



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:56 PM UTC

PDB ID : 9IWA / pdb_00009iwa
EMDB ID : EMD-60945
Title : Structure of apo AsfvPrimPol with dodecamer
Authors : Xu, K.E.; Chen, Y.T.
Deposited on : 2024-07-25
Resolution : 3.70 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:

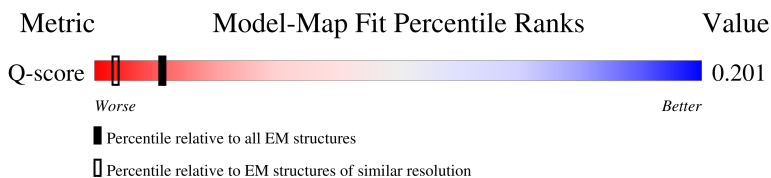
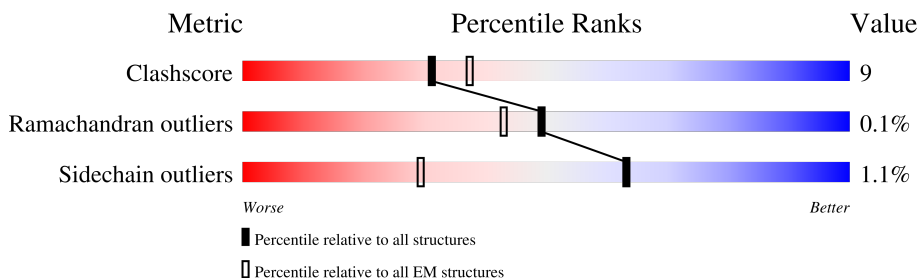
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.70 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	11569 (3.20 - 4.20)

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	962	8% 70% 16% 13%
1	B	962	13% 70% 17% 12%
1	C	962	10% 73% 16% 11%
1	D	962	12% 73% 16% 11%

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Mol	Chain	Length	Quality of chain
1	E	962	
1	F	962	
1	G	962	
1	H	962	
1	I	962	
1	J	962	
1	K	962	
1	L	962	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 81790 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.

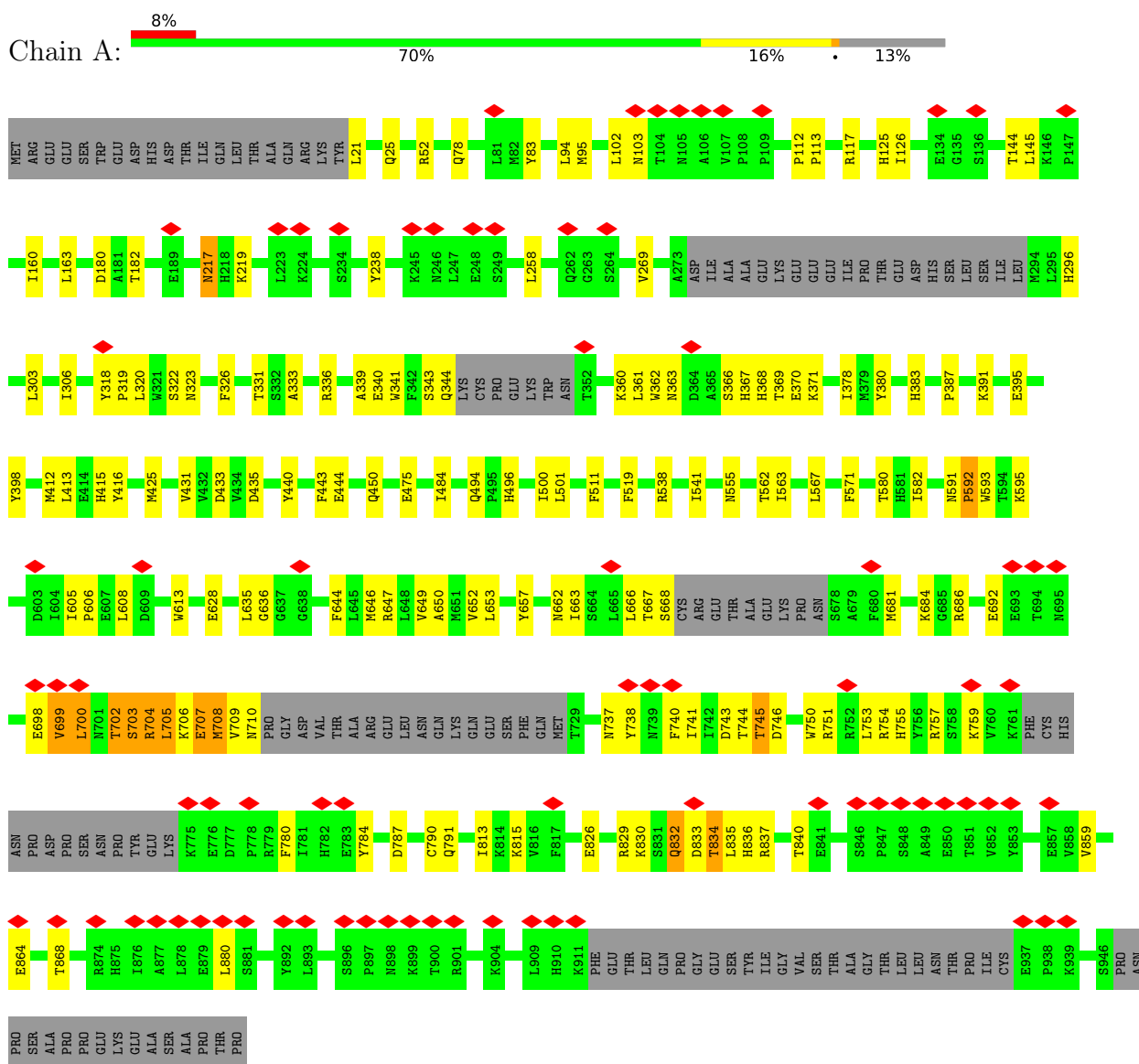
- Molecule 1 is a protein called Putative primase C962R.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	834	Total	C	N	O	S	0	0
			6763	4366	1148	1222	27		
1	B	848	Total	C	N	O	S	0	0
			6867	4431	1162	1247	27		
1	C	860	Total	C	N	O	S	0	0
			6981	4503	1183	1266	29		
1	D	856	Total	C	N	O	S	0	0
			6960	4489	1181	1260	30		
1	E	844	Total	C	N	O	S	0	0
			6854	4426	1164	1235	29		
1	F	796	Total	C	N	O	S	0	0
			6470	4176	1097	1170	27		
1	G	834	Total	C	N	O	S	0	0
			6763	4366	1148	1222	27		
1	H	848	Total	C	N	O	S	0	0
			6867	4431	1162	1247	27		
1	I	860	Total	C	N	O	S	0	0
			6981	4503	1183	1266	29		
1	J	856	Total	C	N	O	S	0	0
			6960	4489	1181	1260	30		
1	K	844	Total	C	N	O	S	0	0
			6854	4426	1164	1235	29		
1	L	796	Total	C	N	O	S	0	0
			6470	4176	1097	1170	27		

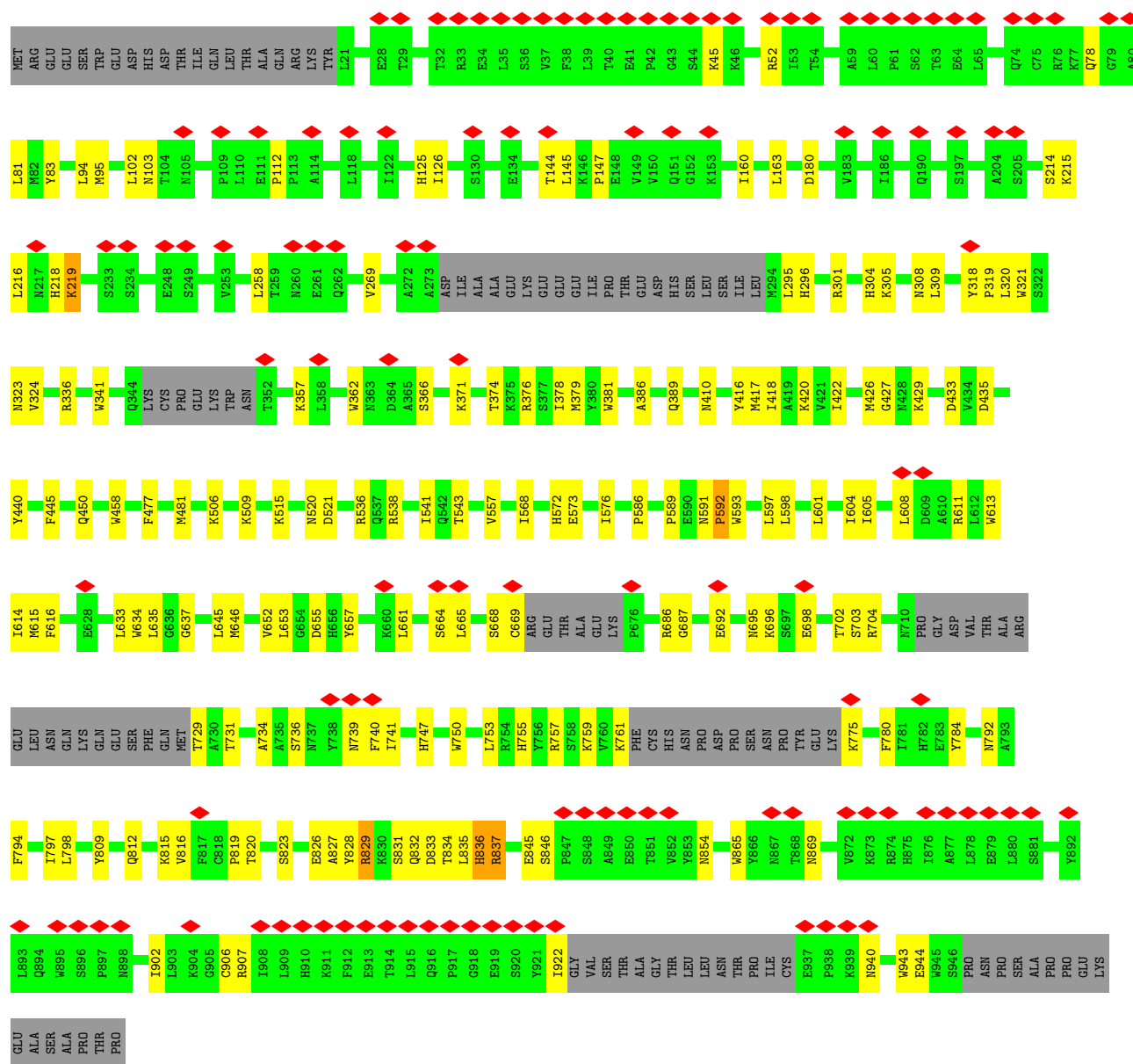
3 Residue-property plots

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.

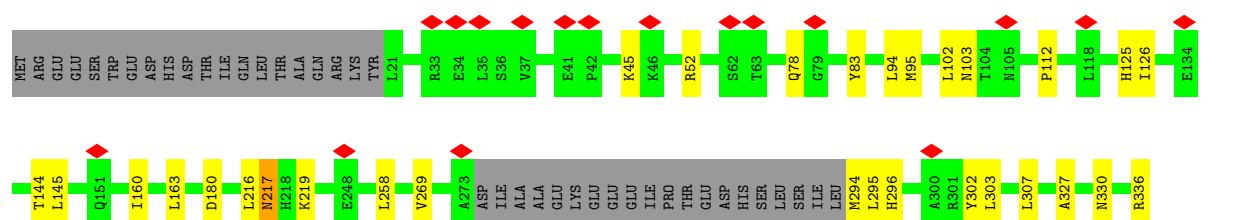
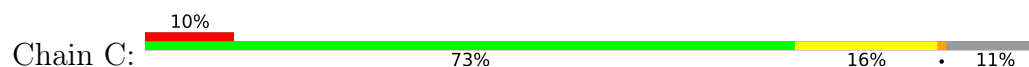
• Molecule 1: Putative primase C962R

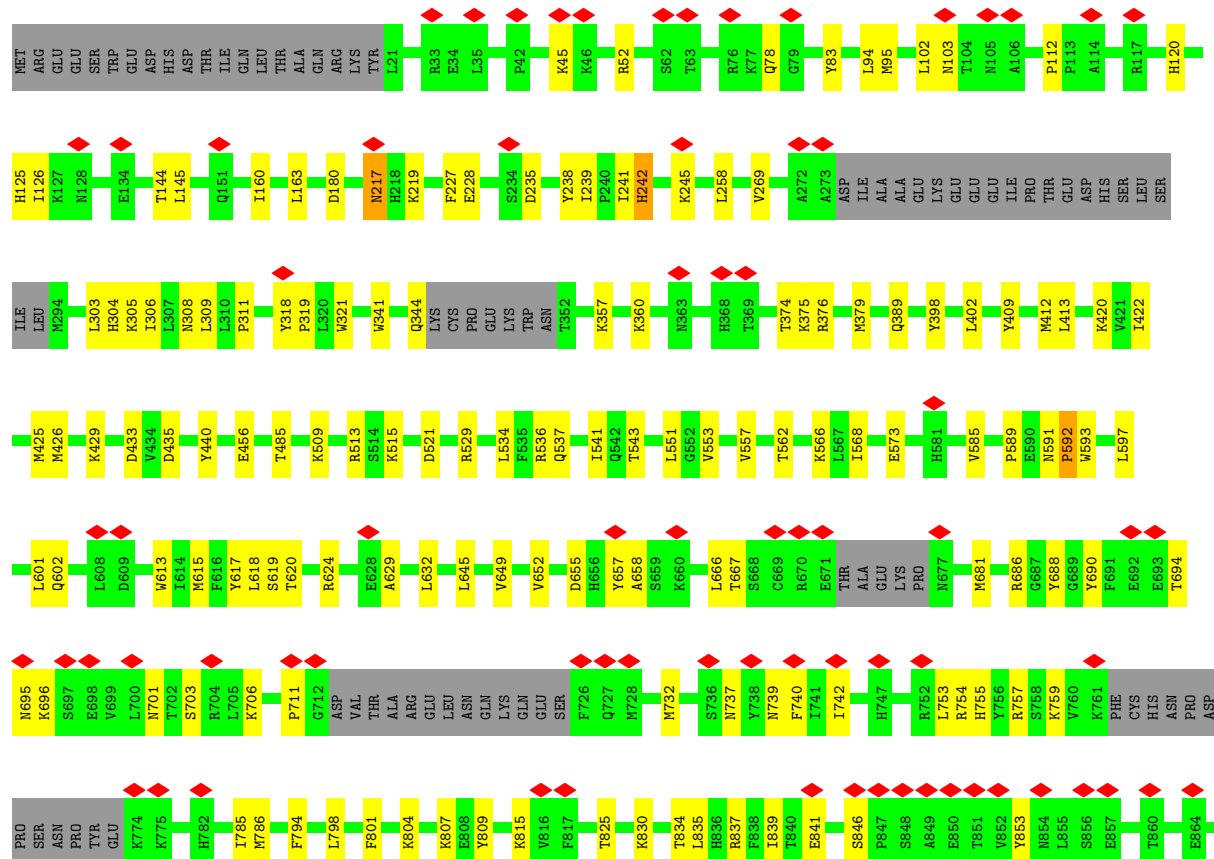


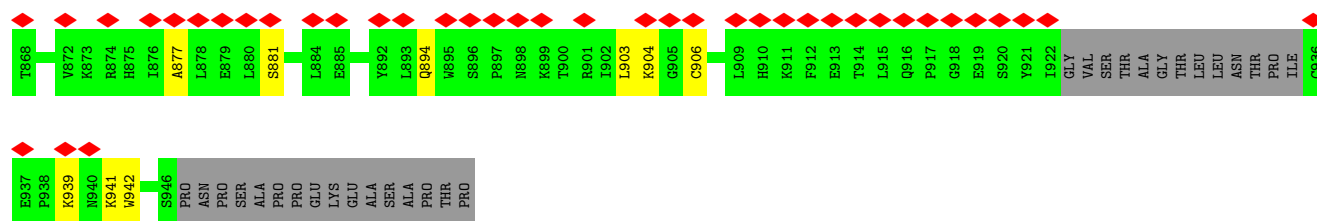
• Molecule 1: Putative primase C962R



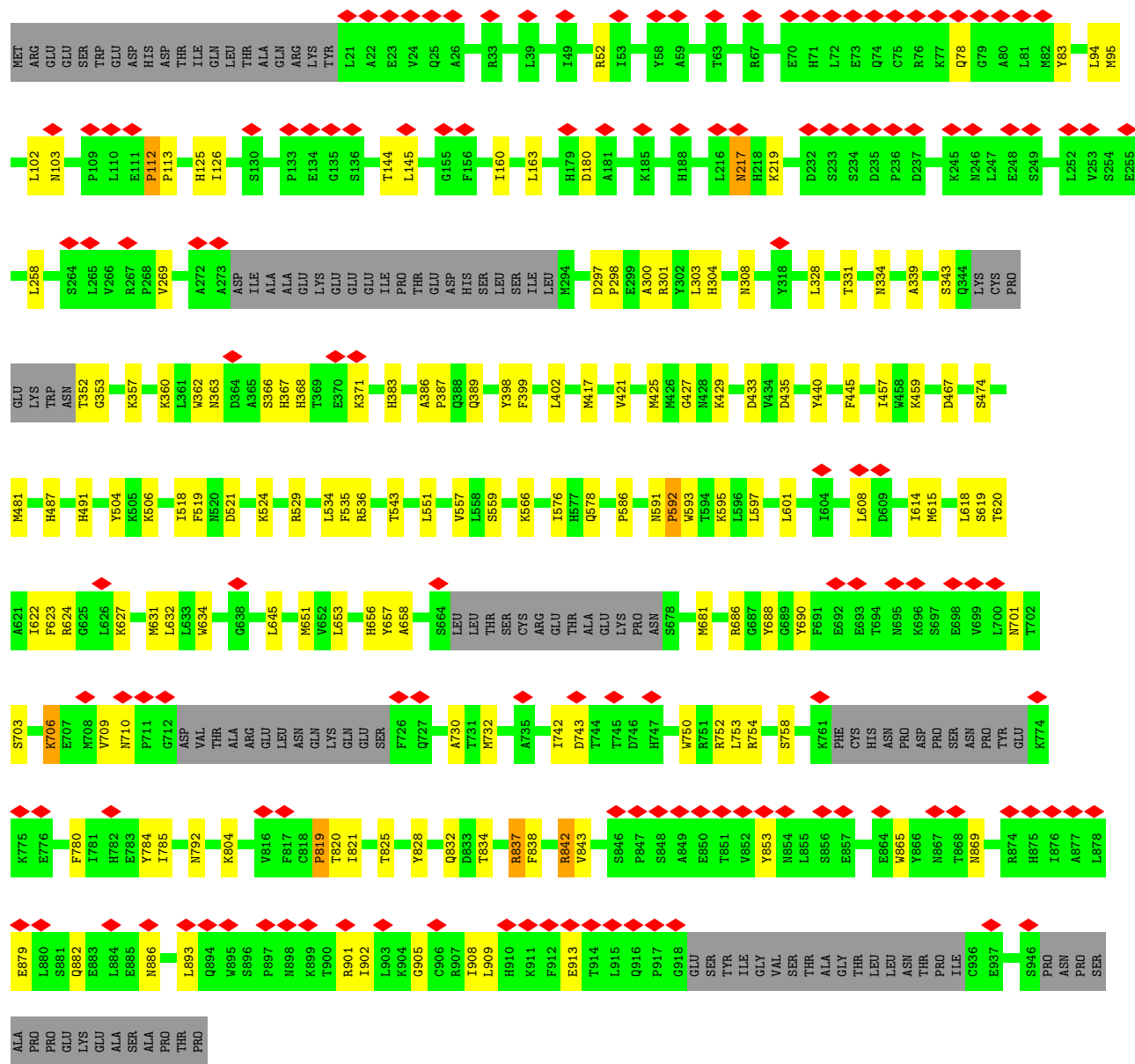
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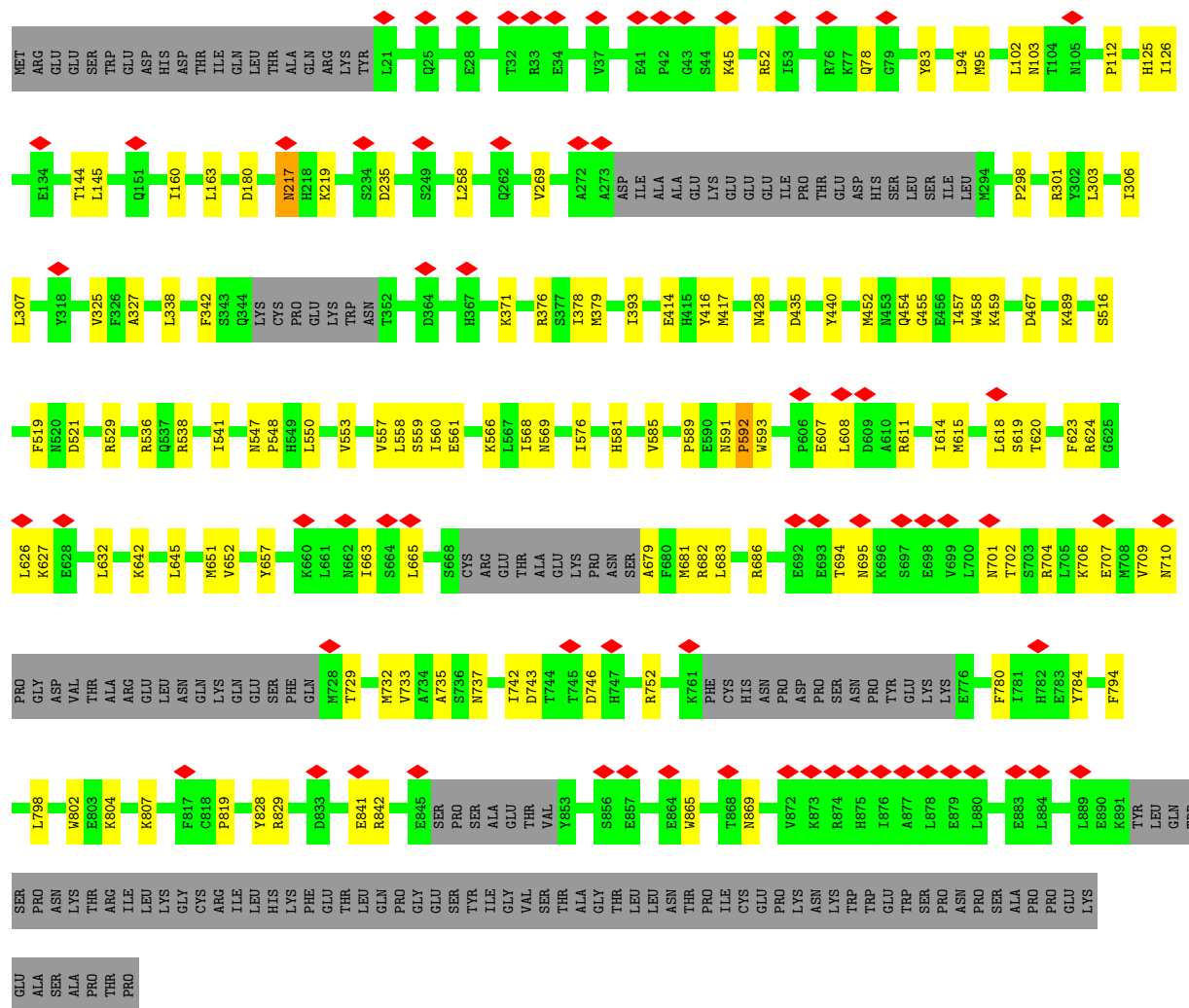


