:593:ALA:CB	2.13	0.60
4:Q:31:SER:OG	4:Q:33:ASP:OD2	2.20	0.60
1:B:824:PHE:CE1	1:B:834:GLY:HA2	2.37	0.59
3:D:550:LEU:HD22	3:D:552:TYR:HD2	1.66	0.59
4:E:289:THR:HG22	4:E:291:THR:HG23	1.83	0.59
6:V:28:ILE:HG13	6:V:32:PHE:CD2	2.36	0.59
1:A:585:ASN:OD1	1:A:588:LEU:HD12	2.03	0.59
1:B:787:LEU:O	3:N:876:ARG:NE	2.28	0.59
1:L:97:ASN:O	1:L:99:LYS:NZ	2.35	0.59
1:L:135:LYS:HZ3	6:V:120:THR:CG2	2.14	0.59
6:U:309:PRO:O	6:U:311:ASP:N	2.33	0.59
1:B:118:THR:HG21	1:B:189:SER:HA	1.84	0.59
1:B:640:MET:SD	1:B:645:ASN:HB3	2.43	0.59
1:L:271:THR:N	1:L:286:LEU:O	2.32	0.59
5:H:115:MET:HE3	5:H:116:TYR:CE2	2.38	0.59
1:L:679:MET:HE3	1:L:679:MET:O	2.03	0.59
6:V:269:GLY:HA2	6:V:303:PHE:CD1	2.37	0.59
4:F:64:THR:HG21	4:F:120:LYS:HD3	1.84	0.59
1:L:103:LEU:HD22	1:L:106:LYS:CE	2.33	0.59
4:E:148:MET:HE1	2:I:732:VAL:HB	1.85	0.59
2:I:38:ALA:HB1	2:I:306:ARG:HE	1.68	0.59
1:K:509:GLY:O	1:K:513:ASN:ND2	2.36	0.59
1:L:409:VAL:HG21	1:L:434:LYS:HD3	1.84	0.59
5:R:282:GLN:HA	5:R:310:VAL:HG13	1.85	0.59
3:N:742:VAL:HG11	5:R:270:ILE:HD12	1.84	0.58
6:U:28:ILE:HG13	6:U:32:PHE:CD1	2.38	0.58
7:X:122:ARG:NH2	7:X:317:GLU:O	2.36	0.58
7:X:441:ASN:O	7:X:445:ARG:NH1	2.37	0.58
2:C:273:MET:O	2:C:275:ASP:N	2.31	0.58
1:B:103:LEU:O	1:B:105:GLY:N	2.36	0.58
1:B:789:LEU:CD2	5:R:115:MET:HE1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:55:THR:HG22	4:G:56:HIS:CD2	2.36	0.58
6:U:183:ARG:HH11	6:U:262:LEU:HG	1.68	0.58
6:V:97:ILE:HD11	6:V:123:ILE:HD11	1.85	0.58
7:Y:390:ARG:HG2	7:Y:458:LEU:HD21	1.84	0.58
2:C:718:ASN:HD21	1:K:736:SER:HB3	1.68	0.58
4:F:119:VAL:HG22	4:F:132:THR:HG22	1.86	0.58
5:R:152:VAL:HA	5:R:170:SER:HA	1.86	0.58
1:B:593:ALA:HA	1:B:596:THR:HG22	1.85	0.58
2:C:720:SER:OG	1:K:732:GLN:O	2.14	0.58
1:L:552:LEU:HD23	1:L:553:ASN:H	1.68	0.58
1:A:640:MET:HE1	1:A:645:ASN:CB	2.34	0.58
1:L:271:THR:OG1	1:L:286:LEU:HD22	2.04	0.58
7:Y:361:GLN:O	7:Y:365:GLU:HG3	2.03	0.58
5:H:305:HIS:ND1	5:H:306:LYS:N	2.52	0.57
1:L:521:TRP:H	1:L:521:TRP:CD1	2.20	0.57
4:G:31:SER:OG	4:G:33:ASP:OD1	2.14	0.57
3:D:691:ASP:OD2	3:D:691:ASP:C	2.47	0.57
6:V:296:TYR:HB3	6:V:307:LEU:HB2	1.87	0.57
2:C:151:ARG:O	2:C:153:LYS:N	2.37	0.57
2:I:231:MET:SD	2:I:247:CYS:SG	3.02	0.57
1:L:268:LYS:NZ	1:L:289:ASP:O	2.37	0.57
6:U:34:PRO:HG2	6:U:35:ARG:NH1	2.19	0.57
5:R:109:VAL:HB	5:R:120:LEU:HD21	1.86	0.57
1:L:363:ILE:HD12	1:L:363:ILE:H	1.69	0.57
1:B:842:TRP:CD1	1:B:850:PRO:HG3	2.40	0.56
4:G:299:ASP:OD1	4:G:299:ASP:N	2.38	0.56
1:K:620:ALA:HA	1:K:624:LEU:HD13	1.85	0.56
1:B:112:HIS:HD2	1:B:136:HIS:CE1	2.23	0.56
2:C:236:ASP:OD1	2:C:236:ASP:C	2.47	0.56
2:C:451:MET:HE2	3:N:701:VAL:HG23	1.88	0.56
1:L:640:MET:HE2	1:L:648:GLY:N	2.21	0.56
6:U:203:ASP:HA	6:U:207:TYR:HD2	1.70	0.56
6:V:177:ILE:CD1	6:V:320:LEU:HB2	2.34	0.56
1:A:74:PRO:HD2	1:A:74:PRO:O	2.05	0.56
3:D:707:LEU:HD21	2:I:447:GLN:HG3	1.87	0.56
1:B:521:TRP:CZ3	1:B:544:GLY:HA2	2.29	0.56
2:C:93:ALA:HB2	2:C:126:VAL:HG13	1.87	0.56
1:L:271:THR:OG1	1:L:286:LEU:O	2.17	0.56
1:L:649:ILE:HD11	1:L:654:LEU:HD23	1.88	0.56
1:B:499:TRP:HA	1:B:511:PHE:CD1	2.40	0.56
2:I:231:MET:HE3	2:I:233:LYS:CE	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:VAL:HG12	1:A:508:VAL:O	2.06	0.56
1:L:228:GLN:OE1	1:L:244:TYR:HA	2.06	0.56
1:A:377:CYS:HA	4:E:5:ARG:HH22	1.71	0.56
3:D:941:CYS:HB3	3:D:943:HIS:CE1	2.41	0.56
1:L:425:SER:O	1:L:429:THR:OG1	2.17	0.56
1:K:372:ARG:NH1	4:O:13:ASP:O	2.39	0.55
4:P:30:CYS:CB	4:P:36:VAL:CG2	2.67	0.55
6:V:31:LEU:O	6:V:31:LEU:HD23	2.05	0.55
6:V:97:ILE:O	6:V:101:VAL:HG12	2.06	0.55
1:L:68:TRP:CD1	1:L:69:TYR:N	2.73	0.55
1:L:723:LEU:HD23	1:L:723:LEU:H	1.71	0.55
1:A:377:CYS:C	4:E:5:ARG:HH22	2.15	0.55
4:E:114:THR:HG22	4:E:115:SER:H	1.71	0.55
4:O:275:ASP:C	4:O:275:ASP:OD1	2.49	0.55
1:B:331:HIS:CD2	1:B:334:SER:H	2.19	0.55
6:V:244:GLU:O	6:V:247:LYS:NZ	2.39	0.55
1:B:69:TYR:CZ	1:B:71:ASN:HB2	2.41	0.55
1:L:135:LYS:HZ3	6:V:120:THR:HG22	1.71	0.55
7:Y:113:HIS:O	7:Y:117:ILE:HG23	2.07	0.55
1:K:74:PRO:HD2	1:K:74:PRO:O	2.06	0.55
4:P:146:ASP:O	4:P:148:MET:N	2.40	0.55
6:U:67:GLU:CD	6:U:67:GLU:H	2.15	0.55
6:U:202:ILE:HG22	6:U:207:TYR:HE2	1.72	0.55
7:Y:162:ILE:HD12	7:Y:181:LEU:CD1	2.34	0.55
7:Y:338:ARG:HH21	7:Y:406:ASP:CG	2.00	0.55
1:L:720:ARG:O	1:L:724:ASP:HB3	2.06	0.55
6:U:108:HIS:O	6:U:109:HIS:ND1	2.39	0.55
1:B:606:LEU:HD11	1:B:624:LEU:HD11	1.88	0.55
7:X:373:LEU:HB3	7:X:454:HIS:NE2	2.22	0.55
1:K:77:LEU:HA	1:K:91:SER:HA	1.89	0.54
1:L:10:TRP:NE1	1:L:339:ILE:HG12	2.19	0.54
7:Y:186:GLU:O	7:Y:187:HIS:ND1	2.38	0.54
3:D:869:ILE:HD11	5:H:318:ILE:HG13	1.90	0.54
1:K:490:ARG:NH1	1:K:621:CYS:O	2.39	0.54
1:L:608:GLU:O	1:L:616:ARG:NH1	2.40	0.54
3:N:914:CYS:SG	3:N:915:ALA:N	2.80	0.54
7:Y:78:ASN:O	7:Y:82:VAL:HG12	2.07	0.54
1:K:640:MET:SD	1:K:645:ASN:HB3	2.47	0.54
1:L:361:SER:OG	1:L:365:SER:O	2.25	0.54
3:D:690:LYS:NZ	2:I:626:SER:O	2.40	0.54
1:L:6:PRO:HB3	1:L:22:ASP:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:LEU:HD12	1:A:838:HIS:HB3	1.89	0.54
1:B:181:LEU:HD22	1:B:216:THR:HG23	1.89	0.54
3:D:690:LYS:HZ3	2:I:626:SER:C	2.14	0.54
4:F:61:TRP:HE1	4:F:79:PHE:HD2	1.55	0.54
1:K:411:ARG:HG2	1:K:414:ILE:HD11	1.89	0.54
1:L:217:SER:O	1:L:217:SER:OG	2.25	0.54
4:P:84:ALA:HB1	4:P:86:TRP:HE1	1.73	0.54
1:L:135:LYS:NZ	6:V:120:THR:HG22	2.17	0.54
2:C:347:LEU:HD12	4:Q:288:ILE:HB	1.90	0.54
6:U:32:PHE:HD2	6:U:194:LEU:HD21	1.73	0.54
6:U:186:VAL:HG22	6:U:240:VAL:HG22	1.89	0.54
4:F:181:MET:O	4:F:182:ILE:HD13	2.08	0.54
7:Y:436:THR:HG23	7:Y:439:MET:HE3	1.90	0.54
2:C:231:MET:HE3	2:C:233:LYS:HE3	1.89	0.53
1:L:61:PRO:HG2	1:L:62:TYR:CE2	2.43	0.53
1:L:523:ARG:O	1:L:527:VAL:HG22	2.08	0.53
1:B:283:LEU:O	1:B:295:LEU:HD12	2.08	0.53
4:E:80:ASP:O	4:E:82:THR:HG23	2.08	0.53
4:F:240:ILE:HG22	4:F:242:THR:HG23	1.88	0.53
1:L:231:THR:HG21	1:L:275:TRP:HD1	1.72	0.53
3:N:960:CYS:SG	3:N:964:CYS:HB3	2.48	0.53
1:A:585:ASN:HD21	1:A:588:LEU:H	1.57	0.53
1:B:669:THR:HG23	1:B:671:ASP:H	1.72	0.53
1:L:338:MET:HE3	1:L:338:MET:HA	1.91	0.53
3:N:923:GLN:HE22	3:N:929:VAL:N	1.99	0.53
4:O:220:ASP:CB	4:O:243:LYS:HZ3	2.21	0.53
7:X:119:ALA:HB2	7:X:201:LEU:HD23	1.89	0.53
2:C:767:GLN:HA	2:C:770:MET:HB3	1.91	0.53
3:D:658:VAL:O	3:D:659:HIS:ND1	2.41	0.53
3:D:690:LYS:CE	2:I:626:SER:O	2.57	0.53
1:K:787:LEU:HD13	1:K:838:HIS:HB3	1.90	0.53
1:K:827:CYS:CB	1:K:858:CYS:SG	2.90	0.53
4:O:62:ARG:NH1	4:O:118:ASP:CG	2.55	0.53
6:U:10:VAL:HG23	6:U:76:TRP:HB2	1.91	0.53
6:V:31:LEU:HD22	6:V:32:PHE:CE2	2.44	0.53
6:V:197:ILE:HG22	6:V:201:LEU:HD23	1.90	0.53
1:A:459:ILE:HG21	1:A:492:LEU:HD23	1.90	0.53
4:O:67:HIS:CG	4:O:68:PRO:HD2	2.44	0.53
1:B:331:HIS:CD2	1:B:333:THR:H	2.27	0.53
3:D:550:LEU:HD23	3:D:551:VAL:N	2.23	0.53
2:C:306:ARG:HH11	2:C:325:GLN:HE22	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:926:ILE:HD11	3:D:953:TRP:HB2	1.90	0.52
4:O:62:ARG:NH1	4:O:117:THR:O	2.41	0.52
6:V:242:ASP:OD2	6:V:242:ASP:N	2.40	0.52
4:F:231:LEU:HD12	4:F:289:THR:O	2.10	0.52
1:L:28:TYR:CE1	1:L:53:LEU:CD2	2.90	0.52
4:O:284:VAL:HG22	4:O:293:LEU:HD11	1.91	0.52
3:D:690:LYS:NZ	2:I:626:SER:OG	2.37	0.52
1:K:778:CYS:HB3	1:K:780:LYS:HG3	1.91	0.52
6:V:254:LEU:HD12	6:V:254:LEU:H	1.73	0.52
4:F:199:ILE:HD11	4:F:238:LEU:HD21	1.90	0.52
6:U:315:SER:O	6:U:319:VAL:HG12	2.10	0.52
2:C:83:HIS:CE1	2:C:85:MET:HB2	2.44	0.52
4:O:122:ALA:HB1	4:O:126:MET:HE1	1.92	0.52
7:Y:443:PHE:CD1	7:Y:444:TRP:HD1	2.23	0.52
1:B:429:THR:HG23	1:B:650:LEU:HD13	1.92	0.52
4:G:312:ASN:O	4:G:314:LYS:NZ	2.43	0.52
4:E:137:GLY:C	4:E:138:ILE:HD13	2.35	0.52
5:H:116:TYR:HD1	5:H:164:LEU:HD13	1.74	0.52
1:K:238:ASP:O	1:K:253:LEU:N	2.41	0.52
1:A:522:GLU:CD	1:A:522:GLU:H	2.15	0.52
1:K:389:ASP:OD1	4:O:292:VAL:CG2	2.58	0.52
1:K:490:ARG:NH2	1:K:626:ASP:OD2	2.43	0.52
1:L:228:GLN:NE2	1:L:244:TYR:HA	2.25	0.52
5:H:105:PRO:HD2	5:H:125:TYR:HB3	1.91	0.51
6:V:176:PRO:O	6:V:176:PRO:HG2	2.09	0.51
1:L:656:LYS:O	1:L:656:LYS:HD3	2.10	0.51
5:R:124:SER:OG	5:R:125:TYR:N	2.43	0.51
2:C:122:THR:HG21	7:Y:340:GLN:HE21	1.75	0.51
4:E:242:THR:O	4:E:281:VAL:HG12	2.11	0.51
1:K:200:LEU:O	1:K:211:PHE:N	2.43	0.51
4:P:91:GLY:O	4:P:102:HIS:N	2.42	0.51
1:L:225:LYS:HG2	1:L:225:LYS:O	2.10	0.51
2:I:46:ARG:NH1	7:X:341:ASP:OD1	2.43	0.51
2:I:776:SER:OG	2:I:777:SER:N	2.44	0.51
3:D:689:ARG:HB3	3:D:692:LEU:HB2	1.93	0.51
3:N:960:CYS:CB	3:N:964:CYS:HB3	2.41	0.51
2:C:106:ARG:NH1	2:C:106:ARG:CB	2.64	0.51
1:K:408:GLN:OE1	1:K:410:TRP:NE1	2.44	0.51
1:K:775:CYS:SG	1:K:778:CYS:HB2	2.50	0.51
1:L:10:TRP:CZ3	1:L:331:HIS:CA	2.90	0.51
6:U:105:LEU:HD22	6:U:110:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:375:PHE:HD2	7:X:389:LEU:HD21	1.76	0.51
3:D:869:ILE:HD11	5:H:318:ILE:CG1	2.41	0.51
1:L:433:MET:SD	1:L:453:TYR:HA	2.51	0.50
4:P:174:SER:O	4:P:174:SER:OG	2.22	0.50
1:B:534:ILE:O	1:B:538:ILE:HG23	2.11	0.50
1:B:619:PHE:CE1	1:B:623:PHE:CD2	2.99	0.50
1:L:457:LYS:NZ	1:L:637:THR:HG21	2.26	0.50
3:N:693:VAL:O	3:N:697:SER:OG	2.26	0.50
6:U:47:THR:HG21	6:U:300:THR:HG21	1.93	0.50
1:A:408:GLN:HB2	1:A:411:ARG:NH2	2.26	0.50
1:B:426:LEU:CD1	1:B:646:LEU:HD13	2.42	0.50
3:N:957:GLN:OE1	3:N:957:GLN:N	2.39	0.50
6:U:7:GLU:N	6:U:7:GLU:OE1	2.44	0.50
1:B:641:LYS:HA	1:B:661:LEU:HD13	1.94	0.50
4:O:274:PHE:HZ	4:O:313:TRP:HB3	1.75	0.50
1:A:535:ARG:HA	1:A:538:ILE:HD12	1.92	0.50
1:K:411:ARG:HG3	1:K:411:ARG:NH1	2.27	0.50
5:R:78:SER:OG	5:R:79:SER:N	2.44	0.50
6:V:268:ILE:HD12	6:V:284:ILE:HG12	1.92	0.50
7:Y:423:VAL:HG12	7:Y:423:VAL:O	2.11	0.50
1:B:619:PHE:CE1	1:B:623:PHE:HD2	2.29	0.50
4:F:222:VAL:HG12	4:F:242:THR:HG22	1.93	0.50
2:I:312:SER:O	2:I:312:SER:OG	2.25	0.50
1:K:67:ALA:N	1:K:79:ALA:O	2.42	0.50
4:P:67:HIS:HB3	4:P:124:LYS:NZ	2.26	0.50
7:X:389:LEU:O	7:X:393:ILE:HG22	2.12	0.50
3:N:849:ARG:HE	3:N:853:PRO:HG3	1.76	0.50
5:R:314:VAL:HB	5:R:323:LEU:HD11	1.93	0.50
2:I:742:MET:HE3	2:I:747:HIS:C	2.37	0.50
4:O:34:GLN:NE2	4:O:58:GLY:O	2.38	0.50
6:U:302:ASN:OD1	6:U:303:PHE:CD1	2.64	0.50
1:A:359:ALA:HB1	4:E:20:PHE:HD2	1.77	0.49
1:A:529:LEU:HD23	1:A:591:MET:HG3	1.93	0.49
1:B:536:ARG:O	1:B:540:ILE:HG22	2.11	0.49
4:F:5:ARG:O	1:L:375:TYR:HB3	2.12	0.49
5:R:289:TRP:H	5:R:289:TRP:CD1	2.30	0.49
1:A:646:LEU:HD21	1:A:662:MET:HE1	1.93	0.49
1:B:492:LEU:HA	1:B:495:GLN:HG3	1.93	0.49
6:V:31:LEU:HD22	6:V:32:PHE:CZ	2.47	0.49
2:C:718:ASN:ND2	1:K:736:SER:HB3	2.27	0.49
4:E:123:PRO:HD2	4:E:126:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:LEU:HA	1:K:212:ASP:HA	1.94	0.49
1:L:103:LEU:HD22	1:L:106:LYS:HE2	1.93	0.49
4:P:200:PHE:HD1	4:P:209:TYR:HB3	1.77	0.49
2:C:42:VAL:HG11	2:C:80:VAL:HG21	1.93	0.49
4:P:238:LEU:HD12	4:P:239:ALA:H	1.78	0.49
1:A:640:MET:HE3	1:A:640:MET:CA	2.38	0.49
3:D:666:TYR:HE1	3:D:680:ASN:HB3	1.77	0.49
4:F:295:SER:O	4:F:302:VAL:HB	2.13	0.49
4:G:82:THR:HG22	4:G:110:VAL:HG12	1.94	0.49
2:I:117:THR:HG22	2:I:117:THR:O	2.12	0.49
3:D:858:GLN:CA	3:D:861:ASP:OD1	2.60	0.49
1:L:637:THR:O	1:L:641:LYS:N	2.45	0.49
7:Y:375:PHE:CZ	7:Y:454:HIS:CE1	3.00	0.49
1:A:788:CYS:SG	1:A:838:HIS:HE1	2.35	0.49
4:G:192:ASN:CB	4:G:194:MET:HE2	2.43	0.49
6:U:109:HIS:ND1	6:U:109:HIS:O	2.43	0.49
7:X:440:TYR:CE2	7:X:452:LYS:HD3	2.47	0.49
3:D:934:SER:HA	1:L:827:CYS:HA	1.95	0.49
4:E:284:VAL:HG12	4:E:293:LEU:HD11	1.94	0.49
2:I:134:HIS:O	2:I:134:HIS:ND1	2.46	0.49
2:I:176:TYR:CE1	2:I:177:PHE:CE2	3.01	0.49
6:U:9:ARG:NH1	6:U:75:THR:HG21	2.27	0.49
2:I:36:ARG:HD3	2:I:84:GLN:O	2.13	0.49
