Full wwPDB EM Validation Report

Mar 10, 2026 – 10:36 AM UTC

PDB ID	:	7EGQ / pdb_00007egq
EMDB ID	:	EMD-31138
Title	:	Co-transcriptional capping machineries in SARS-CoV-2 RTC: Coupling of N7-methyltransferase and 3'-5' exoribonuclease with polymerase reveals mechanisms for capping and proofreading
Authors	:	Yan, L.M.; Yang, Y.X.; Li, M.Y.; Zhang, Y.; Zheng, L.T.; Ge, J.; Huang, Y.C.; Liu, Z.Y.; Wang, T.; Gao, S.; Zhang, R.; Huang, Y.Y.; Guddat, L.W.; Gao, Y.; Rao, Z.H.; Lou, Z.Y.
Deposited on	:	2021-03-25
Resolution	:	3.35 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 (i) 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 (i)) were used in the production of this report:

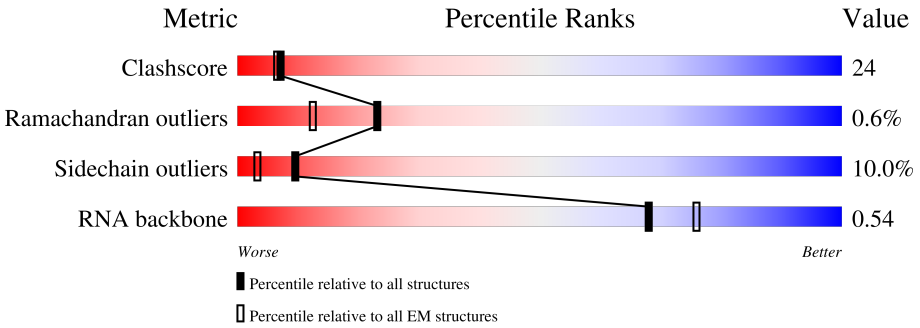
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

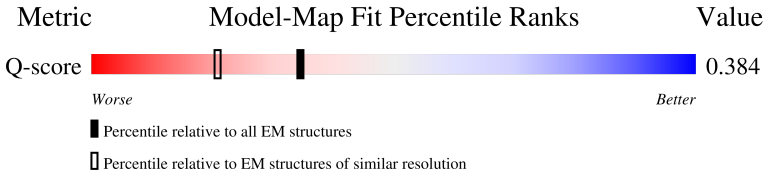
1 Overall quality at a glance

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

The reported resolution of this entry is 3.35 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	14390 (2.85 - 3.85)

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 <=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	932	62% 28% 8%
1	N	932	61% 29% 8%
2	B	198	10% 55% 35% 6%

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Mol	Chain	Length	Quality of chain
2	D	198	8% 54% 38% 6%
2	O	198	67% 25% 6%
2	Q	198	5% 53% 37% 6%
3	C	83	48% 31% 6% 13%
3	P	83	52% 28% 6% 13%
4	E	601	18% 43% 52%
4	F	601	64% 49% 47%
4	R	601	6% 43% 49% 5%
4	S	601	39% 43% 50% 6%
5	G	117	41% 39% 14%
5	T	117	41% 38% 15%
6	H	139	49% 41% 6%
6	U	139	42% 44% 6% 6%
7	K	527	57% 35% 7%
7	X	527	53% 38% 7%
8	I	25	40% 52% 8%
8	L	25	40% 52% 8%
9	J	33	39% 48% 12%
9	M	33	36% 48% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ZN	X	600	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 54547 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	926	Total	C	N	O	S	0	0
			7462	4766	1252	1390	54		
1	N	926	Total	C	N	O	S	0	0
			7462	4766	1252	1390	54		

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1400	873	241	275	11		
2	D	186	Total	C	N	O	S	0	0
			1418	892	243	272	11		
2	O	187	Total	C	N	O	S	0	0
			1400	873	241	275	11		
2	Q	186	Total	C	N	O	S	0	0
			1418	892	243	272	11		

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	72	Total	C	N	O	S	0	0
			553	349	91	107	6		
3	P	72	Total	C	N	O	S	0	0
			553	349	91	107	6		

- Molecule 4 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	588	Total	C	N	O	S	1	0
			4567	2908	767	857	35		
4	R	588	Total	C	N	O	S	1	0
			4567	2908	767	857	35		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	596	Total	C	N	O	S	0	0
			4630	2940	787	869	34		
4	S	596	Total	C	N	O	S	0	0
			4630	2940	787	869	34		

- Molecule 5 is a protein called Non-structural protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	113	Total	C	N	O	S	0	0
			868	549	150	164	5		
5	T	113	Total	C	N	O	S	0	0
			868	549	150	164	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	SER	-	expression tag	UNP P0DTD1
G	-2	ASN	-	expression tag	UNP P0DTD1
G	-1	ALA	-	expression tag	UNP P0DTD1
G	0	MET	-	expression tag	UNP P0DTD1
T	-3	SER	-	expression tag	UNP P0DTD1
T	-2	ASN	-	expression tag	UNP P0DTD1
T	-1	ALA	-	expression tag	UNP P0DTD1
T	0	MET	-	expression tag	UNP P0DTD1

- Molecule 6 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			955	593	160	186	16		
6	U	130	Total	C	N	O	S	0	0
			947	589	159	183	16		

- Molecule 7 is a protein called Proofreading exoribonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	523	Total	C	N	O	S	0	0
			4169	2674	710	749	36		
7	X	524	Total	C	N	O	S	0	0
			4177	2679	710	752	36		

- Molecule 8 is a RNA chain called primer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	25	Total 545	C 242	N 105	O 173	P 25	0	0
8	L	25	Total 545	C 242	N 105	O 173	P 25	0	0

- Molecule 9 is a RNA chain called Template RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	33	Total 692	C 310	N 116	O 233	P 33	0	0
9	M	33	Total 692	C 310	N 116	O 233	P 33	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total 2	Zn 2	0
10	E	3	Total 3	Zn 3	0
10	H	2	Total 2	Zn 2	0
10	K	3	Total 3	Zn 3	0
10	N	2	Total 2	Zn 2	0
10	R	3	Total 3	Zn 3	0
10	U	2	Total 2	Zn 2	0
10	X	3	Total 3	Zn 3	0
10	F	3	Total 3	Zn 3	0
10	S	3	Total 3	Zn 3	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