• Molecule 1: Putative primase C962R

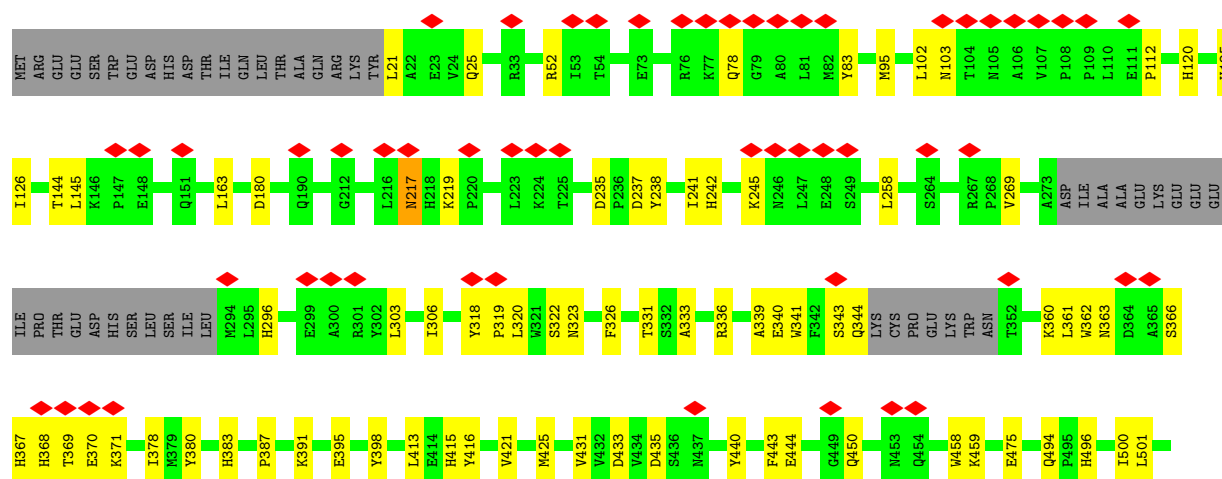


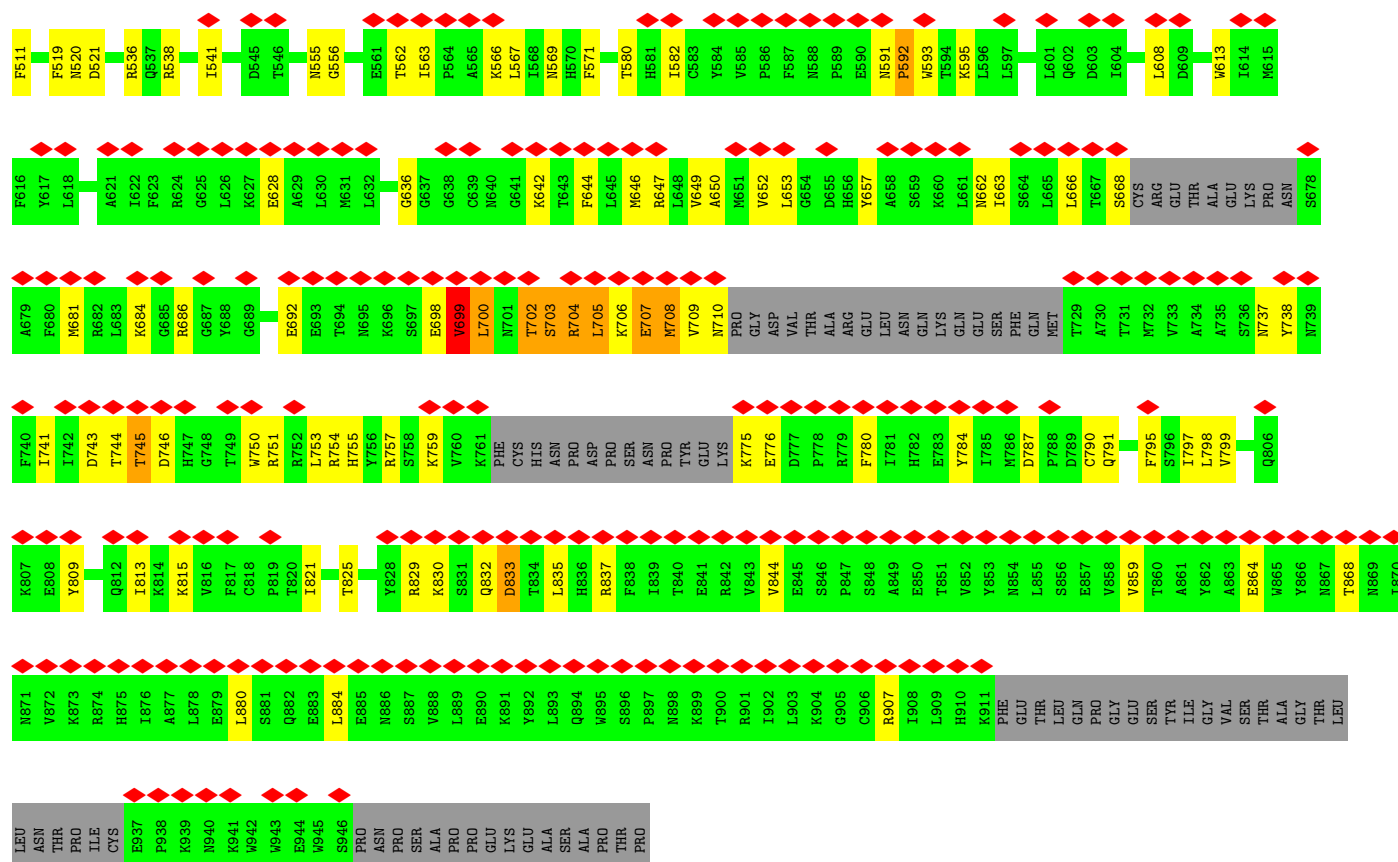
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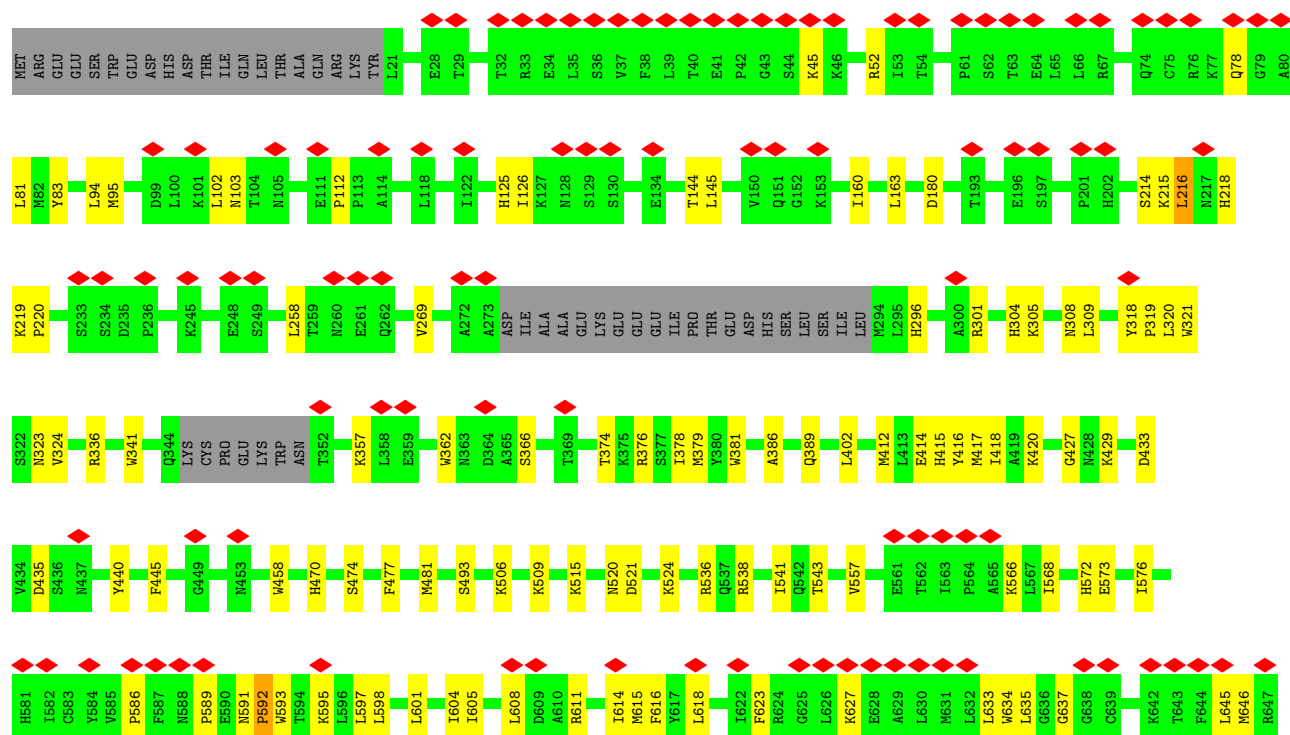


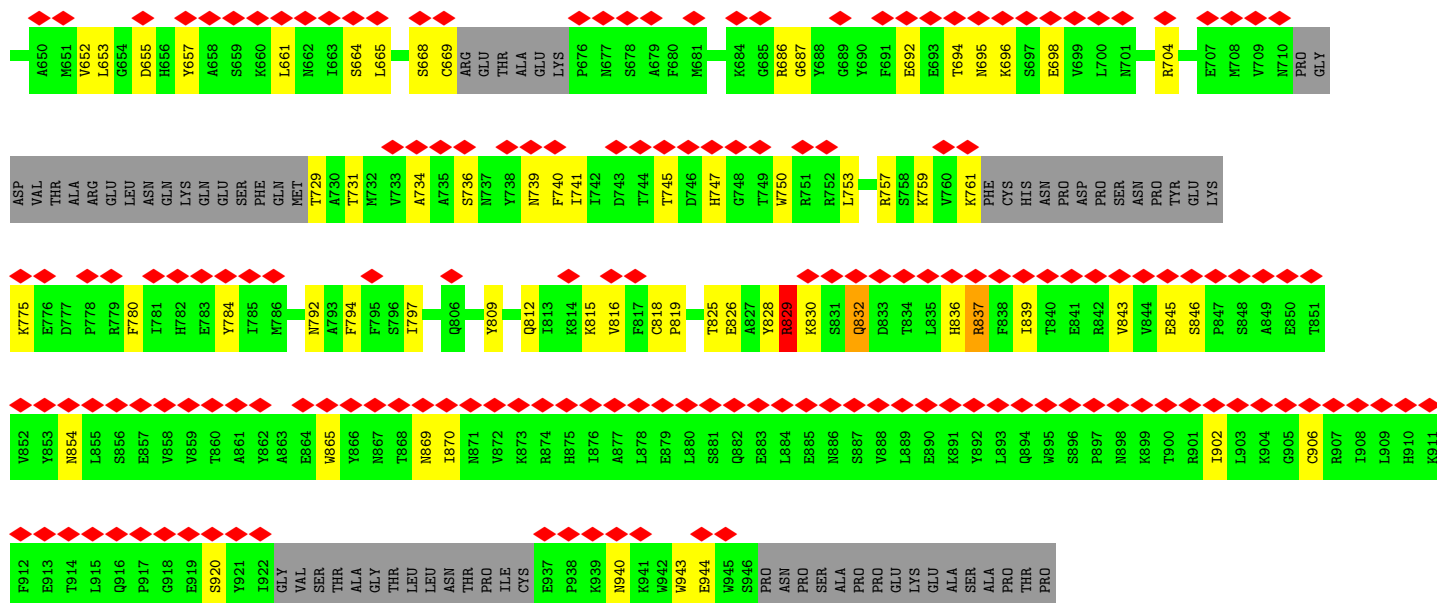
● Molecule 1: Putative primase C962R



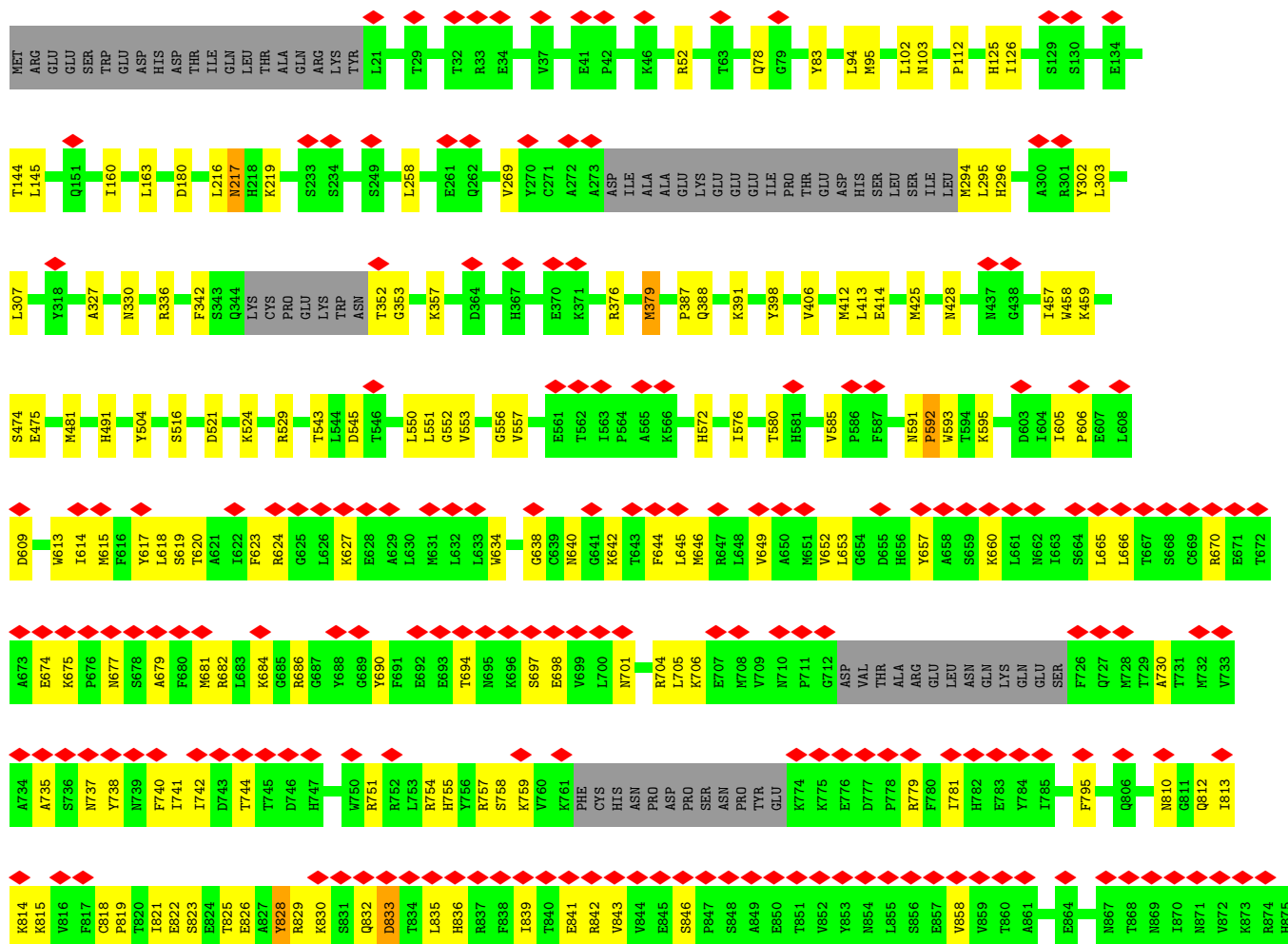


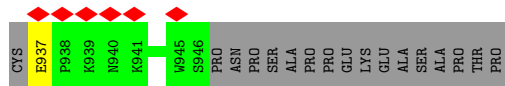
• Molecule 1: Putative primase C962R



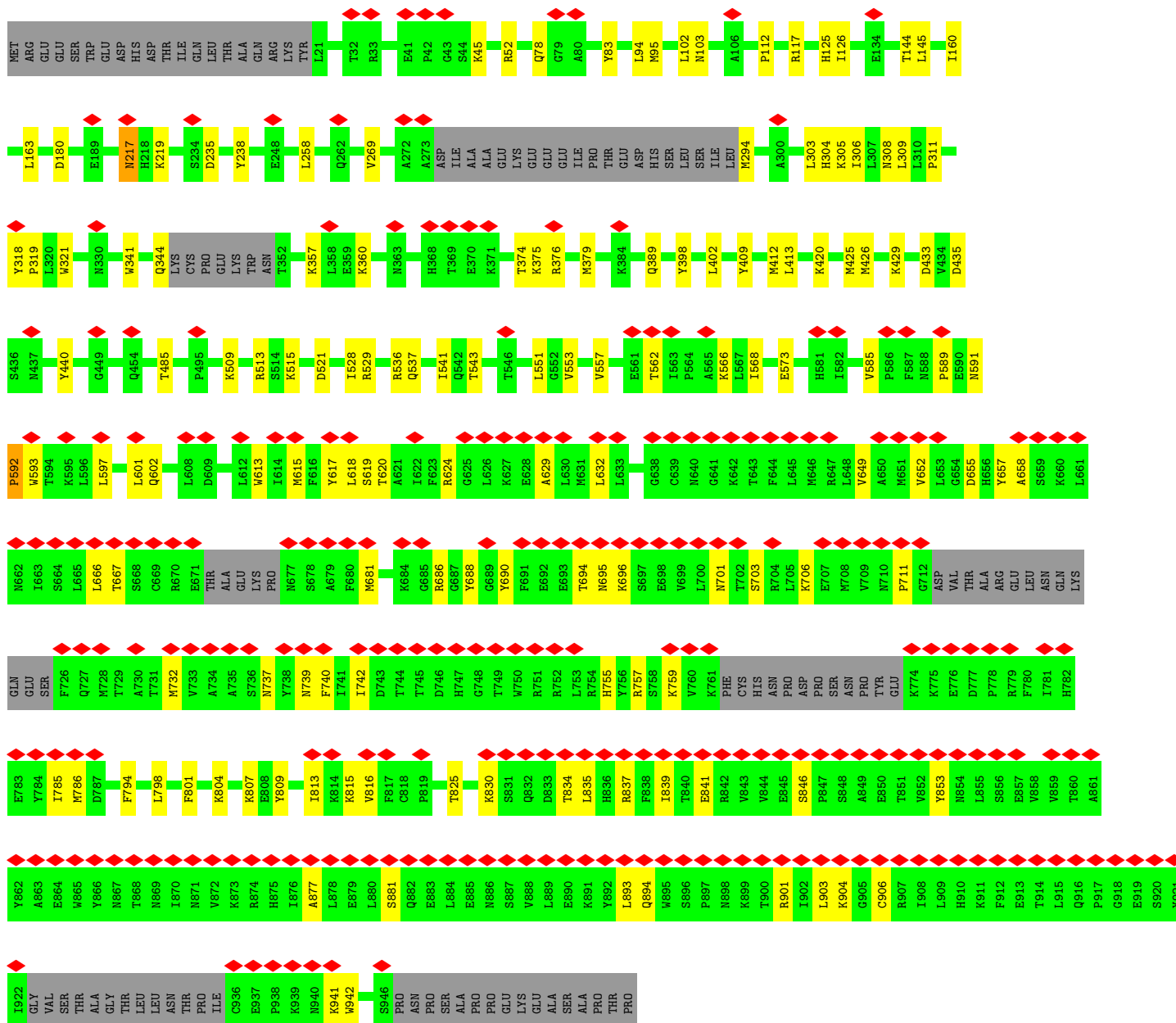
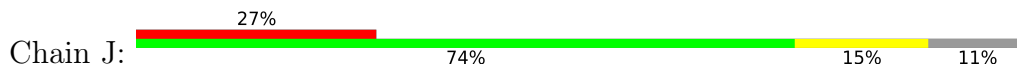


• Molecule 1: Putative primase C962R



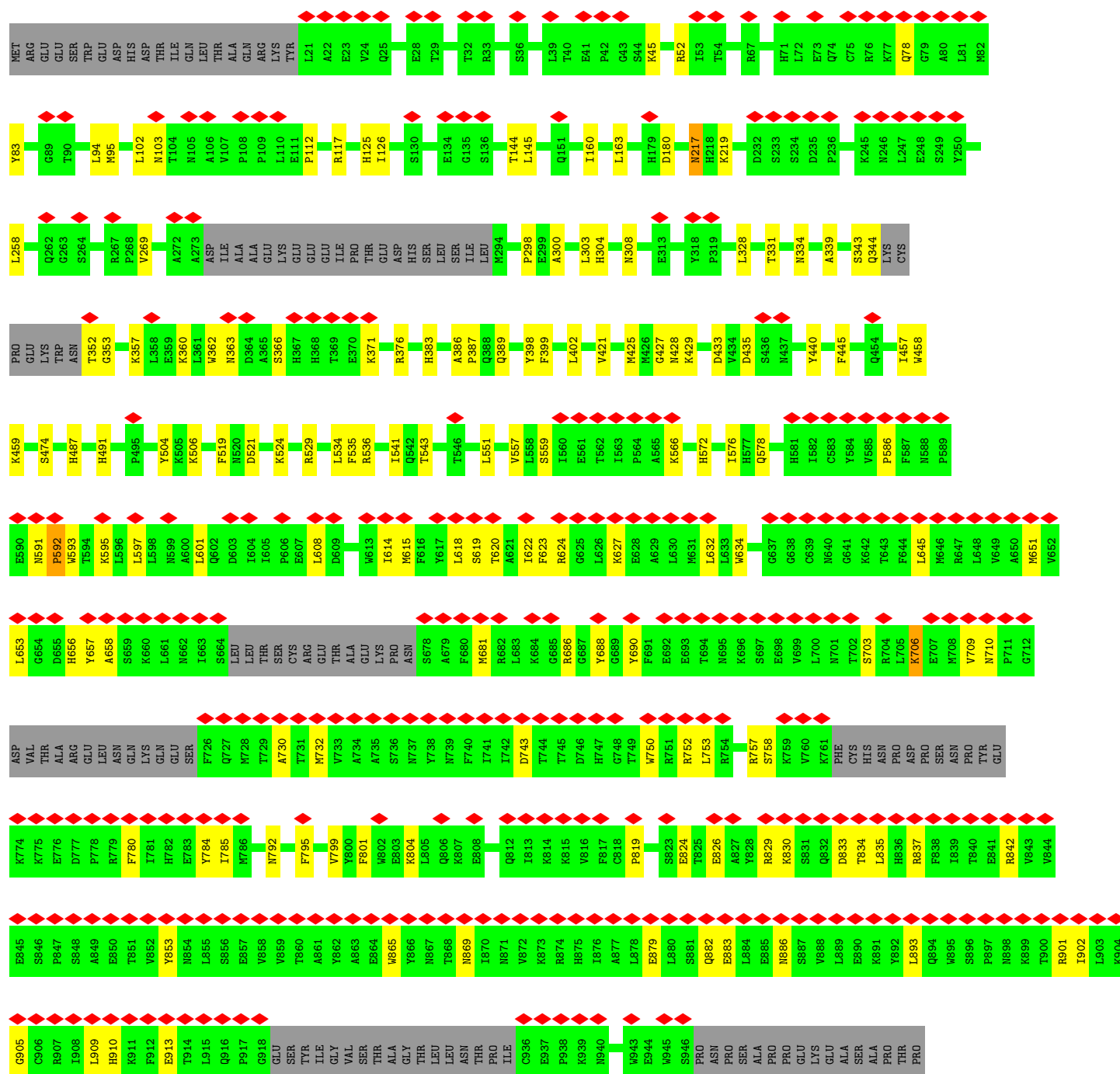


- Molecule 1: Putative primase C962R



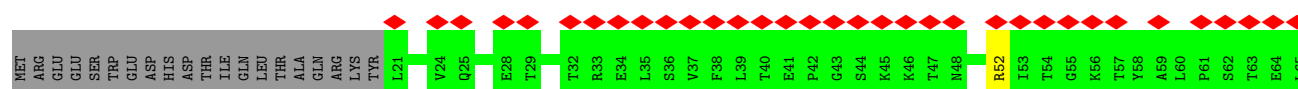
- Molecule 1: Putative primase C962R

Chain K: 



• Molecule 1: Putative primase C962R

Chain L: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136167	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.691	Depositor
Minimum map value	-0.356	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.142	Depositor
Map size ($\text{\AA}$)	410.0, 410.0, 410.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	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	0.58	0/6942	0.92	14/9406 (0.1%)
1	B	0.59	0/7048	0.88	6/9554 (0.1%)
1	C	0.58	0/7163	0.88	7/9705 (0.1%)
1	D	0.56	0/7144	0.85	5/9677 (0.1%)
1	E	0.58	0/7035	0.86	5/9531 (0.1%)
1	F	0.57	0/6637	0.86	5/8990 (0.1%)
1	G	0.59	0/6942	0.92	15/9406 (0.2%)
1	H	0.58	0/7048	0.87	6/9554 (0.1%)
1	I	0.58	0/7163	0.88	6/9705 (0.1%)
1	J	0.55	0/7144	0.85	5/9677 (0.1%)
1	K	0.57	0/7035	0.85	5/9531 (0.1%)
1	L	0.57	0/6637	0.86	5/8990 (0.1%)
All	All	0.58	0/83938	0.87	84/113726 (0.1%)

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
1	D	0	2
1	E	0	1
1	H	0	2
1	J	0	2
1	K	0	1
All	All	0	8

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	704	ARG	N-CA-C	-12.17	97.95	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	704	ARG	N-CA-C	-12.16	97.97	112.92
1	A	705	LEU	N-CA-C	-9.18	100.40	111.69
1	G	705	LEU	N-CA-C	-9.15	100.43	111.69
1	K	592	PRO	CA-N-CD	-9.15	99.18	112.00
1	A	592	PRO	CA-N-CD	-9.15	99.19	112.00
1	G	592	PRO	CA-N-CD	-9.13	99.21	112.00
1	E	592	PRO	CA-N-CD	-9.13	99.22	112.00
1	C	592	PRO	CA-N-CD	-9.09	99.28	112.00
1	B	592	PRO	CA-N-CD	-9.08	99.28	112.00
1	D	592	PRO	CA-N-CD	-9.08	99.29	112.00
1	H	592	PRO	CA-N-CD	-9.08	99.29	112.00
1	I	592	PRO	CA-N-CD	-9.07	99.30	112.00
1	J	592	PRO	CA-N-CD	-9.06	99.32	112.00
1	L	592	PRO	CA-N-CD	-9.04	99.34	112.00
1	F	592	PRO	CA-N-CD	-9.03	99.36	112.00
1	A	700	LEU	N-CA-C	-8.70	87.56	107.48
1	G	702	THR	N-CA-C	7.52	121.48	109.83
1	A	702	THR	N-CA-C	7.48	121.42	109.83
1	G	703	SER	N-CA-C	7.30	122.95	114.62
1	A	703	SER	N-CA-C	7.28	122.92	114.62
1	A	704	ARG	CB-CA-C	-6.78	99.11	110.56
1	G	704	ARG	CB-CA-C	-6.77	99.12	110.56
1	G	700	LEU	N-CA-C	-6.71	100.35	109.54
1	G	703	SER	CB-CA-C	-6.39	100.78	109.28
1	A	703	SER	CB-CA-C	-6.36	100.83	109.28
1	A	703	SER	N-CA-CB	-6.12	101.50	111.18
1	G	703	SER	N-CA-CB	-6.11	101.53	111.18
1	H	589	PRO	CA-N-CD	-5.70	104.03	112.00
1	B	589	PRO	CA-N-CD	-5.67	104.06	112.00
1	C	379	MET	CB-CG-SD	5.67	129.72	112.70
1	I	379	MET	CB-CG-SD	5.67	129.70	112.70
1	H	102	LEU	CA-C-N	5.56	128.49	120.38
1	H	102	LEU	C-N-CA	5.56	128.49	120.38
1	I	102	LEU	CA-C-N	5.56	128.49	120.38
1	I	102	LEU	C-N-CA	5.56	128.49	120.38
1	A	102	LEU	CA-C-N	5.55	128.48	120.38
1	A	102	LEU	C-N-CA	5.55	128.48	120.38
1	C	102	LEU	CA-C-N	5.54	128.47	120.38
1	C	102	LEU	C-N-CA	5.54	128.47	120.38
1	G	102	LEU	CA-C-N	5.54	128.46	120.38
1	G	102	LEU	C-N-CA	5.54	128.46	120.38
1	B	102	LEU	CA-C-N	5.53	128.45	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	LEU	C-N-CA	5.53	128.45	120.38
1	D	102	LEU	CA-C-N	5.53	128.45	120.38
1	D	102	LEU	C-N-CA	5.53	128.45	120.38
1	L	102	LEU	CA-C-N	5.53	128.45	120.38
1	L	102	LEU	C-N-CA	5.53	128.45	120.38
1	J	102	LEU	CA-C-N	5.52	128.44	120.38
1	J	102	LEU	C-N-CA	5.52	128.44	120.38
1	F	102	LEU	CA-C-N	5.51	128.43	120.38
1	F	102	LEU	C-N-CA	5.51	128.43	120.38
1	E	102	LEU	CA-C-N	5.50	128.41	120.38
1	E	102	LEU	C-N-CA	5.50	128.41	120.38
1	K	102	LEU	CA-C-N	5.50	128.41	120.38
1	K	102	LEU	C-N-CA	5.50	128.41	120.38
1	G	361	LEU	CA-CB-CG	5.42	135.28	116.30
1	A	361	LEU	CA-CB-CG	5.41	135.25	116.30
1	G	699	VAL	CB-CA-C	5.41	120.16	111.29
1	J	112	PRO	N-CA-C	5.27	117.13	110.70
1	D	112	PRO	N-CA-C	5.26	117.12	110.70
1	A	112	PRO	N-CA-C	5.23	117.08	110.70
1	G	112	PRO	N-CA-C	5.21	117.06	110.70
1	F	112	PRO	N-CA-C	5.20	117.04	110.70
1	I	112	PRO	N-CA-C	5.19	117.03	110.70
1	H	112	PRO	N-CA-C	5.18	117.02	110.70
1	E	112	PRO	N-CA-C	5.17	117.01	110.70
1	K	112	PRO	N-CA-C	5.17	117.01	110.70
1	L	112	PRO	N-CA-C	5.16	116.99	110.70
1	C	112	PRO	N-CA-C	5.15	116.99	110.70
1	B	112	PRO	N-CA-C	5.14	116.97	110.70
1	I	103	ASN	CB-CA-C	-5.13	100.51	110.46
1	B	103	ASN	CB-CA-C	-5.12	100.53	110.46
1	E	103	ASN	CB-CA-C	-5.12	100.53	110.46
1	A	103	ASN	CB-CA-C	-5.12	100.53	110.46
1	F	103	ASN	CB-CA-C	-5.12	100.53	110.46
1	H	103	ASN	CB-CA-C	-5.12	100.54	110.46
1	C	103	ASN	CB-CA-C	-5.11	100.54	110.46
1	G	103	ASN	CB-CA-C	-5.11	100.54	110.46
1	L	103	ASN	CB-CA-C	-5.10	100.56	110.46
1	D	103	ASN	CB-CA-C	-5.10	100.57	110.46
1	J	103	ASN	CB-CA-C	-5.09	100.58	110.46
1	K	103	ASN	CB-CA-C	-5.09	100.58	110.46
1	C	45	LYS	N-CA-C	-5.06	106.95	113.23