2:I:104:LEU:HD23	2:I:111:LYS:HD2	1.95	0.49
6:V:269:GLY:HA2	6:V:303:PHE:HE1	1.78	0.49
4:F:286:TRP:CZ3	4:F:293:LEU:HB2	2.47	0.49
2:I:239:THR:HG23	2:I:241:ARG:O	2.12	0.49
4:P:283:ARG:HG3	4:P:283:ARG:HH11	1.78	0.49
5:R:141:LYS:HE2	5:R:143:HIS:C	2.37	0.49
6:U:34:PRO:HD2	6:U:35:ARG:HH22	1.78	0.49
1:B:111:LYS:HZ3	1:B:112:HIS:CG	2.31	0.48
2:C:345:TYR:CD1	2:C:347:LEU:HD21	2.47	0.48
2:C:345:TYR:CE1	2:C:347:LEU:HD21	2.48	0.48
1:L:204:MET:HA	1:L:204:MET:HE2	1.95	0.48
4:Q:17:ASP:OD2	4:Q:62:ARG:HG3	2.13	0.48
7:Y:440:TYR:CE1	7:Y:452:LYS:HD3	2.48	0.48
1:B:111:LYS:HG3	1:B:112:HIS:N	2.27	0.48
1:B:684:PRO:HA	1:B:688:LEU:HD22	1.94	0.48
1:L:619:PHE:CE1	1:L:623:PHE:HD2	2.27	0.48
1:B:512:LEU:HD11	1:B:528:ALA:HB2	1.95	0.48
2:C:719:CYS:HA	1:K:733:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:876:ARG:HH22	3:N:879:ARG:HH11	1.59	0.48
2:C:122:THR:HG21	7:Y:340:GLN:NE2	2.28	0.48
1:L:554:LEU:N	1:L:554:LEU:HD23	2.29	0.48
3:D:928:HIS:HD2	1:L:713:ARG:HH12	1.60	0.48
4:O:274:PHE:CD1	4:O:305:TRP:CE3	3.02	0.48
4:P:228:ALA:HB3	4:P:237:ILE:HB	1.94	0.48
7:X:433:GLU:H	7:X:433:GLU:CD	2.16	0.48
1:A:411:ARG:CZ	1:A:411:ARG:HB2	2.43	0.48
1:K:67:ALA:O	1:K:79:ALA:N	2.46	0.48
1:L:326:ALA:HB3	1:L:341:VAL:HG23	1.94	0.48
4:P:16:HIS:H	4:P:31:SER:CB	2.27	0.48
1:A:665:TYR:O	1:A:669:THR:HG22	2.13	0.48
1:B:13:HIS:CD2	1:B:72:TYR:CE2	3.02	0.48
1:B:70:LEU:HD12	1:B:70:LEU:N	2.29	0.48
4:F:228:ALA:HB3	4:F:237:ILE:HB	1.96	0.48
5:H:72:THR:HG22	5:H:89:ARG:HD3	1.96	0.48
1:K:369:ALA:HB2	1:K:374:LEU:HD23	1.95	0.48
1:L:558:ALA:O	1:L:562:SER:N	2.42	0.48
1:L:701:ARG:O	1:L:705:ASP:OD1	2.32	0.48
5:R:88:VAL:HG12	5:R:88:VAL:O	2.13	0.48
4:F:289:THR:HG23	4:F:291:THR:HG23	1.96	0.48
4:G:113:ARG:NH1	4:G:113:ARG:HB2	2.29	0.48
4:E:81:ARG:HG3	4:E:114:THR:O	2.14	0.48
1:K:374:LEU:HD12	4:O:9:ALA:HB3	1.96	0.48
1:L:10:TRP:CE3	1:L:331:HIS:CA	2.96	0.48
4:Q:58:GLY:N	4:Q:80:ASP:OD1	2.47	0.48
7:X:152:ALA:O	7:X:157:ARG:NH1	2.47	0.48
1:B:70:LEU:HD13	1:B:121:TRP:HB3	1.95	0.48
4:G:55:THR:HG23	4:G:86:TRP:CZ2	2.49	0.48
1:L:112:HIS:ND1	1:L:139:ASP:OD1	2.46	0.48
1:L:839:MET:HE3	1:L:850:PRO:HG2	1.96	0.48
6:U:93:GLY:O	6:U:97:ILE:HG22	2.14	0.48
6:V:24:THR:O	6:V:28:ILE:HG22	2.13	0.48
7:X:393:ILE:O	7:X:397:ILE:HG22	2.14	0.48
1:B:220:MET:SD	1:B:220:MET:N	2.87	0.47
1:B:509:GLY:O	1:B:512:LEU:N	2.47	0.47
1:L:106:LYS:HE3	1:L:147:ILE:O	2.14	0.47
7:X:47:PHE:HB3	7:X:440:TYR:CD1	2.49	0.47
1:B:499:TRP:HA	1:B:511:PHE:HD1	1.78	0.47
1:B:673:GLN:O	1:B:676:SER:OG	2.28	0.47
2:C:760:CYS:O	2:C:762:HIS:ND1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:189:GLN:O	2:I:190:LEU:HD12	2.14	0.47
1:L:656:LYS:HD3	1:L:656:LYS:C	2.38	0.47
3:N:876:ARG:NH1	3:N:879:ARG:HD3	2.27	0.47
2:C:214:ASP:OD2	2:C:215:TRP:N	2.47	0.47
4:F:286:TRP:CE3	4:F:293:LEU:HB2	2.50	0.47
1:A:862:ASP:OD2	2:I:765:HIS:NE2	2.43	0.47
2:C:127:CYS:SG	2:C:128:PHE:N	2.87	0.47
1:K:534:ILE:O	1:K:538:ILE:HG12	2.14	0.47
4:Q:17:ASP:OD1	4:Q:18:VAL:N	2.47	0.47
4:Q:21:ASP:OD1	4:Q:24:GLY:N	2.45	0.47
6:V:80:ASN:OD1	6:V:81:VAL:N	2.47	0.47
1:A:17:ARG:HA	1:A:29:HIS:HA	1.95	0.47
2:C:742:MET:HE3	2:C:747:HIS:C	2.40	0.47
4:O:220:ASP:CB	4:O:243:LYS:NZ	2.77	0.47
6:U:28:ILE:HG23	6:V:207:TYR:OH	2.14	0.47
6:V:67:GLU:O	6:V:67:GLU:CD	2.57	0.47
1:A:367:MET:SD	4:E:27:MET:HE1	2.53	0.47
1:A:529:LEU:CD2	1:A:591:MET:HG3	2.45	0.47
4:G:268:ILE:N	4:G:268:ILE:HD12	2.29	0.47
1:L:325:ILE:HG12	1:L:340:VAL:HG11	1.96	0.47
4:Q:63:VAL:HG22	4:Q:74:LEU:HD22	1.95	0.47
4:Q:107:THR:HG21	4:Q:153:TRP:NE1	2.30	0.47
5:R:145:HIS:ND1	5:R:178:LEU:HD11	2.29	0.47
7:X:169:ARG:HG2	7:X:171:TRP:CZ2	2.50	0.47
1:A:722:LYS:HE2	1:A:722:LYS:HB2	1.71	0.47
1:B:336:ASN:O	1:B:351:THR:HA	2.14	0.47
1:B:662:MET:HE3	1:B:679:MET:HE1	1.97	0.47
1:B:684:PRO:O	1:B:688:LEU:HB2	2.15	0.47
2:C:164:GLU:N	2:C:164:GLU:OE1	2.48	0.47
3:D:538:ARG:HD2	5:H:312:TRP:HB3	1.96	0.47
3:D:553:PHE:HB3	3:D:647:VAL:HG12	1.96	0.47
5:H:73:ARG:NH1	5:H:111:TRP:CZ3	2.82	0.47
2:I:61:GLU:O	2:I:61:GLU:HG2	2.14	0.47
1:L:28:TYR:HD1	1:L:51:ALA:HB1	1.80	0.47
3:N:944:GLY:HA2	3:N:950:MET:HE1	1.96	0.47
6:U:182:ASN:OD1	6:U:182:ASN:N	2.47	0.47
6:U:203:ASP:OD2	6:U:203:ASP:N	2.47	0.47
1:A:522:GLU:OE1	1:A:522:GLU:N	2.42	0.47
1:B:792:MET:HA	1:B:824:PHE:CE2	2.49	0.47
2:I:70:LYS:O	2:I:72:SER:N	2.42	0.47
2:I:97:GLY:HA2	2:I:123:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:300:THR:HG22	6:U:301:PHE:H	1.80	0.47
1:A:574:GLU:CD	1:B:535:ARG:HH22	2.20	0.47
1:A:585:ASN:ND2	1:A:588:LEU:H	2.13	0.47
1:A:590:VAL:HG21	1:A:611:VAL:HG21	1.95	0.47
1:B:665:TYR:O	1:B:669:THR:HG22	2.15	0.47
2:I:207:ASN:OD1	2:I:207:ASN:C	2.58	0.47
1:L:619:PHE:CD1	1:L:619:PHE:C	2.91	0.47
3:N:956:THR:OG1	3:N:957:GLN:OE1	2.30	0.47
6:V:317:ILE:O	6:V:321:GLN:HG2	2.15	0.47
2:I:273:MET:O	2:I:275:ASP:N	2.37	0.47
1:K:557:VAL:HG11	1:K:588:LEU:HD22	1.97	0.47
1:L:86:ARG:NH1	1:L:86:ARG:CB	2.78	0.47
1:L:487:ASN:O	1:L:491:ILE:HG13	2.15	0.47
6:U:44:LEU:HD12	6:U:45:THR:N	2.30	0.47
1:A:580:ARG:NH2	1:A:593:ALA:HA	2.30	0.46
1:B:221:PHE:CE2	1:B:223:ASN:OD1	2.67	0.46
5:H:68:ASP:CG	5:H:73:ARG:H	2.23	0.46
1:L:410:TRP:O	1:L:413:HIS:HD2	1.98	0.46
1:B:779:ARG:O	5:R:182:GLY:HA3	2.15	0.46
1:B:835:HIS:O	1:B:839:MET:HG2	2.15	0.46
4:G:54:LYS:NZ	4:G:56:HIS:O	2.39	0.46
6:U:103:ALA:O	6:U:107:GLU:HG2	2.15	0.46
6:V:3:LEU:HD23	6:V:143:ILE:HD12	1.97	0.46
1:B:619:PHE:HE1	1:B:623:PHE:CD2	2.34	0.46
2:C:82:TRP:HA	2:C:90:LEU:HD23	1.97	0.46
2:C:347:LEU:CD1	4:Q:288:ILE:H	2.28	0.46
1:K:833:GLY:HA2	1:K:839:MET:HE2	1.98	0.46
6:V:12:VAL:C	6:V:13:LEU:HD23	2.40	0.46
4:E:275:ASP:O	4:E:275:ASP:OD1	2.34	0.46
1:K:781:PRO:HA	4:Q:148:MET:HE1	1.98	0.46
4:P:177:ALA:O	4:P:178:HIS:ND1	2.48	0.46
1:K:665:TYR:O	1:K:669:THR:HG22	2.16	0.46
1:L:10:TRP:HE1	1:L:339:ILE:CD1	2.29	0.46
1:L:86:ARG:CB	1:L:86:ARG:HH11	2.28	0.46
1:L:215:ASN:OD1	1:L:215:ASN:C	2.59	0.46
5:R:80:ASP:O	5:R:81:ARG:NE	2.30	0.46
6:U:310:GLU:O	6:U:313:ILE:HG22	2.16	0.46
6:V:114:MET:HE3	6:V:297:TYR:HB2	1.97	0.46
3:D:674:GLN:O	3:D:678:GLN:HG3	2.16	0.46
4:G:241:ALA:HB2	4:G:284:VAL:HG13	1.98	0.46
5:H:240:TRP:CZ3	5:H:250:GLU:OE1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:41:PHE:CD2	6:V:233:ILE:HD12	2.50	0.46
7:X:154:GLU:O	7:X:154:GLU:CD	2.53	0.46
4:E:16:HIS:HB2	4:E:30:CYS:SG	2.56	0.46
2:I:25:LEU:N	2:I:25:LEU:CD1	2.79	0.46
1:L:671:ASP:OD2	1:L:671:ASP:C	2.59	0.46
1:L:705:ASP:OD1	1:L:705:ASP:N	2.48	0.46
3:N:973:THR:O	3:N:973:THR:OG1	2.33	0.46
5:R:63:HIS:NE2	5:R:79:SER:HB2	2.31	0.46
6:U:198:ALA:O	6:U:202:ILE:HG13	2.16	0.46
3:D:914:CYS:HB3	3:D:919:GLY:H	1.81	0.46
1:L:112:HIS:HD1	1:L:136:HIS:CE1	2.34	0.46
7:Y:342:TYR:HE2	7:Y:473:ARG:HA	1.80	0.46
3:N:900:VAL:O	3:N:909:VAL:N	2.37	0.46
5:R:130:ILE:HD12	5:R:130:ILE:H	1.81	0.46
5:R:175:ILE:HD12	5:R:175:ILE:N	2.30	0.46
6:U:126:ARG:HH21	6:U:128:GLN:CD	2.23	0.46
6:V:15:VAL:HG12	6:V:69:LEU:HD12	1.97	0.46
1:A:771:LYS:NZ	4:G:148:MET:HA	2.32	0.45
1:A:849:CYS:HB3	1:A:854:CYS:HB3	1.98	0.45
3:D:936:ASN:OD1	3:D:936:ASN:N	2.49	0.45
4:F:181:MET:C	4:F:182:ILE:HD13	2.40	0.45
1:A:845:ASP:OD1	1:A:846:HIS:ND1	2.42	0.45
1:B:820:PHE:HD2	3:N:951:MET:CE	2.29	0.45
4:F:287:ASN:ND2	4:F:289:THR:HG22	2.28	0.45
1:A:201:LEU:HA	1:A:210:ILE:HA	1.97	0.45
1:B:734:PHE:N	3:N:899:GLY:O	2.37	0.45
4:E:273:GLN:C	4:E:274:PHE:HD1	2.25	0.45
1:L:249:ALA:C	1:L:250:ILE:HD12	2.42	0.45
3:N:876:ARG:NH2	3:N:879:ARG:HH11	2.15	0.45
4:Q:85:VAL:HB	4:Q:107:THR:HG22	1.99	0.45
6:U:133:VAL:HG13	6:U:137:LEU:HD13	1.97	0.45
7:Y:375:PHE:CE1	7:Y:454:HIS:ND1	2.85	0.45
1:B:566:ASP:OD1	1:B:566:ASP:N	2.46	0.45
1:L:103:LEU:HD23	1:L:106:LYS:HZ1	1.82	0.45
1:L:229:GLY:O	1:L:242:SER:HA	2.16	0.45
4:Q:250:LEU:HD22	4:Q:268:ILE:HG13	1.98	0.45
5:R:312:TRP:H	5:R:327:GLY:HA2	1.81	0.45
6:U:181:GLN:HA	6:U:264:ARG:HH12	1.81	0.45
6:U:250:PRO:HG2	6:U:253:LEU:HD12	1.99	0.45
1:B:389:ASP:OD1	1:B:390:ILE:N	2.48	0.45
1:L:55:SER:O	1:L:56:ILE:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:195:HIS:HD2	5:R:232:GLY:HA3	1.80	0.45
7:X:440:TYR:CZ	7:X:452:LYS:HD3	2.52	0.45
1:B:105:GLY:O	1:B:106:LYS:HD3	2.17	0.45
1:B:235:TYR:C	1:B:236:PHE:HD1	2.25	0.45
1:B:535:ARG:O	1:B:538:ILE:HG12	2.17	0.45
3:D:550:LEU:HD23	3:D:551:VAL:H	1.82	0.45
4:F:130:LEU:HD23	4:F:131:ALA:H	1.82	0.45
4:G:140:ARG:NH1	4:G:158:GLU:OE2	2.50	0.45
5:H:240:TRP:CE3	5:H:250:GLU:OE1	2.70	0.45
1:L:146:ASP:CB	1:L:178:LEU:HD11	2.47	0.45
6:U:80:ASN:OD1	6:U:81:VAL:N	2.50	0.45
7:Y:454:HIS:O	7:Y:454:HIS:CG	2.70	0.45
1:A:640:MET:CE	1:A:645:ASN:CB	2.94	0.45
1:B:624:LEU:HD22	1:B:628:GLN:HG2	1.97	0.45
2:C:431:ASP:OD1	2:C:432:HIS:N	2.49	0.45
3:D:935:SER:N	1:L:826:TRP:O	2.42	0.45
1:L:554:LEU:CD2	1:L:554:LEU:H	2.30	0.45
1:L:724:ASP:OD1	1:L:724:ASP:C	2.60	0.45
4:O:102:HIS:O	4:O:102:HIS:CG	2.70	0.45
1:A:738:ASN:OD1	2:I:716:HIS:CD2	2.70	0.45
4:G:108:THR:HG22	4:G:110:VAL:HG13	1.99	0.45
6:U:67:GLU:OE1	6:U:67:GLU:N	2.50	0.45
6:U:183:ARG:NH1	6:U:262:LEU:HG	2.31	0.45
6:U:202:ILE:HG22	6:U:207:TYR:CE2	2.50	0.45
7:X:122:ARG:NH2	7:X:164:LYS:HG2	2.31	0.45
1:B:78:LEU:HD23	1:B:78:LEU:HA	1.81	0.44
1:L:433:MET:HG2	1:L:452:VAL:HG22	1.99	0.44
4:P:284:VAL:HB	4:P:293:LEU:HD11	1.98	0.44
6:V:15:VAL:HG22	6:V:51:TYR:HB2	1.99	0.44
4:F:26:ARG:NH1	4:F:72:GLN:OE1	2.50	0.44
5:H:260:TRP:O	5:H:282:GLN:N	2.50	0.44
1:K:534:ILE:HD12	1:K:534:ILE:H	1.82	0.44
1:A:408:GLN:HB2	1:A:411:ARG:HH21	1.83	0.44
1:L:44:ARG:HH12	1:L:47:GLU:CA	2.19	0.44
6:V:175:HIS:HB3	6:V:176:PRO:HD2	1.99	0.44
7:X:137:LEU:HD23	7:X:137:LEU:HA	1.83	0.44
1:A:367:MET:HE3	1:A:367:MET:HB2	1.95	0.44
1:A:436:TYR:HE1	1:A:452:VAL:HG22	1.82	0.44
1:B:111:LYS:HG3	1:B:112:HIS:H	1.82	0.44
4:G:15:ILE:HG13	2:I:395:SER:HB2	1.99	0.44
5:H:73:ARG:NH1	5:H:111:TRP:HZ3	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:226:ALA:O	1:L:242:SER:OG	2.30	0.44
5:R:145:HIS:CD2	5:R:147:GLY:H	2.36	0.44
6:V:6:LEU:HD13	6:V:78:VAL:HG12	1.98	0.44
7:X:83:MET:HE3	7:X:90:PHE:CE2	2.52	0.44
3:D:953:TRP:NE1	3:D:961:PRO:HG3	2.33	0.44
1:K:408:GLN:CD	1:K:410:TRP:NE1	2.75	0.44
1:K:788:CYS:SG	1:K:838:HIS:HE1	2.41	0.44
1:L:641:LYS:HE3	1:L:641:LYS:HB2	1.82	0.44
3:N:872:ARG:HD3	5:R:69:TYR:CE2	2.53	0.44
4:O:67:HIS:CG	4:O:124:LYS:HD3	2.53	0.44
1:A:356:ILE:HB	4:E:296:SER:OG	2.17	0.44
2:C:25:LEU:HD11	2:C:323:LEU:HB2	2.00	0.44
2:C:750:VAL:HG22	2:C:765:HIS:CD2	2.52	0.44
3:D:726:ARG:HG2	3:D:730:GLU:OE2	2.18	0.44
3:D:923:GLN:NE2	3:D:928:HIS:CA	2.81	0.44
4:E:299:ASP:OD2	4:E:299:ASP:C	2.60	0.44
2:I:76:SER:O	2:I:76:SER:OG	2.26	0.44
1:L:838:HIS:O	1:L:841:SER:OG	2.33	0.44
3:N:923:GLN:HE22	3:N:928:HIS:CA	2.19	0.44
4:O:140:ARG:HG2	4:O:158:GLU:OE1	2.17	0.44
1:A:580:ARG:HH22	1:A:593:ALA:HA	1.81	0.44
1:A:771:LYS:NZ	4:G:147:VAL:O	2.31	0.44
4:G:55:THR:HG23	4:G:86:TRP:HZ2	1.82	0.44
5:H:67:MET:CE	5:H:71:GLY:HA2	2.48	0.44
1:L:193:LEU:HD12	1:L:199:LEU:HD23	2.00	0.44
1:B:426:LEU:HD12	1:B:646:LEU:HD13	1.98	0.44
4:F:303:ARG:CB	4:F:318:ILE:HG12	2.48	0.44
1:L:422:GLN:O	1:L:425:SER:OG	2.33	0.44
5:R:254:LEU:HD13	5:R:289:TRP:CE3	2.53	0.44
5:H:152:VAL:HA	5:H:170:SER:HA	1.99	0.44
4:O:242:THR:OG1	4:O:243:LYS:N	2.51	0.44
6:V:126:ARG:HG3	6:V:127:GLU:N	2.33	0.44
6:V:186:VAL:HG22	6:V:240:VAL:HG22	1.98	0.44
7:Y:162:ILE:CD1	7:Y:181:LEU:HD11	2.38	0.44
1:A:422:GLN:OE1	1:A:646:LEU:N	2.50	0.43
1:B:780:LYS:HA	1:B:781:PRO:HD3	1.77	0.43
1:L:8:ILE:CD1	1:L:339:ILE:CD1	2.61	0.43