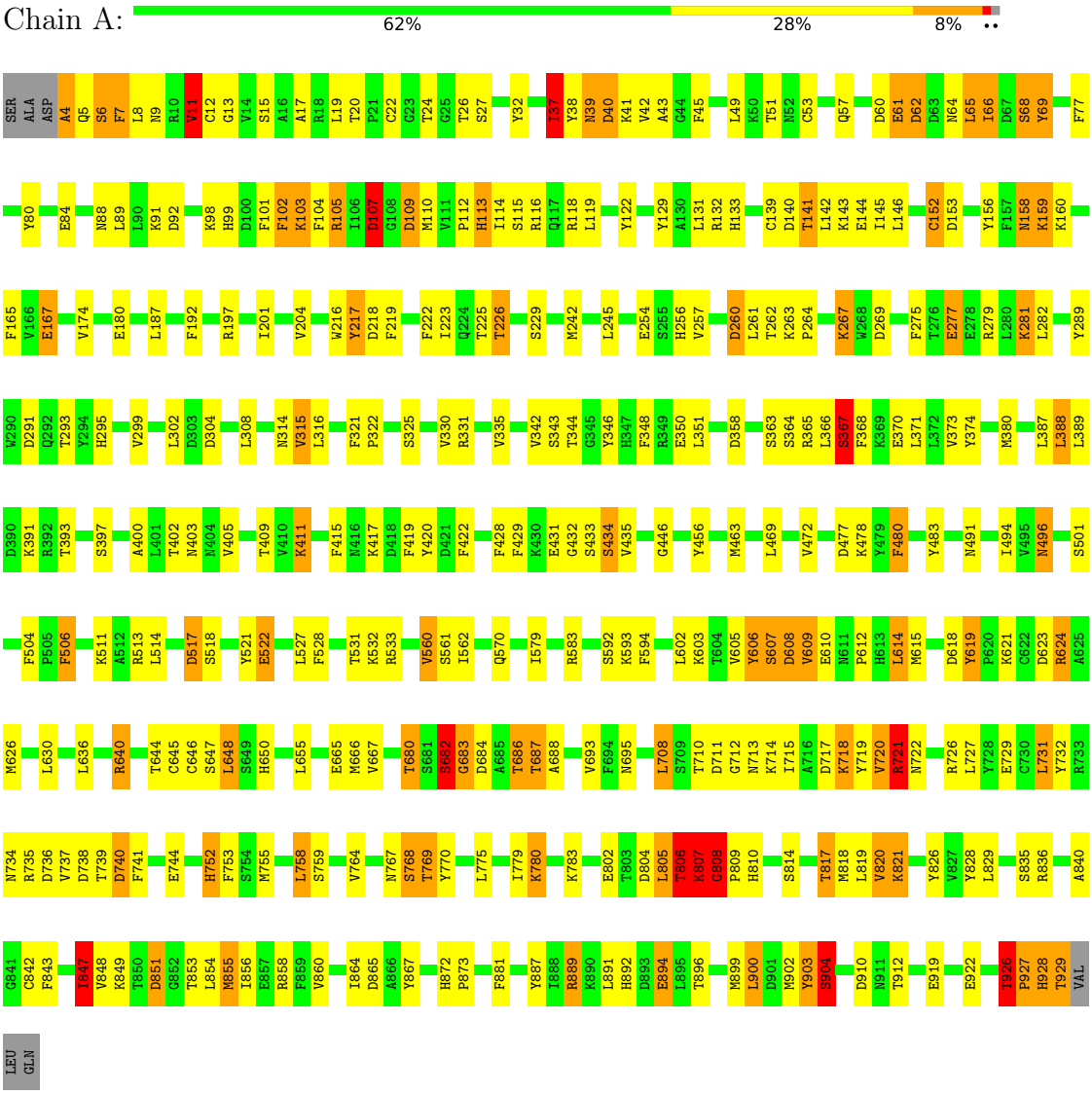
Mol	Chain	Residues	Atoms	AltConf
11	K	2	Total Mg 2 2	0
11	X	1	Total Mg 1 1	0

3 Residue-property plots (i)

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

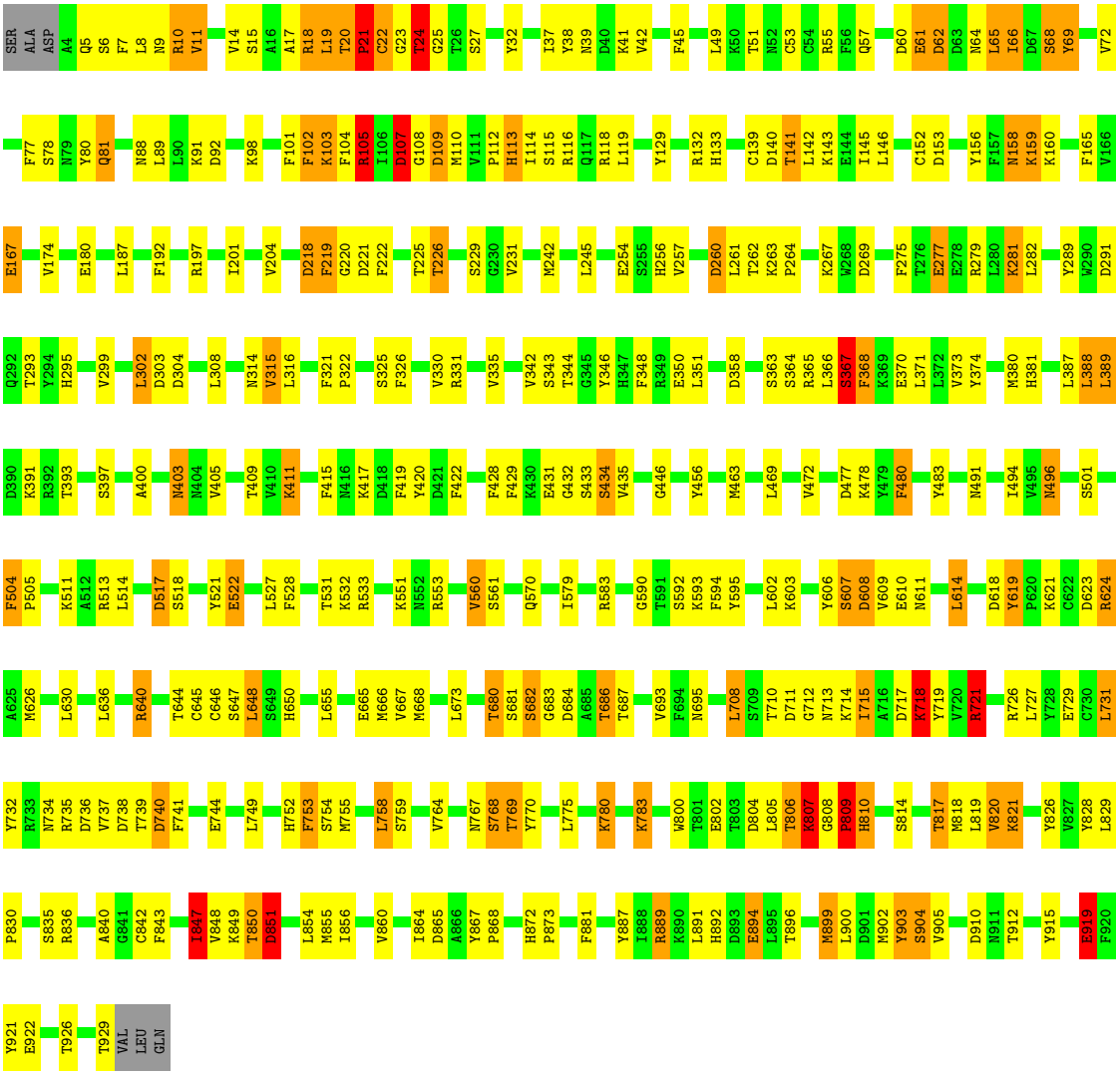
• Molecule 1: RNA-directed RNA polymerase