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	409	TYR	Peptide
1	D	839	ILE	Peptide
1	E	842	ARG	Sidechain
1	H	829	ARG	Sidechain
1	H	837	ARG	Sidechain
1	J	409	TYR	Peptide
1	J	839	ILE	Peptide
1	K	833	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6763	0	6640	176	0
1	B	6867	0	6740	134	0
1	C	6981	0	6900	114	0
1	D	6960	0	6849	141	0
1	E	6854	0	6761	109	0
1	F	6470	0	6384	102	0
1	G	6763	0	6642	189	0
1	H	6867	0	6740	139	0
1	I	6981	0	6900	113	0
1	J	6960	0	6848	131	0
1	K	6854	0	6761	113	0
1	L	6470	0	6385	112	0
All	All	81790	0	80550	1431	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 (1431) 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:D:245:LYS:HE2	1:G:245:LYS:CE	1.32	1.52
1:A:117:ARG:HB2	1:J:238:TYR:CZ	1.54	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LYS:CE	1:G:245:LYS:CE	1.98	1.41
1:D:238:TYR:HB2	1:G:120:HIS:NE2	1.30	1.39
1:D:238:TYR:CD2	1:G:120:HIS:CD2	2.14	1.35
1:K:865:TRP:CD1	1:K:869:ASN:HD21	1.47	1.33
1:D:245:LYS:CE	1:G:245:LYS:HE3	1.57	1.30
1:D:238:TYR:HB2	1:G:120:HIS:CE1	1.75	1.22
1:K:865:TRP:CD1	1:K:869:ASN:ND2	2.07	1.22
1:D:245:LYS:CE	1:G:245:LYS:HE2	1.64	1.18
1:A:591:ASN:OD1	1:A:592:PRO:HD2	1.46	1.16
1:L:591:ASN:OD1	1:L:592:PRO:HD2	1.45	1.15
1:D:238:TYR:CG	1:G:120:HIS:CD2	2.35	1.14
1:F:591:ASN:OD1	1:F:592:PRO:HD2	1.45	1.14
1:G:591:ASN:OD1	1:G:592:PRO:HD2	1.46	1.14
1:A:238:TYR:CE2	1:J:117:ARG:HG3	1.82	1.12
1:A:117:ARG:HG3	1:J:238:TYR:CD2	1.69	1.12
1:C:591:ASN:OD1	1:C:592:PRO:HD2	1.49	1.12
1:C:592:PRO:HD2	1:C:593:TRP:H	1.14	1.11
1:H:592:PRO:HD2	1:H:593:TRP:H	1.12	1.11
1:A:238:TYR:CD2	1:J:117:ARG:HG3	1.86	1.11
1:A:238:TYR:CZ	1:J:117:ARG:HB2	1.86	1.10
1:D:238:TYR:CB	1:G:120:HIS:NE2	2.14	1.10
1:K:865:TRP:NE1	1:K:869:ASN:ND2	2.00	1.10
1:I:591:ASN:HB3	1:I:592:PRO:HD3	1.18	1.10
1:A:117:ARG:HE	1:J:238:TYR:CB	1.31	1.09
1:A:117:ARG:CB	1:J:238:TYR:CZ	2.34	1.09
1:D:120:HIS:CD2	1:G:238:TYR:HB2	1.86	1.09
1:B:591:ASN:OD1	1:B:592:PRO:HD2	1.50	1.09
1:A:238:TYR:CE2	1:J:117:ARG:CG	2.34	1.09
1:H:591:ASN:OD1	1:H:592:PRO:HD2	1.50	1.08
1:K:592:PRO:HD2	1:K:593:TRP:H	1.15	1.08
1:F:592:PRO:HD2	1:F:593:TRP:H	1.12	1.07
1:I:592:PRO:HD2	1:I:593:TRP:H	1.14	1.07
1:B:592:PRO:HD2	1:B:593:TRP:H	1.13	1.07
1:L:591:ASN:OD1	1:L:592:PRO:CD	2.02	1.07
1:L:592:PRO:HD2	1:L:593:TRP:H	1.12	1.07
1:F:591:ASN:OD1	1:F:592:PRO:CD	2.02	1.06
1:A:117:ARG:CB	1:J:238:TYR:CE2	2.38	1.06
1:G:592:PRO:HD2	1:G:593:TRP:H	1.17	1.06
1:A:592:PRO:HD2	1:A:593:TRP:H	1.17	1.05
1:A:591:ASN:OD1	1:A:592:PRO:CD	2.05	1.05
1:G:591:ASN:OD1	1:G:592:PRO:CD	2.05	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:592:PRO:HD2	1:J:593:TRP:H	1.16	1.03
1:D:592:PRO:HD2	1:D:593:TRP:H	1.16	1.03
1:E:592:PRO:HD2	1:E:593:TRP:H	1.15	1.03
1:E:591:ASN:OD1	1:E:592:PRO:HD2	1.57	1.03
1:K:591:ASN:OD1	1:K:592:PRO:HD2	1.57	1.02
1:D:245:LYS:HE3	1:G:245:LYS:HE3	1.42	1.02
1:C:591:ASN:OD1	1:C:592:PRO:CD	2.06	1.02
1:D:245:LYS:HE2	1:G:245:LYS:HE2	1.21	1.02
1:A:238:TYR:CZ	1:J:117:ARG:CD	2.22	1.01
1:F:235:ASP:OD1	1:K:117:ARG:NH1	1.93	1.01
1:D:245:LYS:CD	1:G:245:LYS:HE2	1.91	1.01
1:A:117:ARG:CG	1:J:238:TYR:CE2	2.45	1.00
1:A:117:ARG:NE	1:J:238:TYR:CB	2.06	1.00
1:A:238:TYR:OH	1:J:117:ARG:HB2	1.61	1.00
1:B:591:ASN:OD1	1:B:592:PRO:CD	2.10	1.00
1:F:235:ASP:OD1	1:K:117:ARG:CZ	2.10	0.99
1:H:591:ASN:OD1	1:H:592:PRO:CD	2.09	0.99
1:D:591:ASN:OD1	1:D:592:PRO:HD2	1.63	0.99
1:A:117:ARG:HE	1:J:238:TYR:HB2	1.25	0.99
1:D:120:HIS:NE2	1:G:238:TYR:HB2	1.77	0.98
1:J:591:ASN:OD1	1:J:592:PRO:HD2	1.63	0.97
1:D:245:LYS:HE2	1:G:245:LYS:HE3	1.11	0.96
1:I:216:LEU:HG	1:I:295:LEU:CD2	1.96	0.95
1:A:238:TYR:CZ	1:J:117:ARG:CG	2.49	0.95
1:I:591:ASN:HB3	1:I:592:PRO:CD	1.96	0.95
1:A:702:THR:HG22	1:A:702:THR:O	1.65	0.95
1:C:216:LEU:CD1	1:C:295:LEU:HD23	1.97	0.95
1:C:216:LEU:HG	1:C:295:LEU:CD2	1.96	0.95
1:A:238:TYR:HB3	1:J:117:ARG:HH11	1.29	0.95
1:G:702:THR:O	1:G:702:THR:HG22	1.65	0.95
1:I:216:LEU:CD1	1:I:295:LEU:HD23	1.96	0.95
1:A:117:ARG:CG	1:J:238:TYR:CD2	2.41	0.94
1:D:238:TYR:CD2	1:G:120:HIS:HD2	1.68	0.94
1:K:591:ASN:OD1	1:K:592:PRO:CD	2.15	0.94
1:A:238:TYR:CZ	1:J:117:ARG:CB	2.50	0.94
1:A:238:TYR:CB	1:J:117:ARG:HH11	1.80	0.93
1:E:591:ASN:OD1	1:E:592:PRO:CD	2.15	0.93
1:I:697:SER:O	1:I:741:ILE:HG12	1.68	0.93
1:C:697:SER:O	1:C:741:ILE:HG12	1.68	0.92
1:C:216:LEU:HD12	1:C:295:LEU:HD23	1.50	0.92
1:K:865:TRP:CE2	1:K:869:ASN:ND2	2.37	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:ASN:HB2	1:C:592:PRO:HD3	1.53	0.90
1:C:216:LEU:CG	1:C:295:LEU:HD23	2.02	0.89
1:D:591:ASN:OD1	1:D:592:PRO:CD	2.20	0.89
1:A:117:ARG:HG3	1:J:238:TYR:CE2	2.07	0.89
1:L:591:ASN:HB2	1:L:592:PRO:HD3	1.54	0.89
1:I:216:LEU:CG	1:I:295:LEU:HD23	2.02	0.89
1:J:591:ASN:OD1	1:J:592:PRO:CD	2.20	0.89
1:H:591:ASN:HB2	1:H:592:PRO:HD3	1.53	0.89
1:K:865:TRP:NE1	1:K:869:ASN:HD21	1.67	0.89
1:I:216:LEU:HD12	1:I:295:LEU:HD23	1.50	0.89
1:B:591:ASN:HB2	1:B:592:PRO:HD3	1.53	0.88
1:D:591:ASN:HB2	1:D:592:PRO:HD3	1.53	0.88
1:H:592:PRO:HD2	1:H:593:TRP:N	1.89	0.88
1:J:591:ASN:HB2	1:J:592:PRO:HD3	1.53	0.88
1:A:238:TYR:HB3	1:J:117:ARG:NH1	1.89	0.87
1:F:591:ASN:HB2	1:F:592:PRO:HD3	1.54	0.87
1:A:117:ARG:HB2	1:J:238:TYR:CE2	2.03	0.87
1:J:592:PRO:HD2	1:J:593:TRP:N	1.91	0.86
1:K:592:PRO:HD2	1:K:593:TRP:N	1.90	0.86
1:D:238:TYR:HB2	1:G:120:HIS:CD2	2.10	0.86
1:D:120:HIS:CE1	1:G:235:ASP:OD1	2.28	0.85
1:B:147:PRO:HG3	1:B:219:LYS:HB2	1.57	0.85
1:C:592:PRO:HD2	1:C:593:TRP:N	1.89	0.85
1:D:238:TYR:CB	1:G:120:HIS:CD2	2.59	0.85
1:A:592:PRO:HD2	1:A:593:TRP:N	1.91	0.85
1:D:245:LYS:HD3	1:G:245:LYS:HE2	1.58	0.85
1:L:592:PRO:HD2	1:L:593:TRP:N	1.89	0.85
1:D:592:PRO:HD2	1:D:593:TRP:N	1.91	0.85
1:B:592:PRO:HD2	1:B:593:TRP:N	1.89	0.84
1:K:591:ASN:HB2	1:K:592:PRO:HD3	1.59	0.84
1:A:117:ARG:HB2	1:J:238:TYR:OH	1.75	0.84
1:E:592:PRO:HD2	1:E:593:TRP:N	1.90	0.84
1:E:591:ASN:HB2	1:E:592:PRO:HD3	1.59	0.84
1:A:117:ARG:NH1	1:J:238:TYR:HB3	1.93	0.84
1:D:120:HIS:HE1	1:G:235:ASP:OD1	1.61	0.84
1:G:592:PRO:HD2	1:G:593:TRP:N	1.91	0.83
1:K:865:TRP:CG	1:K:869:ASN:ND2	2.48	0.82
1:D:245:LYS:HE2	1:G:245:LYS:CD	2.10	0.81
1:D:120:HIS:CD2	1:G:238:TYR:CB	2.62	0.81
1:A:238:TYR:CE2	1:J:117:ARG:CB	2.62	0.81
1:A:666:LEU:HD21	1:A:705:LEU:HG	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:LEU:HG	1:I:295:LEU:HD23	1.62	0.80
1:G:666:LEU:HD21	1:G:705:LEU:HG	1.63	0.80
1:G:835:LEU:HD21	1:G:884:LEU:CB	2.11	0.80
1:H:305:LYS:O	1:H:309:LEU:HB2	1.81	0.80
1:A:833:ASP:HA	1:A:837:ARG:HG3	1.62	0.80
1:D:245:LYS:HE3	1:G:245:LYS:CE	1.99	0.80
1:I:592:PRO:HD2	1:I:593:TRP:N	1.89	0.80
1:A:591:ASN:HB2	1:A:592:PRO:HD3	1.64	0.80
1:B:305:LYS:O	1:B:309:LEU:HB2	1.81	0.80
1:C:846:SER:H	1:C:906:CYS:HA	1.46	0.79
1:F:591:ASN:CB	1:F:592:PRO:HD3	2.12	0.79
1:E:113:PRO:HG3	1:L:238:TYR:CE1	2.18	0.79
1:G:591:ASN:HB2	1:G:592:PRO:HD3	1.64	0.79
1:L:591:ASN:CB	1:L:592:PRO:HD3	2.12	0.79
1:A:113:PRO:O	1:J:238:TYR:OH	2.02	0.77
1:C:216:LEU:HG	1:C:295:LEU:HD23	1.62	0.77
1:D:238:TYR:CE2	1:G:241:ILE:HD12	2.19	0.77
1:A:117:ARG:CA	1:J:238:TYR:CE2	2.68	0.77
1:G:755:HIS:HB3	1:G:825:THR:HA	1.66	0.76
1:F:592:PRO:HD2	1:F:593:TRP:N	1.89	0.76
1:L:592:PRO:CD	1:L:593:TRP:H	1.97	0.76
1:A:117:ARG:HA	1:J:238:TYR:CE2	2.20	0.76
1:D:238:TYR:CZ	1:G:241:ILE:HD12	2.20	0.76
1:C:591:ASN:CB	1:C:592:PRO:HD3	2.14	0.76
1:D:433:ASP:O	1:D:440:TYR:HA	1.86	0.76
1:A:238:TYR:CD2	1:J:117:ARG:CG	2.62	0.76
1:J:433:ASP:O	1:J:440:TYR:HA	1.86	0.76
1:F:592:PRO:CD	1:F:593:TRP:H	1.97	0.75
1:G:703:SER:O	1:G:706:LYS:HE2	1.86	0.75
1:H:591:ASN:CB	1:H:592:PRO:HD3	2.16	0.75
1:B:591:ASN:CB	1:B:592:PRO:HD3	2.16	0.75
1:A:703:SER:O	1:A:706:LYS:HE2	1.86	0.75
1:I:592:PRO:CD	1:I:593:TRP:H	1.98	0.74
1:C:592:PRO:CD	1:C:593:TRP:H	1.98	0.74
1:G:835:LEU:CD2	1:G:884:LEU:HA	2.18	0.74
1:G:835:LEU:HD21	1:G:884:LEU:CA	2.17	0.74
1:H:837:ARG:NH2	1:H:870:ILE:HD11	2.01	0.74
1:F:591:ASN:OD1	1:F:592:PRO:HD3	1.88	0.74
1:L:591:ASN:OD1	1:L:592:PRO:HD3	1.88	0.74
1:A:25:GLN:NE2	1:F:489:LYS:HD2	2.03	0.74
1:D:238:TYR:OH	1:G:241:ILE:HD12	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:HIS:HA	1:G:242:HIS:CE1	2.23	0.73
1:A:702:THR:HA	1:A:705:LEU:HD13	1.69	0.73
1:B:592:PRO:CD	1:B:593:TRP:H	1.97	0.73
1:H:865:TRP:O	1:H:869:ASN:HB2	1.88	0.73
1:G:25:GLN:NE2	1:L:489:LYS:HD2	2.03	0.73
1:G:702:THR:HA	1:G:705:LEU:HD13	1.69	0.73
1:A:700:LEU:HG	1:A:741:ILE:O	1.89	0.73
1:G:703:SER:O	1:G:706:LYS:HG2	1.89	0.73
1:A:703:SER:O	1:A:706:LYS:HG2	1.89	0.72
1:D:591:ASN:CB	1:D:592:PRO:HD3	2.19	0.72
1:A:238:TYR:CB	1:J:117:ARG:NH1	2.46	0.72
1:B:319:PRO:HD2	1:B:320:LEU:HD22	1.72	0.72
1:B:865:TRP:O	1:B:869:ASN:HB2	1.88	0.72
1:E:592:PRO:CD	1:E:593:TRP:H	1.99	0.72
1:A:117:ARG:CZ	1:J:238:TYR:CB	2.67	0.72
1:J:591:ASN:CB	1:J:592:PRO:HD3	2.19	0.72
1:G:709:VAL:HG11	1:G:753:LEU:HD21	1.71	0.71
1:B:81:LEU:HD21	1:B:216:LEU:HD13	1.72	0.71
1:G:700:LEU:HG	1:G:741:ILE:O	1.89	0.71
1:H:81:LEU:HD11	1:H:216:LEU:HD22	1.71	0.71
1:H:319:PRO:HD2	1:H:320:LEU:HD22	1.72	0.71
1:A:709:VAL:HG11	1:A:753:LEU:HD21	1.71	0.71
1:A:700:LEU:HD22	1:A:744:THR:HG23	1.73	0.71
1:A:592:PRO:CD	1:A:593:TRP:H	2.01	0.71
1:H:592:PRO:CD	1:H:593:TRP:H	1.97	0.70
1:C:615:MET:HA	1:C:618:LEU:HB2	1.73	0.70
1:G:592:PRO:CD	1:G:593:TRP:H	2.01	0.70
1:I:591:ASN:CB	1:I:592:PRO:HD3	2.11	0.70
1:A:750:TRP:HE1	1:A:829:ARG:HG3	1.58	0.69
1:D:238:TYR:HD2	1:G:120:HIS:CD2	2.04	0.69
1:G:700:LEU:HD22	1:G:744:THR:HG23	1.73	0.69
1:D:553:VAL:HG11	1:D:585:VAL:HG12	1.75	0.69
1:H:83:TYR:HB2	1:H:216:LEU:HD21	1.75	0.69
1:G:591:ASN:CB	1:G:592:PRO:HD3	2.22	0.69
1:G:835:LEU:HD21	1:G:884:LEU:HA	1.75	0.69
1:I:615:MET:HA	1:I:618:LEU:HB2	1.74	0.69
1:J:553:VAL:HG11	1:J:585:VAL:HG12	1.75	0.69
1:A:117:ARG:CZ	1:J:238:TYR:HB3	2.23	0.69
1:F:591:ASN:CG	1:F:592:PRO:CD	2.65	0.69
1:K:591:ASN:CB	1:K:592:PRO:HD3	2.22	0.68
1:I:294:MET:SD	1:I:336:ARG:NH1	2.67	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:615:MET:HA	1:D:618:LEU:HB2	1.74	0.68
1:L:591:ASN:CG	1:L:592:PRO:CD	2.65	0.68
1:E:591:ASN:CB	1:E:592:PRO:HD3	2.22	0.68
1:G:25:GLN:NE2	1:L:489:LYS:CD	2.56	0.68
1:A:25:GLN:NE2	1:F:489:LYS:CD	2.56	0.68
1:J:615:MET:HA	1:J:618:LEU:HB2	1.74	0.68
1:J:357:LYS:HE2	1:J:360:LYS:HE2	1.75	0.68
1:K:592:PRO:CD	1:K:593:TRP:H	1.99	0.68
1:B:81:LEU:HD11	1:B:216:LEU:HD22	1.76	0.67
1:A:591:ASN:CB	1:A:592:PRO:HD3	2.23	0.67
1:E:112:PRO:HB2	1:L:238:TYR:OH	1.94	0.67
1:H:597:LEU:O	1:H:601:LEU:HB2	1.95	0.67
1:A:117:ARG:HB2	1:J:238:TYR:HH	1.58	0.67
1:B:597:LEU:O	1:B:601:LEU:HB2	1.95	0.67
1:C:294:MET:SD	1:C:336:ARG:NH1	2.67	0.67
1:D:357:LYS:HE2	1:D:360:LYS:HE2	1.76	0.67
1:G:591:ASN:OD1	1:G:592:PRO:HD3	1.95	0.67
1:H:825:THR:O	1:H:829:ARG:N	2.27	0.67
1:I:653:LEU:HD13	1:I:657:TYR:HB2	1.77	0.67
1:G:835:LEU:CD2	1:G:884:LEU:CA	2.73	0.67
1:C:653:LEU:HD13	1:C:657:TYR:HB2	1.77	0.67
1:J:592:PRO:CD	1:J:593:TRP:H	2.00	0.66
1:H:830:LYS:HD2	1:H:837:ARG:HG2	1.77	0.66
1:E:608:LEU:HD22	1:E:819:PRO:HG2	1.77	0.66
1:L:592:PRO:CD	1:L:593:TRP:N	2.58	0.66
1:I:592:PRO:CD	1:I:593:TRP:N	2.58	0.66
1:B:592:PRO:CD	1:B:593:TRP:N	2.58	0.66
1:C:591:ASN:OD1	1:C:592:PRO:HD3	1.96	0.66
1:E:113:PRO:HG3	1:L:238:TYR:CD1	2.30	0.66
1:F:235:ASP:CG	1:K:117:ARG:CZ	2.68	0.65
1:F:235:ASP:OD2	1:K:117:ARG:NH2	2.28	0.65
1:I:591:ASN:CB	1:I:592:PRO:CD	2.73	0.65
1:D:238:TYR:CG	1:G:120:HIS:CG	2.84	0.65
1:E:592:PRO:CD	1:E:593:TRP:N	2.59	0.65
1:I:216:LEU:CG	1:I:295:LEU:CD2	2.67	0.65
1:A:591:ASN:OD1	1:A:592:PRO:HD3	1.95	0.65
1:G:591:ASN:CG	1:G:592:PRO:CD	2.70	0.65
1:F:592:PRO:CD	1:F:593:TRP:N	2.58	0.65
1:A:702:THR:O	1:A:702:THR:CG2	2.38	0.65
1:F:591:ASN:CB	1:F:592:PRO:CD	2.75	0.64
1:G:592:PRO:CD	1:G:593:TRP:N	2.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:547:ASN:HD21	1:F:550:LEU:HB2	1.62	0.64
1:L:547:ASN:HD21	1:L:550:LEU:HB2	1.63	0.64
1:D:592:PRO:CD	1:D:593:TRP:H	2.00	0.64
1:F:235:ASP:CG	1:K:117:ARG:NH2	2.54	0.64
1:L:591:ASN:CB	1:L:592:PRO:CD	2.75	0.64
1:J:592:PRO:CD	1:J:593:TRP:N	2.60	0.64
1:K:834:THR:HA	1:K:837:ARG:HE	1.63	0.63
1:A:591:ASN:CG	1:A:592:PRO:CD	2.70	0.63
1:D:120:HIS:CE1	1:G:238:TYR:HB2	2.32	0.63
1:D:592:PRO:CD	1:D:593:TRP:N	2.60	0.63
1:D:241:ILE:HG13	1:G:238:TYR:HE2	1.64	0.63
1:H:592:PRO:CD	1:H:593:TRP:N	2.58	0.63
1:A:117:ARG:NH1	1:J:238:TYR:CB	2.61	0.63
1:C:591:ASN:CB	1:C:592:PRO:CD	2.77	0.63
1:F:414:GLU:H	1:F:417:MET:HE3	1.64	0.63
1:A:238:TYR:CE2	1:J:117:ARG:CD	2.67	0.62
1:J:562:THR:OG1	1:J:566:LYS:NZ	2.32	0.62
1:F:561:GLU:HB2	1:F:566:LYS:HZ1	1.63	0.62
1:H:591:ASN:CB	1:H:592:PRO:CD	2.78	0.62
1:L:701:ASN:HB3	1:L:742:ILE:HA	1.81	0.62
1:B:591:ASN:CB	1:B:592:PRO:CD	2.78	0.62
1:D:755:HIS:H	1:D:825:THR:HG22	1.64	0.62
1:J:755:HIS:H	1:J:825:THR:HG22	1.64	0.62
1:C:591:ASN:CG	1:C:592:PRO:CD	2.72	0.62
1:A:182:THR:HG23	1:J:235:ASP:OD2	1.99	0.62
1:L:414:GLU:H	1:L:417:MET:HE3	1.64	0.62
1:E:865:TRP:O	1:E:869:ASN:HB2	2.00	0.61
1:H:745:THR:HB	1:H:832:GLN:HE22	1.64	0.61
1:H:45:LYS:HA	1:H:45:LYS:HE2	1.83	0.61
1:A:555:ASN:HB2	1:A:567:LEU:HD11	1.83	0.61
1:C:550:LEU:O	1:C:624:ARG:NH2	2.34	0.61
1:I:474:SER:OG	1:I:524:LYS:NZ	2.33	0.61
1:F:701:ASN:HB3	1:F:742:ILE:HA	1.81	0.61
1:A:743:ASP:HB3	1:A:832:GLN:HB3	1.82	0.61
1:D:658:ALA:H	1:D:686:ARG:HD3	1.66	0.61
1:C:592:PRO:CD	1:C:593:TRP:N	2.58	0.61
1:E:491:HIS:HD1	1:E:504:TYR:HH	1.48	0.61
1:G:555:ASN:HB2	1:G:567:LEU:HD11	1.83	0.61
1:I:550:LEU:O	1:I:624:ARG:NH2	2.34	0.61
1:D:562:THR:OG1	1:D:566:LYS:NZ	2.32	0.60
1:D:695:ASN:HB2	1:D:696:LYS:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:LEU:HB2	1:B:829:ARG:HH22	1.65	0.60
1:J:658:ALA:H	1:J:686:ARG:HD3	1.66	0.60
1:B:635:LEU:HD21	1:B:828:TYR:HE2	1.65	0.60
1:B:845:GLU:HB2	1:B:922:ILE:HG12	1.82	0.60
1:B:591:ASN:CG	1:B:592:PRO:CD	2.75	0.60
1:E:853:TYR:HB2	1:E:905:GLY:HA3	1.83	0.60
1:A:750:TRP:NE1	1:A:829:ARG:HG3	2.16	0.60
1:A:21:LEU:HD13	1:A:500:ILE:HD11	1.84	0.60
1:A:592:PRO:CD	1:A:593:TRP:N	2.60	0.60
1:C:474:SER:OG	1:C:524:LYS:NZ	2.33	0.60
1:B:698:GLU:HA	1:B:741:ILE:HG23	1.84	0.60
1:J:695:ASN:HB2	1:J:696:LYS:HD2	1.83	0.60
1:A:238:TYR:HB2	1:J:117:ARG:HH11	1.65	0.59
1:B:826:GLU:HA	1:B:829:ARG:HB2	1.84	0.59
1:D:238:TYR:CB	1:G:120:HIS:CE1	2.68	0.59
1:C:376:ARG:HA	1:C:379:MET:HB2	1.84	0.59
1:E:681:MET:SD	1:E:681:MET:N	2.75	0.59
1:H:591:ASN:CG	1:H:592:PRO:CD	2.75	0.59
1:K:853:TYR:HB2	1:K:905:GLY:HA3	1.83	0.59
1:A:698:GLU:HG2	1:A:699:VAL:HG23	1.85	0.59
1:C:839:ILE:HG21	1:C:888:VAL:HG12	1.83	0.59
1:F:865:TRP:O	1:F:869:ASN:HB2	2.03	0.59
1:C:606:PRO:HD2	1:C:759:LYS:HG3	1.85	0.59
1:G:360:LYS:HG3	1:G:363:ASN:H	1.68	0.59
1:G:780:PHE:HA	1:G:784:TYR:HB2	1.84	0.59
1:H:357:LYS:HE3	1:H:362:TRP:H	1.67	0.59
1:A:780:PHE:HA	1:A:784:TYR:HB2	1.84	0.59
1:D:591:ASN:CB	1:D:592:PRO:CD	2.80	0.59
1:D:681:MET:SD	1:D:681:MET:N	2.76	0.59
1:G:21:LEU:HD13	1:G:500:ILE:HD11	1.84	0.59
1:J:591:ASN:CB	1:J:592:PRO:CD	2.80	0.59
1:K:681:MET:SD	1:K:681:MET:N	2.75	0.59
1:I:376:ARG:HA	1:I:379:MET:HB2	1.84	0.59
1:G:698:GLU:HG2	1:G:699:VAL:HG23	1.85	0.59
1:L:865:TRP:O	1:L:869:ASN:HB2	2.02	0.59
1:D:120:HIS:CD2	1:G:238:TYR:CG	2.91	0.58
1:H:591:ASN:OD1	1:H:592:PRO:HD3	2.02	0.58
1:K:435:ASP:N	1:K:435:ASP:OD1	2.36	0.58
1:K:592:PRO:CD	1:K:593:TRP:N	2.59	0.58
1:D:238:TYR:CE2	1:G:241:ILE:CD1	2.87	0.58
1:F:435:ASP:HB3	1:F:541:ILE:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:698:GLU:HA	1:H:741:ILE:HG23	1.84	0.58
1:J:681:MET:SD	1:J:681:MET:N	2.76	0.58
1:G:303:LEU:O	1:G:306:ILE:HB	2.03	0.58
1:A:303:LEU:O	1:A:306:ILE:HB	2.03	0.58
1:I:606:PRO:HD2	1:I:759:LYS:HG3	1.84	0.58
1:B:357:LYS:HE3	1:B:362:TRP:H	1.67	0.58
1:B:536:ARG:HH21	1:B:538:ARG:HD3	1.68	0.58
1:H:536:ARG:HH21	1:H:538:ARG:HD3	1.68	0.58
1:D:238:TYR:HD2	1:G:120:HIS:HD2	1.38	0.58
1:D:801:PHE:HA	1:D:804:LYS:HB2	1.86	0.58
1:E:435:ASP:OD1	1:E:435:ASP:N	2.36	0.58
1:G:608:LEU:HD21	1:G:759:LYS:HG3	1.86	0.58
1:H:521:ASP:OD2	1:I:529:ARG:NH1	2.37	0.58
1:L:619:SER:OG	1:L:620:THR:N	2.36	0.58
1:G:591:ASN:CB	1:G:592:PRO:CD	2.82	0.58
1:G:835:LEU:HD23	1:G:884:LEU:HA	1.85	0.58
1:E:591:ASN:CB	1:E:592:PRO:CD	2.82	0.58
1:K:521:ASP:OD2	1:L:529:ARG:NH1	2.37	0.58
1:K:591:ASN:CB	1:K:592:PRO:CD	2.82	0.58
1:L:435:ASP:HB3	1:L:541:ILE:HG13	1.86	0.58
1:A:25:GLN:HE21	1:F:489:LYS:CD	2.17	0.57
1:B:846:SER:H	1:B:906:CYS:HA	1.68	0.57
1:D:120:HIS:CD2	1:G:238:TYR:CD2	2.91	0.57
1:H:214:SER:O	1:H:215:LYS:C	2.46	0.57
1:A:681:MET:SD	1:A:681:MET:N	2.70	0.57
1:E:754:ARG:HD3	1:E:825:THR:HG21	1.86	0.57
1:H:520:ASN:ND2	1:I:414:GLU:OE2	2.35	0.57
1:J:801:PHE:HA	1:J:804:LYS:HB2	1.86	0.57
1:A:591:ASN:CB	1:A:592:PRO:CD	2.82	0.57
1:H:81:LEU:CD1	1:H:216:LEU:HD22	2.35	0.57
1:L:591:ASN:CG	1:L:592:PRO:HD3	2.26	0.57
1:F:591:ASN:CG	1:F:592:PRO:HD3	2.27	0.57
1:B:521:ASP:OD2	1:C:529:ARG:NH1	2.37	0.57
1:A:360:LYS:HG3	1:A:363:ASN:H	1.68	0.57
1:H:653:LEU:HD13	1:H:657:TYR:HE1	1.70	0.57
1:H:846:SER:H	1:H:906:CYS:HA	1.70	0.57
1:I:681:MET:SD	1:I:681:MET:N	2.77	0.57
1:A:117:ARG:HA	1:J:238:TYR:HE2	1.70	0.57
1:E:709:VAL:O	1:E:752:ARG:NH2	2.38	0.57
1:F:663:ILE:HG12	1:F:695:ASN:HB2	1.87	0.57
1:F:780:PHE:HA	1:F:784:TYR:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:780:PHE:HA	1:L:784:TYR:HB2	1.86	0.57
1:K:709:VAL:O	1:K:752:ARG:NH2	2.38	0.57
1:C:681:MET:SD	1:C:681:MET:N	2.77	0.56
1:E:113:PRO:HG3	1:L:238:TYR:HE1	1.65	0.56
1:J:877:ALA:O	1:J:881:SER:HB3	2.05	0.56
1:G:666:LEU:HD21	1:G:705:LEU:CG	2.35	0.56
1:I:755:HIS:HB3	1:I:825:THR:HA	1.86	0.56
1:A:613:TRP:HD1	1:A:815:LYS:HG2	1.71	0.56
1:A:628:GLU:HG3	1:A:813:ILE:HG12	1.88	0.56
1:E:521:ASP:OD2	1:F:529:ARG:NH1	2.37	0.56
1:E:591:ASN:CG	1:E:592:PRO:CD	2.78	0.56
1:F:619:SER:OG	1:F:620:THR:N	2.36	0.56
1:G:444:GLU:OE2	1:G:450:GLN:NE2	2.39	0.56
1:K:491:HIS:HD1	1:K:504:TYR:HH	1.51	0.56
1:L:307:LEU:HD13	1:L:393:ILE:HD11	1.88	0.56
1:L:663:ILE:HG12	1:L:695:ASN:HB2	1.87	0.56
1:C:660:LYS:HG2	1:C:682:ARG:HH22	1.71	0.56
1:D:235:ASP:OD2	1:G:120:HIS:CE1	2.58	0.56
1:G:628:GLU:HG3	1:G:813:ILE:HG12	1.88	0.56
1:I:660:LYS:HG2	1:I:682:ARG:HH22	1.71	0.56
1:K:591:ASN:CG	1:K:592:PRO:CD	2.78	0.56
1:F:307:LEU:HD13	1:F:393:ILE:HD11	1.88	0.56
1:K:627:LYS:HE3	1:K:730:ALA:HB3	1.88	0.56
1:L:561:GLU:HB2	1:L:566:LYS:HZ1	1.69	0.56
1:A:608:LEU:HD21	1:A:759:LYS:HG3	1.86	0.56
1:C:747:HIS:CD2	1:C:835:LEU:HB3	2.40	0.56
1:E:653:LEU:HD13	1:E:657:TYR:HB2	1.88	0.56
1:G:613:TRP:HD1	1:G:815:LYS:HG2	1.71	0.56
1:B:653:LEU:HD13	1:B:657:TYR:HE1	1.70	0.56
1:H:474:SER:OG	1:H:524:LYS:NZ	2.36	0.56
1:K:331:THR:O	1:K:334:ASN:ND2	2.38	0.56
1:K:429:LYS:NZ	1:K:445:PHE:O	2.39	0.56
1:D:877:ALA:O	1:D:881:SER:HB3	2.05	0.56
1:J:341:TRP:O	1:J:344:GLN:NE2	2.39	0.56
1:J:402:LEU:HD11	1:J:413:LEU:HD21	1.88	0.56
1:L:701:ASN:OD1	1:L:701:ASN:N	2.39	0.56
1:A:707:GLU:HA	1:A:710:ASN:HB3	1.88	0.55
1:D:402:LEU:HD11	1:D:413:LEU:HD21	1.88	0.55
1:D:426:MET:HE3	1:D:429:LYS:HD3	1.88	0.55
1:G:25:GLN:HE21	1:L:489:LYS:CD	2.17	0.55
1:A:444:GLU:OE2	1:A:450:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:LEU:HD21	1:A:705:LEU:CG	2.35	0.55
1:K:591:ASN:OD1	1:K:592:PRO:HD3	2.04	0.55
1:B:750:TRP:CZ2	1:B:829:ARG:HB3	2.41	0.55
1:D:521:ASP:OD2	1:E:529:ARG:NH1	2.40	0.55
1:E:331:THR:O	1:E:334:ASN:ND2	2.38	0.55
1:J:426:MET:HE3	1:J:429:LYS:HD3	1.88	0.55
1:A:431:VAL:HG23	1:A:443:PHE:HB2	1.89	0.55
1:B:655:ASP:O	1:B:686:ARG:NH1	2.40	0.55
1:A:666:LEU:HD12	1:A:704:ARG:HB2	1.89	0.55
1:G:707:GLU:HA	1:G:710:ASN:HB3	1.88	0.55
1:H:301:ARG:O	1:H:301:ARG:NH1	2.38	0.55
1:K:842:ARG:NH1	1:K:910:HIS:O	2.40	0.55
1:B:696:LYS:NZ	1:B:739:ASN:OD1	2.40	0.55
1:J:613:TRP:HB2	1:J:815:LYS:HE2	1.89	0.55
1:D:228:GLU:O	1:D:242:HIS:N	2.39	0.55
1:D:830:LYS:HD3	1:D:837:ARG:HH12	1.72	0.55
1:H:655:ASP:O	1:H:686:ARG:NH1	2.40	0.55
1:I:413:LEU:HD12	1:I:481:MET:HE1	1.87	0.55
1:J:557:VAL:HB	1:J:568:ILE:HB	1.89	0.55
1:A:702:THR:CG2	1:A:745:THR:HG22	2.37	0.55
1:C:413:LEU:HD12	1:C:481:MET:HE1	1.88	0.55
1:C:591:ASN:CG	1:C:592:PRO:HD3	2.32	0.55
1:C:645:LEU:HB3	1:C:646:MET:HE2	1.89	0.55
1:J:521:ASP:OD2	1:K:529:ARG:NH1	2.40	0.55
1:L:679:ALA:N	1:L:681:MET:SD	2.80	0.55
1:K:653:LEU:HD13	1:K:657:TYR:HB2	1.88	0.54
1:C:406:VAL:HG12	1:C:413:LEU:HD21	1.89	0.54
1:D:120:HIS:CE1	1:G:235:ASP:CG	2.85	0.54
1:E:112:PRO:CB	1:L:238:TYR:OH	2.55	0.54
1:E:627:LYS:HE3	1:E:730:ALA:HB3	1.88	0.54
1:G:702:THR:CG2	1:G:745:THR:HG22	2.37	0.54
1:H:83:TYR:HB2	1:H:216:LEU:CD2	2.37	0.54
1:H:376:ARG:NH1	1:H:427:GLY:O	2.40	0.54
1:I:818:CYS:SG	1:I:821:ILE:HB	2.46	0.54
1:K:865:TRP:CD2	1:K:869:ASN:ND2	2.65	0.54
1:L:732:MET:SD	1:L:732:MET:N	2.80	0.54
1:A:580:THR:HG22	1:A:582:ILE:H	1.72	0.54
1:F:558:LEU:HD13	1:F:585:VAL:HG11	1.89	0.54
1:F:611:ARG:HH12	1:F:614:ILE:HG22	1.72	0.54
1:F:701:ASN:OD1	1:F:701:ASN:N	2.39	0.54
1:L:553:VAL:HG21	1:L:585:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:TYR:HB3	1:A:686:ARG:HB3	1.90	0.54
1:E:843:VAL:HG22	1:E:908:ILE:HG22	1.88	0.54
1:F:679:ALA:N	1:F:681:MET:SD	2.80	0.54
1:F:694:THR:OG1	1:F:737:ASN:ND2	2.39	0.54
1:I:645:LEU:HB3	1:I:646:MET:HE2	1.89	0.54
1:L:694:THR:OG1	1:L:737:ASN:ND2	2.39	0.54
1:A:706:LYS:HA	1:A:709:VAL:HG22	1.90	0.54
1:F:746:ASP:OD1	1:F:746:ASP:N	2.40	0.54
1:B:304:HIS:O	1:B:308:ASN:ND2	2.41	0.54
1:B:591:ASN:OD1	1:B:592:PRO:HD3	2.02	0.54
1:F:553:VAL:HG21	1:F:585:VAL:HG12	1.89	0.54
1:H:304:HIS:O	1:H:308:ASN:ND2	2.41	0.54
1:B:301:ARG:NH1	1:B:301:ARG:O	2.38	0.54
1:F:732:MET:SD	1:F:732:MET:N	2.80	0.54
1:G:580:THR:HG22	1:G:582:ILE:H	1.72	0.54
1:G:702:THR:O	1:G:702:THR:CG2	2.38	0.54
1:H:657:TYR:HB3	1:H:686:ARG:HB3	1.89	0.54
1:I:406:VAL:HG12	1:I:413:LEU:HD21	1.89	0.54
1:L:611:ARG:HH12	1:L:614:ILE:HG22	1.72	0.54
1:L:657:TYR:HA	1:L:686:ARG:HG3	1.88	0.54