1:L:28:TYR:CD1	1:L:51:ALA:HB1	2.53	0.43
1:L:554:LEU:N	1:L:554:LEU:CD2	2.81	0.43
4:O:62:ARG:NH1	4:O:118:ASP:CA	2.70	0.43
4:P:265:LYS:C	4:P:266:PHE:HD1	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:305:TRP:CZ3	4:Q:315:CYS:HB2	2.53	0.43
2:I:427:ALA:O	2:I:431:ASP:OD1	2.36	0.43
7:X:428:VAL:HG12	7:X:459:LEU:CD2	2.48	0.43
7:Y:126:SER:OG	7:Y:312:MET:HE1	2.17	0.43
4:G:249:THR:HG21	4:G:251:LYS:HE2	1.99	0.43
4:P:289:THR:H	4:P:289:THR:HG1	1.62	0.43
1:B:102:ASP:OD1	1:B:102:ASP:N	2.42	0.43
2:C:23:CYS:HB3	2:C:59:PHE:HD2	1.83	0.43
2:C:176:TYR:HD2	2:C:177:PHE:CE2	2.37	0.43
2:C:685:GLN:HG2	2:C:690:TRP:CZ3	2.53	0.43
4:F:27:MET:SD	4:F:39:TRP:HB2	2.58	0.43
4:P:84:ALA:CB	4:P:86:TRP:HE1	2.31	0.43
5:R:199:CYS:H	5:R:232:GLY:HA3	1.83	0.43
6:U:302:ASN:OD1	6:U:303:PHE:HD1	2.01	0.43
6:V:53:LEU:HD23	6:V:53:LEU:HA	1.85	0.43
1:B:542:ASN:OD1	1:B:543:GLU:N	2.52	0.43
4:E:306:LYS:HB3	4:E:306:LYS:HE2	1.72	0.43
1:L:8:ILE:C	1:L:9:LEU:HD23	2.44	0.43
1:L:14:HIS:HB3	1:L:17:ARG:HG2	2.01	0.43
1:L:693:VAL:HA	1:L:696:TRP:CE3	2.53	0.43
5:H:178:LEU:HD22	5:H:186:TRP:HB3	1.99	0.43
2:I:125:LYS:HA	2:I:125:LYS:HD2	1.82	0.43
2:I:177:PHE:CD1	2:I:194:ARG:NH1	2.86	0.43
1:L:69:TYR:OH	1:L:71:ASN:HB2	2.19	0.43
4:P:181:MET:C	4:P:182:ILE:HD12	2.43	0.43
1:B:180:GLU:C	1:B:181:LEU:HD23	2.44	0.43
2:C:451:MET:HG2	3:N:701:VAL:HG21	2.00	0.43
3:D:923:GLN:NE2	3:D:928:HIS:HA	2.34	0.43
4:E:274:PHE:CD1	4:E:274:PHE:N	2.84	0.43
4:F:243:LYS:HA	4:F:243:LYS:HD2	1.94	0.43
1:L:215:ASN:OD1	1:L:215:ASN:O	2.37	0.43
1:L:246:GLY:HA2	1:L:270:LEU:HD13	2.00	0.43
3:N:699:ALA:O	3:N:703:THR:OG1	2.30	0.43
7:X:415:GLN:OE1	7:X:415:GLN:N	2.51	0.43
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.85	0.43
1:A:646:LEU:HD23	1:A:646:LEU:HA	1.84	0.43
2:C:282:ASP:OD2	2:C:282:ASP:C	2.61	0.43
4:F:249:THR:C	4:F:250:LEU:HD12	2.43	0.43
1:L:8:ILE:HD12	1:L:341:VAL:HG13	2.00	0.43
1:L:295:LEU:C	1:L:296:TYR:HD1	2.27	0.43
1:L:545:ALA:HB2	1:L:554:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:56:ASP:OD1	6:V:58:GLU:N	2.50	0.43
7:Y:149:LEU:HD22	7:Y:157:ARG:HG2	2.00	0.43
5:H:283:ASP:OD1	5:H:284:GLY:N	2.52	0.43
1:K:377:CYS:SG	4:O:2:PHE:HB3	2.59	0.43
1:L:102:ASP:O	1:L:106:LYS:NZ	2.52	0.43
7:Y:198:LEU:O	7:Y:202:THR:HG23	2.19	0.43
1:B:68:TRP:CZ3	1:B:76:CYS:HA	2.53	0.43
1:B:411:ARG:O	1:B:414:ILE:HG12	2.19	0.43
1:K:355:ARG:HH22	4:O:282:TRP:NE1	2.03	0.43
1:K:408:GLN:NE2	1:K:410:TRP:NE1	2.66	0.43
1:K:433:MET:HG2	1:K:452:VAL:HG22	2.01	0.43
3:D:840:GLU:OE2	4:G:312:ASN:ND2	2.51	0.42
3:D:962:THR:O	1:L:729:PRO:HG3	2.19	0.42
4:G:276:ASN:OD1	4:G:303:ARG:NE	2.52	0.42
1:L:200:LEU:O	1:L:210:ILE:HD12	2.18	0.42
1:L:422:GLN:OE1	1:L:646:LEU:HB2	2.19	0.42
7:X:414:ASN:OD1	7:X:422:LYS:NZ	2.51	0.42
1:B:824:PHE:HE1	1:B:834:GLY:HA2	1.82	0.42
1:K:827:CYS:HB2	1:K:858:CYS:SG	2.58	0.42
4:Q:148:MET:HE2	4:Q:148:MET:HB3	1.53	0.42
6:U:34:PRO:HG2	6:U:35:ARG:HH12	1.84	0.42
6:V:261:GLU:O	6:V:262:LEU:HD23	2.19	0.42
1:A:378:THR:N	4:E:5:ARG:HH22	2.16	0.42
1:B:69:TYR:HB2	1:B:77:LEU:HB3	2.01	0.42
1:B:687:VAL:HG13	1:B:688:LEU:HD13	2.00	0.42
3:D:552:TYR:CE1	3:D:648:ILE:HD11	2.54	0.42
5:H:164:LEU:HD12	5:H:164:LEU:HA	1.84	0.42
5:R:157:TRP:CZ3	5:R:166:LEU:HB2	2.54	0.42
6:U:295:ALA:HB3	6:U:297:TYR:CE2	2.55	0.42
1:B:825:THR:O	1:B:833:GLY:HA3	2.20	0.42
4:E:251:LYS:HE2	4:E:251:LYS:HB2	1.95	0.42
2:I:16:LEU:N	2:I:16:LEU:HD23	2.35	0.42
1:K:734:PHE:CE2	1:K:743:SER:HB2	2.55	0.42
1:L:62:TYR:HB2	1:L:82:GLN:OE1	2.19	0.42
1:L:68:TRP:HD1	1:L:69:TYR:N	2.18	0.42
3:N:869:ILE:HD11	5:R:318:ILE:HD11	2.00	0.42
1:B:8:ILE:HD12	1:B:20:VAL:HG22	2.01	0.42
1:B:223:ASN:OD1	1:B:223:ASN:N	2.53	0.42
4:F:228:ALA:HB2	4:F:286:TRP:CE2	2.54	0.42
1:L:286:LEU:HD12	1:L:328:PHE:HD2	1.84	0.42
4:P:266:PHE:N	4:P:266:PHE:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:106:VAL:HA	5:R:124:SER:HA	2.02	0.42
5:R:302:LYS:NZ	5:R:302:LYS:HB2	2.34	0.42
6:U:43:SER:HA	6:U:231:SER:HA	2.01	0.42
7:Y:413:VAL:O	7:Y:417:LEU:HB2	2.20	0.42
2:C:42:VAL:HG22	2:C:51:ILE:HD13	2.02	0.42
2:C:640:MET:HE3	2:C:640:MET:HB3	1.81	0.42
4:E:244:ASP:OD1	4:E:244:ASP:N	2.53	0.42
4:F:51:ALA:HB1	4:F:53:TRP:HZ3	1.85	0.42
1:K:640:MET:HE2	1:K:640:MET:HB2	1.92	0.42
1:L:325:ILE:HG12	1:L:340:VAL:CG1	2.49	0.42
1:L:535:ARG:HD3	1:L:535:ARG:HA	1.84	0.42
1:B:336:ASN:OD1	1:B:336:ASN:N	2.53	0.42
2:C:307:HIS:ND1	2:C:308:PRO:HD2	2.35	0.42
3:D:666:TYR:CE1	3:D:680:ASN:HB3	2.54	0.42
4:E:26:ARG:NH1	4:E:72:GLN:OE1	2.51	0.42
1:K:646:LEU:HD21	1:K:662:MET:HE2	2.02	0.42
1:L:713:ARG:O	1:L:716:PHE:HB3	2.20	0.42
4:Q:168:ILE:HG22	4:Q:184:VAL:HG22	2.01	0.42
5:R:141:LYS:HD2	5:R:142:SER:N	2.35	0.42
4:F:70:PHE:CD2	4:F:128:LEU:HD13	2.55	0.42
1:K:662:MET:HG3	1:K:679:MET:HE3	2.01	0.42
1:L:523:ARG:HD3	1:L:587:TYR:CE2	2.55	0.42
1:L:701:ARG:HE	1:L:713:ARG:HE	1.68	0.42
5:R:58:HIS:CE1	5:R:78:SER:HB2	2.54	0.42
1:A:363:ILE:HD12	1:A:363:ILE:HA	1.89	0.42
2:I:319:LYS:O	2:I:319:LYS:HG2	2.20	0.42
1:L:103:LEU:CD2	1:L:106:LYS:HZ1	2.32	0.42
1:L:646:LEU:HD11	1:L:665:TYR:CE2	2.55	0.42
1:B:327:SER:O	1:B:341:VAL:HG12	2.20	0.42
5:H:87:ASP:OD1	5:H:87:ASP:C	2.63	0.42
1:L:114:ARG:HD3	1:L:136:HIS:HB2	2.02	0.42
4:Q:34:GLN:HG2	4:Q:58:GLY:O	2.20	0.42
7:Y:99:LEU:HD22	7:Y:362:LEU:HD12	2.00	0.42
1:B:201:LEU:HD12	1:B:210:ILE:HB	2.01	0.41
2:C:177:PHE:HD1	2:C:194:ARG:CZ	2.32	0.41
2:C:402:THR:HG22	4:Q:2:PHE:N	2.35	0.41
2:I:222:TRP:CE2	2:I:245:MET:HE1	2.54	0.41
1:L:193:LEU:HA	1:L:194:PRO:HD3	1.94	0.41
4:P:266:PHE:HD1	4:P:266:PHE:N	2.17	0.41
5:R:81:ARG:HD3	5:R:81:ARG:HA	1.89	0.41
7:X:207:LEU:HD12	7:X:207:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:94:ALA:HB3	2:I:98:VAL:HG22	2.02	0.41
2:I:339:ASN:HA	2:I:340:PRO:HD3	1.85	0.41
1:K:773:THR:HG23	1:K:792:MET:O	2.20	0.41
1:L:27:LEU:HD12	1:L:28:TYR:H	1.86	0.41
1:L:374:LEU:HD23	1:L:374:LEU:HA	1.88	0.41
5:R:100:ARG:HE	5:R:100:ARG:HB3	1.55	0.41
6:U:28:ILE:HG13	6:U:32:PHE:CE1	2.54	0.41
7:X:122:ARG:CZ	7:X:164:LYS:HG2	2.51	0.41
7:Y:375:PHE:CD2	7:Y:389:LEU:HD23	2.56	0.41
1:B:58:SER:O	1:B:58:SER:OG	2.38	0.41
2:I:89:LEU:O	2:I:90:LEU:HD12	2.21	0.41
1:K:724:ASP:HA	1:K:725:PRO:HD3	1.89	0.41
4:Q:207:ARG:HG3	4:Q:207:ARG:NH1	2.32	0.41
7:X:438:ARG:O	7:X:442:LEU:HG	2.21	0.41
7:X:442:LEU:HA	7:X:445:ARG:NH1	2.35	0.41
1:B:13:HIS:CD2	1:B:72:TYR:CD2	3.08	0.41
5:H:116:TYR:CD1	5:H:164:LEU:HD13	2.55	0.41
1:L:553:ASN:O	1:L:557:VAL:N	2.44	0.41
4:P:124:LYS:O	4:P:127:GLY:N	2.47	0.41
6:U:223:SER:O	6:U:223:SER:OG	2.27	0.41
1:B:363:ILE:O	1:B:364:THR:OG1	2.28	0.41
3:D:923:GLN:OE1	3:D:928:HIS:HA	2.18	0.41
4:E:3:VAL:HG23	4:E:5:ARG:NH1	2.35	0.41
4:E:4:ALA:C	4:E:5:ARG:HG3	2.46	0.41
4:G:149:ASN:OD1	4:G:149:ASN:N	2.54	0.41
1:L:223:ASN:OD1	1:L:223:ASN:C	2.62	0.41
6:U:132:VAL:O	6:U:136:THR:HG23	2.21	0.41
1:B:118:THR:O	1:B:119:LEU:HD23	2.20	0.41
1:B:178:LEU:HB3	1:B:179:TYR:CD1	2.52	0.41
1:B:679:MET:HE2	1:B:679:MET:HB2	1.86	0.41
4:F:166:SER:N	4:F:185:GLY:O	2.43	0.41
1:K:773:THR:HG22	1:K:773:THR:O	2.20	0.41
5:R:66:GLN:NE2	5:R:109:VAL:O	2.54	0.41
1:B:511:PHE:CD2	1:B:511:PHE:C	2.96	0.41
2:C:74:ASN:C	2:C:75:LEU:HD23	2.45	0.41
2:I:137:LEU:HD23	2:I:137:LEU:HA	1.87	0.41
4:P:66:ALA:HB2	4:P:121:PHE:CE2	2.55	0.41
6:V:31:LEU:HD23	6:V:31:LEU:C	2.46	0.41
1:B:394:MET:CE	1:B:672:VAL:H	2.33	0.41
2:C:743:CYS:HB3	2:C:746:CYS:HB2	1.86	0.41
4:E:164:SER:O	4:E:164:SER:OG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:126:ARG:HH21	6:U:128:GLN:NE2	2.18	0.41
6:V:114:MET:CE	6:V:297:TYR:HB2	2.50	0.41
6:V:268:ILE:HD12	6:V:284:ILE:CG1	2.50	0.41
1:A:455:GLY:O	1:A:459:ILE:HG13	2.21	0.41
1:A:730:LEU:HD12	1:A:730:LEU:HA	1.85	0.41
1:B:295:LEU:HB3	1:B:316:ARG:O	2.20	0.41
1:B:404:LEU:HD23	1:B:404:LEU:HA	1.90	0.41
2:C:21:MET:HE3	2:C:325:GLN:OE1	2.20	0.41
2:C:689:LEU:HB3	2:C:692:VAL:HG12	2.01	0.41
4:E:87:GLU:HG3	4:E:88:GLU:N	2.36	0.41
5:H:125:TYR:C	5:H:127:ARG:H	2.29	0.41
1:L:231:THR:CG2	1:L:275:TRP:HD1	2.33	0.41
4:Q:107:THR:HG21	4:Q:153:TRP:CD1	2.56	0.41
7:X:83:MET:HE3	7:X:90:PHE:CD2	2.56	0.41
7:X:409:ASP:OD1	7:X:409:ASP:C	2.61	0.41
7:Y:166:LEU:HD22	7:Y:467:ALA:HB1	2.03	0.41
2:C:106:ARG:HH11	2:C:106:ARG:HB3	1.81	0.41
4:F:199:ILE:HG22	4:F:212:ALA:HB3	2.03	0.41
4:F:230:ASN:O	4:F:233:ARG:HG3	2.21	0.41
4:G:122:ALA:HB1	4:G:126:MET:HE2	2.02	0.41
1:K:408:GLN:OE1	1:K:411:ARG:NH1	2.53	0.41
1:K:521:TRP:CE2	1:K:544:GLY:HA2	2.56	0.41
1:K:534:ILE:HD12	1:K:534:ILE:N	2.36	0.41
1:B:125:ASP:OD2	1:B:125:ASP:N	2.54	0.40
1:B:456:ILE:HD11	1:B:650:LEU:HG	2.03	0.40
2:C:339:ASN:HA	2:C:340:PRO:HD3	1.91	0.40
2:C:428:GLU:O	2:C:431:ASP:OD1	2.39	0.40
3:D:864:LYS:NZ	3:D:864:LYS:HB2	2.36	0.40
4:P:230:ASN:O	4:P:233:ARG:HG3	2.20	0.40
6:U:192:GLU:O	6:U:195:PRO:HD2	2.20	0.40
3:D:662:LEU:HD23	3:D:662:LEU:HA	1.96	0.40
2:I:213:CYS:HA	2:I:224:ALA:O	2.21	0.40
1:L:77:LEU:HD12	1:L:77:LEU:HA	1.91	0.40
3:N:948:SER:O	3:N:951:MET:HB2	2.20	0.40
4:P:92:GLU:HA	4:P:102:HIS:N	2.36	0.40
4:Q:171:ASN:HB2	4:Q:181:MET:HB2	2.01	0.40
7:X:362:LEU:HD23	7:X:362:LEU:HA	1.86	0.40
7:Y:162:ILE:CD1	7:Y:181:LEU:CD1	2.98	0.40
7:Y:239:SER:HA	7:Y:240:PRO:HD3	1.90	0.40
7:Y:416:LEU:HA	7:Y:416:LEU:HD23	1.77	0.40
1:B:233:ASP:OD1	1:B:233:ASP:N	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:114:GLN:H	2:C:114:GLN:HG3	1.60	0.40
3:D:690:LYS:HE2	2:I:626:SER:O	2.22	0.40
2:I:214:ASP:OD2	2:I:215:TRP:N	2.54	0.40
1:K:541:LEU:HD23	1:K:541:LEU:HA	1.82	0.40
1:L:144:ILE:CD1	1:L:213:LEU:HD11	2.51	0.40
4:O:286:TRP:CE2	4:O:293:LEU:HD13	2.56	0.40
5:R:81:ARG:NH1	5:R:103:GLU:O	2.54	0.40
6:U:268:ILE:HD11	6:U:280:ILE:HG22	2.03	0.40
7:Y:78:ASN:O	7:Y:81:VAL:HG22	2.21	0.40
2:C:257:VAL:HG23	2:C:269:THR:HG22	2.04	0.40
2:C:328:PHE:HD2	2:C:328:PHE:O	2.04	0.40
4:G:142:TYR:CE2	4:G:155:LEU:HD13	2.56	0.40
2:I:104:LEU:HA	2:I:111:LYS:HD3	2.04	0.40
1:L:228:GLN:OE1	1:L:243:PHE:O	2.39	0.40
3:N:948:SER:HA	3:N:951:MET:HB2	2.02	0.40
4:O:163:LEU:HD23	4:O:163:LEU:HA	1.80	0.40
4:F:24:GLY:O	4:F:25:ARG:HD3	2.22	0.40
1:K:74:PRO:O	1:K:74:PRO:CD	2.69	0.40
1:K:780:LYS:HE2	1:K:780:LYS:HB3	1.78	0.40
1:L:118:THR:HG21	1:L:189:SER:HA	2.04	0.40
1:L:513:ASN:OD1	1:L:513:ASN:N	2.54	0.40
5:R:145:HIS:CD2	5:R:145:HIS:C	2.98	0.40
6:U:320:LEU:HD23	6:U:320:LEU:HA	1.98	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	733/875 (84%)	681 (93%)	50 (7%)	2 (0%)	36 65
1	B	703/875 (80%)	620 (88%)	76 (11%)	7 (1%)	12 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	728/875 (83%)	704 (97%)	24 (3%)	0	100	100
1	L	707/875 (81%)	620 (88%)	83 (12%)	4 (1%)	21	49
2	C	560/790 (71%)	509 (91%)	45 (8%)	6 (1%)	11	37
2	I	565/790 (72%)	522 (92%)	42 (7%)	1 (0%)	43	71
3	D	256/974 (26%)	248 (97%)	8 (3%)	0	100	100
3	N	256/974 (26%)	244 (95%)	12 (5%)	0	100	100
4	E	297/421 (70%)	282 (95%)	15 (5%)	0	100	100
4	F	296/421 (70%)	255 (86%)	40 (14%)	1 (0%)	36	65
4	G	298/421 (71%)	286 (96%)	11 (4%)	1 (0%)	36	65
4	O	296/421 (70%)	284 (96%)	12 (4%)	0	100	100
4	P	287/421 (68%)	256 (89%)	31 (11%)	0	100	100
4	Q	296/421 (70%)	289 (98%)	7 (2%)	0	100	100
5	H	279/368 (76%)	258 (92%)	21 (8%)	0	100	100
5	R	280/368 (76%)	258 (92%)	22 (8%)	0	100	100
6	U	280/329 (85%)	266 (95%)	14 (5%)	0	100	100
6	V	268/329 (82%)	257 (96%)	11 (4%)	0	100	100
7	X	310/480 (65%)	297 (96%)	12 (4%)	1 (0%)	36	65
7	Y	300/480 (62%)	282 (94%)	16 (5%)	2 (1%)	18	47
All	All	7995/11908 (67%)	7418 (93%)	552 (7%)	25 (0%)	37	65