1:D:655:ASP:OD1	1:D:655:ASP:N	2.41	0.54
1:H:747:HIS:HA	1:H:750:TRP:HB2	1.89	0.54
1:B:757:ARG:O	1:B:759:LYS:NZ	2.41	0.54
1:D:613:TRP:HB2	1:D:815:LYS:HE2	1.89	0.54
1:G:706:LYS:HA	1:G:709:VAL:HG22	1.90	0.54
1:H:435:ASP:HB3	1:H:541:ILE:HG13	1.89	0.54
1:B:376:ARG:NH1	1:B:427:GLY:O	2.40	0.54
1:D:341:TRP:O	1:D:344:GLN:NE2	2.39	0.54
1:G:666:LEU:HD12	1:G:704:ARG:HB2	1.89	0.54
1:B:435:ASP:HB3	1:B:541:ILE:HG13	1.89	0.53
1:E:357:LYS:HD2	1:E:360:LYS:HE3	1.91	0.53
1:C:387:PRO:HG2	1:C:388:GLN:HE21	1.73	0.53
1:D:557:VAL:HB	1:D:568:ILE:HB	1.89	0.53
1:H:696:LYS:NZ	1:H:739:ASN:OD1	2.40	0.53
1:J:509:LYS:O	1:J:513:ARG:NH1	2.41	0.53
1:J:837:ARG:HH21	1:J:841:GLU:HB2	1.74	0.53
1:G:657:TYR:HB3	1:G:686:ARG:HB3	1.90	0.53
1:H:616:PHE:HB3	1:H:812:GLN:HE22	1.74	0.53
1:B:747:HIS:HA	1:B:750:TRP:HB2	1.89	0.53
1:H:757:ARG:O	1:H:759:LYS:NZ	2.41	0.53
1:I:387:PRO:HG2	1:I:388:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:701:ASN:OD1	1:I:744:THR:N	2.41	0.53
1:L:710:ASN:HD22	1:L:752:ARG:HH22	1.55	0.53
1:C:701:ASN:OD1	1:C:744:THR:N	2.41	0.53
1:D:591:ASN:OD1	1:D:592:PRO:HD3	2.08	0.53
1:E:893:LEU:HB3	1:E:901:ARG:HB2	1.90	0.53
1:F:657:TYR:HA	1:F:686:ARG:HG3	1.88	0.53
1:I:640:ASN:HD21	1:I:642:LYS:HD2	1.74	0.53
1:K:893:LEU:HB3	1:K:901:ARG:HB2	1.90	0.53
1:B:832:GLN:HA	1:B:837:ARG:HH21	1.73	0.53
1:D:374:THR:OG1	1:D:573:GLU:OE1	2.27	0.53
1:H:652:VAL:HG13	1:H:653:LEU:HG	1.91	0.53
1:I:557:VAL:HG22	1:I:576:ILE:HD11	1.90	0.53
1:J:830:LYS:HD3	1:J:837:ARG:HH12	1.72	0.53
1:B:652:VAL:HG13	1:B:653:LEU:HG	1.91	0.53
1:D:837:ARG:HH21	1:D:841:GLU:HB2	1.73	0.53
1:E:300:ALA:HA	1:E:303:LEU:HB2	1.91	0.53
1:J:624:ARG:NH1	1:J:657:TYR:OH	2.39	0.53
1:B:657:TYR:HB3	1:B:686:ARG:HB3	1.90	0.53
1:D:509:LYS:O	1:D:513:ARG:NH1	2.41	0.53
1:G:431:VAL:HG23	1:G:443:PHE:HB2	1.89	0.53
1:H:815:LYS:NZ	1:H:816:VAL:O	2.38	0.53
1:C:557:VAL:HG22	1:C:576:ILE:HD11	1.90	0.53
1:F:710:ASN:HD22	1:F:752:ARG:HH22	1.55	0.53
1:I:521:ASP:OD2	1:J:529:ARG:NH1	2.42	0.53
1:J:376:ARG:HH12	1:J:537:GLN:HE22	1.57	0.53
1:K:300:ALA:HA	1:K:303:LEU:HB2	1.91	0.53
1:K:357:LYS:HD2	1:K:360:LYS:HE3	1.91	0.53
1:D:591:ASN:CG	1:D:592:PRO:CD	2.82	0.52
1:D:688:TYR:HE2	1:D:690:TYR:HB3	1.73	0.52
1:G:754:ARG:HA	1:G:825:THR:HG23	1.91	0.52
1:I:83:TYR:HE2	1:I:295:LEU:HD22	1.74	0.52
1:J:701:ASN:HD21	1:J:742:ILE:HA	1.73	0.52
1:J:894:GLN:HE22	1:J:904:LYS:HB3	1.74	0.52
1:L:558:LEU:HD13	1:L:585:VAL:HG11	1.90	0.52
1:L:702:THR:OG1	1:L:706:LYS:NZ	2.41	0.52
1:B:687:GLY:O	1:B:731:THR:OG1	2.27	0.52
1:C:83:TYR:HE2	1:C:295:LEU:HD22	1.74	0.52
1:D:376:ARG:HH12	1:D:537:GLN:HE22	1.58	0.52
1:G:700:LEU:HD23	1:G:743:ASP:H	1.75	0.52
1:H:669:CYS:O	1:H:704:ARG:NH1	2.42	0.52
1:H:687:GLY:O	1:H:731:THR:OG1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:640:ASN:ND2	1:I:758:SER:OG	2.43	0.52
1:J:688:TYR:HE2	1:J:690:TYR:HB3	1.73	0.52
1:A:702:THR:HG23	1:A:745:THR:HG22	1.92	0.52
1:B:520:ASN:ND2	1:C:414:GLU:OE2	2.35	0.52
1:B:815:LYS:NZ	1:B:816:VAL:O	2.38	0.52
1:C:640:ASN:ND2	1:C:758:SER:OG	2.43	0.52
1:D:894:GLN:HE22	1:D:904:LYS:HB3	1.74	0.52
1:L:338:LEU:HD22	1:L:342:PHE:HE2	1.73	0.52
1:B:669:CYS:O	1:B:704:ARG:NH1	2.42	0.52
1:C:521:ASP:OD2	1:D:529:ARG:NH1	2.42	0.52
1:C:640:ASN:HD21	1:C:642:LYS:HD2	1.74	0.52
1:J:619:SER:OG	1:J:620:THR:N	2.42	0.52
1:L:428:ASN:OD1	1:L:428:ASN:N	2.39	0.52
1:L:746:ASP:N	1:L:746:ASP:OD1	2.40	0.52
1:A:737:ASN:OD1	1:A:738:TYR:N	2.43	0.52
1:B:433:ASP:O	1:B:440:TYR:HA	2.10	0.52
1:E:474:SER:OG	1:E:524:LYS:NZ	2.42	0.52
1:J:591:ASN:CG	1:J:592:PRO:CD	2.82	0.52
1:A:646:MET:HE1	1:A:692:GLU:HB2	1.92	0.52
1:D:701:ASN:HD21	1:D:742:ILE:HA	1.73	0.52
1:F:298:PRO:O	1:F:301:ARG:NH1	2.43	0.52
1:F:702:THR:OG1	1:F:706:LYS:NZ	2.41	0.52
1:E:614:ILE:HD11	1:E:821:ILE:HD11	1.91	0.52
1:G:737:ASN:OD1	1:G:738:TYR:N	2.43	0.52
1:H:750:TRP:CE2	1:H:829:ARG:HG3	2.45	0.52
1:A:296:HIS:NE2	1:A:333:ALA:O	2.41	0.52
1:A:700:LEU:HD23	1:A:743:ASP:H	1.75	0.52
1:C:459:LYS:NZ	1:C:556:GLY:O	2.43	0.52
1:F:683:LEU:HB3	1:F:729:THR:HG21	1.92	0.52
1:G:702:THR:HG23	1:G:745:THR:HG22	1.92	0.52
1:J:591:ASN:OD1	1:J:592:PRO:HD3	2.08	0.52
1:B:386:ALA:HB3	1:B:389:GLN:HE21	1.75	0.51
1:C:858:VAL:HG22	1:C:908:ILE:HD11	1.93	0.51
1:H:433:ASP:O	1:H:440:TYR:HA	2.10	0.51
1:K:879:GLU:OE2	1:K:882:GLN:N	2.41	0.51
1:D:619:SER:OG	1:D:620:THR:N	2.42	0.51
1:E:519:PHE:HD1	1:F:416:TYR:HB3	1.75	0.51
1:F:338:LEU:HD22	1:F:342:PHE:HE2	1.73	0.51
1:G:646:MET:HE1	1:G:692:GLU:HB2	1.92	0.51
1:L:683:LEU:HB3	1:L:729:THR:HG21	1.92	0.51
1:B:81:LEU:HD11	1:B:216:LEU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:829:ARG:HD2	1:H:832:GLN:HG2	1.91	0.51
1:B:736:SER:HB2	1:B:741:ILE:HD12	1.92	0.51
1:E:429:LYS:NZ	1:E:445:PHE:O	2.39	0.51
1:L:608:LEU:HD11	1:L:819:PRO:HG2	1.91	0.51
1:D:227:PHE:HB3	1:D:241:ILE:HG22	1.92	0.51
1:D:667:THR:HG22	1:D:701:ASN:HB3	1.92	0.51
1:F:632:LEU:HB3	1:F:733:VAL:HG12	1.92	0.51
1:I:657:TYR:HA	1:I:686:ARG:HG3	1.93	0.51
1:J:667:THR:HG22	1:J:701:ASN:HB3	1.92	0.51
1:K:634:TRP:HH2	1:K:645:LEU:HD12	1.76	0.51
1:E:703:SER:O	1:E:706:LYS:NZ	2.44	0.51
1:K:352:THR:OG1	1:K:353:GLY:N	2.44	0.51
1:A:657:TYR:HA	1:A:686:ARG:HD3	1.93	0.51
1:B:616:PHE:HB3	1:B:812:GLN:HE22	1.74	0.51
1:E:352:THR:OG1	1:E:353:GLY:N	2.44	0.51
1:E:743:ASP:OD1	1:E:743:ASP:N	2.42	0.51
1:F:327:ALA:HB1	1:F:378:ILE:HD11	1.93	0.51
1:F:435:ASP:N	1:F:435:ASP:OD1	2.43	0.51
1:K:519:PHE:HD1	1:L:416:TYR:HB3	1.75	0.51
1:K:743:ASP:N	1:K:743:ASP:OD1	2.42	0.51
1:A:709:VAL:HG11	1:A:753:LEU:CD2	2.39	0.51
1:C:657:TYR:HA	1:C:686:ARG:HG3	1.93	0.51
1:F:608:LEU:HD11	1:F:819:PRO:HG2	1.91	0.51
1:I:459:LYS:NZ	1:I:556:GLY:O	2.43	0.51
1:L:298:PRO:O	1:L:301:ARG:NH1	2.43	0.51
1:F:804:LYS:HA	1:F:807:LYS:HE3	1.93	0.51
1:H:591:ASN:CG	1:H:592:PRO:HD3	2.36	0.51
1:K:909:LEU:HD22	1:K:913:GLU:HB2	1.92	0.51
1:E:909:LEU:HD22	1:E:913:GLU:HB2	1.92	0.51
1:H:646:MET:HE1	1:H:692:GLU:HB2	1.93	0.51
1:I:858:VAL:HG22	1:I:908:ILE:HD11	1.93	0.51
1:J:804:LYS:HD2	1:J:807:LYS:HZ1	1.76	0.51
1:K:623:PHE:HB3	1:K:627:LYS:HD3	1.93	0.51
1:L:632:LEU:HB3	1:L:733:VAL:HG12	1.93	0.51
1:A:238:TYR:CE2	1:J:117:ARG:HA	2.46	0.50
1:E:634:TRP:HH2	1:E:645:LEU:HD12	1.76	0.50
1:E:710:ASN:HA	1:E:752:ARG:HH22	1.76	0.50
1:J:374:THR:OG1	1:J:573:GLU:OE1	2.27	0.50
1:J:655:ASP:OD1	1:J:655:ASP:N	2.41	0.50
1:L:455:GLY:O	1:L:459:LYS:NZ	2.44	0.50
1:F:95:MET:HB2	1:F:258:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:638:GLY:HA2	1:I:738:TYR:HD2	1.77	0.50
1:I:698:GLU:HA	1:I:741:ILE:HA	1.93	0.50
1:I:543:THR:O	1:I:543:THR:OG1	2.29	0.50
1:D:239:ILE:HD12	1:G:237:ASP:O	2.11	0.50
1:E:95:MET:HB2	1:E:258:LEU:HD11	1.94	0.50
1:H:386:ALA:HB3	1:H:389:GLN:HE21	1.75	0.50
1:D:305:LYS:O	1:D:309:LEU:HB2	2.11	0.50
1:G:95:MET:HB2	1:G:258:LEU:HD11	1.94	0.50
1:H:435:ASP:N	1:H:435:ASP:OD1	2.43	0.50
1:D:95:MET:HB2	1:D:258:LEU:HD11	1.94	0.50
1:G:709:VAL:HG11	1:G:753:LEU:CD2	2.39	0.50
1:I:95:MET:HB2	1:I:258:LEU:HD11	1.94	0.50
1:K:703:SER:O	1:K:706:LYS:NZ	2.44	0.50
1:L:548:PRO:HB3	1:L:624:ARG:H	1.77	0.50
1:B:435:ASP:OD1	1:B:435:ASP:N	2.43	0.50
1:C:95:MET:HB2	1:C:258:LEU:HD11	1.94	0.50
1:H:736:SER:HB2	1:H:741:ILE:HD12	1.92	0.50
1:J:305:LYS:O	1:J:309:LEU:HB2	2.11	0.50
1:L:95:MET:HB2	1:L:258:LEU:HD11	1.94	0.50
1:B:835:LEU:O	1:B:836:HIS:C	2.54	0.50
1:C:352:THR:OG1	1:C:353:GLY:N	2.45	0.50
1:E:623:PHE:HB3	1:E:627:LYS:HD3	1.94	0.50
1:F:548:PRO:HB3	1:F:624:ARG:H	1.77	0.50
1:I:352:THR:OG1	1:I:353:GLY:N	2.45	0.50
1:I:516:SER:HB3	1:J:412:MET:HE2	1.94	0.50
1:L:435:ASP:OD1	1:L:435:ASP:N	2.43	0.50
1:H:837:ARG:HH22	1:H:870:ILE:HD11	1.76	0.50
1:A:834:THR:HG22	1:A:835:LEU:H	1.76	0.49
1:B:95:MET:HB2	1:B:258:LEU:HD11	1.94	0.49
1:D:120:HIS:CG	1:G:238:TYR:HB2	2.43	0.49
1:G:435:ASP:HB3	1:G:541:ILE:HG13	1.93	0.49
1:J:666:LEU:O	1:J:703:SER:OG	2.24	0.49
1:L:327:ALA:HB1	1:L:378:ILE:HD11	1.93	0.49
1:K:651:MET:HG3	1:K:785:ILE:HD11	1.94	0.49
1:A:440:TYR:OH	1:F:467:ASP:OD1	2.28	0.49
1:C:638:GLY:HA2	1:C:738:TYR:HD2	1.77	0.49
1:C:644:PHE:HB2	1:C:781:ILE:HG22	1.94	0.49
1:F:455:GLY:O	1:F:459:LYS:NZ	2.44	0.49
1:K:710:ASN:HA	1:K:752:ARG:HH22	1.76	0.49
1:B:318:TYR:O	1:B:321:TRP:NE1	2.44	0.49
1:B:608:LEU:HD13	1:B:819:PRO:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:MET:HE1	1:B:692:GLU:HB2	1.93	0.49
1:C:823:SER:O	1:C:826:GLU:HG2	2.11	0.49
1:D:737:ASN:ND2	1:D:739:ASN:OD1	2.45	0.49
1:E:651:MET:HG3	1:E:785:ILE:HD11	1.94	0.49
1:A:435:ASP:HB3	1:A:541:ILE:HG13	1.93	0.49
1:B:320:LEU:HA	1:B:323:ASN:HB2	1.95	0.49
1:C:552:GLY:O	1:C:580:THR:N	2.43	0.49
1:J:737:ASN:ND2	1:J:739:ASN:OD1	2.45	0.49
1:B:215:LYS:O	1:B:216:LEU:C	2.56	0.49
1:G:657:TYR:HA	1:G:686:ARG:HD3	1.93	0.49
1:G:833:ASP:HA	1:G:837:ARG:HD3	1.94	0.49
1:H:215:LYS:O	1:H:218:HIS:N	2.43	0.49
1:H:608:LEU:HD13	1:H:819:PRO:HG2	1.95	0.49
1:A:829:ARG:O	1:A:832:GLN:HG3	2.13	0.49
1:C:516:SER:HB3	1:D:412:MET:HE2	1.94	0.49
1:D:853:TYR:HB2	1:D:903:LEU:HB2	1.95	0.49
1:B:81:LEU:HD11	1:B:216:LEU:CB	2.43	0.49
1:B:147:PRO:CG	1:B:219:LYS:HB2	2.36	0.49
1:J:95:MET:HB2	1:J:258:LEU:HD11	1.94	0.49
1:A:668:SER:O	1:A:704:ARG:HD2	2.13	0.49
1:C:83:TYR:CE2	1:C:295:LEU:HD22	2.48	0.49
1:G:652:VAL:HA	1:G:791:GLN:HG2	1.95	0.49
1:K:360:LYS:NZ	1:K:363:ASN:OD1	2.46	0.49
1:L:325:VAL:HG23	1:L:338:LEU:HD21	1.95	0.49
1:K:750:TRP:HB3	1:K:753:LEU:HD13	1.94	0.49
1:E:750:TRP:HB3	1:E:753:LEU:HD13	1.94	0.48
1:G:591:ASN:CG	1:G:592:PRO:HD3	2.37	0.48
1:G:750:TRP:CD1	1:G:829:ARG:HE	2.31	0.48
1:A:95:MET:HB2	1:A:258:LEU:HD11	1.94	0.48
1:B:664:SER:O	1:B:668:SER:OG	2.29	0.48
1:C:698:GLU:HA	1:C:741:ILE:HA	1.93	0.48
1:D:602:GLN:HG3	1:D:942:TRP:HE1	1.78	0.48
1:E:591:ASN:OD1	1:E:592:PRO:HD3	2.04	0.48
1:G:125:HIS:HE1	1:G:180:ASP:OD2	1.97	0.48
1:H:81:LEU:HD11	1:H:216:LEU:HB3	1.94	0.48
1:I:613:TRP:CE3	1:I:821:ILE:HG12	2.48	0.48
1:L:804:LYS:HA	1:L:807:LYS:HE3	1.93	0.48
1:B:755:HIS:CD2	1:B:828:TYR:HD2	2.32	0.48
1:C:819:PRO:O	1:C:822:GLU:HG3	2.13	0.48
1:D:624:ARG:NH1	1:D:657:TYR:OH	2.39	0.48
1:E:113:PRO:CG	1:L:238:TYR:CE1	2.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:TRP:O	1:E:366:SER:OG	2.30	0.48
1:G:296:HIS:NE2	1:G:333:ALA:O	2.41	0.48
1:G:336:ARG:NH1	1:G:340:GLU:OE1	2.44	0.48
1:H:95:MET:HB2	1:H:258:LEU:HD11	1.94	0.48
1:H:750:TRP:CZ2	1:H:829:ARG:HB3	2.48	0.48
1:G:751:ARG:O	1:G:754:ARG:NH2	2.46	0.48
1:H:320:LEU:HA	1:H:323:ASN:HB2	1.94	0.48
1:H:686:ARG:O	1:H:729:THR:OG1	2.31	0.48
1:H:695:ASN:HD22	1:I:706:LYS:HE2	1.78	0.48
1:I:823:SER:O	1:I:826:GLU:HG2	2.12	0.48
1:K:95:MET:HB2	1:K:258:LEU:HD11	1.94	0.48
1:C:835:LEU:HD21	1:C:884:LEU:HA	1.95	0.48
1:D:235:ASP:OD1	1:G:120:HIS:HE1	1.96	0.48
1:I:644:PHE:HB2	1:I:781:ILE:HG22	1.94	0.48
1:K:125:HIS:HE1	1:K:180:ASP:OD2	1.97	0.48
1:K:386:ALA:HB1	1:K:389:GLN:HB2	1.95	0.48
1:B:828:TYR:O	1:B:833:ASP:HB2	2.13	0.48
1:C:623:PHE:HB3	1:C:627:LYS:HE2	1.96	0.48
1:E:360:LYS:NZ	1:E:363:ASN:OD1	2.46	0.48
1:G:668:SER:O	1:G:704:ARG:HD2	2.13	0.48
1:H:125:HIS:HE1	1:H:180:ASP:OD2	1.97	0.48
1:H:634:TRP:HH2	1:H:645:LEU:HD23	1.79	0.48
1:I:83:TYR:CE2	1:I:295:LEU:HD22	2.48	0.48
1:A:125:HIS:HE1	1:A:180:ASP:OD2	1.97	0.48
1:A:666:LEU:CD1	1:A:704:ARG:HB2	2.44	0.48
1:B:695:ASN:HD22	1:C:706:LYS:HE2	1.78	0.48
1:E:402:LEU:HD13	1:E:421:VAL:HG21	1.96	0.48
1:F:325:VAL:HG23	1:F:338:LEU:HD21	1.95	0.48
1:I:125:HIS:HE1	1:I:180:ASP:OD2	1.97	0.48
1:I:552:GLY:O	1:I:580:THR:N	2.43	0.48
1:I:819:PRO:O	1:I:822:GLU:HG3	2.14	0.48
1:K:658:ALA:O	1:K:686:ARG:NH1	2.46	0.48
1:F:376:ARG:HA	1:F:379:MET:HE1	1.96	0.48
1:G:440:TYR:OH	1:L:467:ASP:OD1	2.28	0.48
1:I:701:ASN:HB3	1:I:742:ILE:HB	1.96	0.48
1:J:602:GLN:HG3	1:J:942:TRP:HE1	1.78	0.48
1:L:125:HIS:HE1	1:L:180:ASP:OD2	1.97	0.48
1:A:653:LEU:HD11	1:A:657:TYR:HE1	1.79	0.48
1:B:125:HIS:HE1	1:B:180:ASP:OD2	1.96	0.48
1:C:826:GLU:O	1:C:830:LYS:N	2.40	0.48
1:E:427:GLY:HA2	1:E:535:PHE:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:383:HIS:HA	1:G:387:PRO:HA	1.96	0.48
1:I:623:PHE:HB3	1:I:627:LYS:HE2	1.96	0.48
1:K:339:ALA:O	1:K:343:SER:OG	2.25	0.48
1:B:216:LEU:HG	1:B:295:LEU:HD23	1.96	0.47
1:B:591:ASN:CG	1:B:592:PRO:HD3	2.36	0.47
1:C:634:TRP:HB3	1:C:735:ALA:HB2	1.96	0.47
1:G:681:MET:HA	1:G:684:LYS:HG2	1.96	0.47
1:H:481:MET:HB3	1:H:515:LYS:HD2	1.96	0.47
1:H:750:TRP:CZ2	1:H:829:ARG:HG3	2.49	0.47
1:I:755:HIS:ND1	1:I:828:TYR:HB2	2.29	0.47
1:J:125:HIS:HE1	1:J:180:ASP:OD2	1.97	0.47
1:K:882:GLN:O	1:K:886:ASN:ND2	2.46	0.47
1:L:683:LEU:HD13	1:L:686:ARG:HB3	1.96	0.47
1:A:25:GLN:NE2	1:F:489:LYS:HD3	2.29	0.47
1:A:383:HIS:HA	1:A:387:PRO:HA	1.96	0.47
1:A:433:ASP:O	1:A:440:TYR:HA	2.15	0.47
1:E:112:PRO:HB2	1:L:238:TYR:CZ	2.49	0.47
1:E:339:ALA:O	1:E:343:SER:OG	2.25	0.47
1:E:658:ALA:O	1:E:686:ARG:NH1	2.47	0.47
1:G:636:GLY:HA3	1:G:757:ARG:HG2	1.96	0.47
1:J:304:HIS:O	1:J:308:ASN:ND2	2.46	0.47
1:K:362:TRP:O	1:K:366:SER:OG	2.30	0.47
1:A:652:VAL:HA	1:A:791:GLN:HG2	1.95	0.47
1:F:683:LEU:HD13	1:F:686:ARG:HB3	1.96	0.47
1:G:25:GLN:NE2	1:L:489:LYS:HD3	2.29	0.47
1:A:322:SER:HB2	1:A:326:PHE:HE1	1.80	0.47
1:A:416:TYR:HB3	1:F:519:PHE:HD2	1.79	0.47
1:B:429:LYS:NZ	1:B:445:PHE:O	2.47	0.47
1:D:125:HIS:HE1	1:D:180:ASP:OD2	1.97	0.47
1:D:304:HIS:O	1:D:308:ASN:ND2	2.47	0.47
1:E:879:GLU:OE2	1:E:882:GLN:N	2.41	0.47
1:F:125:HIS:HE1	1:F:180:ASP:OD2	1.97	0.47
1:G:322:SER:HB2	1:G:326:PHE:HE1	1.80	0.47
1:H:854:ASN:HA	1:H:902:ILE:HG22	1.95	0.47
1:K:304:HIS:O	1:K:308:ASN:ND2	2.47	0.47
1:K:402:LEU:HD13	1:K:421:VAL:HG21	1.96	0.47
1:A:519:PHE:HD1	1:B:416:TYR:HB3	1.80	0.47
1:B:846:SER:HB3	1:B:907:ARG:HB3	1.96	0.47
1:C:125:HIS:HE1	1:C:180:ASP:OD2	1.97	0.47
1:C:459:LYS:NZ	1:C:553:VAL:O	2.45	0.47
1:C:701:ASN:HB3	1:C:742:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:882:GLN:O	1:E:886:ASN:ND2	2.46	0.47
1:G:520:ASN:ND2	1:H:414:GLU:OE1	2.38	0.47
1:H:543:THR:O	1:H:543:THR:OG1	2.31	0.47
1:A:636:GLY:HA3	1:A:757:ARG:HG2	1.96	0.47
1:B:657:TYR:HA	1:B:686:ARG:HD3	1.97	0.47
1:C:428:ASN:OD1	1:C:428:ASN:N	2.45	0.47
1:E:619:SER:OG	1:E:620:THR:N	2.48	0.47
1:G:331:THR:HG22	1:G:333:ALA:H	1.78	0.47
1:I:694:THR:HG21	1:I:737:ASN:HD22	1.79	0.47
1:K:427:GLY:HA2	1:K:535:PHE:HE1	1.78	0.47
1:L:376:ARG:HA	1:L:379:MET:HE1	1.95	0.47
1:A:331:THR:HG22	1:A:333:ALA:H	1.78	0.47
1:A:391:LYS:O	1:A:395:GLU:HG3	2.15	0.47
1:A:681:MET:HA	1:A:684:LYS:HG2	1.96	0.47
1:A:751:ARG:O	1:A:754:ARG:NH2	2.46	0.47
1:B:854:ASN:HA	1:B:902:ILE:HG22	1.95	0.47
1:C:665:LEU:HD21	1:C:679:ALA:HA	1.97	0.47
1:E:304:HIS:O	1:E:308:ASN:ND2	2.47	0.47
1:E:557:VAL:HG22	1:E:576:ILE:HD11	1.97	0.47
1:G:844:VAL:HG13	1:G:907:ARG:HB3	1.95	0.47
1:H:591:ASN:HB2	1:H:592:PRO:CD	2.34	0.47
1:H:828:TYR:O	1:H:832:GLN:N	2.47	0.47
1:J:853:TYR:HB2	1:J:903:LEU:HB2	1.95	0.47
1:A:815:LYS:HA	1:A:815:LYS:HD3	1.79	0.47
1:B:543:THR:O	1:B:543:THR:OG1	2.30	0.47
1:E:125:HIS:HE1	1:E:180:ASP:OD2	1.97	0.47
1:F:559:SER:HB3	1:F:566:LYS:HB2	1.96	0.47
1:F:841:GLU:HG3	1:F:842:ARG:HG2	1.96	0.47
1:G:519:PHE:HD1	1:H:416:TYR:HB3	1.80	0.47
1:H:828:TYR:O	1:H:832:GLN:HB3	2.15	0.47
1:K:619:SER:OG	1:K:620:THR:N	2.48	0.47
1:B:215:LYS:O	1:B:218:HIS:N	2.48	0.47
1:E:586:PRO:HD3	1:E:792:ASN:HB3	1.97	0.47
1:G:433:ASP:O	1:G:440:TYR:HA	2.15	0.47
1:I:634:TRP:HB3	1:I:735:ALA:HB2	1.96	0.47
1:L:559:SER:HB3	1:L:566:LYS:HB2	1.96	0.47
1:A:371:LYS:HA	1:A:371:LYS:HD2	1.69	0.47
1:C:619:SER:OG	1:C:620:THR:N	2.48	0.47
1:E:386:ALA:HB1	1:E:389:GLN:HB2	1.95	0.47
1:F:428:ASN:OD1	1:F:428:ASN:N	2.39	0.47
1:F:623:PHE:HB3	1:F:627:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:653:LEU:HD11	1:G:657:TYR:HE1	1.79	0.47
1:H:429:LYS:NZ	1:H:445:PHE:O	2.47	0.47
1:H:470:HIS:O	1:H:524:LYS:NZ	2.35	0.47
1:L:339:ALA:O	1:L:343:SER:OG	2.30	0.47
1:A:398:TYR:CE2	1:A:425:MET:HG2	2.50	0.46
1:A:837:ARG:HE	1:A:837:ARG:HA	1.79	0.46
1:B:481:MET:HB3	1:B:515:LYS:HD2	1.97	0.46
1:E:615:MET:HA	1:E:618:LEU:HG	1.97	0.46
1:F:557:VAL:O	1:F:568:ILE:N	2.48	0.46
1:F:651:MET:SD	1:F:651:MET:N	2.88	0.46
1:G:775:LYS:HA	1:G:775:LYS:HD2	1.77	0.46
1:H:694:THR:O	1:H:694:THR:OG1	2.33	0.46
1:K:615:MET:HA	1:K:618:LEU:HG	1.97	0.46
1:L:841:GLU:HG3	1:L:842:ARG:HG2	1.96	0.46
1:A:367:HIS:ND1	1:A:368:HIS:O	2.48	0.46
1:B:634:TRP:HH2	1:B:645:LEU:HD23	1.79	0.46
1:C:591:ASN:HB2	1:C:592:PRO:CD	2.35	0.46
1:C:694:THR:HG21	1:C:737:ASN:HD22	1.79	0.46
1:F:615:MET:HA	1:F:618:LEU:HB2	1.97	0.46
1:G:666:LEU:CD1	1:G:704:ARG:HB2	2.44	0.46
1:H:318:TYR:O	1:H:321:TRP:NE1	2.44	0.46
1:I:619:SER:OG	1:I:620:THR:N	2.48	0.46
1:J:311:PRO:HG3	1:J:389:GLN:HE22	1.80	0.46
1:B:702:THR:OG1	1:B:703:SER:N	2.48	0.46
1:E:624:ARG:HG3	1:E:657:TYR:HE1	1.80	0.46
1:I:595:LYS:HD2	1:I:595:LYS:HA	1.78	0.46
1:I:665:LEU:HD21	1:I:679:ALA:HA	1.97	0.46
1:C:835:LEU:O	1:C:839:ILE:HG13	2.15	0.46
1:D:941:LYS:HA	1:D:941:LYS:HD3	1.83	0.46
1:H:604:ILE:HD12	1:H:605:ILE:HG23	1.97	0.46
1:B:604:ILE:HD12	1:B:605:ILE:HG23	1.97	0.46
1:C:216:LEU:CG	1:C:295:LEU:CD2	2.67	0.46
1:C:828:TYR:O	1:C:831:SER:HB3	2.15	0.46
1:D:589:PRO:HB2	1:D:591:ASN:HD22	1.80	0.46
1:F:454:GLN:HB3	1:F:581:HIS:HB2	1.98	0.46
1:G:416:TYR:HB3	1:L:519:PHE:HD2	1.79	0.46
1:H:657:TYR:HA	1:H:686:ARG:HD3	1.97	0.46
1:J:589:PRO:HB2	1:J:591:ASN:HD22	1.80	0.46
1:K:826:GLU:O	1:K:830:LYS:HG2	2.16	0.46
1:C:675:LYS:HD3	1:C:704:ARG:HD2	1.97	0.46
1:E:627:LYS:HB2	1:E:730:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:303:LEU:O	1:I:307:LEU:HD12	2.16	0.46
1:J:846:SER:H	1:J:906:CYS:HA	1.81	0.46
1:J:941:LYS:HA	1:J:941:LYS:HD3	1.83	0.46
1:B:698:GLU:OE2	1:B:739:ASN:ND2	2.45	0.46
1:B:836:HIS:O	1:B:837:ARG:C	2.58	0.46
1:E:383:HIS:HA	1:E:387:PRO:HA	1.98	0.46
1:E:536:ARG:HD2	1:E:536:ARG:HA	1.77	0.46
1:K:433:ASP:O	1:K:440:TYR:HA	2.16	0.46
1:K:586:PRO:HD3	1:K:792:ASN:HB3	1.97	0.46
1:K:624:ARG:HG3	1:K:657:TYR:HE1	1.80	0.46
1:L:557:VAL:O	1:L:568:ILE:N	2.48	0.46
1:L:623:PHE:HB3	1:L:627:LYS:HE2	1.97	0.46
1:L:742:ILE:O	1:L:828:TYR:OH	2.30	0.46
1:C:551:LEU:HD11	1:C:657:TYR:HE1	1.81	0.46
1:D:649:VAL:HG23	1:D:798:LEU:HD11	1.97	0.46
1:D:846:SER:H	1:D:906:CYS:HA	1.81	0.46
1:E:838:PHE:HB2	1:E:865:TRP:CZ3	2.51	0.46
1:H:586:PRO:HG3	1:H:792:ASN:HB3	1.97	0.46
1:B:591:ASN:HB2	1:B:592:PRO:CD	2.35	0.46
1:C:609:ASP:OD1	1:C:937:GLU:N	2.49	0.46
1:C:740:PHE:HZ	1:C:757:ARG:HH21	1.64	0.46
1:G:369:THR:OG1	1:G:370:GLU:N	2.48	0.46
1:G:391:LYS:O	1:G:395:GLU:HG3	2.15	0.46
1:L:651:MET:SD	1:L:651:MET:N	2.88	0.46
1:D:311:PRO:HG3	1:D:389:GLN:HE22	1.80	0.46
1:I:458:TRP:O	1:I:572:HIS:NE2	2.47	0.46
1:I:755:HIS:CG	1:I:828:TYR:HB2	2.51	0.46
1:L:452:MET:HE3	1:L:452:MET:HB3	1.81	0.46
1:L:557:VAL:HG22	1:L:576:ILE:HD11	1.98	0.46
1:L:560:ILE:HB	1:L:802:TRP:HE1	1.81	0.46
1:A:378:ILE:HD12	1:A:378:ILE:H	1.81	0.45
1:B:214:SER:O	1:B:215:LYS:C	2.58	0.45
1:B:586:PRO:HG3	1:B:792:ASN:HB3	1.97	0.45
1:C:303:LEU:O	1:C:307:LEU:HD12	2.16	0.45
1:D:536:ARG:HD2	1:D:536:ARG:HA	1.75	0.45
1:F:457:ILE:H	1:F:459:LYS:HZ2	1.65	0.45
1:G:681:MET:SD	1:G:681:MET:N	2.71	0.45
1:H:618:LEU:HD23	1:H:618:LEU:HA	1.83	0.45
1:H:839:ILE:O	1:H:843:VAL:HB	2.16	0.45
1:I:609:ASP:OD1	1:I:937:GLU:N	2.49	0.45
1:I:675:LYS:HD3	1:I:704:ARG:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:557:VAL:HG22	1:K:576:ILE:HD11	1.97	0.45
1:A:369:THR:OG1	1:A:370:GLU:N	2.48	0.45
1:A:836:HIS:O	1:A:840:THR:HG23	2.16	0.45
1:B:357:LYS:HB2	1:B:357:LYS:HE2	1.75	0.45
1:C:813:ILE:HD12	1:C:813:ILE:H	1.82	0.45
1:G:398:TYR:CE2	1:G:425:MET:HG2	2.50	0.45
1:G:754:ARG:HA	1:G:825:THR:CG2	2.47	0.45
1:L:457:ILE:H	1:L:459:LYS:HZ2	1.64	0.45
1:A:238:TYR:CE2	1:J:117:ARG:CA	3.00	0.45
1:A:362:TRP:O	1:A:366:SER:OG	2.32	0.45
1:F:682:ARG:O	1:F:686:ARG:NH1	2.49	0.45
1:I:475:GLU:OE1	1:J:420:LYS:NZ	2.36	0.45
1:I:813:ILE:HD12	1:I:813:ILE:H	1.82	0.45
1:J:694:THR:OG1	1:J:737:ASN:ND2	2.50	0.45
1:L:454:GLN:HB3	1:L:581:HIS:HB2	1.98	0.45
1:B:45:LYS:HD3	1:B:45:LYS:HA	1.86	0.45
1:H:566:LYS:HD3	1:H:566:LYS:HA	1.82	0.45
1:I:681:MET:HA	1:I:684:LYS:HB2	1.98	0.45
1:J:649:VAL:HG23	1:J:798:LEU:HD11	1.98	0.45
1:K:627:LYS:HB2	1:K:730:ALA:HB3	1.98	0.45
1:K:757:ARG:NE	1:K:824:GLU:OE1	2.50	0.45
1:L:706:LYS:HA	1:L:709:VAL:HG22	1.97	0.45
1:B:834:THR:HG22	1:B:835:LEU:H	1.80	0.45
1:I:551:LEU:HD11	1:I:657:TYR:HE1	1.80	0.45
1:K:383:HIS:HA	1:K:387:PRO:HA	1.98	0.45
1:L:615:MET:HA	1:L:618:LEU:HB2	1.98	0.45
1:A:787:ASP:OD2	1:A:790:CYS:N	2.46	0.45
1:B:686:ARG:O	1:B:729:THR:OG1	2.31	0.45
1:D:228:GLU:O	1:D:241:ILE:HA	2.17	0.45
1:F:303:LEU:HA	1:F:306:ILE:HD12	1.98	0.45
1:J:591:ASN:HB2	1:J:592:PRO:CD	2.35	0.45
1:A:538:ARG:HE	1:A:538:ARG:HB3	1.51	0.45
1:A:684:LYS:HD2	1:A:684:LYS:HA	1.69	0.45
1:C:412:MET:HE2	1:C:412:MET:HB3	1.91	0.45
1:I:829:ARG:O	1:I:833:ASP:HB3	2.16	0.45
1:J:536:ARG:HD2	1:J:536:ARG:HA	1.75	0.45
1:J:551:LEU:HD11	1:J:657:TYR:HE2	1.81	0.45
1:K:835:LEU:HD11	1:K:883:GLU:HB3	1.99	0.45
1:B:740:PHE:HE2	1:B:831:SER:HG	1.63	0.45
1:E:433:ASP:O	1:E:440:TYR:HA	2.16	0.45
1:G:797:ILE:HD12	1:G:797:ILE:HA	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:740:PHE:HZ	1:I:757:ARG:HH21	1.64	0.45
1:J:834:THR:OG1	1:J:835:LEU:N	2.44	0.45
1:K:608:LEU:HD22	1:K:819:PRO:HG2	1.99	0.45
1:A:25:GLN:HE21	1:F:489:LYS:HD3	1.82	0.45
1:E:842:ARG:HG3	1:E:865:TRP:CD1	2.52	0.45
1:F:557:VAL:HG22	1:F:576:ILE:HD11	1.98	0.45
1:G:702:THR:HG21	1:G:744:THR:O	2.17	0.45
1:H:940:ASN:ND2	1:H:944:GLU:OE2	2.50	0.45
1:I:459:LYS:NZ	1:I:553:VAL:O	2.45	0.45
1:I:839:ILE:HG22	1:I:922:ILE:HG21	1.99	0.45
1:J:318:TYR:CG	1:J:319:PRO:HD3	2.52	0.45
1:K:536:ARG:HD2	1:K:536:ARG:HA	1.77	0.45
1:A:380:TYR:HB2	1:A:571:PHE:HD2	1.82	0.45
1:D:551:LEU:HD11	1:D:657:TYR:HE2	1.81	0.45
1:F:704:ARG:O	1:F:707:GLU:HG3	2.17	0.45
1:L:682:ARG:O	1:L:686:ARG:NH1	2.49	0.45
1:A:339:ALA:O	1:A:343:SER:OG	2.35	0.44
1:B:379:MET:SD	1:B:379:MET:N	2.91	0.44
1:C:617:TYR:HA	1:C:812:GLN:HE22	1.83	0.44
1:E:506:LYS:HA	1:E:506:LYS:HD3	1.80	0.44
1:E:828:TYR:O	1:E:832:GLN:N	2.46	0.44
1:A:318:TYR:HB2	1:A:319:PRO:HD3	1.99	0.44
1:B:506:LYS:HA	1:B:509:LYS:HG2	1.99	0.44
1:B:611:ARG:HD3	1:B:820:THR:OG1	2.17	0.44
1:E:328:LEU:HD13	1:E:334:ASN:HB2	2.00	0.44
1:F:458:TRP:NE1	1:F:569:ASN:OD1	2.50	0.44
1:F:560:ILE:HB	1:F:802:TRP:HE1	1.81	0.44
1:F:706:LYS:HA	1:F:709:VAL:HG22	1.97	0.44
1:G:320:LEU:HD23	1:G:323:ASN:HD21	1.82	0.44
1:G:362:TRP:O	1:G:366:SER:OG	2.32	0.44
1:H:362:TRP:O	1:H:366:SER:OG	2.31	0.44
1:L:305:LYS:HD3	1:L:305:LYS:HA	1.85	0.44
1:L:607:GLU:OE1	1:L:611:ARG:NE	2.51	0.44
1:A:336:ARG:NH1	1:A:340:GLU:OE1	2.44	0.44
1:A:702:THR:HG21	1:A:744:THR:O	2.17	0.44
1:C:296:HIS:O	1:C:336:ARG:NH2	2.51	0.44
1:C:342:PHE:HB3	1:C:357:LYS:HG2	1.99	0.44
1:C:681:MET:HA	1:C:684:LYS:HB2	1.98	0.44
1:C:826:GLU:HA	1:C:829:ARG:HB2	1.98	0.44
1:G:859:VAL:HG22	1:G:880:LEU:HG	2.00	0.44
1:L:642:LYS:HE3	1:L:735:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:TYR:HB2	1:B:319:PRO:HD3	1.99	0.44
1:B:324:VAL:HG21	1:B:341:TRP:HE1	1.83	0.44
1:B:823:SER:O	1:B:827:ALA:N	2.41	0.44
1:C:458:TRP:O	1:C:572:HIS:NE2	2.47	0.44
1:D:694:THR:OG1	1:D:737:ASN:ND2	2.50	0.44
1:E:578:GLN:HB3	1:E:656:HIS:HD2	1.82	0.44
1:H:506:LYS:HA	1:H:509:LYS:HG2	2.00	0.44
1:I:342:PHE:HB3	1:I:357:LYS:HG2	1.99	0.44
1:I:428:ASN:OD1	1:I:428:ASN:N	2.45	0.44
1:K:298:PRO:HA	1:K:303:LEU:HD13	1.99	0.44
1:B:611:ARG:HH12	1:B:614:ILE:HG22	1.82	0.44
1:D:318:TYR:CG	1:D:319:PRO:HD3	2.52	0.44
1:D:666:LEU:O	1:D:703:SER:OG	2.24	0.44
1:F:607:GLU:OE1	1:F:611:ARG:NE	2.51	0.44
1:G:318:TYR:HB2	1:G:319:PRO:HD3	1.99	0.44
1:H:318:TYR:HB2	1:H:319:PRO:HD3	1.99	0.44
1:L:624:ARG:NH1	1:L:657:TYR:OH	2.51	0.44
1:A:859:VAL:HG22	1:A:880:LEU:HG	2.00	0.44
1:E:457:ILE:H	1:E:459:LYS:HZ3	1.63	0.44
1:F:642:LYS:HE3	1:F:735:ALA:HB1	2.00	0.44
1:H:379:MET:SD	1:H:379:MET:N	2.91	0.44
1:K:614:ILE:H	1:K:614:ILE:HD12	1.83	0.44
1:B:557:VAL:O	1:B:568:ILE:N	2.51	0.44
1:C:847:PRO:C	1:C:849:ALA:H	2.26	0.44
1:F:624:ARG:NH1	1:F:657:TYR:OH	2.51	0.44
1:H:418:ILE:HG23	1:H:477:PHE:HE2	1.83	0.44
1:I:617:TYR:HA	1:I:812:GLN:HE22	1.83	0.44
1:K:328:LEU:HD13	1:K:334:ASN:HB2	2.00	0.44
1:B:450:GLN:HE21	1:B:450:GLN:HB2	1.61	0.44
1:E:298:PRO:HA	1:E:303:LEU:HD13	1.99	0.44
1:E:398:TYR:CZ	1:E:425:MET:HA	2.53	0.44
1:E:614:ILE:HD12	1:E:614:ILE:H	1.83	0.44
1:E:834:THR:O	1:E:837:ARG:HB3	2.18	0.44
1:H:214:SER:HB3	1:H:220:PRO:HA	1.98	0.44
1:I:296:HIS:O	1:I:336:ARG:NH2	2.51	0.44
1:I:613:TRP:HD1	1:I:815:LYS:HD3	1.83	0.44
1:I:670:ARG:HH21	1:I:704:ARG:HH11	1.66	0.44
1:K:506:LYS:HA	1:K:506:LYS:HD3	1.80	0.44
1:A:412:MET:SD	1:F:516:SER:OG	2.71	0.44
1:C:674:GLU:HG2	1:C:677:ASN:HB2	1.99	0.44
1:G:705:LEU:O	1:G:709:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:296:HIS:HA	1:H:336:ARG:HD2	2.00	0.44
1:H:324:VAL:HG21	1:H:341:TRP:HE1	1.82	0.44
1:H:557:VAL:O	1:H:568:ILE:N	2.51	0.44
1:H:780:PHE:HA	1:H:784:TYR:HD1	1.83	0.44
1:K:45:LYS:HD3	1:K:45:LYS:HA	1.80	0.44
1:L:618:LEU:HD23	1:L:618:LEU:HA	1.89	0.44
1:A:705:LEU:O	1:A:709:VAL:N	2.51	0.43
1:B:216:LEU:N	1:B:216:LEU:HD23	2.33	0.43
1:B:940:ASN:ND2	1:B:944:GLU:OE2	2.50	0.43
1:F:742:ILE:O	1:F:828:TYR:OH	2.30	0.43
1:G:378:ILE:HD12	1:G:378:ILE:H	1.81	0.43
1:I:674:GLU:HG2	1:I:677:ASN:HB2	1.99	0.43
1:K:634:TRP:HE1	1:K:758:SER:HB3	1.82	0.43
1:L:303:LEU:HA	1:L:306:ILE:HD12	1.98	0.43
1:L:618:LEU:HD11	1:L:645:LEU:HD21	2.00	0.43
1:B:296:HIS:HA	1:B:336:ARG:HD2	2.00	0.43
1:B:362:TRP:O	1:B:366:SER:OG	2.31	0.43
1:H:458:TRP:O	1:H:572:HIS:NE2	2.45	0.43
1:L:458:TRP:NE1	1:L:569:ASN:OD1	2.51	0.43
1:B:418:ILE:HG23	1:B:477:PHE:HE2	1.83	0.43
1:D:757:ARG:O	1:D:759:LYS:NZ	2.50	0.43
1:G:339:ALA:O	1:G:343:SER:OG	2.35	0.43
1:J:757:ARG:O	1:J:759:LYS:NZ	2.50	0.43
1:A:591:ASN:CG	1:A:592:PRO:HD3	2.37	0.43
1:B:829:ARG:HA	1:B:829:ARG:HD3	1.59	0.43
1:E:417:MET:H	1:E:417:MET:HG3	1.64	0.43
1:E:634:TRP:HE1	1:E:758:SER:HB3	1.83	0.43
1:H:357:LYS:HE2	1:H:357:LYS:HB2	1.74	0.43
1:K:457:ILE:H	1:K:459:LYS:HZ3	1.66	0.43
1:K:474:SER:OG	1:K:524:LYS:NZ	2.42	0.43
1:K:780:PHE:HA	1:K:784:TYR:HB2	2.00	0.43
1:A:344:GLN:H	1:A:344:GLN:HG2	1.65	0.43
1:B:216:LEU:HG	1:B:295:LEU:CD2	2.48	0.43
1:B:661:LEU:HD23	1:B:665:LEU:HD23	2.01	0.43
1:G:341:TRP:O	1:G:344:GLN:NE2	2.52	0.43
1:G:755:HIS:HE1	1:G:757:ARG:HE	1.67	0.43
1:H:215:LYS:O	1:H:216:LEU:C	2.61	0.43
1:H:611:ARG:HH12	1:H:614:ILE:HG22	1.82	0.43
1:H:745:THR:N	1:H:832:GLN:OE1	2.48	0.43
1:K:597:LEU:O	1:K:601:LEU:HD22	2.18	0.43
1:L:126:ILE:HG21	1:L:163:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLU:OE1	1:B:420:LYS:NZ	2.51	0.43
1:B:536:ARG:HD2	1:B:536:ARG:HA	1.84	0.43
1:B:780:PHE:HA	1:B:784:TYR:HD1	1.83	0.43
1:C:670:ARG:HH21	1:C:704:ARG:HH11	1.66	0.43
1:D:534:LEU:HD12	1:D:534:LEU:HA	1.89	0.43
1:D:754:ARG:HA	1:D:754:ARG:HD3	1.85	0.43
1:F:618:LEU:HD23	1:F:618:LEU:HA	1.89	0.43
1:G:380:TYR:HB2	1:G:571:PHE:HD2	1.82	0.43
1:G:536:ARG:HA	1:G:536:ARG:HD2	1.84	0.43
1:H:412:MET:HE2	1:H:412:MET:HB2	1.95	0.43
1:K:126:ILE:HG21	1:K:163:LEU:HD21	2.01	0.43
1:K:578:GLN:HB3	1:K:656:HIS:HD2	1.82	0.43
1:K:829:ARG:HD2	1:K:829:ARG:HA	1.69	0.43
1:A:320:LEU:HD23	1:A:323:ASN:HD21	1.83	0.43
1:A:708:MET:HE3	1:A:708:MET:HB2	1.75	0.43
1:A:746:ASP:OD1	1:A:746:ASP:N	2.50	0.43
1:A:755:HIS:HE1	1:A:757:ARG:HE	1.67	0.43
1:C:376:ARG:HG2	1:C:428:ASN:HB3	2.01	0.43
1:G:595:LYS:HA	1:G:595:LYS:HD3	1.77	0.43
1:H:81:LEU:HD21	1:H:216:LEU:HD13	2.00	0.43
1:H:615:MET:HB2	1:H:615:MET:HE2	1.72	0.43
1:H:826:GLU:HA	1:H:829:ARG:HB2	2.00	0.43
1:I:126:ILE:HG21	1:I:163:LEU:HD21	2.01	0.43
1:I:412:MET:HE2	1:I:412:MET:HB3	1.91	0.43
1:L:591:ASN:HB2	1:L:592:PRO:CD	2.36	0.43
1:L:704:ARG:O	1:L:707:GLU:HG3	2.17	0.43
1:A:662:ASN:OD1	1:A:663:ILE:N	2.52	0.43
1:B:126:ILE:HG21	1:B:163:LEU:HD21	2.01	0.43
1:B:635:LEU:HD11	1:B:740:PHE:HD1	1.83	0.43
1:C:126:ILE:HG21	1:C:163:LEU:HD21	2.01	0.43
1:C:589:PRO:HB2	1:C:591:ASN:HD22	1.84	0.43
1:D:227:PHE:HB3	1:D:241:ILE:CG2	2.48	0.43
1:E:399:PHE:HZ	1:E:487:HIS:HB2	1.84	0.43
1:E:595:LYS:HA	1:E:595:LYS:HD2	1.80	0.43
1:E:597:LEU:O	1:E:601:LEU:HD22	2.18	0.43
1:E:631:MET:HE3	1:E:631:MET:HB3	1.88	0.43
1:E:688:TYR:HE1	1:E:690:TYR:HB3	1.84	0.43
1:H:635:LEU:HD11	1:H:740:PHE:HD1	1.83	0.43
1:I:376:ARG:HG2	1:I:428:ASN:HB3	2.01	0.43
1:J:321:TRP:H	1:J:321:TRP:CD1	2.36	0.43
1:J:376:ARG:HA	1:J:379:MET:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:398:TYR:CZ	1:K:425:MET:HA	2.53	0.43
1:L:652:VAL:HG21	1:L:794:PHE:HD2	1.84	0.43
1:D:398:TYR:CZ	1:D:425:MET:HA	2.54	0.43
1:D:939:LYS:HD3	1:D:939:LYS:HA	1.81	0.43
1:F:45:LYS:HD3	1:F:45:LYS:HA	1.80	0.43
1:F:371:LYS:HD3	1:F:371:LYS:HA	1.75	0.43
1:F:618:LEU:HD11	1:F:645:LEU:HD21	2.00	0.43
1:H:633:LEU:HD13	1:H:734:ALA:HB3	2.00	0.43
1:K:344:GLN:H	1:K:344:GLN:HG2	1.64	0.43
1:K:402:LEU:HD12	1:K:402:LEU:HA	1.87	0.43
1:A:217:ASN:N	1:A:217:ASN:HD22	2.17	0.43
1:A:484:ILE:HD13	1:A:484:ILE:HA	1.94	0.43
1:B:775:LYS:HD2	1:B:775:LYS:HA	1.86	0.43
1:C:847:PRO:C	1:C:849:ALA:N	2.77	0.43
1:D:321:TRP:CD1	1:D:321:TRP:H	2.36	0.43
1:D:591:ASN:CG	1:D:592:PRO:HD3	2.43	0.43
1:E:126:ILE:HG21	1:E:163:LEU:HD21	2.01	0.43
1:G:708:MET:HE3	1:G:708:MET:HB2	1.75	0.43
1:G:859:VAL:HG13	1:G:880:LEU:HD23	2.01	0.43
1:H:661:LEU:HD23	1:H:665:LEU:HD23	2.01	0.43
1:J:126:ILE:HG21	1:J:163:LEU:HD21	2.01	0.43
1:A:702:THR:CA	1:A:705:LEU:HD13	2.45	0.42
1:C:217:ASN:N	1:C:217:ASN:HD22	2.17	0.42
1:G:217:ASN:HD22	1:G:217:ASN:N	2.17	0.42
1:H:417:MET:H	1:H:417:MET:HG2	1.55	0.42
1:H:759:LYS:O	1:I:895:TRP:NE1	2.37	0.42
1:H:775:LYS:HD2	1:H:775:LYS:HA	1.86	0.42
1:I:216:LEU:HG	1:I:295:LEU:HD21	1.94	0.42
1:J:305:LYS:HE3	1:J:375:LYS:HG3	2.01	0.42
1:K:399:PHE:HZ	1:K:487:HIS:HB2	1.84	0.42
1:K:543:THR:O	1:K:543:THR:OG1	2.34	0.42
1:K:688:TYR:HE1	1:K:690:TYR:HB3	1.84	0.42
1:L:746:ASP:OD2	1:L:829:ARG:NH1	2.52	0.42
1:B:633:LEU:HD13	1:B:734:ALA:HB3	2.00	0.42
1:C:595:LYS:HD2	1:C:595:LYS:HA	1.78	0.42
1:G:798:LEU:HD23	1:G:798:LEU:HA	1.85	0.42
1:L:371:LYS:HA	1:L:371:LYS:HD3	1.75	0.42
1:D:52:ARG:HB3	1:D:83:TYR:CD2	2.55	0.42
1:E:367:HIS:ND1	1:E:368:HIS:O	2.50	0.42
1:G:367:HIS:ND1	1:G:368:HIS:O	2.48	0.42
1:G:459:LYS:NZ	1:G:556:GLY:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:815:LYS:HA	1:G:815:LYS:HD3	1.79	0.42
1:H:52:ARG:HB3	1:H:83:TYR:CD2	2.55	0.42
1:I:457:ILE:HG13	1:I:458:TRP:CD1	2.55	0.42
1:J:217:ASN:N	1:J:217:ASN:HD22	2.17	0.42
1:J:815:LYS:NZ	1:J:816:VAL:O	2.43	0.42
1:A:52:ARG:HB3	1:A:83:TYR:CD2	2.55	0.42
1:B:52:ARG:HB3	1:B:83:TYR:CD2	2.55	0.42
1:B:410:ASN:OD1	1:B:410:ASN:N	2.52	0.42
1:C:457:ILE:HG13	1:C:458:TRP:CD1	2.55	0.42
1:C:613:TRP:HD1	1:C:815:LYS:HD3	1.83	0.42
1:C:666:LEU:HD21	1:C:705:LEU:HB2	2.02	0.42
1:D:241:ILE:C	1:G:242:HIS:HE1	2.27	0.42
1:D:695:ASN:HD22	1:D:696:LYS:HG2	1.85	0.42
1:D:785:ILE:HG13	1:D:786:MET:HE2	2.01	0.42
1:D:834:THR:OG1	1:D:835:LEU:N	2.44	0.42
1:E:780:PHE:HA	1:E:784:TYR:HB2	2.00	0.42
1:F:452:MET:HB3	1:F:452:MET:HE3	1.81	0.42
1:G:25:GLN:HE21	1:L:489:LYS:HD3	1.82	0.42
1:G:52:ARG:HB3	1:G:83:TYR:CD2	2.55	0.42
1:G:475:GLU:OE1	1:H:420:LYS:NZ	2.51	0.42
1:G:494:GLN:HB2	1:G:496:HIS:CE1	2.54	0.42
1:H:374:THR:OG1	1:H:573:GLU:OE1	2.37	0.42
1:H:637:GLY:HA2	1:H:761:LYS:HD3	2.02	0.42
1:I:52:ARG:HB3	1:I:83:TYR:CD2	2.55	0.42
1:I:327:ALA:O	1:I:330:ASN:ND2	2.52	0.42
1:I:751:ARG:O	1:I:754:ARG:NH2	2.41	0.42
1:K:551:LEU:HD11	1:K:622:ILE:HB	2.01	0.42
1:K:591:ASN:CG	1:K:592:PRO:HD3	2.43	0.42
1:K:902:ILE:HB	1:K:905:GLY:H	1.85	0.42
1:L:52:ARG:HB3	1:L:83:TYR:CD2	2.55	0.42
1:A:494:GLN:HB2	1:A:496:HIS:CE1	2.54	0.42
1:B:417:MET:H	1:B:417:MET:HG2	1.55	0.42
1:C:475:GLU:OE1	1:D:420:LYS:NZ	2.36	0.42
1:D:305:LYS:HE3	1:D:375:LYS:HG3	2.01	0.42
1:E:217:ASN:N	1:E:217:ASN:HD22	2.17	0.42
1:E:551:LEU:HD11	1:E:622:ILE:HB	2.01	0.42
1:E:804:LYS:HB3	1:E:804:LYS:HE3	1.79	0.42
1:F:126:ILE:HG21	1:F:163:LEU:HD21	2.01	0.42
1:G:322:SER:HB2	1:G:326:PHE:CE1	2.55	0.42
1:G:787:ASP:OD2	1:G:790:CYS:N	2.46	0.42
1:H:698:GLU:OE2	1:H:739:ASN:ND2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:217:ASN:N	1:K:217:ASN:HD22	2.17	0.42
1:K:559:SER:HB3	1:K:566:LYS:HB3	2.02	0.42
1:L:217:ASN:HD22	1:L:217:ASN:N	2.17	0.42
1:A:238:TYR:HE2	1:J:117:ARG:HA	1.84	0.42
1:A:647:ARG:O	1:A:650:ALA:HB3	2.20	0.42
1:D:804:LYS:HD2	1:D:807:LYS:HZ1	1.84	0.42
1:E:371:LYS:HD3	1:E:371:LYS:HA	1.86	0.42
1:F:52:ARG:HB3	1:F:83:TYR:CD2	2.55	0.42
1:I:666:LEU:HD21	1:I:705:LEU:HB2	2.02	0.42
1:J:398:TYR:CZ	1:J:425:MET:HA	2.54	0.42
1:L:358:LEU:HD23	1:L:358:LEU:HA	1.88	0.42
1:L:375:LYS:HB3	1:L:375:LYS:HE2	1.81	0.42
1:L:536:ARG:HD2	1:L:536:ARG:HA	1.92	0.42
1:A:653:LEU:HD21	1:A:657:TYR:CD1	2.55	0.42
1:B:829:ARG:HA	1:B:833:ASP:HB3	2.00	0.42
1:C:627:LYS:HD2	1:C:730:ALA:HB3	2.02	0.42
1:E:113:PRO:HA	1:L:238:TYR:CD1	2.55	0.42
1:I:645:LEU:O	1:I:649:VAL:HG23	2.20	0.42
1:A:322:SER:HB2	1:A:326:PHE:CE1	2.55	0.42
1:A:341:TRP:O	1:A:344:GLN:NE2	2.52	0.42
1:A:859:VAL:HG13	1:A:880:LEU:HD23	2.01	0.42
1:D:126:ILE:HG21	1:D:163:LEU:HD21	2.01	0.42
1:F:652:VAL:HG21	1:F:794:PHE:HD2	1.84	0.42
1:F:743:ASP:OD1	1:F:743:ASP:N	2.52	0.42
1:G:323:ASN:OD1	1:G:323:ASN:N	2.53	0.42
1:G:562:THR:OG1	1:G:563:ILE:N	2.53	0.42
1:K:865:TRP:O	1:K:869:ASN:HB2	2.20	0.42
1:A:126:ILE:HG21	1:A:163:LEU:HD21	2.01	0.42
1:A:813:ILE:HD13	1:A:813:ILE:HA	1.88	0.42
1:B:637:GLY:HA2	1:B:761:LYS:HD3	2.02	0.42
1:D:144:THR:C	1:D:145:LEU:HD12	2.45	0.42
1:D:732:MET:N	1:D:732:MET:SD	2.93	0.42
1:E:144:THR:C	1:E:145:LEU:HD12	2.45	0.42
1:F:217:ASN:N	1:F:217:ASN:HD22	2.17	0.42
1:G:371:LYS:HD2	1:G:371:LYS:HA	1.69	0.42
1:G:830:LYS:HD3	1:G:830:LYS:HA	1.78	0.42
1:H:144:THR:C	1:H:145:LEU:HD12	2.45	0.42
1:H:829:ARG:HD2	1:H:829:ARG:HA	1.87	0.42
1:J:144:THR:C	1:J:145:LEU:HD12	2.45	0.42
1:K:52:ARG:HB3	1:K:83:TYR:CD2	2.55	0.42
1:A:144:THR:C	1:A:145:LEU:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:TYR:HA	1:A:686:ARG:HH11	1.85	0.42
1:B:374:THR:OG1	1:B:573:GLU:OE1	2.37	0.42
1:C:52:ARG:HB3	1:C:83:TYR:CD2	2.55	0.42
1:C:327:ALA:O	1:C:330:ASN:ND2	2.52	0.42
1:D:217:ASN:N	1:D:217:ASN:HD22	2.17	0.42
1:E:52:ARG:HB3	1:E:83:TYR:CD2	2.55	0.42
1:F:746:ASP:OD2	1:F:829:ARG:NH1	2.52	0.42
1:G:391:LYS:HE3	1:G:391:LYS:HB3	1.90	0.42
1:H:81:LEU:HD11	1:H:216:LEU:CD2	2.47	0.42
1:I:627:LYS:HD2	1:I:730:ALA:HB3	2.02	0.42
1:J:52:ARG:HB3	1:J:83:TYR:CD2	2.55	0.42
1:J:617:TYR:CE2	1:J:632:LEU:HB2	2.55	0.42
1:L:144:THR:C	1:L:145:LEU:HD12	2.45	0.42
1:L:425:MET:HE3	1:L:425:MET:HB2	1.86	0.42
1:C:545:ASP:HB3	1:C:624:ARG:NH1	2.35	0.41
1:C:645:LEU:O	1:C:649:VAL:HG23	2.20	0.41
1:D:376:ARG:HA	1:D:379:MET:HB2	2.01	0.41
1:E:467:ASP:OD1	1:F:440:TYR:OH	2.36	0.41
1:F:144:THR:C	1:F:145:LEU:HD12	2.45	0.41
1:F:798:LEU:HD23	1:F:798:LEU:HA	1.90	0.41
1:G:657:TYR:HA	1:G:686:ARG:HH11	1.85	0.41
1:G:684:LYS:HD2	1:G:684:LYS:HA	1.69	0.41
1:G:700:LEU:HD23	1:G:743:ASP:HB2	2.02	0.41
1:H:623:PHE:O	1:H:627:LYS:NZ	2.45	0.41
1:J:45:LYS:HA	1:J:45:LYS:HD3	1.87	0.41
1:K:732:MET:HE3	1:K:732:MET:HB3	1.77	0.41
1:A:635:LEU:HD11	1:A:740:PHE:HD1	1.86	0.41
1:D:456:GLU:H	1:D:456:GLU:HG2	1.65	0.41
1:G:458:TRP:NE1	1:G:569:ASN:OD1	2.53	0.41
1:G:653:LEU:HD21	1:G:657:TYR:CD1	2.55	0.41
1:G:662:ASN:OD1	1:G:663:ILE:N	2.52	0.41
1:G:746:ASP:N	1:G:746:ASP:OD1	2.50	0.41
1:H:794:PHE:HA	1:H:797:ILE:HG12	2.02	0.41
1:I:217:ASN:HD22	1:I:217:ASN:N	2.17	0.41
1:L:759:LYS:HA	1:L:759:LYS:HD3	1.92	0.41
1:B:657:TYR:HB3	1:B:687:GLY:H	1.86	0.41
1:C:398:TYR:OH	1:C:425:MET:HA	2.20	0.41
1:C:751:ARG:O	1:C:754:ARG:NH2	2.41	0.41
1:D:94:LEU:HD23	1:D:160:ILE:HD12	2.03	0.41
1:G:421:VAL:HG12	1:G:425:MET:HE3	2.03	0.41
1:G:644:PHE:CD2	1:G:780:PHE:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:ILE:HG21	1:H:163:LEU:HD21	2.01	0.41
1:I:144:THR:C	1:I:145:LEU:HD12	2.45	0.41
1:J:732:MET:SD	1:J:732:MET:N	2.93	0.41
1:K:94:LEU:HD23	1:K:160:ILE:HD12	2.03	0.41
1:K:614:ILE:HG23	1:K:632:LEU:HD21	2.02	0.41
1:A:663:ILE:O	1:A:667:THR:N	2.54	0.41
1:A:826:GLU:O	1:A:830:LYS:HG2	2.21	0.41
1:B:371:LYS:HE3	1:B:371:LYS:HB3	1.89	0.41
1:B:794:PHE:HA	1:B:797:ILE:HG12	2.02	0.41
1:D:652:VAL:HG21	1:D:794:PHE:HD2	1.86	0.41
1:E:402:LEU:HD12	1:E:402:LEU:HA	1.87	0.41
1:E:543:THR:O	1:E:543:THR:OG1	2.34	0.41
1:E:742:ILE:O	1:E:832:GLN:NE2	2.51	0.41
1:H:830:LYS:HD3	1:H:836:HIS:CD2	2.55	0.41
1:H:845:GLU:N	1:H:920:SER:O	2.52	0.41
1:I:614:ILE:HG13	1:I:821:ILE:HD11	2.02	0.41
1:J:303:LEU:HA	1:J:306:ILE:HD12	2.01	0.41
1:J:695:ASN:HD22	1:J:696:LYS:HG2	1.85	0.41
1:A:391:LYS:NZ	1:A:395:GLU:OE2	2.53	0.41
1:A:605:ILE:HA	1:A:606:PRO:HD3	1.91	0.41
1:C:846:SER:N	1:C:906:CYS:HA	2.24	0.41
1:E:559:SER:HB3	1:E:566:LYS:HB3	2.02	0.41
1:G:391:LYS:NZ	1:G:395:GLU:OE2	2.53	0.41
1:G:864:GLU:O	1:G:868:THR:HG23	2.20	0.41
1:H:818:CYS:HA	1:H:819:PRO:HD3	1.97	0.41
1:J:94:LEU:HD23	1:J:160:ILE:HD12	2.03	0.41
1:J:597:LEU:O	1:J:601:LEU:HB3	2.21	0.41
1:A:562:THR:OG1	1:A:563:ILE:N	2.53	0.41
1:A:666:LEU:HD21	1:A:705:LEU:CD1	2.51	0.41
1:B:759:LYS:O	1:C:895:TRP:NE1	2.37	0.41
1:C:94:LEU:HD23	1:C:160:ILE:HD12	2.03	0.41
1:D:45:LYS:HD3	1:D:45:LYS:HA	1.81	0.41
1:D:804:LYS:HE2	1:D:804:LYS:HB3	1.86	0.41
1:E:902:ILE:HB	1:E:905:GLY:H	1.85	0.41
1:F:94:LEU:HD23	1:F:160:ILE:HD12	2.03	0.41
1:H:493:SER:O	1:H:493:SER:OG	2.34	0.41
1:I:94:LEU:HD23	1:I:160:ILE:HD12	2.03	0.41
1:I:398:TYR:OH	1:I:425:MET:HA	2.20	0.41
1:I:491:HIS:HD1	1:I:504:TYR:HH	1.64	0.41
1:I:826:GLU:O	1:I:830:LYS:HG2	2.20	0.41
1:I:833:ASP:OD1	1:I:836:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:785:ILE:HG13	1:J:786:MET:HE2	2.01	0.41
1:K:376:ARG:HG2	1:K:428:ASN:HB3	2.03	0.41
1:B:144:THR:C	1:B:145:LEU:HD12	2.45	0.41
1:B:557:VAL:HG22	1:B:576:ILE:HD11	2.03	0.41
1:D:617:TYR:CE2	1:D:632:LEU:HB2	2.55	0.41
1:F:665:LEU:HD11	1:F:682:ARG:HH21	1.86	0.41
1:G:398:TYR:CZ	1:G:425:MET:HG2	2.56	0.41
1:H:750:TRP:HH2	1:H:836:HIS:CD2	2.38	0.41
1:J:652:VAL:HG21	1:J:794:PHE:HD2	1.86	0.41
1:L:587:PHE:HB3	1:L:588:ASN:H	1.55	0.41
1:A:864:GLU:O	1:A:868:THR:HG23	2.20	0.41
1:B:378:ILE:HA	1:B:381:TRP:CD1	2.56	0.41
1:B:633:LEU:HD21	1:B:753:LEU:HD23	2.03	0.41
1:C:847:PRO:O	1:C:849:ALA:N	2.54	0.41
1:F:589:PRO:HG2	1:F:591:ASN:HD22	1.86	0.41
1:G:413:LEU:HD11	1:G:511:PHE:HE1	1.86	0.41
1:G:647:ARG:O	1:G:650:ALA:HB3	2.20	0.41
1:G:666:LEU:HD21	1:G:705:LEU:CD1	2.51	0.41
1:I:585:VAL:HB	1:I:795:PHE:HD2	1.86	0.41
1:J:629:ALA:HB2	1:J:711:PRO:HD3	2.02	0.41
1:K:144:THR:C	1:K:145:LEU:HD12	2.45	0.41
1:L:536:ARG:HH21	1:L:538:ARG:HA	1.85	0.41
1:L:754:ARG:HA	1:L:754:ARG:HD3	1.90	0.41
1:A:323:ASN:OD1	1:A:323:ASN:N	2.53	0.41
1:B:598:LEU:HD13	1:B:943:TRP:CD1	2.56	0.41
1:B:615:MET:HE2	1:B:615:MET:HB2	1.72	0.41
1:C:585:VAL:HB	1:C:795:PHE:HD2	1.86	0.41
1:C:833:ASP:HB3	1:C:834:THR:H	1.53	0.41
1:D:597:LEU:O	1:D:601:LEU:HB3	2.21	0.41
1:E:481:MET:HG3	1:E:518:ILE:HD13	2.03	0.41
1:F:536:ARG:HH21	1:F:538:ARG:HA	1.85	0.41
1:G:126:ILE:HG21	1:G:163:LEU:HD21	2.01	0.41
1:G:144:THR:C	1:G:145:LEU:HD12	2.45	0.41
1:G:415:HIS:CD2	1:L:521:ASP:H	2.39	0.41
1:G:613:TRP:CZ3	1:G:821:ILE:HG21	2.55	0.41
1:G:775:LYS:HB3	1:G:776:GLU:H	1.71	0.41
1:H:657:TYR:HB3	1:H:687:GLY:H	1.86	0.41
1:I:391:LYS:HE3	1:I:391:LYS:HB3	1.86	0.41
1:I:545:ASP:HB3	1:I:624:ARG:NH1	2.35	0.41
1:I:810:ASN:O	1:I:814:LYS:NZ	2.45	0.41
1:J:528:ILE:HD13	1:J:528:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:813:ILE:HD13	1:J:813:ILE:HA	1.90	0.41
1:K:566:LYS:HB2	1:K:566:LYS:HE2	1.81	0.41
1:L:743:ASP:OD1	1:L:743:ASP:N	2.52	0.41
1:A:700:LEU:HD23	1:A:743:ASP:N	2.36	0.41
1:C:144:THR:C	1:C:145:LEU:HD12	2.45	0.41
1:C:216:LEU:HG	1:C:295:LEU:HD21	1.94	0.41
1:D:303:LEU:HA	1:D:306:ILE:HD12	2.01	0.41
1:D:435:ASP:HB3	1:D:541:ILE:HG13	2.03	0.41
1:G:646:MET:O	1:G:649:VAL:HB	2.21	0.41
1:G:700:LEU:HD23	1:G:743:ASP:N	2.36	0.41
1:H:664:SER:O	1:H:668:SER:OG	2.28	0.41
1:J:804:LYS:HE2	1:J:804:LYS:HB3	1.86	0.41
1:L:665:LEU:HD11	1:L:682:ARG:HH21	1.86	0.41
1:A:94:LEU:HD23	1:A:160:ILE:HD12	2.03	0.40
1:A:415:HIS:CD2	1:F:521:ASP:H	2.39	0.40
1:A:644:PHE:CD2	1:A:780:PHE:HB3	2.55	0.40
1:E:297:ASP:HB2	1:E:301:ARG:HH22	1.86	0.40
1:H:378:ILE:HA	1:H:381:TRP:CD1	2.56	0.40
1:H:597:LEU:O	1:H:601:LEU:CB	2.68	0.40
1:J:435:ASP:HB3	1:J:541:ILE:HG13	2.03	0.40
1:L:624:ARG:HD3	1:L:624:ARG:HA	1.88	0.40
1:A:646:MET:O	1:A:649:VAL:HB	2.21	0.40
1:B:94:LEU:HD23	1:B:160:ILE:HD12	2.03	0.40
1:B:458:TRP:O	1:B:572:HIS:NE2	2.45	0.40
1:B:613:TRP:HD1	1:B:815:LYS:HE3	1.87	0.40
1:C:403:ALA:HA	1:C:406:VAL:HG22	2.03	0.40
1:D:422:ILE:HD13	1:D:422:ILE:HA	1.94	0.40
1:D:629:ALA:HB2	1:D:711:PRO:HD3	2.02	0.40
1:E:94:LEU:HD23	1:E:160:ILE:HD12	2.03	0.40
1:E:614:ILE:HG23	1:E:632:LEU:HD21	2.02	0.40
1:E:732:MET:HE3	1:E:732:MET:HB3	1.77	0.40
1:G:521:ASP:H	1:H:415:HIS:CD2	2.40	0.40
1:G:566:LYS:HD3	1:G:566:LYS:HA	1.88	0.40
1:H:94:LEU:HD23	1:H:160:ILE:HD12	2.03	0.40
1:H:633:LEU:HD21	1:H:753:LEU:HD23	2.03	0.40
1:I:660:LYS:HA	1:I:690:TYR:CE2	2.56	0.40
1:I:779:ARG:H	1:I:779:ARG:HG3	1.61	0.40
1:I:822:GLU:HA	1:I:825:THR:HB	2.03	0.40
1:K:458:TRP:O	1:K:572:HIS:NE2	2.52	0.40
1:A:398:TYR:CZ	1:A:425:MET:HG2	2.56	0.40
1:A:700:LEU:HD23	1:A:743:ASP:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ILE:HD13	1:B:422:ILE:HA	1.92	0.40
1:B:798:LEU:HD23	1:B:798:LEU:HA	1.93	0.40
1:D:238:TYR:HE2	1:G:241:ILE:CD1	2.31	0.40
1:D:485:THR:HG21	1:D:515:LYS:HE2	2.04	0.40
1:G:642:LYS:H	1:G:642:LYS:HG3	1.76	0.40
1:H:595:LYS:HB3	1:H:595:LYS:HE2	1.98	0.40
1:I:846:SER:H	1:I:906:CYS:HA	1.86	0.40
1:J:294:MET:HE2	1:J:294:MET:HA	2.03	0.40
1:J:485:THR:HG21	1:J:515:LYS:HE2	2.04	0.40
1:K:435:ASP:HB3	1:K:541:ILE:HD12	2.03	0.40
1:K:578:GLN:HB3	1:K:656:HIS:CD2	2.57	0.40
1:K:795:PHE:O	1:K:799:VAL:HG12	2.22	0.40
1:A:413:LEU:HD11	1:A:511:PHE:HE1	1.86	0.40
1:A:595:LYS:HA	1:A:595:LYS:HD3	1.77	0.40
1:D:601:LEU:HD11	1:D:645:LEU:HD13	2.04	0.40
1:D:753:LEU:HD12	1:D:753:LEU:HA	1.91	0.40
1:E:701:ASN:HD22	1:E:742:ILE:HG23	1.87	0.40
1:G:795:PHE:O	1:G:799:VAL:HG12	2.22	0.40
1:H:402:LEU:HD12	1:H:402:LEU:HA	1.92	0.40
1:I:841:GLU:C	1:I:843:VAL:H	2.29	0.40
1:J:893:LEU:HB3	1:J:901:ARG:HD2	2.04	0.40
1:K:371:LYS:HA	1:K:371:LYS:HD3	1.86	0.40
1:K:595:LYS:HD2	1:K:595:LYS:HA	1.80	0.40
1:B:597:LEU:O	1:B:601:LEU:CB	2.68	0.40
1:B:780:PHE:HA	1:B:784:TYR:CD1	2.57	0.40
1:C:660:LYS:HA	1:C:690:TYR:CE2	2.57	0.40
1:D:798:LEU:HD23	1:D:798:LEU:HA	1.94	0.40
1:G:538:ARG:HE	1:G:538:ARG:HB3	1.51	0.40
1:H:557:VAL:HG22	1:H:576:ILE:HD11	2.03	0.40
1:H:598:LEU:HD13	1:H:943:TRP:CD1	2.56	0.40
1:H:780:PHE:HA	1:H:784:TYR:CD1	2.57	0.40
1:I:835:LEU:O	1:I:839:ILE:HG13	2.22	0.40
1:K:801:PHE:HA	1:K:804:LYS:HB2	2.04	0.40
1:L:589:PRO:HG2	1:L:591:ASN:HD22	1.86	0.40
1:L:797:ILE:HD13	1:L:797:ILE:HA	1.95	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	820/962 (85%)	735 (90%)	84 (10%)	1 (0%)	48	78
1	B	834/962 (87%)	750 (90%)	82 (10%)	2 (0%)	43	72
1	C	848/962 (88%)	761 (90%)	85 (10%)	2 (0%)	43	72
1	D	842/962 (88%)	771 (92%)	71 (8%)	0	100	100
1	E	830/962 (86%)	753 (91%)	76 (9%)	1 (0%)	48	78
1	F	782/962 (81%)	722 (92%)	60 (8%)	0	100	100
1	G	820/962 (85%)	733 (89%)	86 (10%)	1 (0%)	48	78
1	H	834/962 (87%)	751 (90%)	83 (10%)	0	100	100
1	I	848/962 (88%)	761 (90%)	86 (10%)	1 (0%)	48	78
1	J	842/962 (88%)	772 (92%)	70 (8%)	0	100	100
1	K	830/962 (86%)	753 (91%)	77 (9%)	0	100	100
1	L	782/962 (81%)	721 (92%)	61 (8%)	0	100	100
All	All	9912/11544 (86%)	8983 (91%)	921 (9%)	8 (0%)	49	78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	699	VAL
1	A	699	VAL
1	C	848	SER
1	I	842	ARG
1	B	837	ARG
1	B	836	HIS
1	C	847	PRO
1	E	819	PRO