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	THR
1	A	553	ASN
1	B	104	ILE
2	C	69	ARG
2	C	153	LYS
2	C	170	GLN
2	C	274	VAL
2	C	708	LEU
1	L	48	ASP
1	L	104	ILE
1	L	352	VAL
7	Y	345	GLU
7	Y	377	THR

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Mol	Chain	Res	Type
1	B	96	HIS
1	L	351	THR
7	X	78	ASN
1	B	217	SER
1	B	245	GLU
1	B	782	LEU
2	C	152	ARG
4	F	21	ASP
1	B	255	LYS
2	I	274	VAL
1	B	781	PRO
4	G	232	GLY

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	285/771 (37%)	282 (99%)	3 (1%)	65	73
1	B	400/771 (52%)	398 (100%)	2 (0%)	81	80
1	K	269/771 (35%)	268 (100%)	1 (0%)	84	82
1	L	400/771 (52%)	397 (99%)	3 (1%)	73	76
2	C	379/677 (56%)	377 (100%)	2 (0%)	81	80
2	I	424/677 (63%)	422 (100%)	2 (0%)	81	80
3	D	173/858 (20%)	172 (99%)	1 (1%)	78	80
3	N	151/858 (18%)	148 (98%)	3 (2%)	48	65
4	E	215/365 (59%)	214 (100%)	1 (0%)	81	80
4	F	131/365 (36%)	129 (98%)	2 (2%)	57	69
4	G	237/365 (65%)	236 (100%)	1 (0%)	84	82
4	O	196/365 (54%)	196 (100%)	0	100	100
4	P	85/365 (23%)	85 (100%)	0	100	100
4	Q	225/365 (62%)	225 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	116/313 (37%)	116 (100%)	0	100	100
5	R	150/313 (48%)	148 (99%)	2 (1%)	61	71
6	U	223/285 (78%)	221 (99%)	2 (1%)	70	75
6	V	186/285 (65%)	184 (99%)	2 (1%)	65	73
7	X	240/410 (58%)	240 (100%)	0	100	100
7	Y	222/410 (54%)	221 (100%)	1 (0%)	81	80
All	All	4707/10360 (45%)	4679 (99%)	28 (1%)	76	80