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	731/869 (84%)	721 (99%)	10 (1%)	59	70
1	B	744/869 (86%)	738 (99%)	6 (1%)	73	76
1	C	762/869 (88%)	754 (99%)	8 (1%)	68	74
1	D	757/869 (87%)	748 (99%)	9 (1%)	63	72
1	E	745/869 (86%)	737 (99%)	8 (1%)	65	73
1	F	704/869 (81%)	699 (99%)	5 (1%)	76	77
1	G	731/869 (84%)	720 (98%)	11 (2%)	57	68
1	H	744/869 (86%)	737 (99%)	7 (1%)	70	75
1	I	762/869 (88%)	752 (99%)	10 (1%)	61	71
1	J	757/869 (87%)	749 (99%)	8 (1%)	65	73
1	K	745/869 (86%)	739 (99%)	6 (1%)	73	76
1	L	704/869 (81%)	697 (99%)	7 (1%)	68	74
All	All	8886/10428 (85%)	8791 (99%)	95 (1%)	63	73

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	217	ASN
1	A	219	LYS
1	A	269	VAL
1	A	501	LEU
1	A	707	GLU
1	A	708	MET
1	A	745	THR
1	A	832	GLN
1	A	834	THR
1	B	78	GLN
1	B	219	LYS
1	B	269	VAL
1	B	426	MET

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Mol	Chain	Res	Type
1	B	809	TYR
1	B	829	ARG
1	C	78	GLN
1	C	217	ASN
1	C	219	LYS
1	C	269	VAL
1	C	302	TYR
1	C	551	LEU
1	C	652	VAL
1	C	828	TYR
1	D	78	GLN
1	D	217	ASN
1	D	219	LYS
1	D	242	HIS
1	D	269	VAL
1	D	543	THR
1	D	706	LYS
1	D	740	PHE
1	D	809	TYR
1	E	78	GLN
1	E	217	ASN
1	E	219	LYS
1	E	269	VAL
1	E	534	LEU
1	E	706	LYS
1	E	820	THR
1	E	837	ARG
1	F	78	GLN
1	F	217	ASN
1	F	219	LYS
1	F	269	VAL
1	F	626	LEU
1	G	78	GLN
1	G	217	ASN
1	G	219	LYS
1	G	269	VAL
1	G	501	LEU
1	G	707	GLU
1	G	708	MET
1	G	745	THR
1	G	809	TYR
1	G	832	GLN

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Mol	Chain	Res	Type
1	G	833	ASP
1	H	78	GLN
1	H	216	LEU
1	H	219	LYS
1	H	269	VAL
1	H	809	TYR
1	H	829	ARG
1	H	832	GLN
1	I	78	GLN
1	I	217	ASN
1	I	219	LYS
1	I	269	VAL
1	I	302	TYR
1	I	605	ILE
1	I	652	VAL
1	I	828	TYR
1	I	832	GLN
1	I	833	ASP
1	J	78	GLN
1	J	217	ASN
1	J	219	LYS
1	J	269	VAL
1	J	543	THR
1	J	706	LYS
1	J	740	PHE
1	J	809	TYR
1	K	78	GLN
1	K	217	ASN
1	K	219	LYS
1	K	269	VAL
1	K	534	LEU
1	K	706	LYS
1	L	78	GLN
1	L	217	ASN
1	L	219	LYS
1	L	269	VAL
1	L	622	ILE
1	L	626	LEU
1	L	738	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (232) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	78	GLN
1	A	103	ASN
1	A	125	HIS
1	A	128	ASN
1	A	137	HIS
1	A	217	ASN
1	A	242	HIS
1	A	330	ASN
1	A	344	GLN
1	A	383	HIS
1	A	496	HIS
1	A	502	ASN
1	A	537	GLN
1	A	701	ASN
1	A	710	ASN
1	A	755	HIS
1	A	782	HIS
1	A	894	GLN
1	B	78	GLN
1	B	103	ASN
1	B	125	HIS
1	B	128	ASN
1	B	137	HIS
1	B	217	ASN
1	B	218	HIS
1	B	242	HIS
1	B	308	ASN
1	B	344	GLN
1	B	389	GLN
1	B	415	HIS
1	B	437	ASN
1	B	465	ASN
1	B	476	ASN
1	B	602	GLN
1	B	677	ASN
1	B	695	ASN
1	B	701	ASN
1	B	869	ASN
1	B	886	ASN
1	C	78	GLN
1	C	103	ASN
1	C	125	HIS

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Mol	Chain	Res	Type
1	C	128	ASN
1	C	137	HIS
1	C	217	ASN
1	C	242	HIS
1	C	330	ASN
1	C	334	ASN
1	C	368	HIS
1	C	388	GLN
1	C	450	GLN
1	C	496	HIS
1	C	530	GLN
1	C	602	GLN
1	C	737	ASN
1	C	782	HIS
1	C	806	GLN
1	C	812	GLN
1	D	78	GLN
1	D	103	ASN
1	D	120	HIS
1	D	125	HIS
1	D	128	ASN
1	D	137	HIS
1	D	217	ASN
1	D	389	GLN
1	D	453	ASN
1	D	476	ASN
1	D	499	ASN
1	D	530	GLN
1	D	537	GLN
1	D	570	HIS
1	D	581	HIS
1	D	737	ASN
1	D	739	ASN
1	D	747	HIS
1	D	871	ASN
1	D	894	GLN
1	E	25	GLN
1	E	78	GLN
1	E	103	ASN
1	E	125	HIS
1	E	128	ASN
1	E	137	HIS

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Mol	Chain	Res	Type
1	E	217	ASN
1	E	242	HIS
1	E	243	GLN
1	E	334	ASN
1	E	389	GLN
1	E	496	HIS
1	E	537	GLN
1	E	588	ASN
1	E	710	ASN
1	E	739	ASN
1	E	886	ASN
1	F	78	GLN
1	F	103	ASN
1	F	125	HIS
1	F	128	ASN
1	F	137	HIS
1	F	217	ASN
1	F	242	HIS
1	F	296	HIS
1	F	330	ASN
1	F	368	HIS
1	F	494	GLN
1	F	502	ASN
1	F	530	GLN
1	F	710	ASN
1	F	737	ASN
1	F	755	HIS
1	F	782	HIS
1	F	791	GLN
1	F	836	HIS
1	G	25	GLN
1	G	78	GLN
1	G	103	ASN
1	G	120	HIS
1	G	125	HIS
1	G	128	ASN
1	G	137	HIS
1	G	217	ASN
1	G	242	HIS
1	G	330	ASN
1	G	344	GLN
1	G	383	HIS

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Mol	Chain	Res	Type
1	G	494	GLN
1	G	496	HIS
1	G	502	ASN
1	G	537	GLN
1	G	701	ASN
1	G	710	ASN
1	G	782	HIS
1	G	894	GLN
1	H	78	GLN
1	H	103	ASN
1	H	125	HIS
1	H	128	ASN
1	H	137	HIS
1	H	217	ASN
1	H	242	HIS
1	H	308	ASN
1	H	385	HIS
1	H	389	GLN
1	H	415	HIS
1	H	437	ASN
1	H	465	ASN
1	H	476	ASN
1	H	494	GLN
1	H	578	GLN
1	H	602	GLN
1	H	677	ASN
1	H	695	ASN
1	H	701	ASN
1	H	886	ASN
1	I	78	GLN
1	I	103	ASN
1	I	125	HIS
1	I	128	ASN
1	I	137	HIS
1	I	217	ASN
1	I	242	HIS
1	I	330	ASN
1	I	334	ASN
1	I	368	HIS
1	I	388	GLN
1	I	450	GLN
1	I	476	ASN

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Mol	Chain	Res	Type
1	I	530	GLN
1	I	602	GLN
1	I	737	ASN
1	I	782	HIS
1	I	806	GLN
1	I	812	GLN
1	J	78	GLN
1	J	103	ASN
1	J	125	HIS
1	J	128	ASN
1	J	137	HIS
1	J	217	ASN
1	J	242	HIS
1	J	308	ASN
1	J	389	GLN
1	J	453	ASN
1	J	476	ASN
1	J	499	ASN
1	J	530	GLN
1	J	537	GLN
1	J	570	HIS
1	J	581	HIS
1	J	737	ASN
1	J	739	ASN
1	J	747	HIS
1	J	871	ASN
1	J	894	GLN
1	K	25	GLN
1	K	78	GLN
1	K	103	ASN
1	K	125	HIS
1	K	128	ASN
1	K	137	HIS
1	K	217	ASN
1	K	242	HIS
1	K	330	ASN
1	K	368	HIS
1	K	389	GLN
1	K	496	HIS
1	K	537	GLN
1	K	588	ASN
1	K	695	ASN

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Mol	Chain	Res	Type
1	K	710	ASN
1	K	739	ASN
1	K	886	ASN
1	L	78	GLN
1	L	103	ASN
1	L	125	HIS
1	L	128	ASN
1	L	137	HIS
1	L	217	ASN
1	L	242	HIS
1	L	296	HIS
1	L	330	ASN
1	L	368	HIS
1	L	494	GLN
1	L	502	ASN
1	L	530	GLN
1	L	710	ASN
1	L	737	ASN
1	L	782	HIS
1	L	791	GLN
1	L	836	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

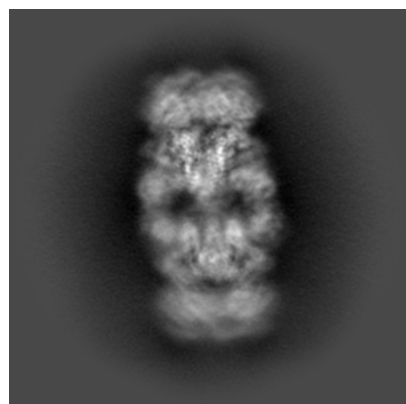
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60945. These allow visual inspection of the internal detail of the map and identification of artifacts.

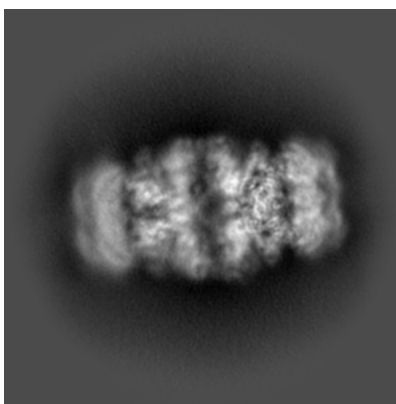
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

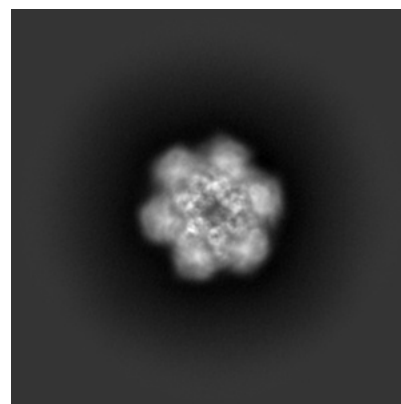
6.1.1 Primary map



X

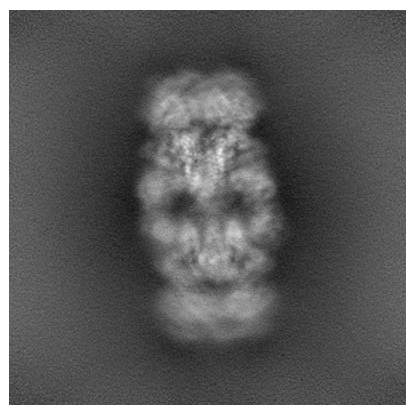


Y

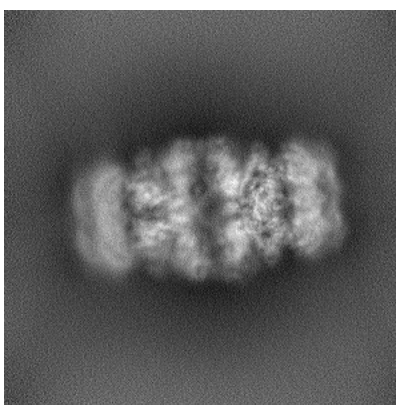


Z

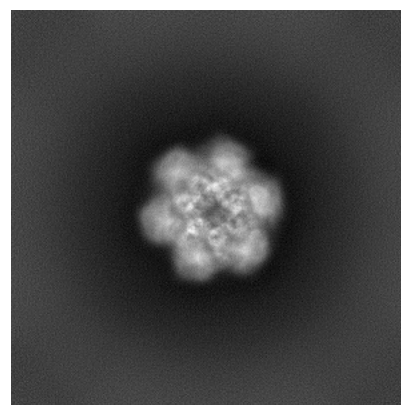
6.1.2 Raw map



X



Y

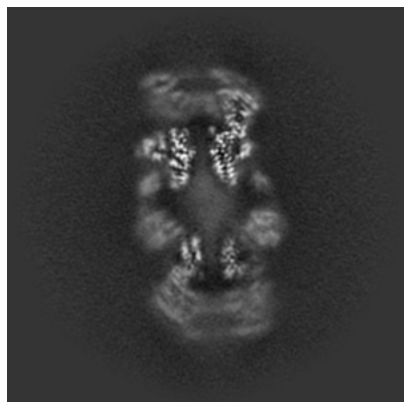


Z

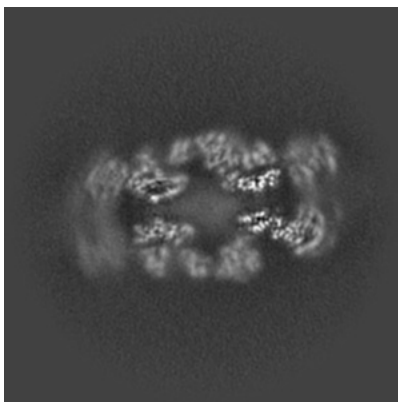
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

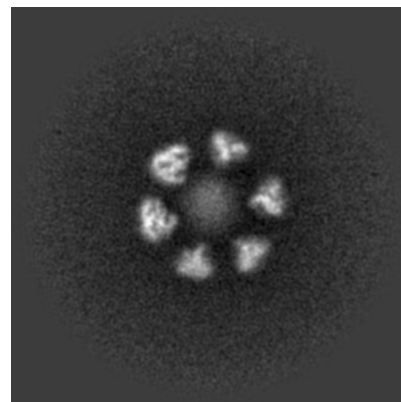
6.2.1 Primary map



X Index: 250

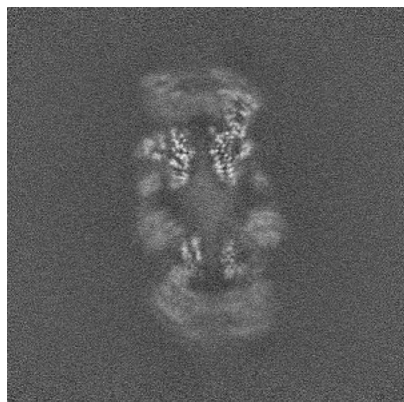


Y Index: 250

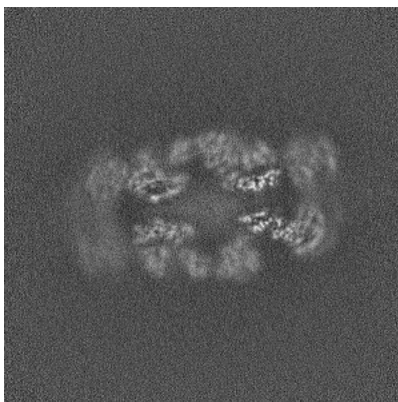


Z Index: 250

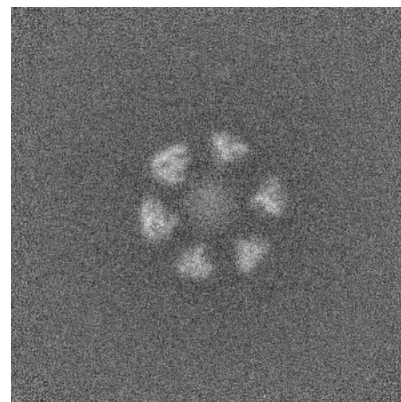
6.2.2 Raw map



X Index: 250



Y Index: 250

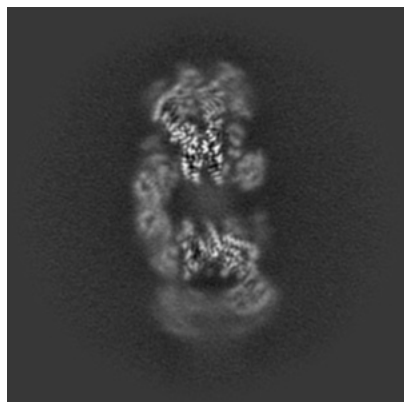


Z Index: 250

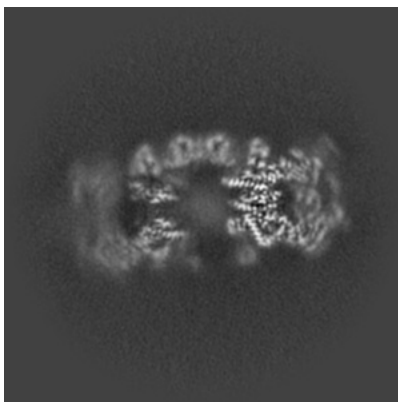
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

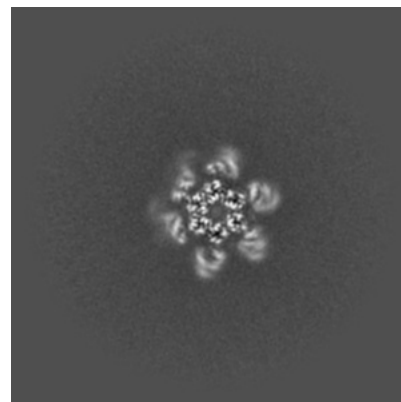
6.3.1 Primary map



X Index: 228

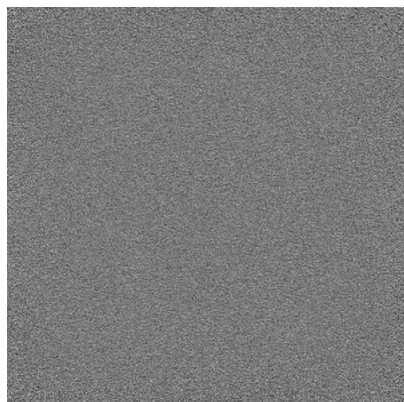


Y Index: 265

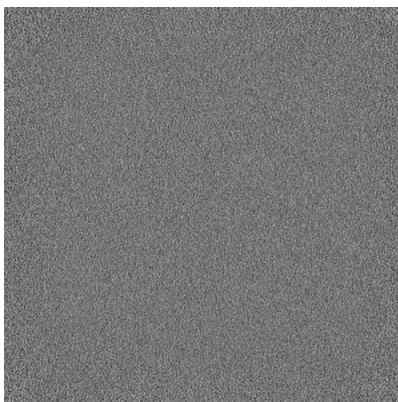


Z Index: 320

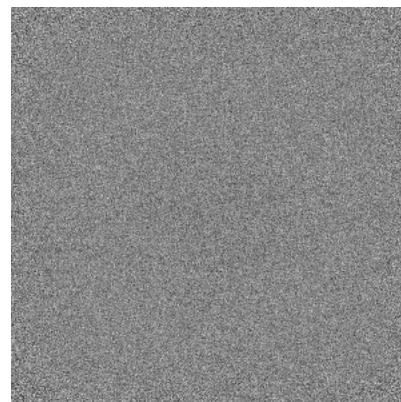
6.3.2 Raw map



X Index: 0



Y Index: 0

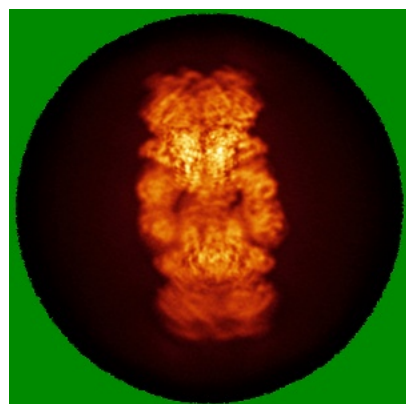


Z Index: 0

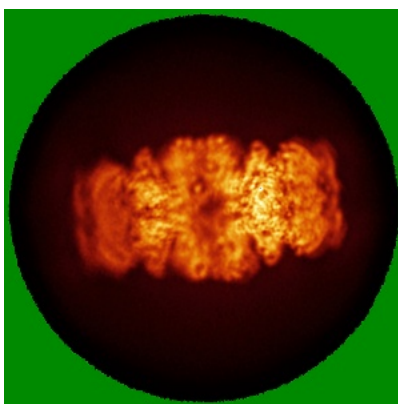
The images above show the largest variance slices of the map in three orthogonal directions.