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	LYS
1	A	452	VAL
1	A	845	ASP
1	B	210	ILE
1	B	244	TYR
2	C	169	VAL
2	C	708	LEU
3	D	717	THR
4	E	282	TRP
4	F	151	SER
4	F	268	ILE
4	G	148	MET
2	I	106	ARG
2	I	767	GLN
1	K	413	HIS
1	L	363	ILE
1	L	396	LEU
1	L	554	LEU
3	N	691	ASP
3	N	951	MET
3	N	959	VAL
5	R	58	HIS
5	R	330	ASN
6	U	62	GLU
6	U	182	ASN
6	V	128	GLN
6	V	174	VAL
7	Y	352	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	GLN
1	A	732	GLN
1	A	791	ASN
1	B	13	HIS
1	B	112	HIS
1	B	115	GLN
1	B	122	ASN
1	B	331	HIS
1	B	673	GLN
2	C	134	HIS
2	C	325	GLN
2	C	447	GLN
2	C	716	HIS
2	C	778	HIS
4	E	11	HIS
4	E	23	HIS
4	E	149	ASN
4	G	16	HIS
4	G	157	HIS
2	I	74	ASN
2	I	96	ASN
2	I	276	HIS
2	I	651	GLN
2	I	716	HIS
2	I	721	HIS
2	I	748	HIS
2	I	767	GLN
1	K	485	ASN
1	K	513	ASN
1	K	517	GLN
1	K	531	ASN
1	K	699	ASN
1	K	791	ASN
1	K	846	HIS
1	L	413	HIS
1	L	422	GLN
1	L	645	ASN
1	L	681	GLN
1	L	699	ASN
3	N	923	GLN
3	N	949	HIS

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Mol	Chain	Res	Type
4	O	23	HIS
4	O	34	GLN
4	O	198	GLN
4	Q	16	HIS
4	Q	23	HIS
4	Q	236	HIS
5	R	66	GLN
5	R	195	HIS
5	R	330	ASN
7	Y	132	HIS
7	Y	340	GLN
7	Y	414	ASN
7	Y	420	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

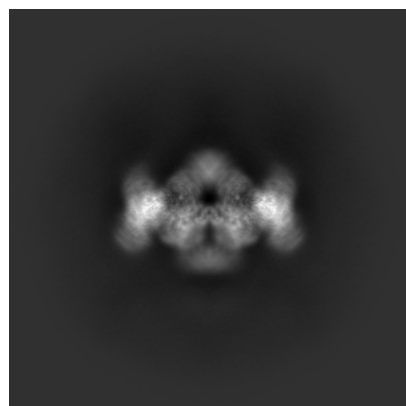
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63442. These allow visual inspection of the internal detail of the map and identification of artifacts.

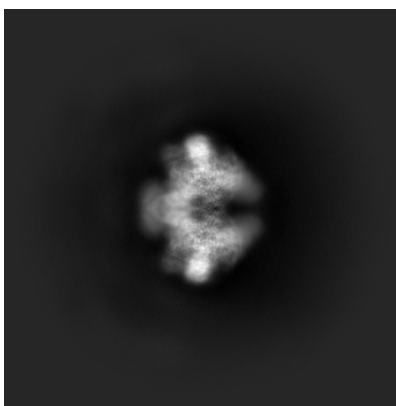
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

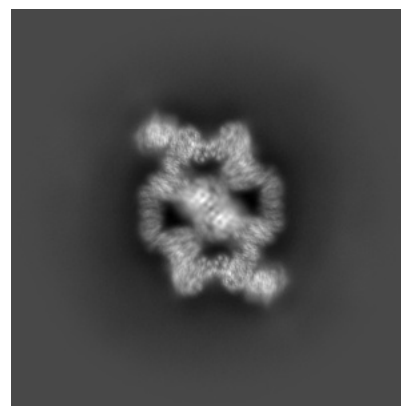
6.1.1 Primary map



X

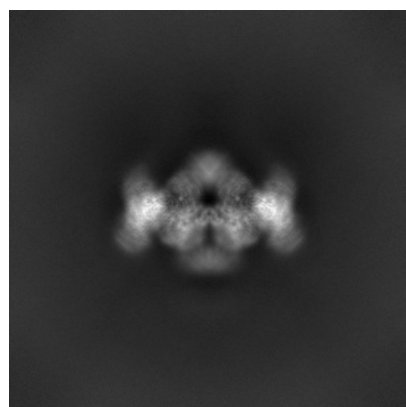


Y

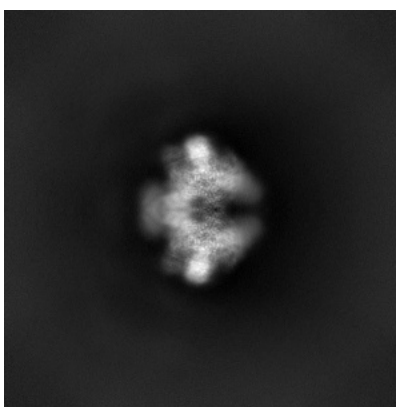


Z

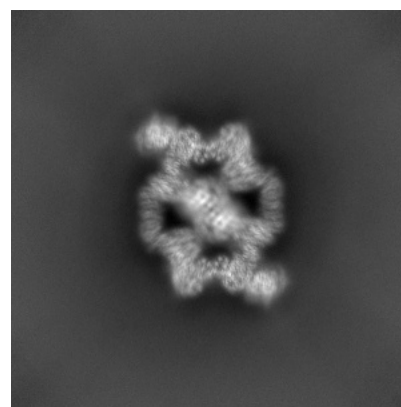
6.1.2 Raw map



X



Y

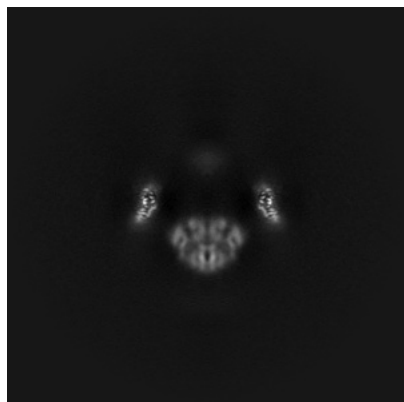


Z

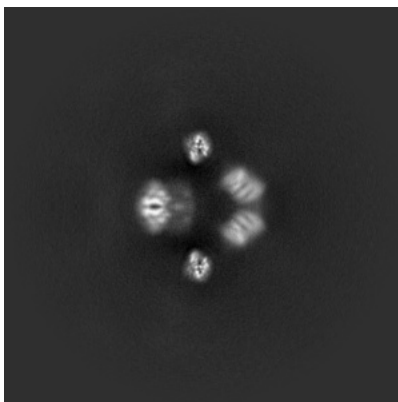
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

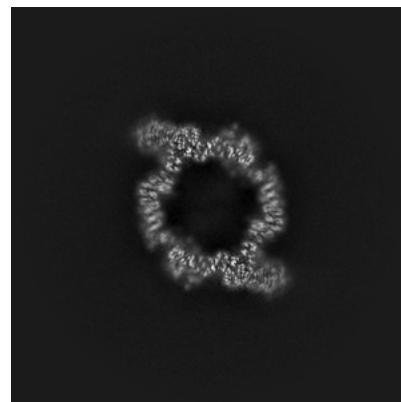
6.2.1 Primary map



X Index: 340

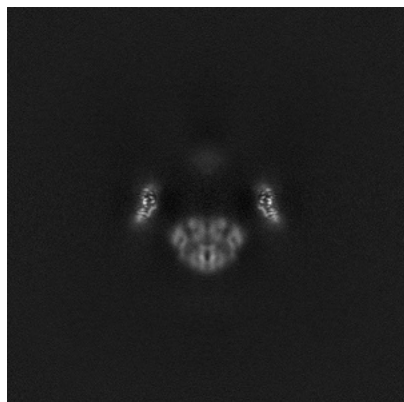


Y Index: 340

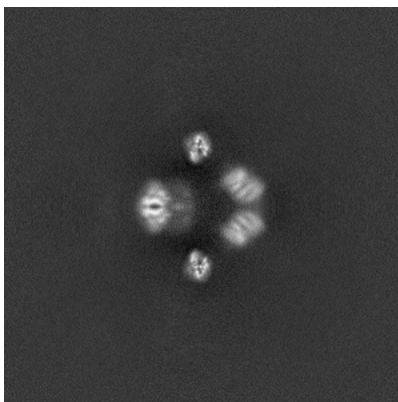


Z Index: 340

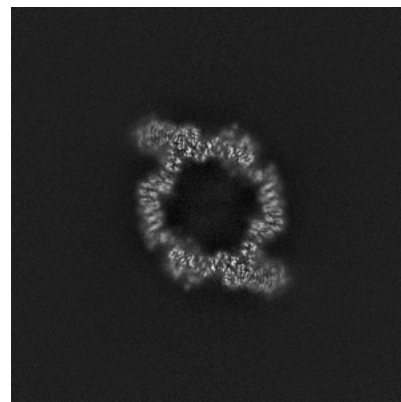
6.2.2 Raw map



X Index: 340



Y Index: 340

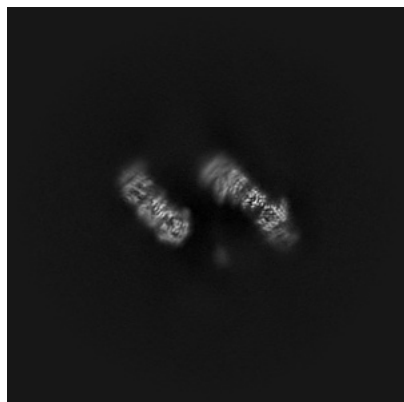


Z Index: 340

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

6.3 Largest variance slices [i](#)

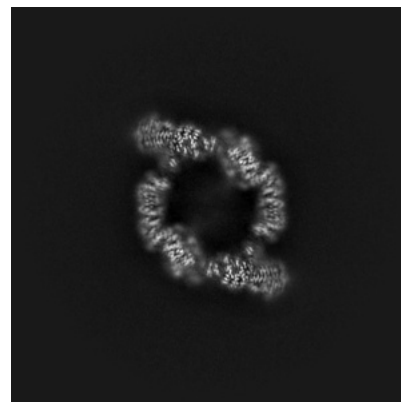
6.3.1 Primary map



X Index: 286

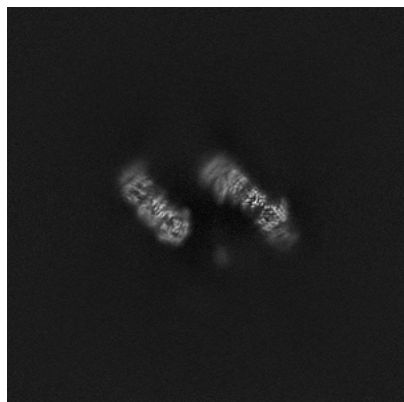


Y Index: 388

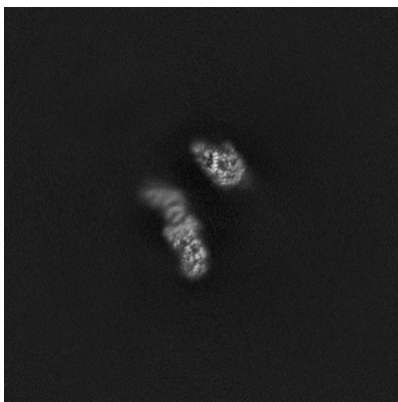


Z Index: 332

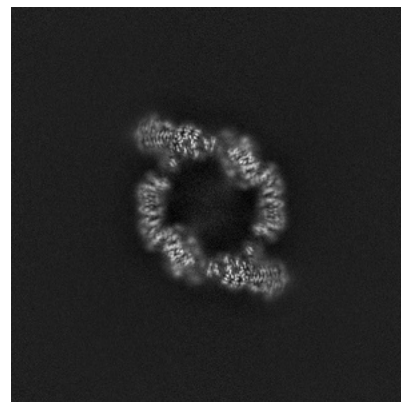
6.3.2 Raw map



X Index: 286



Y Index: 292

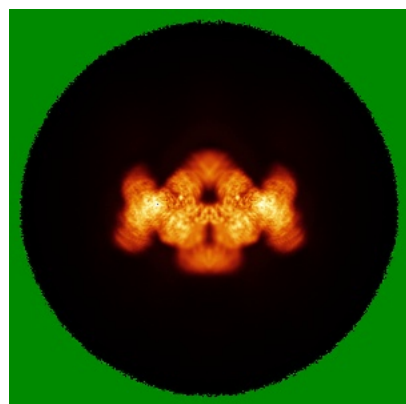


Z Index: 332

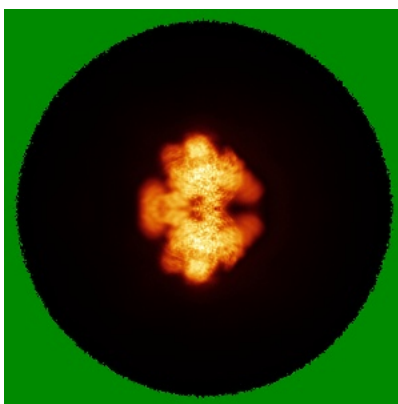
The images above show the largest variance slices of the map in three orthogonal directions.

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

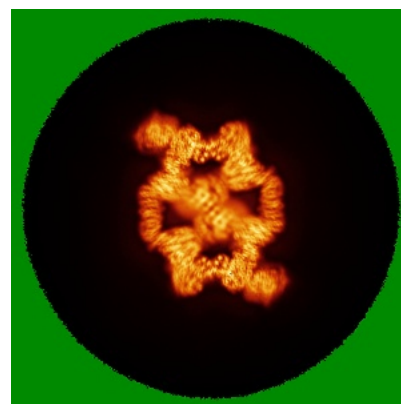
6.4.1 Primary map



X

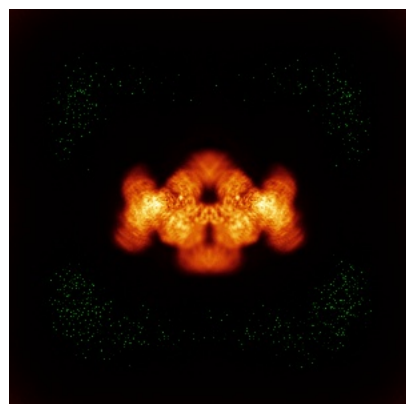


Y

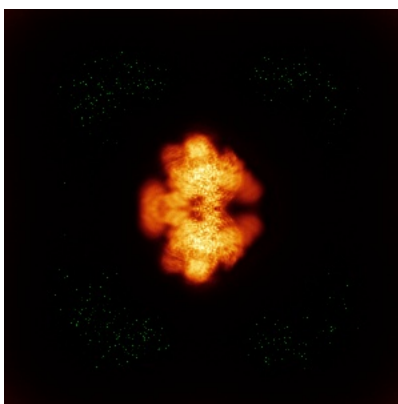


Z

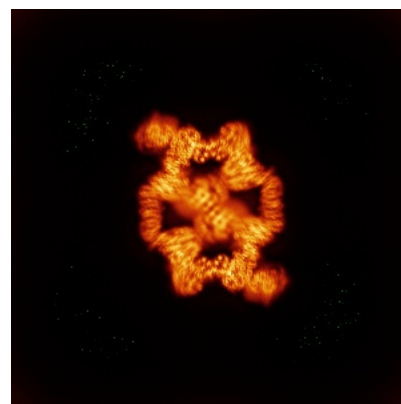
6.4.2 Raw map



X



Y



Z

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

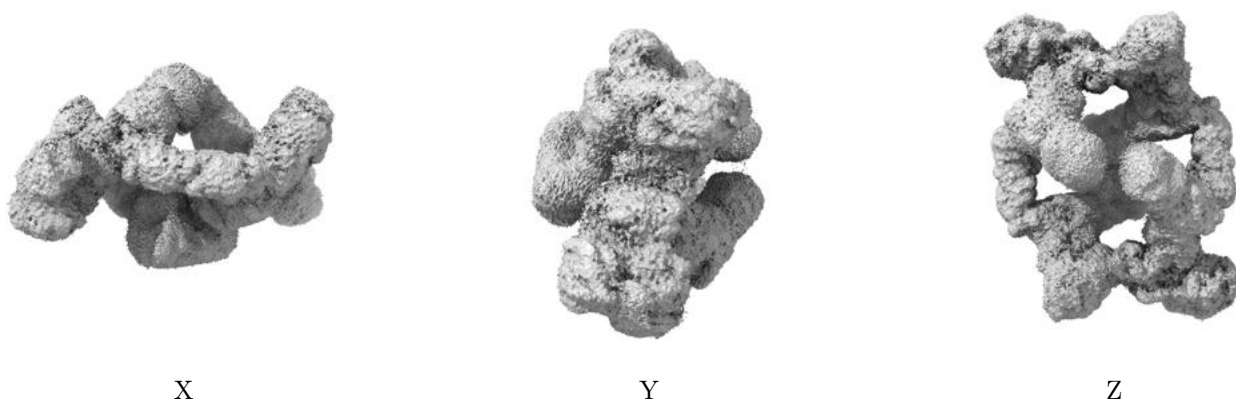
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.103. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation [i](#)

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

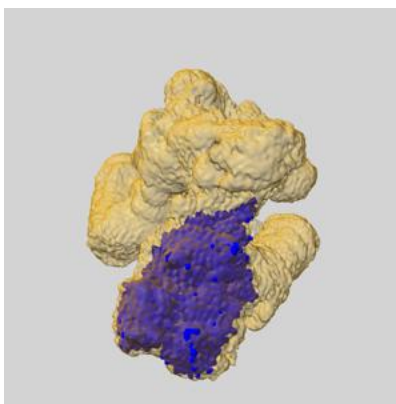
A mask typically either:

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

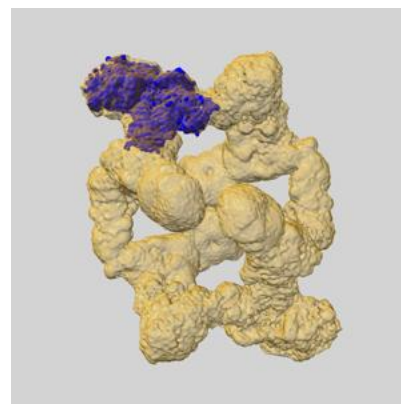
6.6.1 emd_63442_msk_1.map [i](#)



X

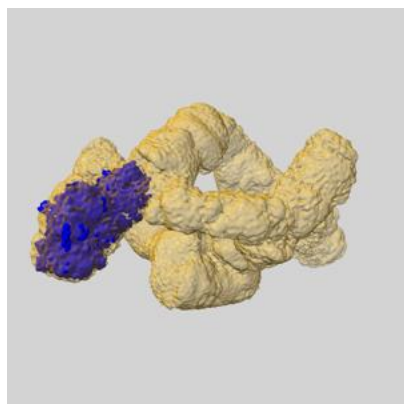


Y

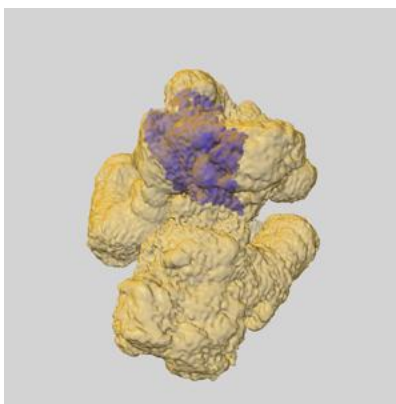


Z

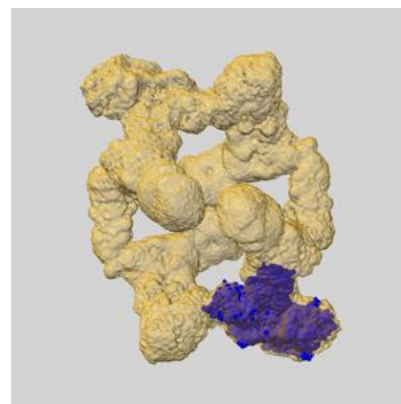
6.6.2 emd_63442_msk_2.map [i](#)



X

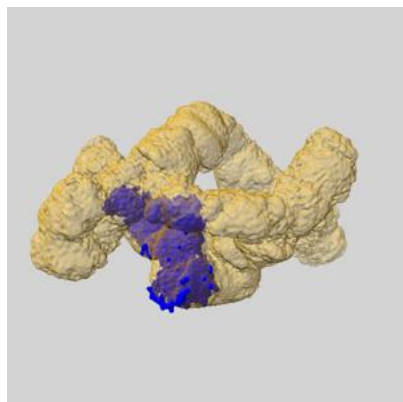


Y

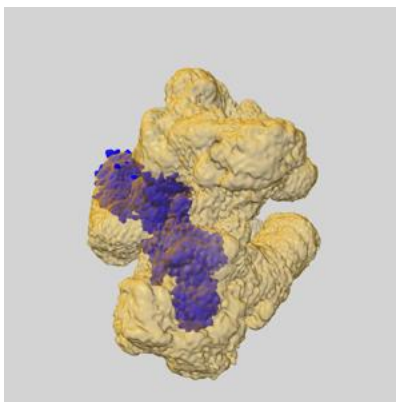


Z

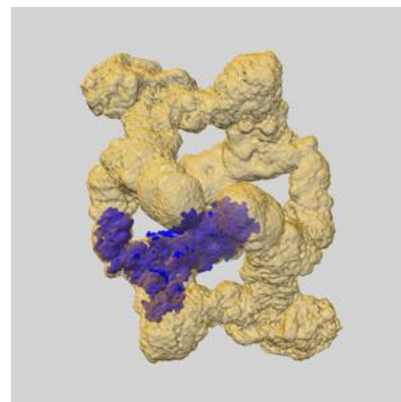
6.6.3 emd_63442_msk_3.map [i](#)



X

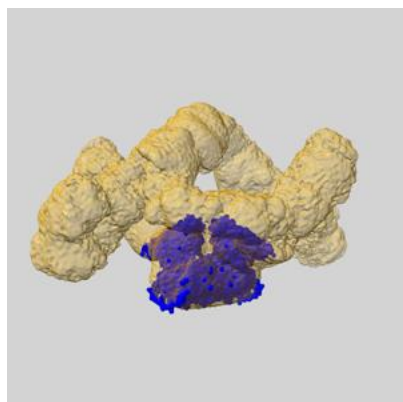


Y

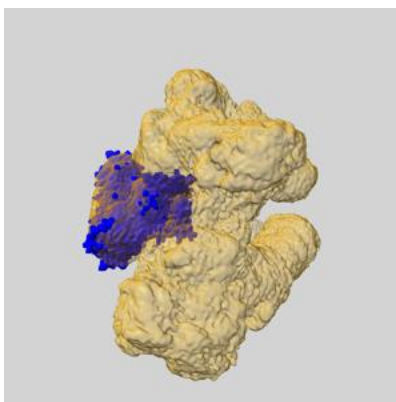


Z

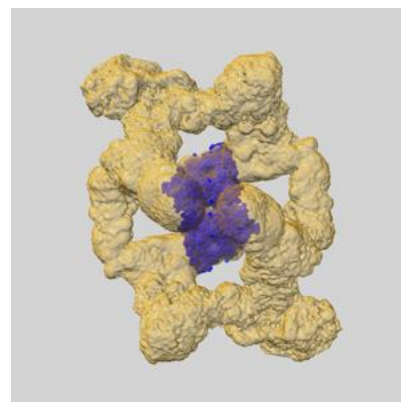
6.6.4 emd_63442_msk_4.map [i](#)



X

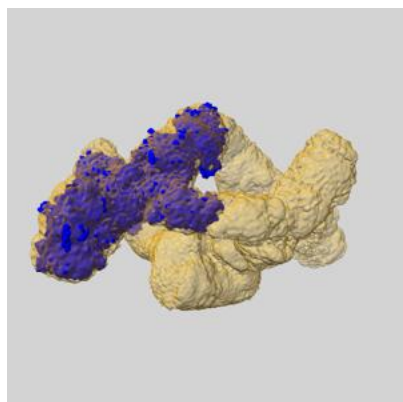


Y

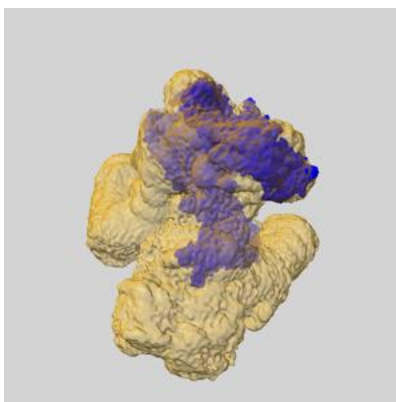


Z

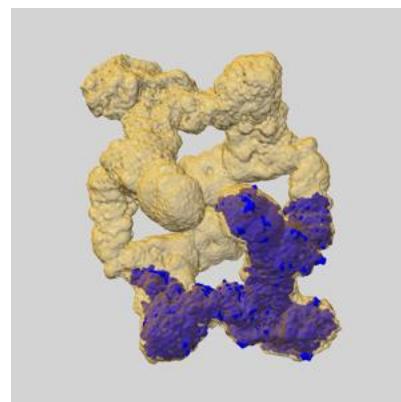
6.6.5 emd_63442_msk_5.map [i](#)