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

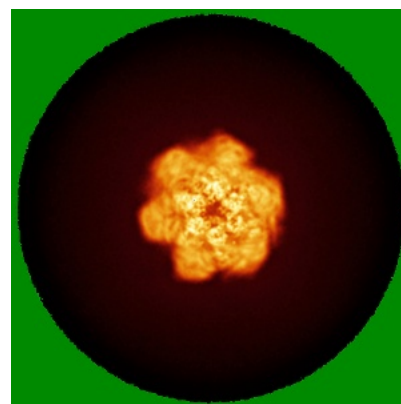
6.4.1 Primary map



X

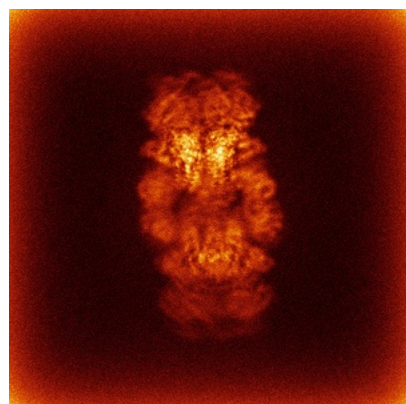


Y

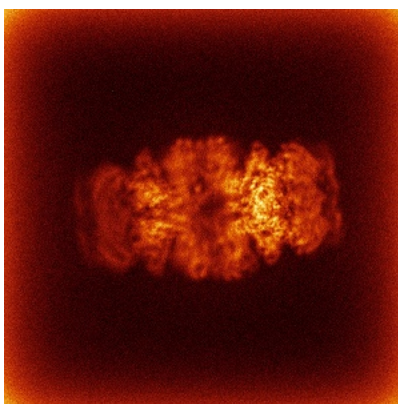


Z

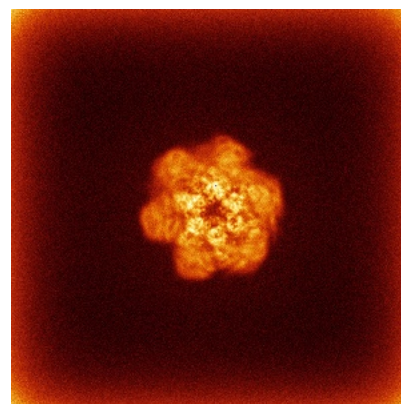
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

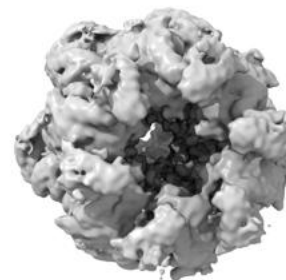
6.5.1 Primary map



X



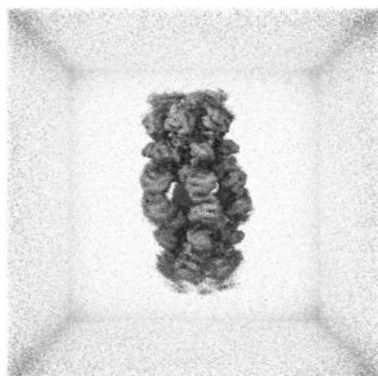
Y



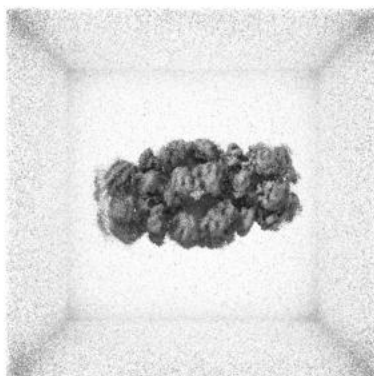
Z

The images above show the 3D surface view of the map at the recommended contour level 0.142. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

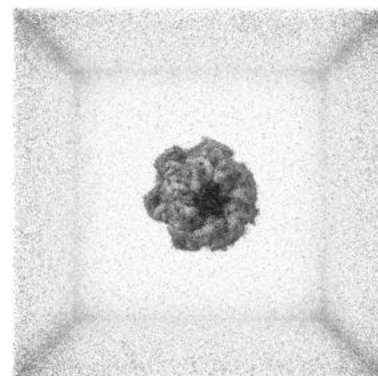
6.5.2 Raw map



X



Y



Z

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

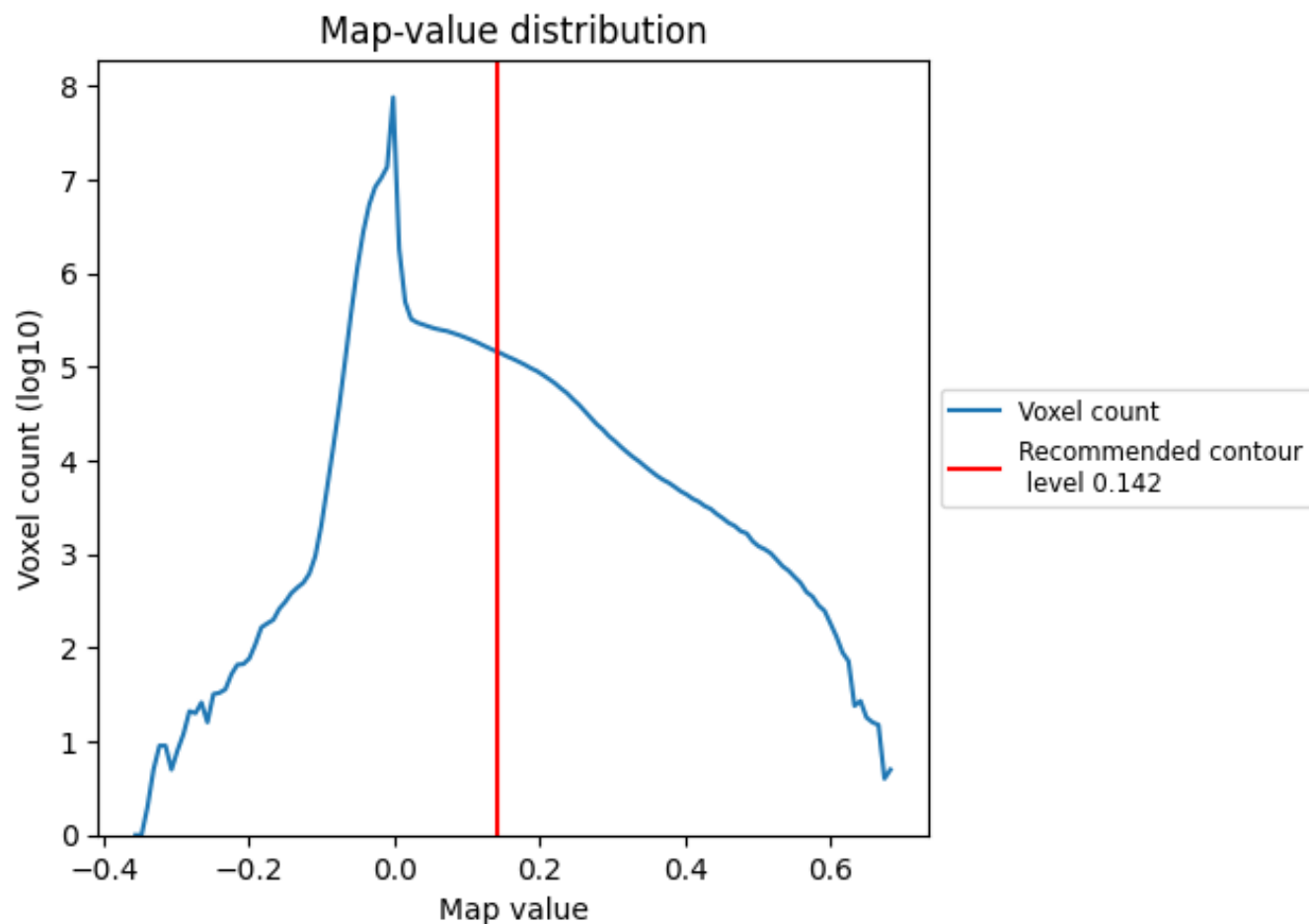
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

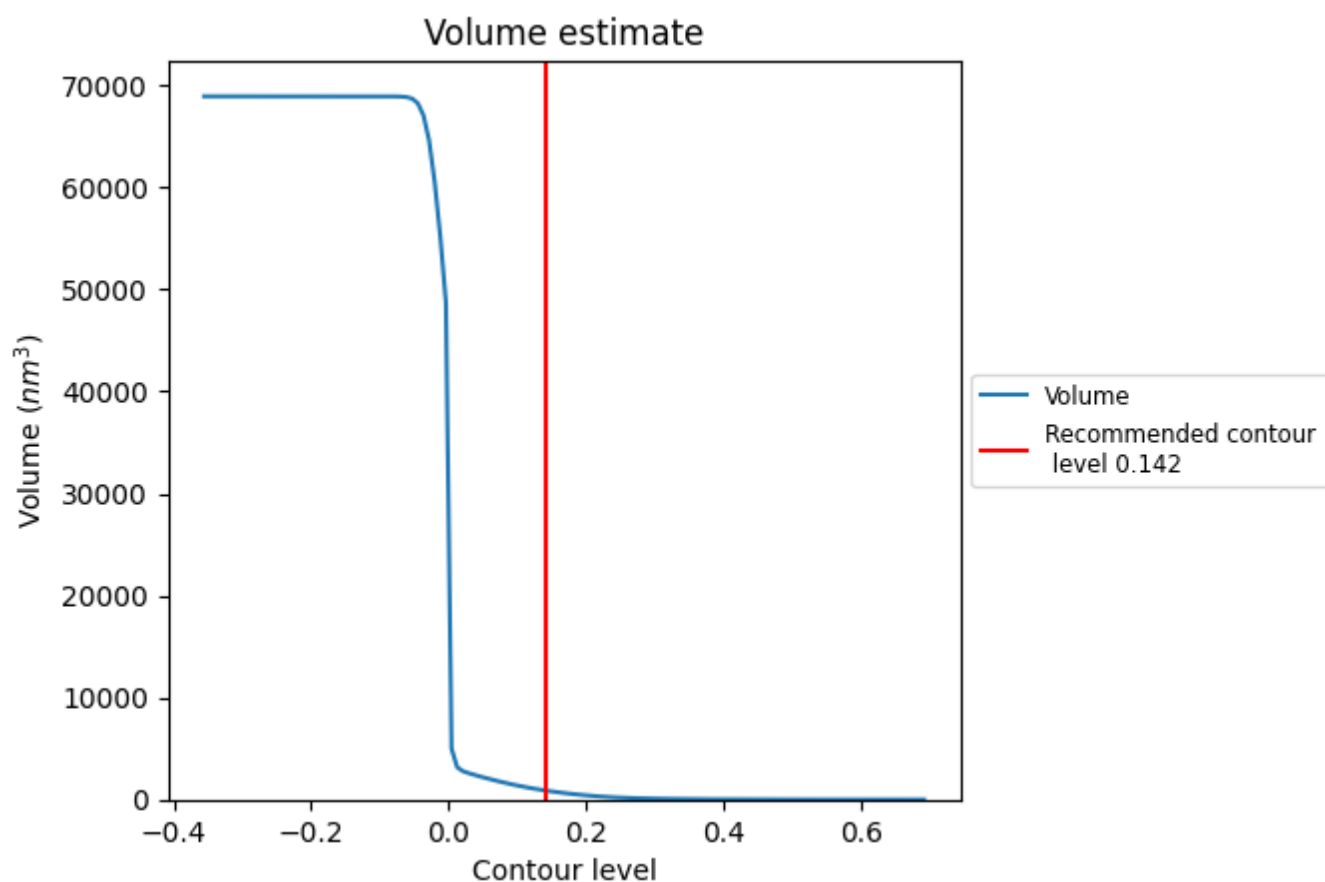
This section contains the results of statistical analysis of the map.

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.

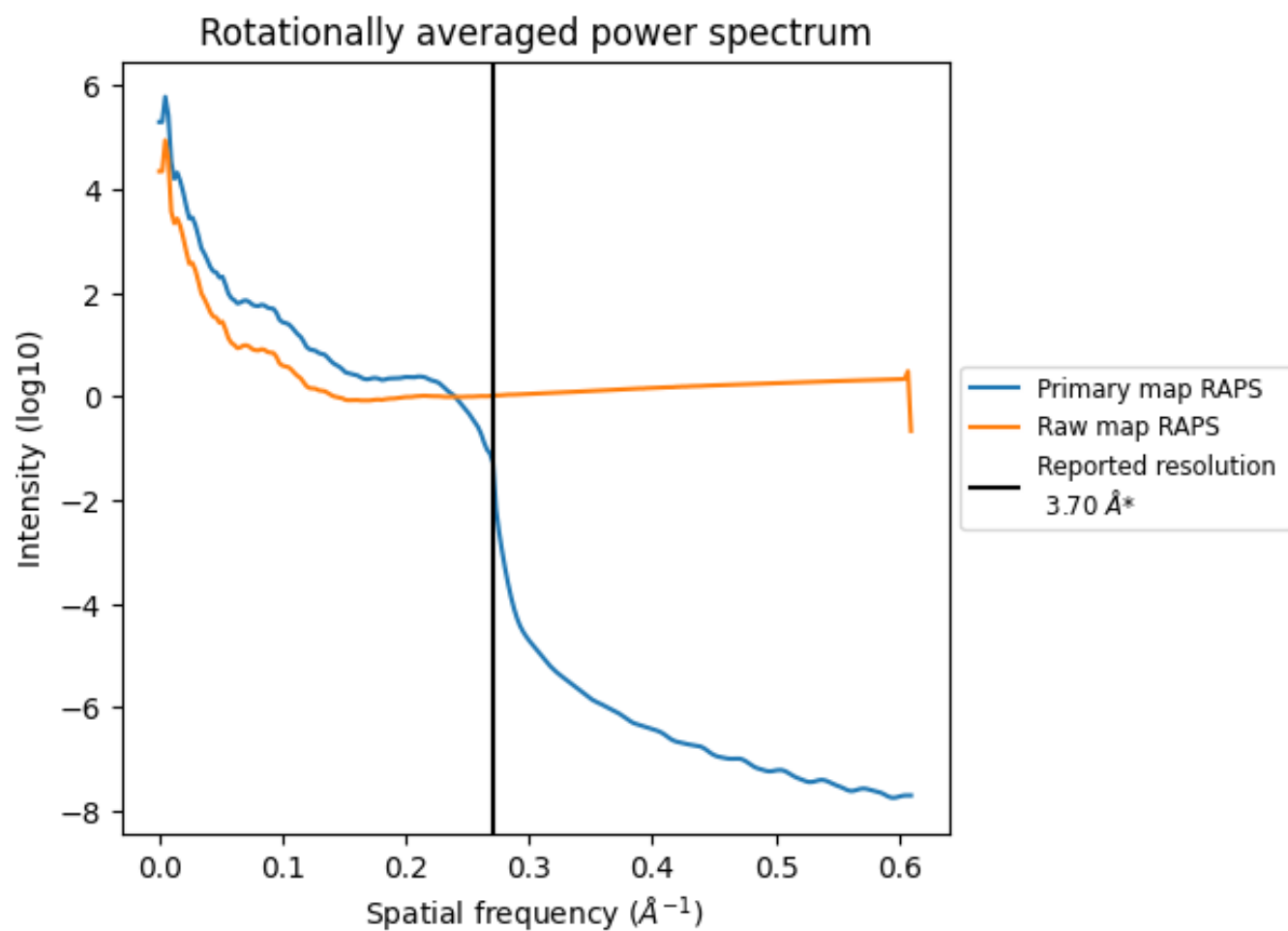
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 869 nm³; this corresponds to an approximate mass of 785 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 ⓘ

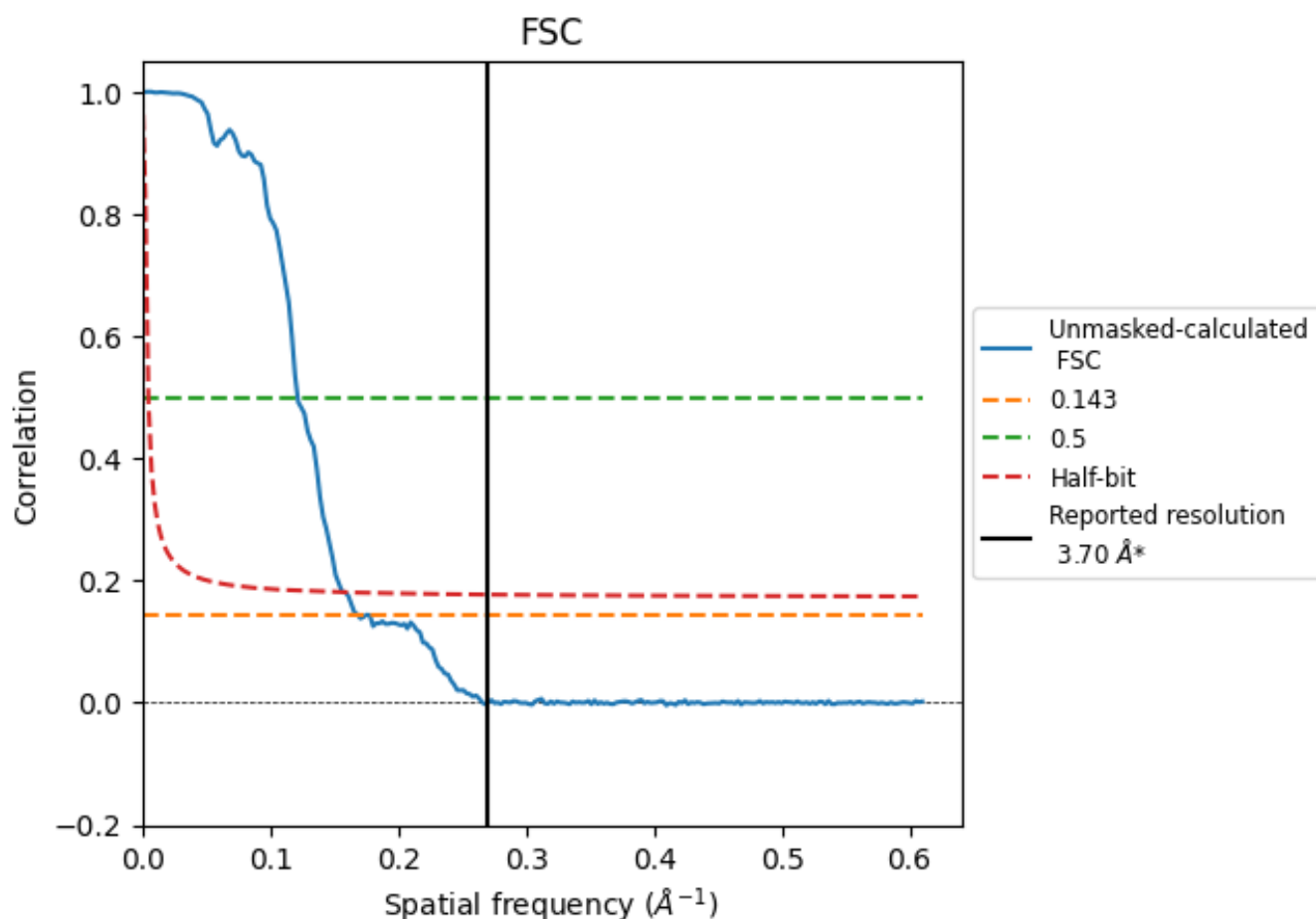


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

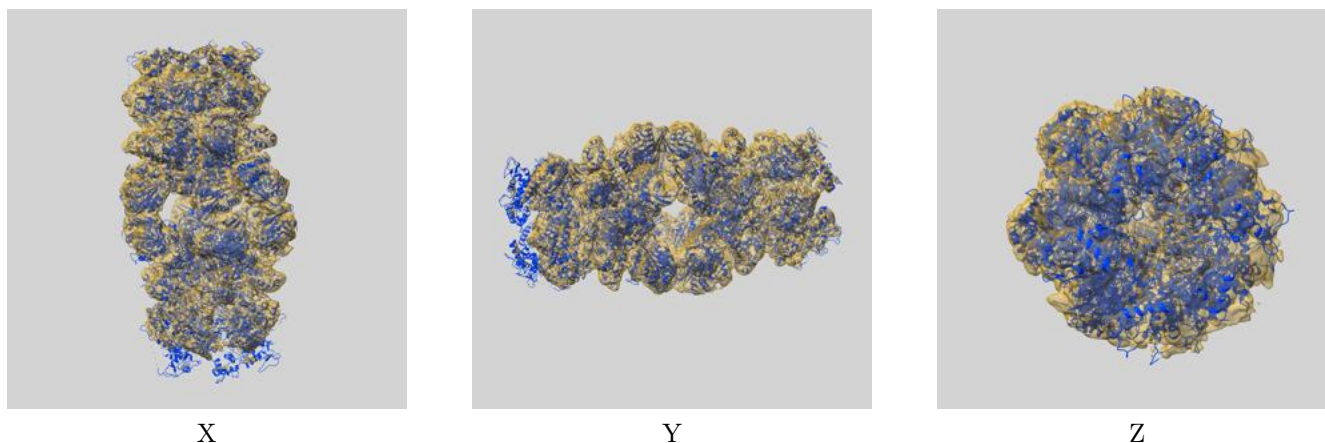
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.92	8.23	6.31

*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 5.92 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

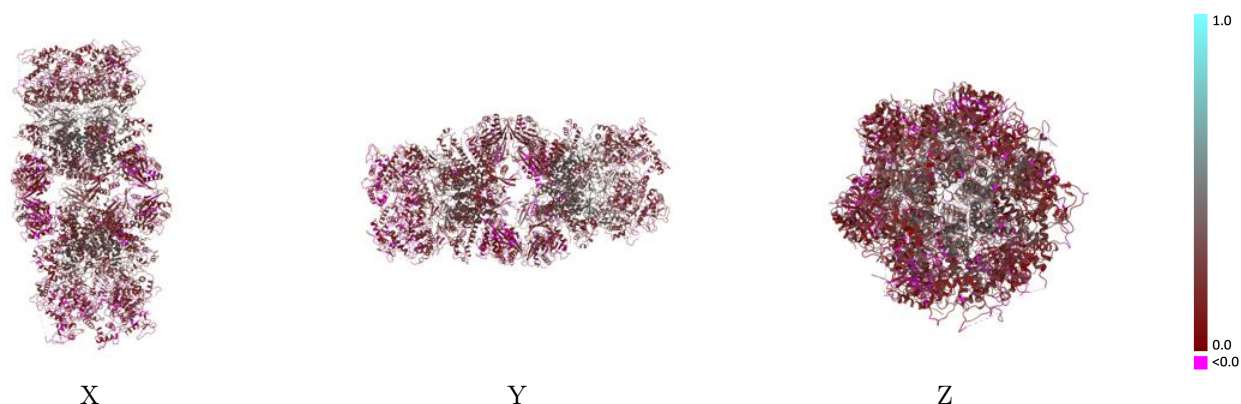
This section contains information regarding the fit between EMDB map EMD-60945 and PDB model 9IWA. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



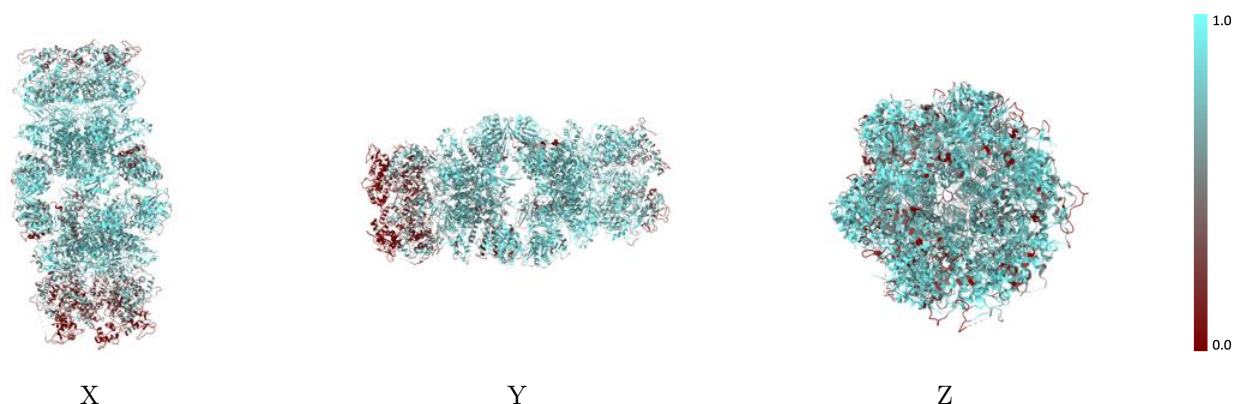
The images above show the 3D surface view of the map at the recommended contour level 0.142 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



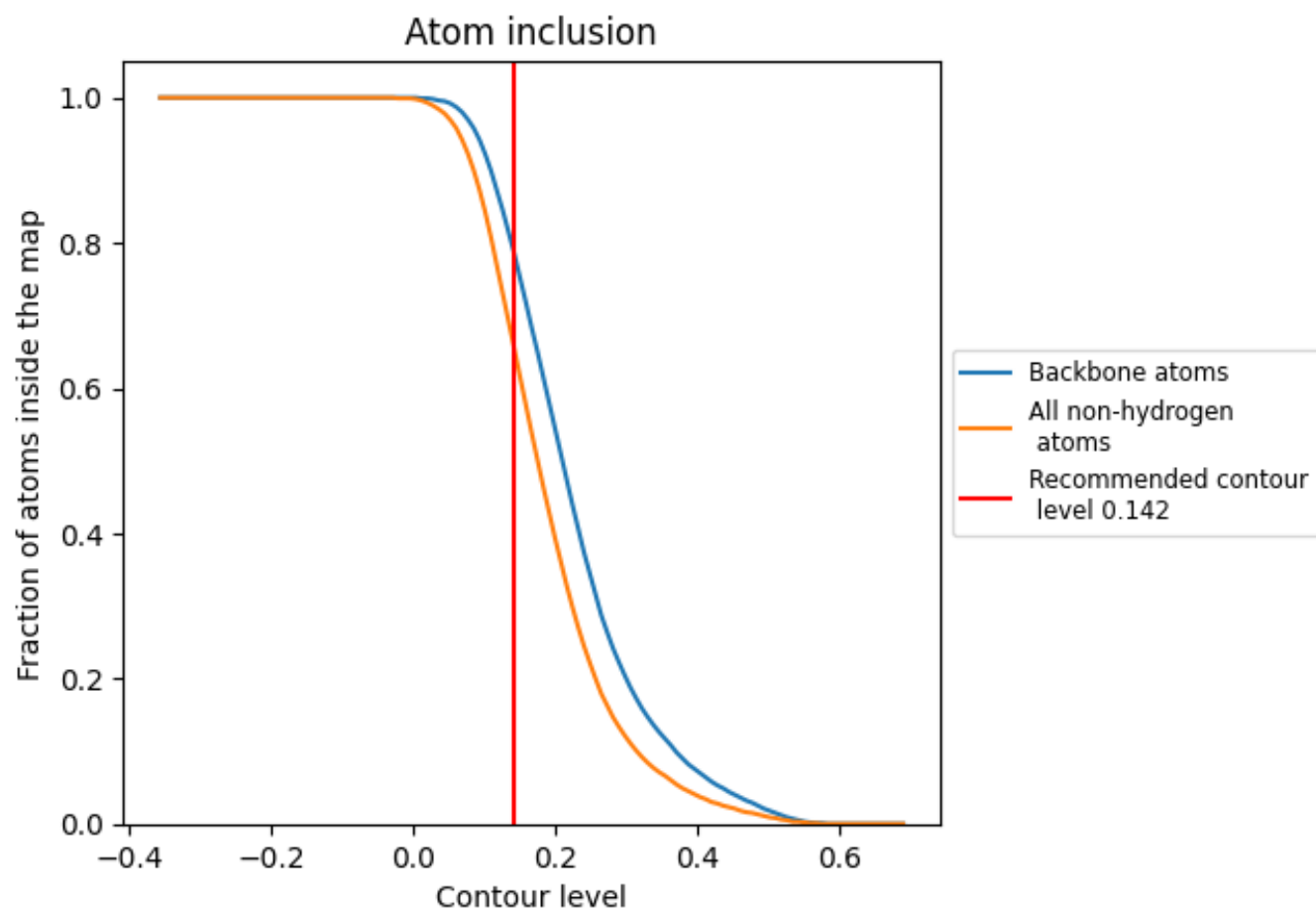
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.142).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 66% 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 (0.142) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6580	0.2010
A	0.7750	0.2520
B	0.7310	0.2200
C	0.7600	0.2410
D	0.7560	0.2280
E	0.7300	0.2110
F	0.7840	0.2360
G	0.5580	0.1860
H	0.5840	0.1700
I	0.6050	0.1860
J	0.5920	0.1840
K	0.5220	0.1560
L	0.4960	0.1350

1.0

0.0

<0.0