X

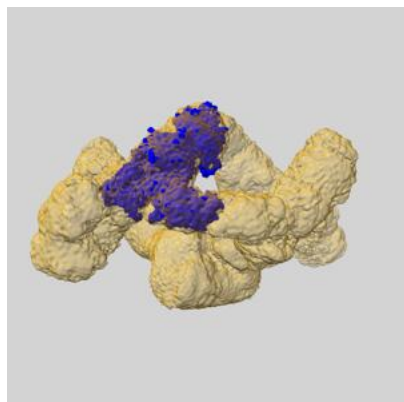


Y

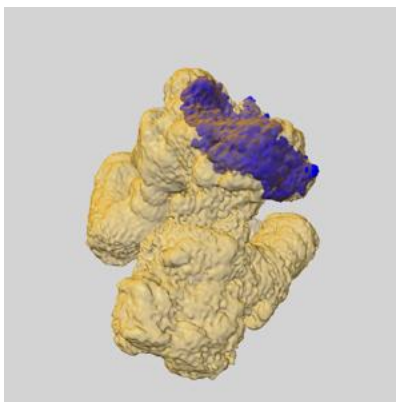


Z

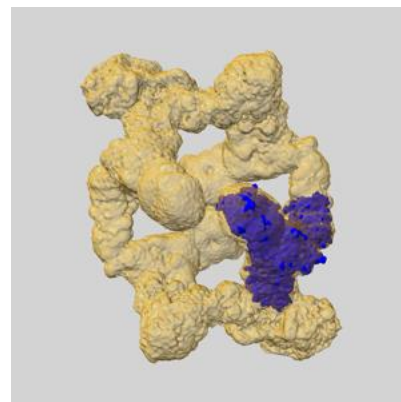
6.6.6 emd_63442_msk_6.map [i](#)



X

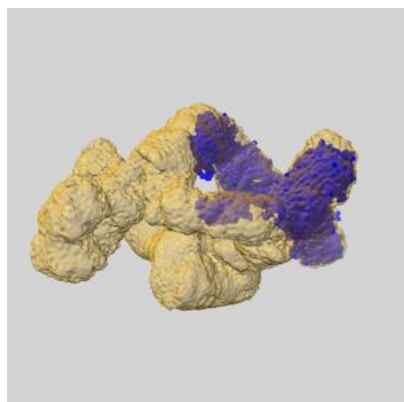


Y

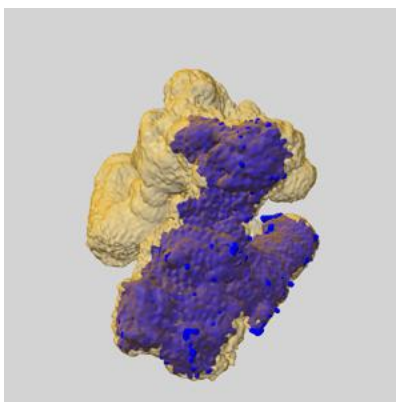


Z

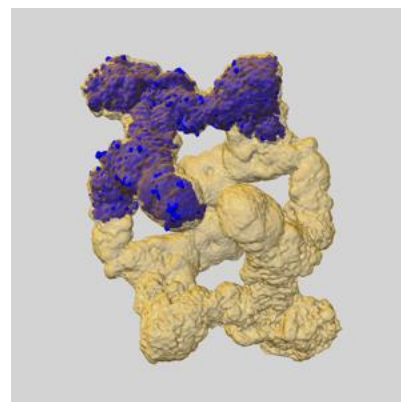
6.6.7 emd_63442_msk_7.map [i](#)



X

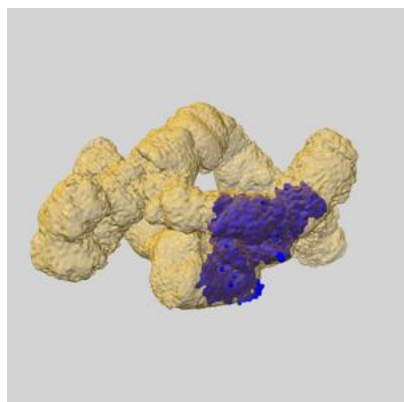


Y

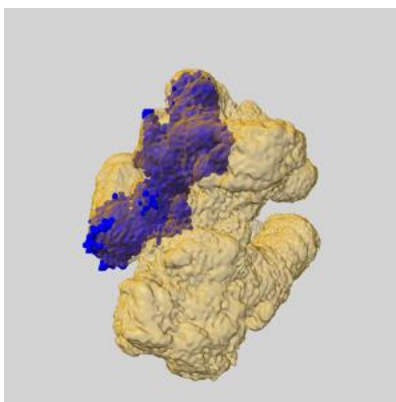


Z

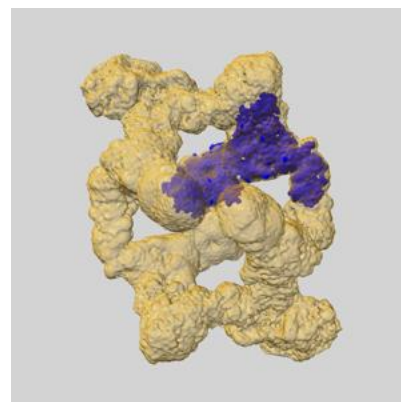
6.6.8 emd_63442_msk_8.map [i](#)



X



Y

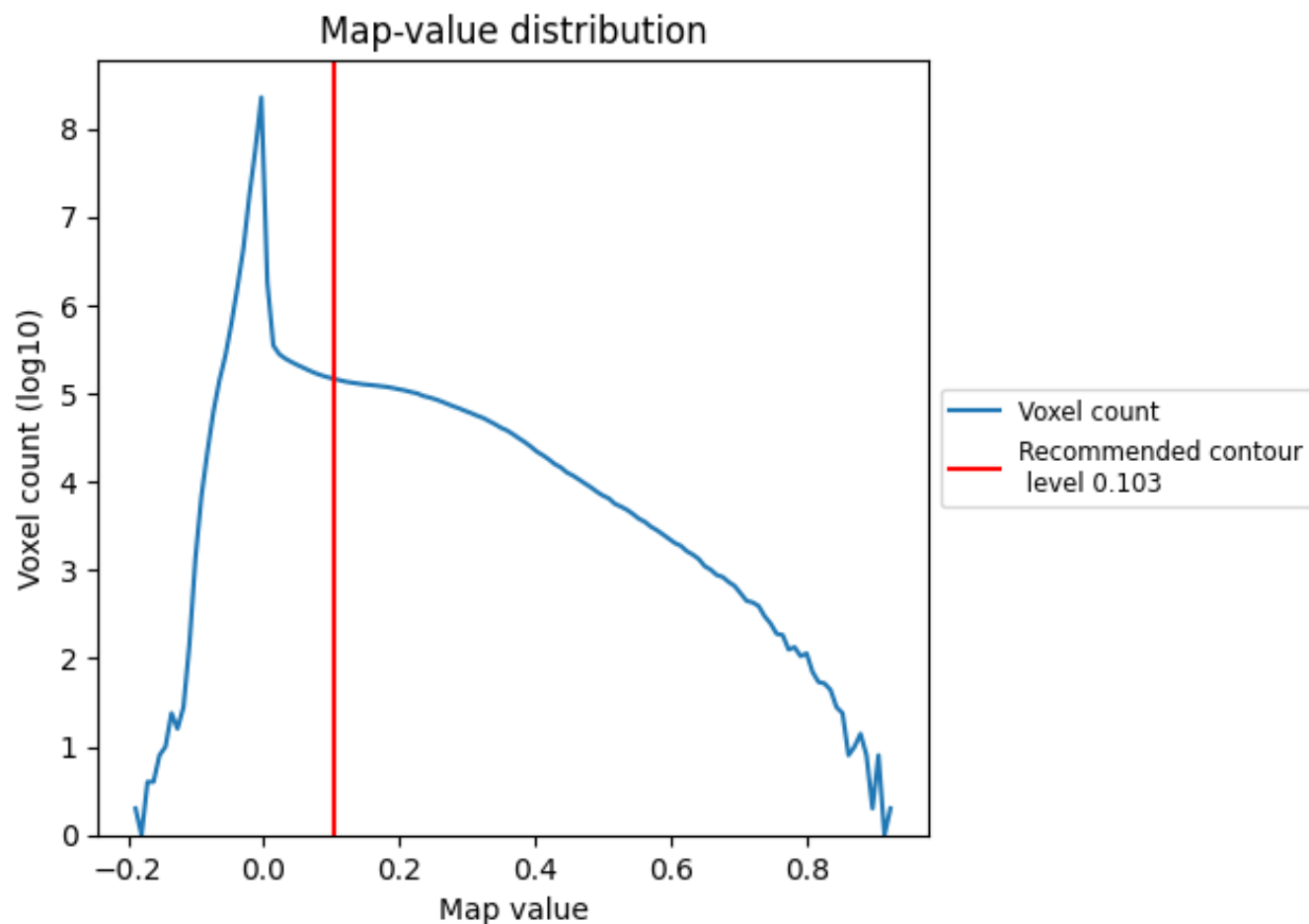


Z

7 Map analysis [i](#)

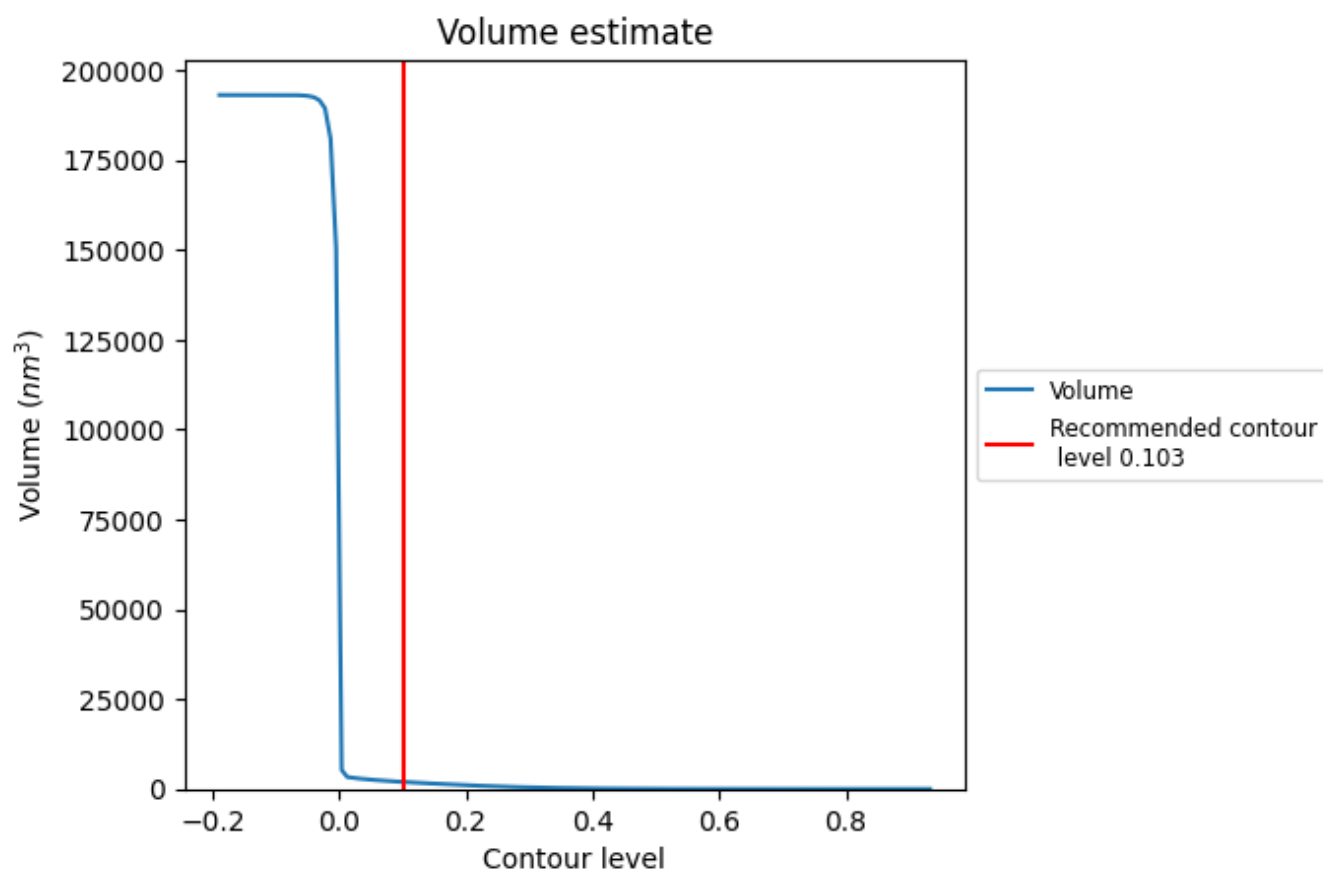
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

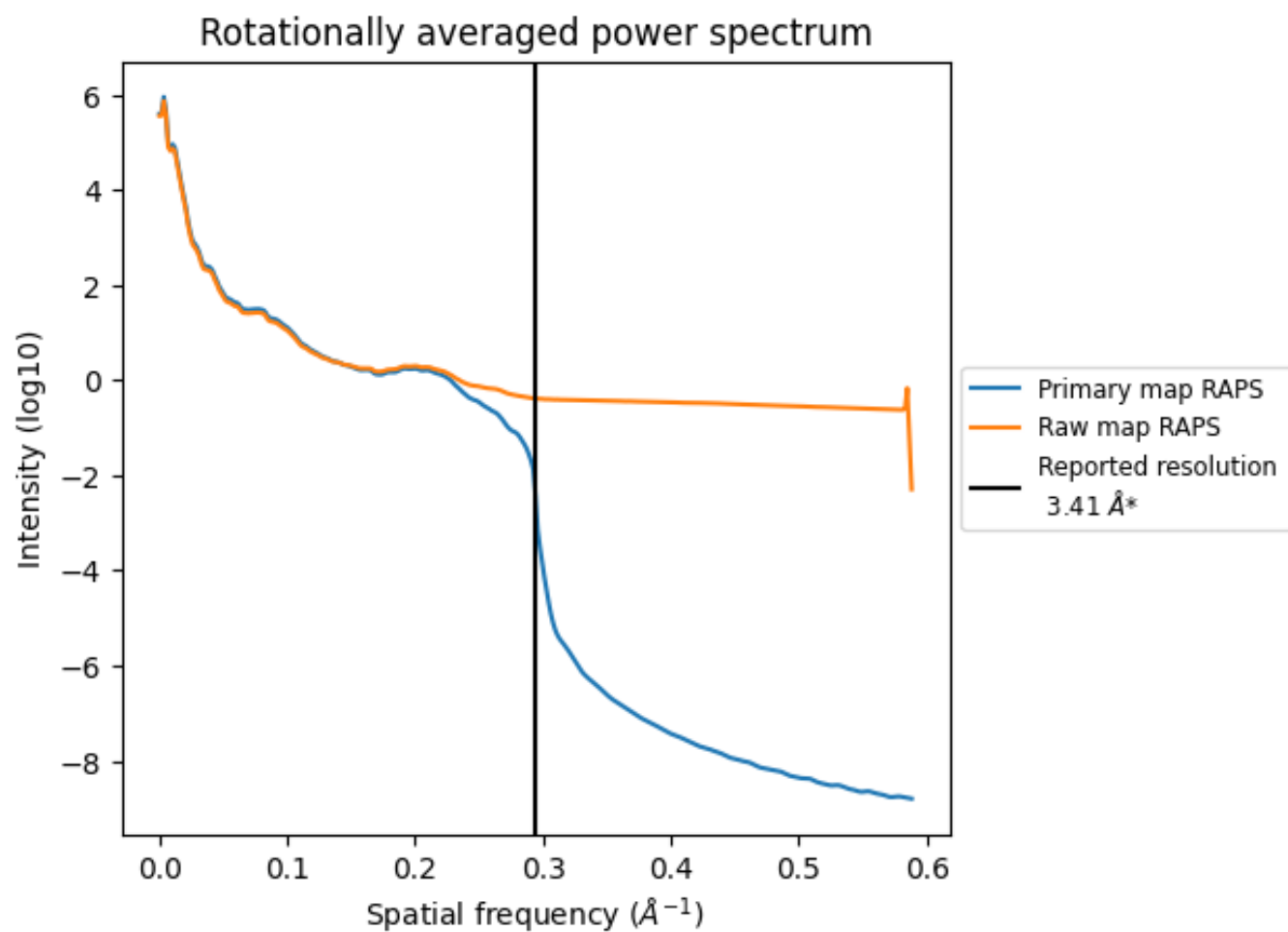
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1932 nm^3 ; this corresponds to an approximate mass of 1745 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 ⓘ

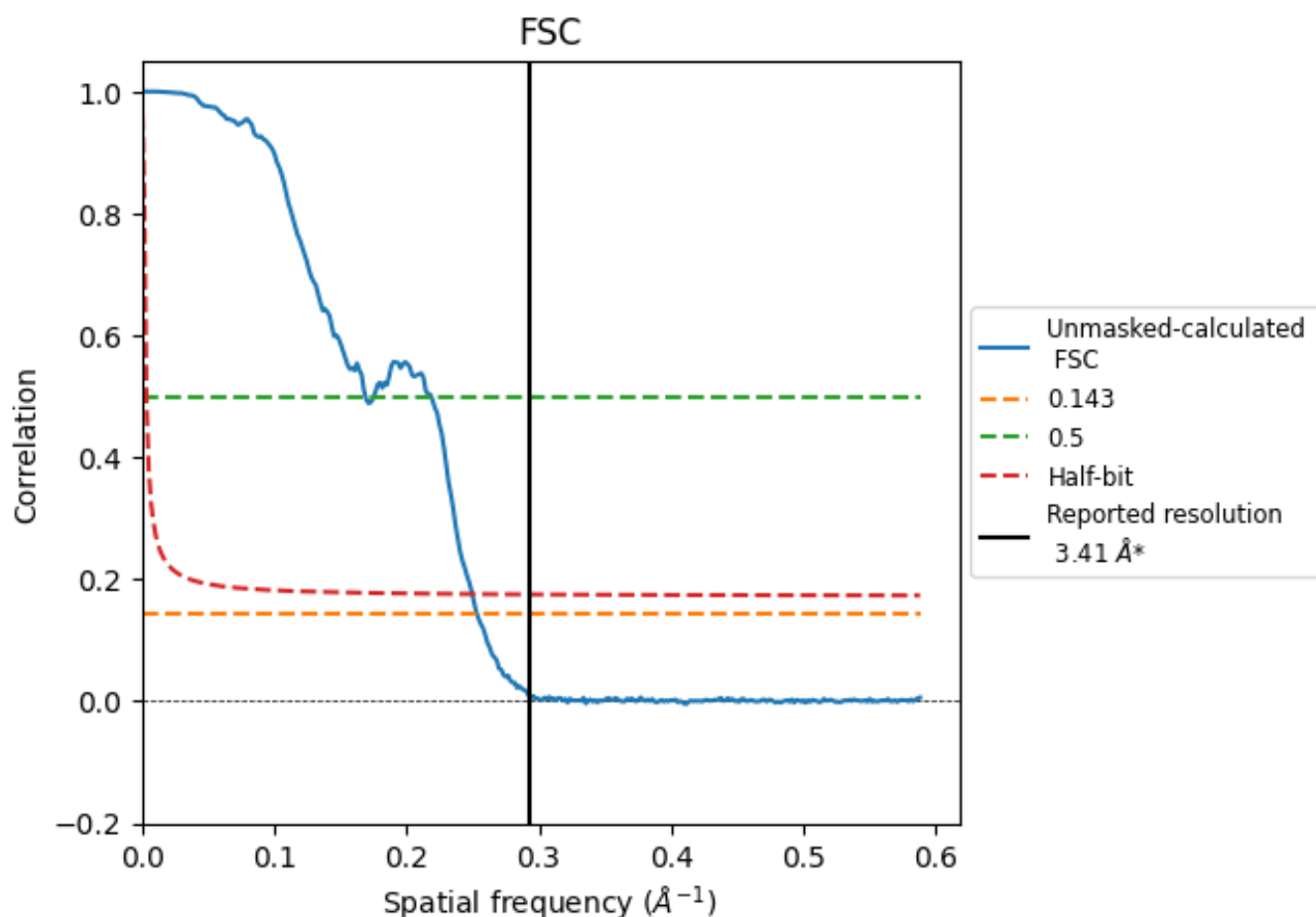


*Reported resolution corresponds to spatial frequency of 0.293 $\text{\AA}^{-1}$

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 $0.293 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

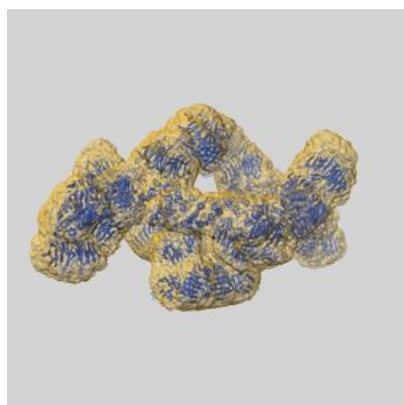
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	5.92	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 3.41 by more than 10 %

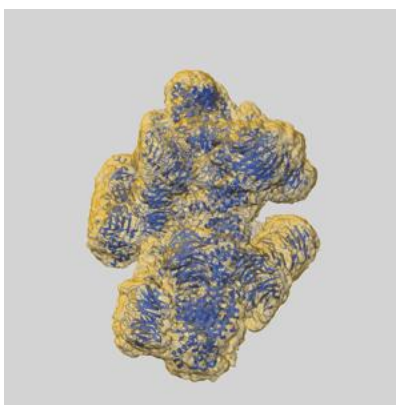
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63442 and PDB model 9LWF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

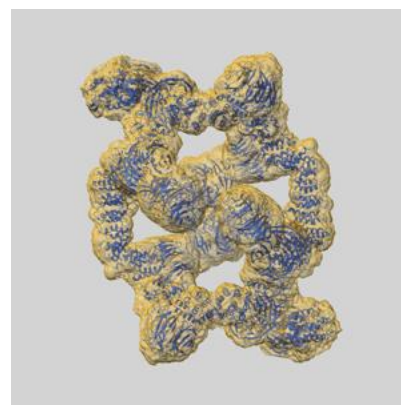
9.1 Map-model overlay [i](#)



X



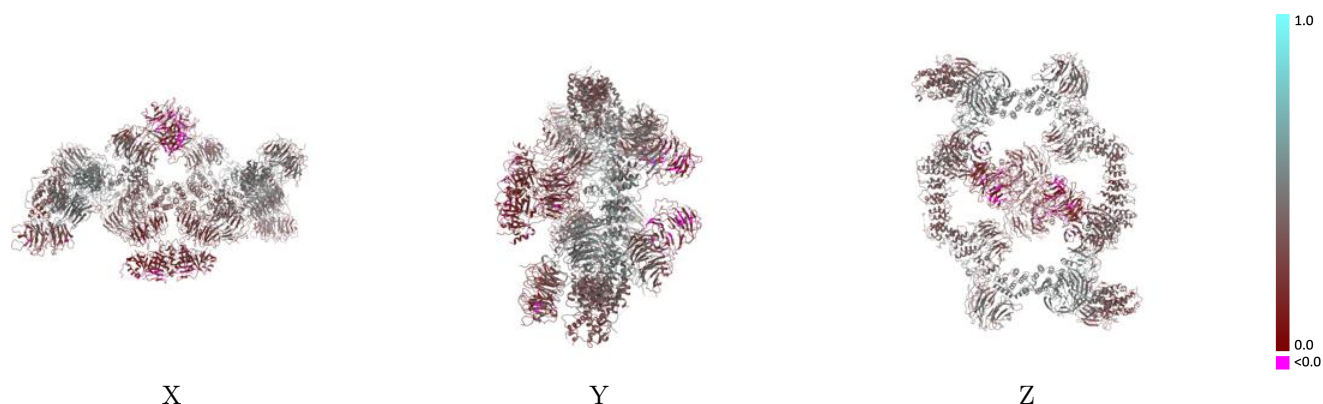
Y



Z

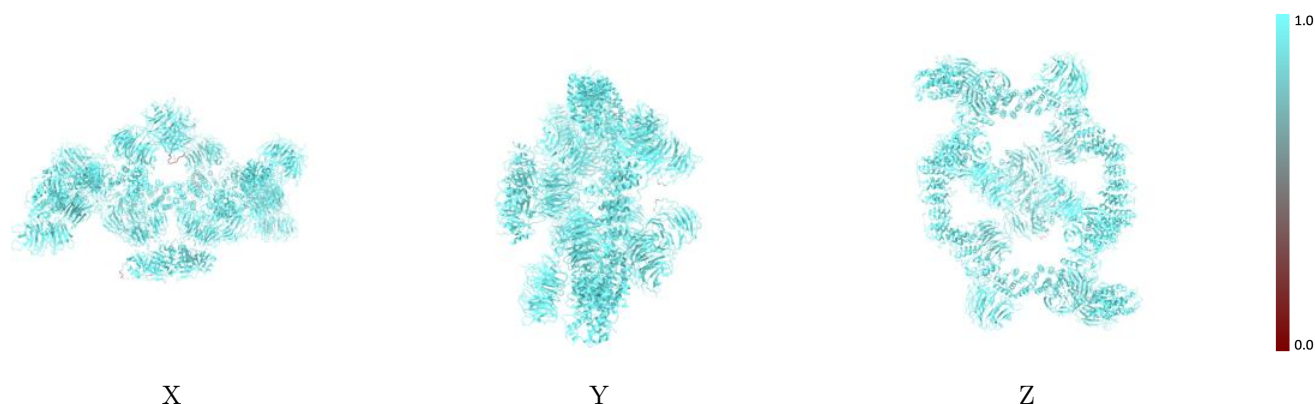
The images above show the 3D surface view of the map at the recommended contour level 0.103 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



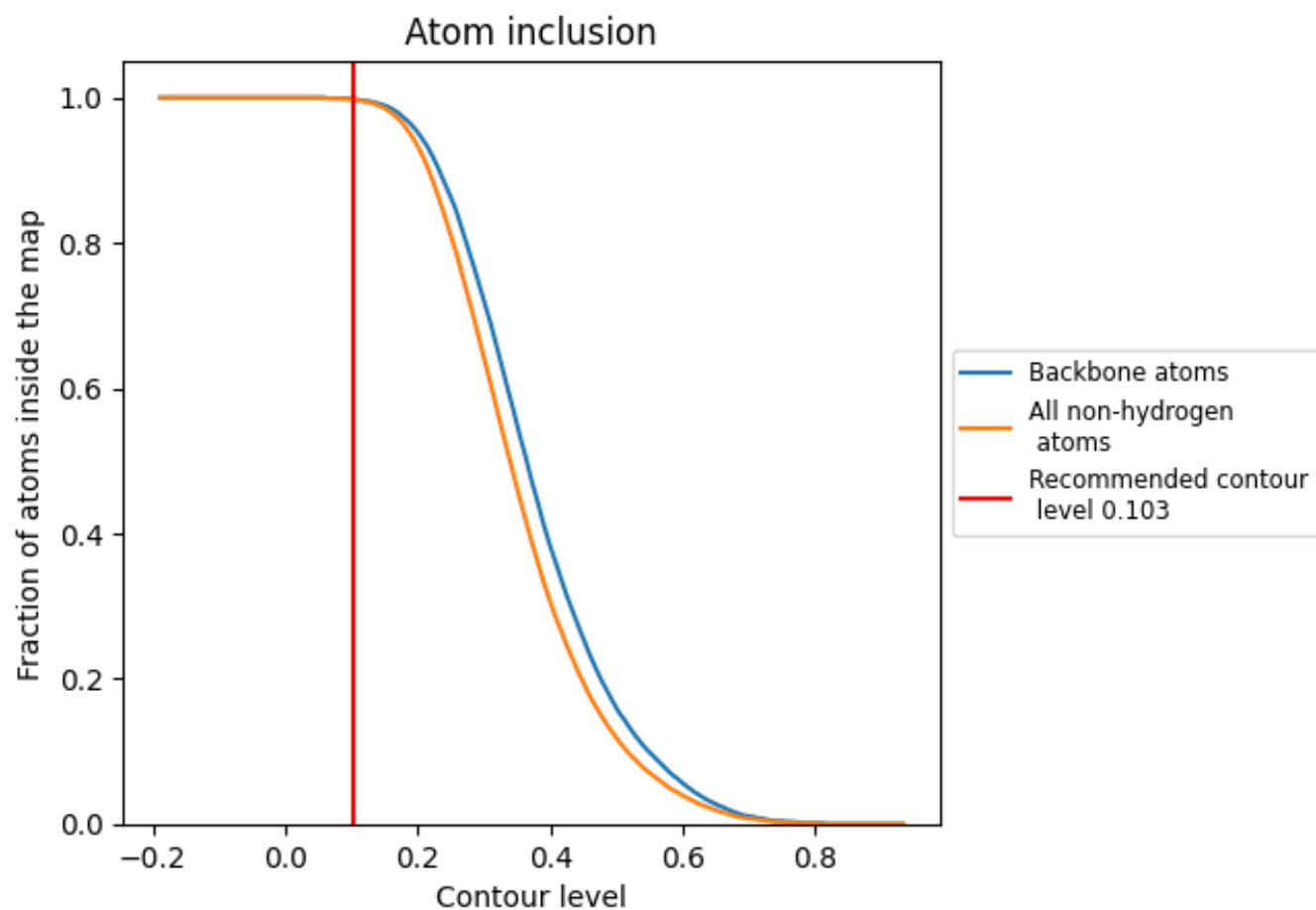
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.103).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9980	 0.3540
A	 0.9960	 0.3260
B	 1.0000	 0.3060
C	 0.9990	 0.3840
D	 1.0000	 0.4400
E	 1.0000	 0.3610
F	 1.0000	 0.3610
G	 1.0000	 0.4800
H	 1.0000	 0.4130
I	 0.9990	 0.3830
K	 0.9860	 0.3220
L	 0.9990	 0.3130
N	 1.0000	 0.4480
O	 1.0000	 0.3650
P	 1.0000	 0.3600
Q	 1.0000	 0.4820
R	 1.0000	 0.4080
U	 0.9850	 0.1680
V	 0.9990	 0.1750
X	 0.9980	 0.3590
Y	 0.9990	 0.3670