Chain A:



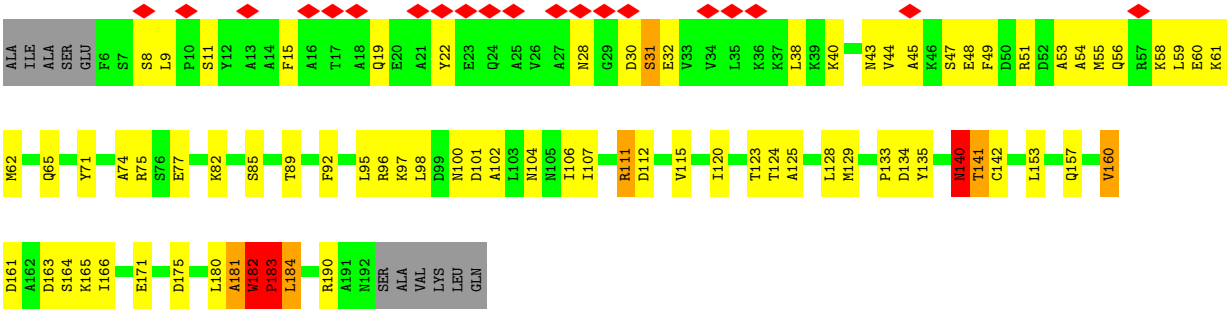
• Molecule 1: RNA-directed RNA polymerase

Chain N:



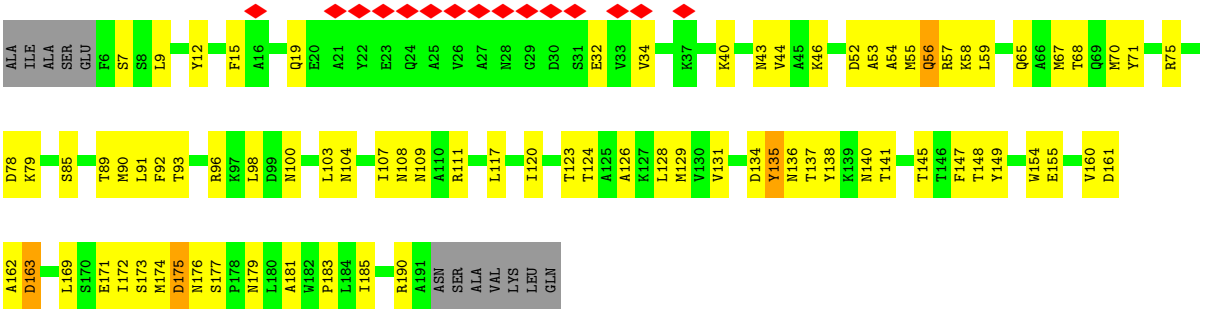
• Molecule 2: Non-structural protein 8

Chain B:



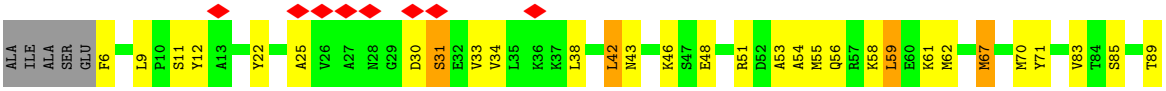
• Molecule 2: Non-structural protein 8

Chain D:



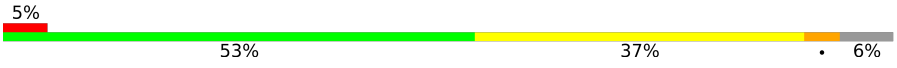
• Molecule 2: Non-structural protein 8

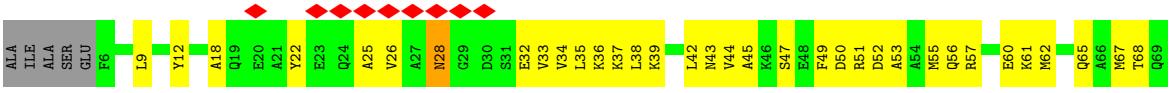
Chain O:

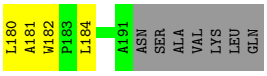


• Molecule 2: Non-structural protein 8

Chain Q:

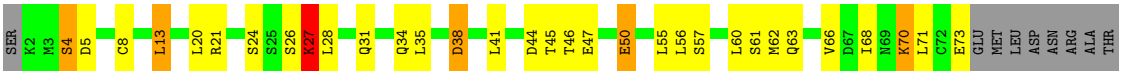






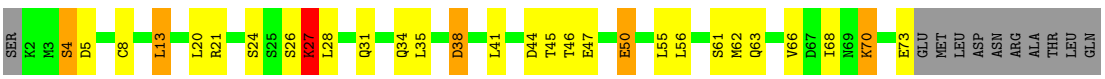
• Molecule 3: Non-structural protein 7

Chain C:



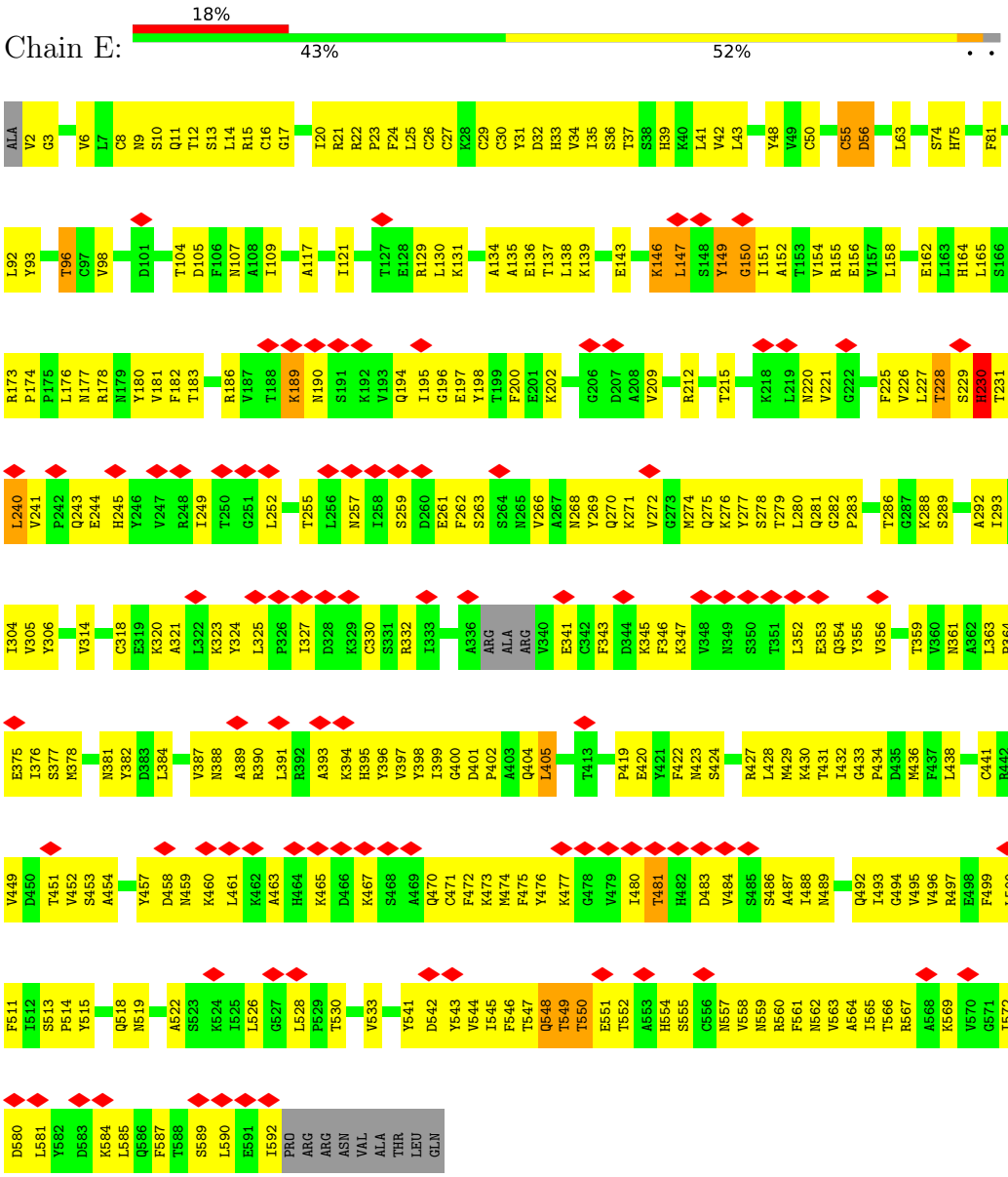
• Molecule 3: Non-structural protein 7

Chain P:



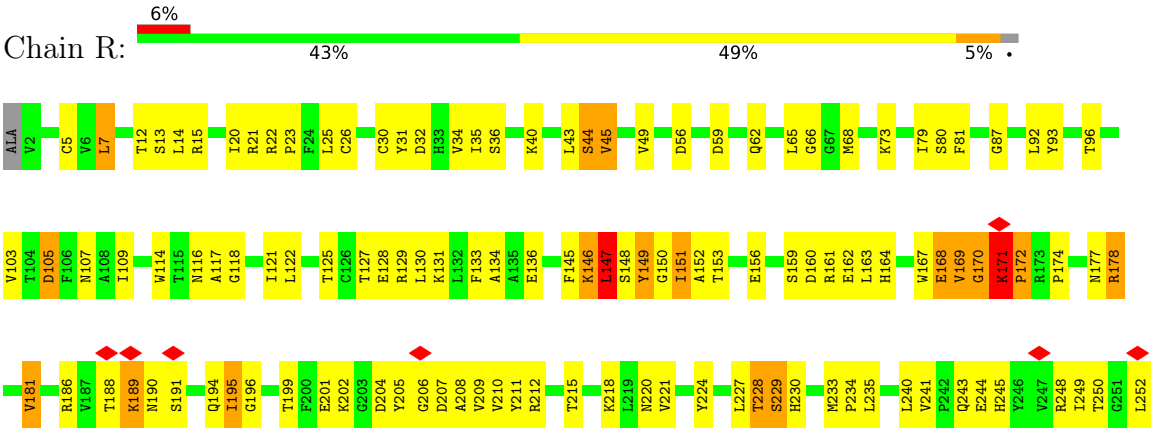
• Molecule 4: Helicase

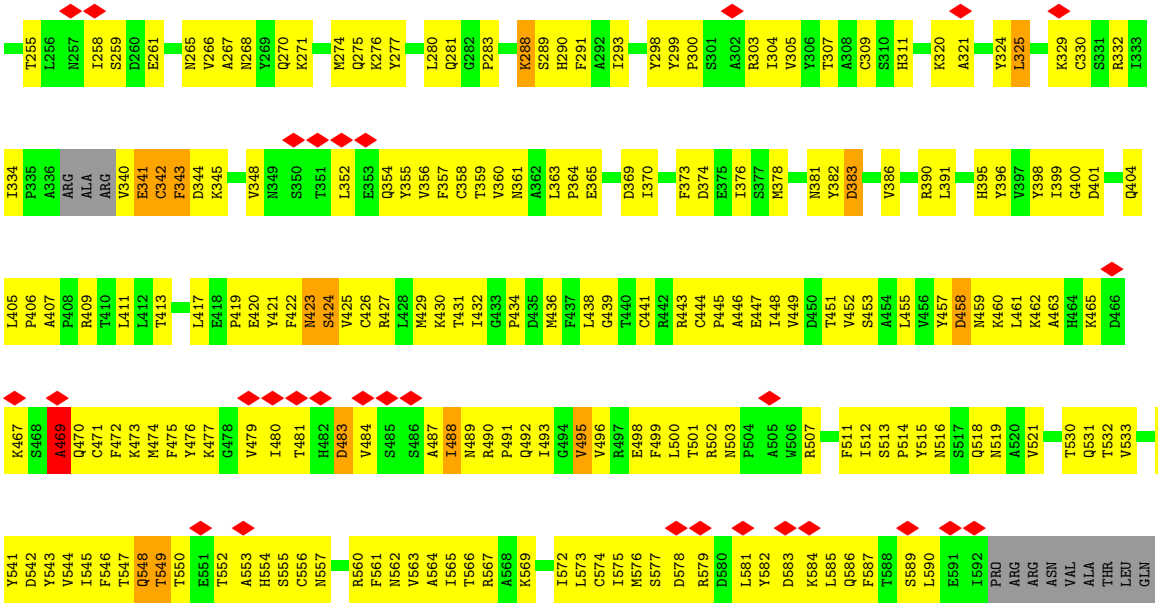
Chain E:



• Molecule 4: Helicase

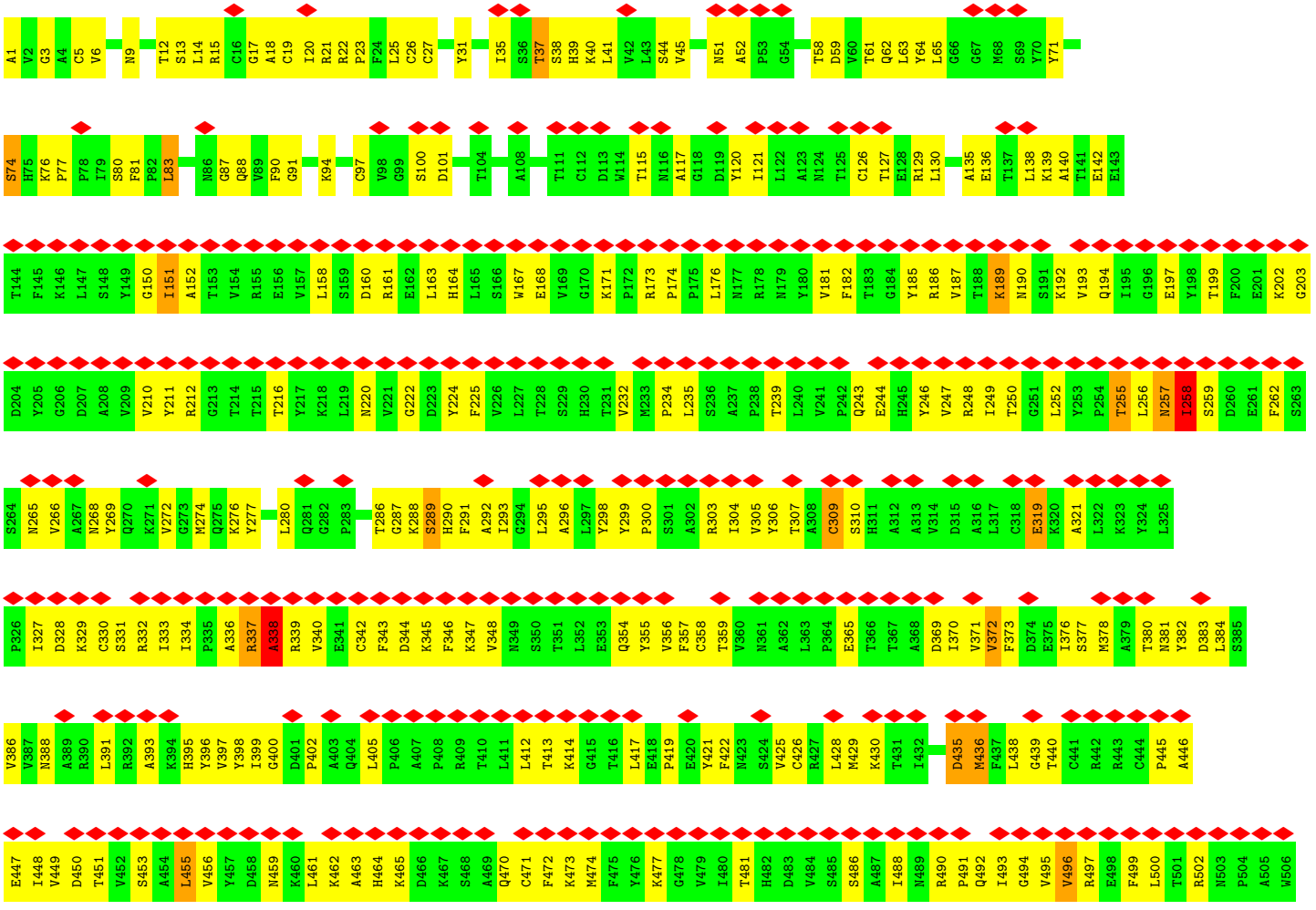
Chain R:

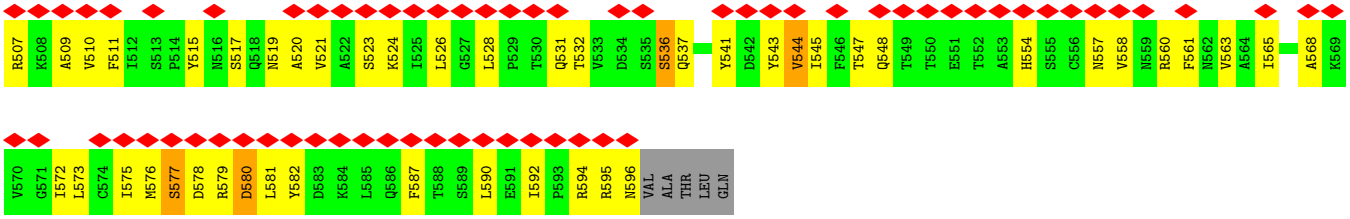




• Molecule 4: Helicase

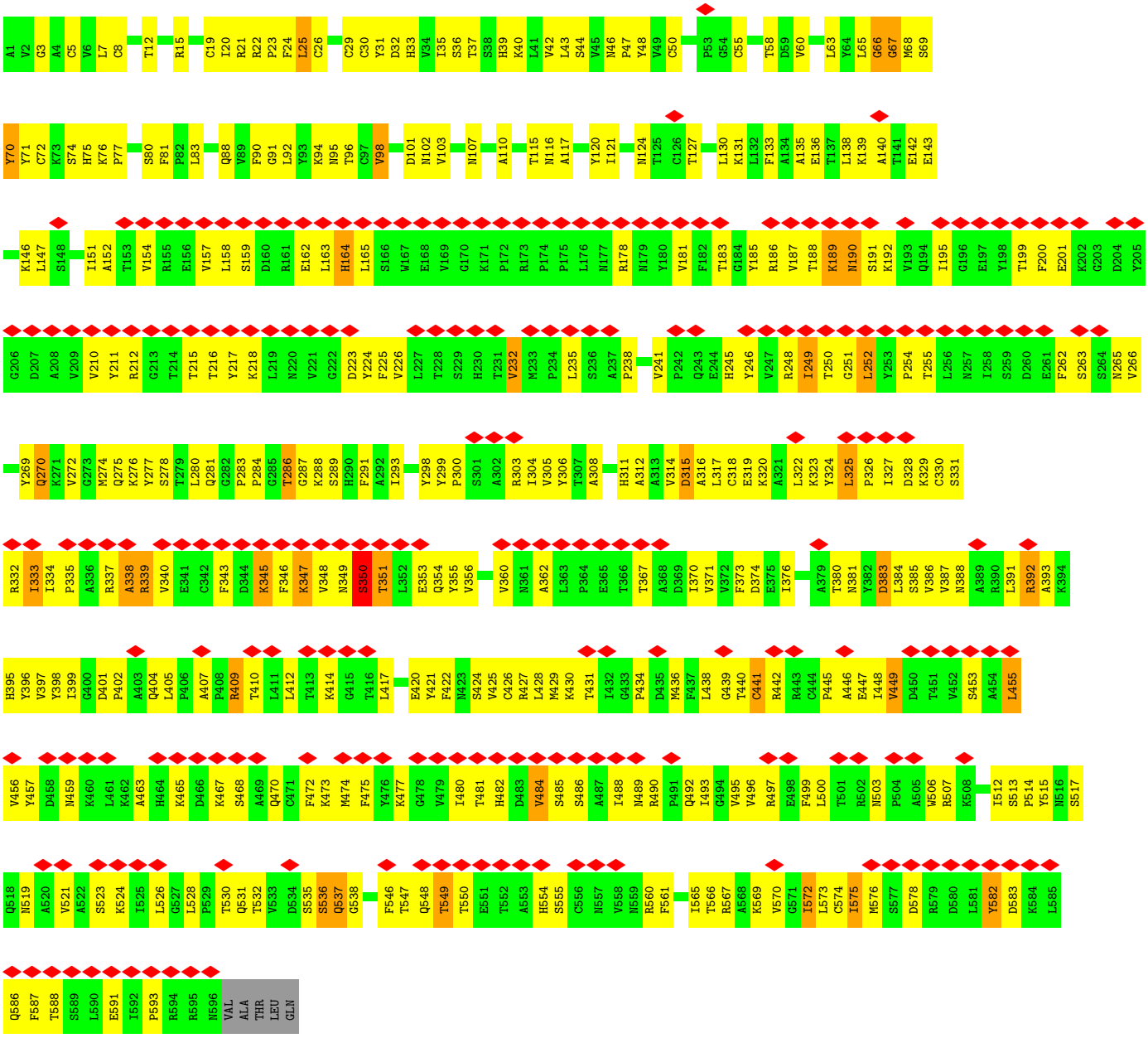
Chain F:





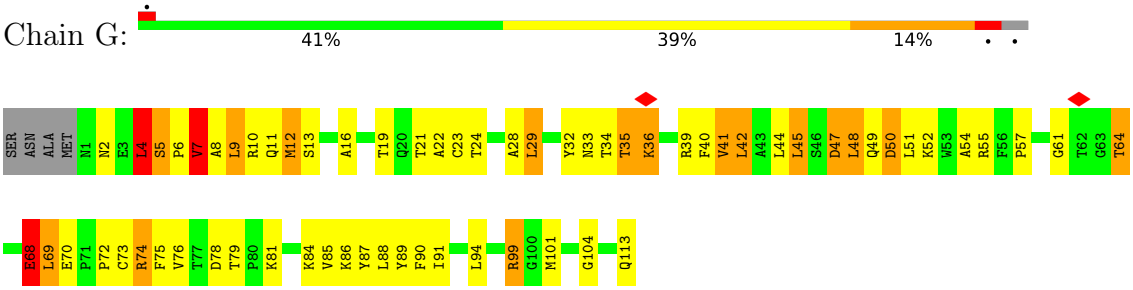
• Molecule 4: Helicase

Chain S:



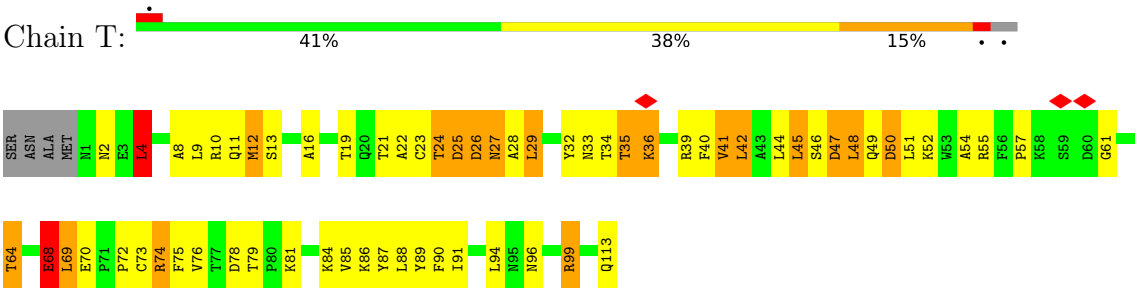
• Molecule 5: Non-structural protein 9

Chain G:



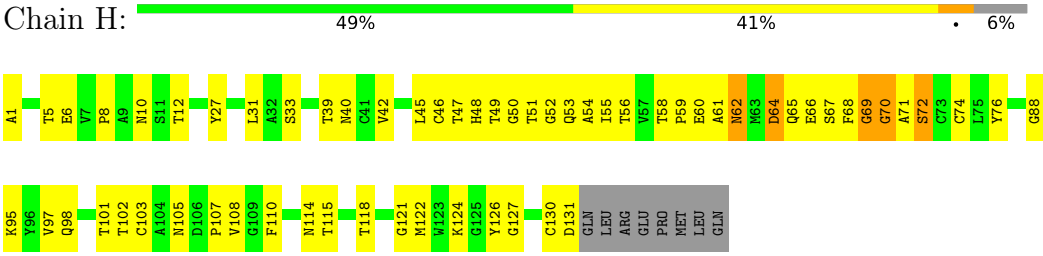
• Molecule 5: Non-structural protein 9

Chain T:



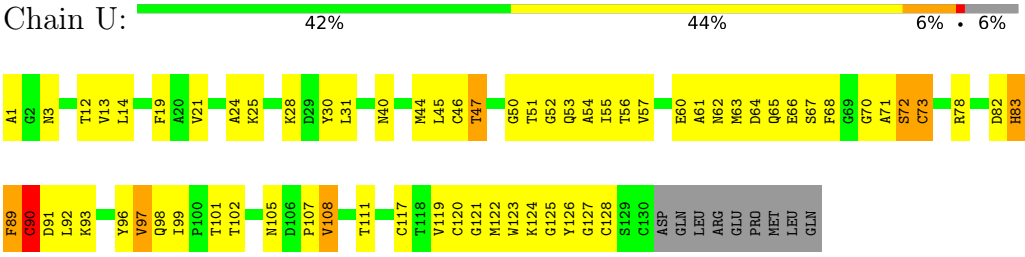
• Molecule 6: Non-structural protein 10

Chain H:



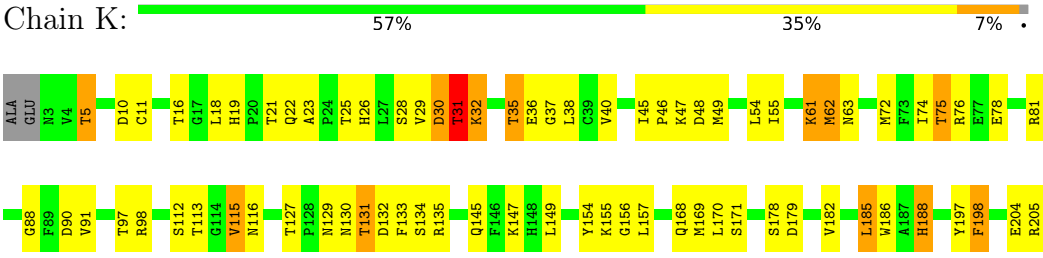
• Molecule 6: Non-structural protein 10

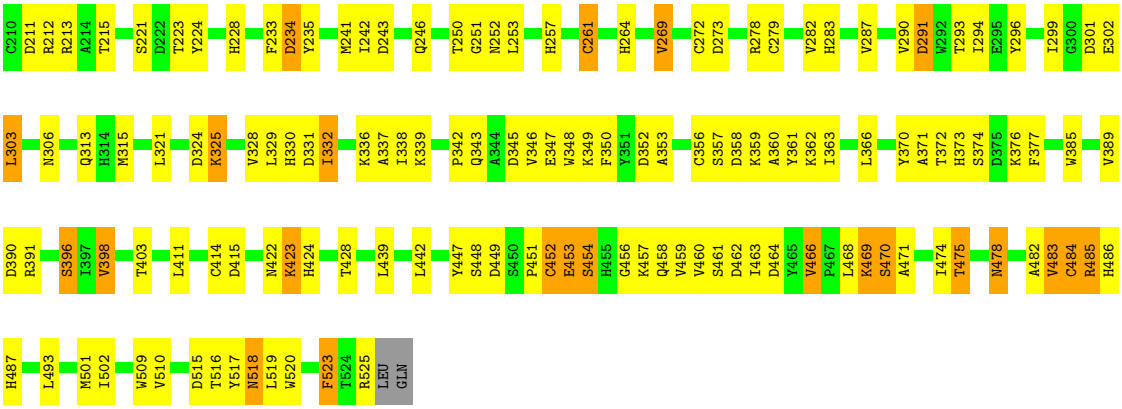
Chain U:



• Molecule 7: Proofreading exoribonuclease

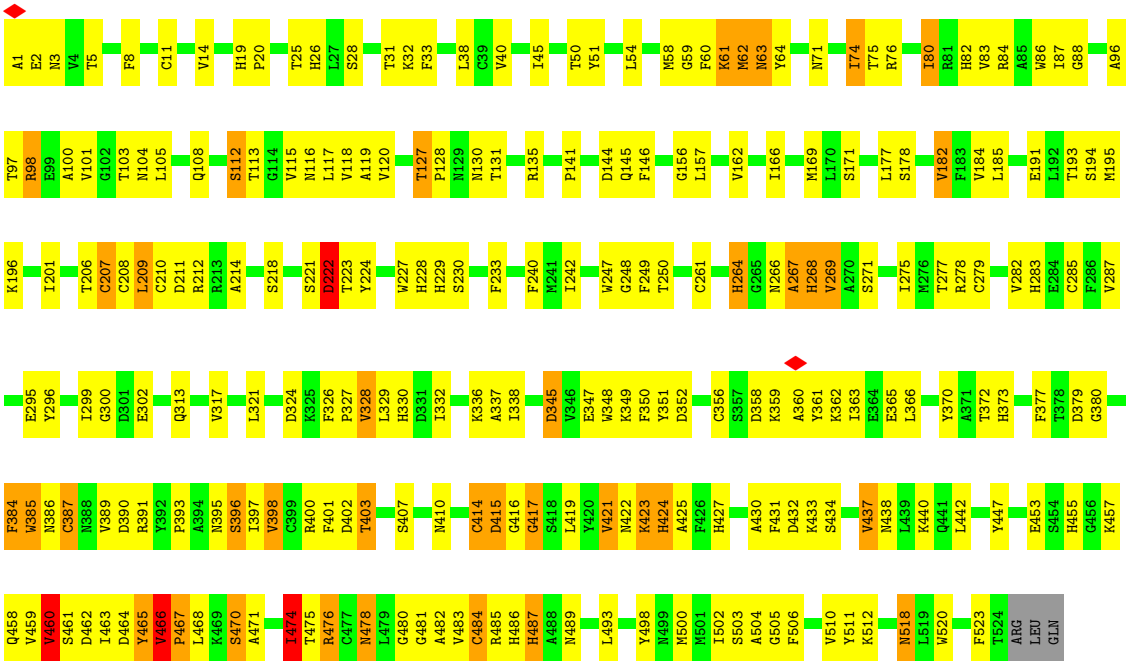
Chain K:





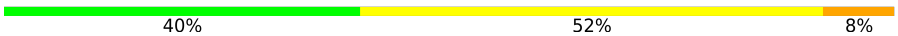
• Molecule 7: Proofreading exoribonuclease

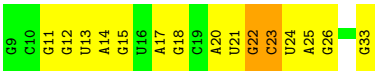
Chain X:



• Molecule 8: primer RNA

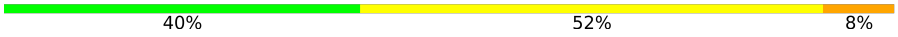
Chain I:

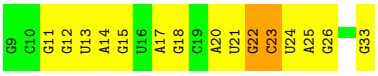




• Molecule 8: primer RNA

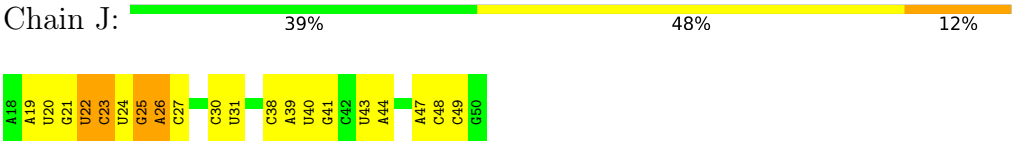
Chain L:





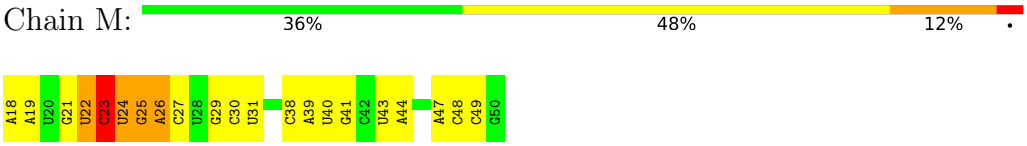
• Molecule 9: Template RNA

Chain J:



• Molecule 9: Template RNA

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.438	Depositor
Minimum map value	-0.945	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	474.87997, 474.87997, 474.87997	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.61	14/7651 (0.2%)	1.19	79/10383 (0.8%)
1	N	0.51	2/7651 (0.0%)	1.00	56/10383 (0.5%)
2	B	0.43	1/1418 (0.1%)	1.16	18/1927 (0.9%)
2	D	0.23	0/1437	0.72	5/1948 (0.3%)
2	O	0.36	0/1418	0.82	10/1927 (0.5%)
2	Q	0.26	0/1437	1.15	14/1948 (0.7%)
3	C	0.35	0/556	0.73	3/749 (0.4%)
3	P	0.35	0/556	0.92	3/749 (0.4%)
4	E	0.21	0/4670	0.66	15/6358 (0.2%)
4	F	0.19	0/4734	0.97	35/6443 (0.5%)
4	R	0.21	0/4670	0.97	32/6358 (0.5%)
4	S	0.19	0/4734	0.95	29/6443 (0.5%)
5	G	0.41	0/884	0.84	6/1200 (0.5%)
5	T	0.35	0/884	1.58	9/1200 (0.8%)
6	H	0.32	0/976	1.11	5/1327 (0.4%)
6	U	0.48	1/968 (0.1%)	1.18	15/1316 (1.1%)
7	K	0.39	1/4288 (0.0%)	0.96	38/5831 (0.7%)
7	X	0.39	1/4297 (0.0%)	1.16	54/5844 (0.9%)
8	I	0.42	0/611	0.34	0/953
8	L	0.42	0/611	0.34	0/953
9	J	0.56	1/770 (0.1%)	0.55	1/1195 (0.1%)
9	M	0.71	5/770 (0.6%)	0.59	2/1195 (0.2%)
All	All	0.40	26/55991 (0.0%)	0.99	429/76630 (0.6%)

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	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
4	E	0	1
4	R	0	2
All	All	0	5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	HIS	CA-C	-8.60	1.41	1.53
1	A	810	HIS	N-CA	-7.69	1.36	1.46
1	A	607	SER	CA-C	-7.60	1.42	1.53
9	M	21	G	C1'-N9	-6.95	1.37	1.48
1	A	810	HIS	C-O	-6.94	1.15	1.23
1	A	927	PRO	N-CD	6.67	1.57	1.47
1	N	810	HIS	C-O	-6.41	1.15	1.24
9	J	26	A	O3'-P	-6.36	1.51	1.61
9	M	26	A	O3'-P	-6.33	1.51	1.61
1	A	608	ASP	N-CA	6.31	1.54	1.46
1	A	810	HIS	CA-CB	-6.02	1.43	1.53
1	A	506	PHE	C-O	-5.99	1.16	1.24
1	A	607	SER	N-CA	5.89	1.55	1.46
9	M	23	C	C1'-N1	5.71	1.56	1.47
9	M	19	A	C1'-N9	-5.68	1.39	1.48
1	N	809	PRO	C-O	-5.62	1.16	1.23
7	K	452	CYS	CA-C	-5.40	1.45	1.52
1	A	809	PRO	CA-C	-5.39	1.44	1.52
9	M	18	A	C1'-N9	-5.39	1.39	1.48
6	U	71	ALA	C-O	-5.38	1.17	1.24
1	A	504	PHE	CA-C	-5.36	1.45	1.52
1	A	806	THR	CA-C	-5.33	1.45	1.52
2	B	184	LEU	C-O	-5.30	1.17	1.23
7	X	484	CYS	CA-C	-5.19	1.46	1.52
1	A	851	ASP	CA-C	-5.15	1.45	1.52
1	A	606	TYR	CA-C	-5.08	1.46	1.52

All (429) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	25	ASP	N-CA-C	42.65	157.46	110.97
4	R	170	GLY	N-CA-C	38.00	158.62	112.64
7	X	208	CYS	N-CA-C	34.16	152.10	111.11
1	A	217	TYR	N-CA-C	32.75	154.65	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	536	SER	N-CA-C	28.41	148.46	113.23
2	Q	125	ALA	N-CA-C	27.61	145.65	111.69
1	A	808	GLY	CA-C-N	27.48	154.19	119.84
1	A	808	GLY	C-N-CA	27.48	154.19	119.84
1	A	926	THR	CA-C-N	27.44	154.14	119.84
1	A	926	THR	C-N-CA	27.44	154.14	119.84
4	S	537	GLN	N-CA-C	-25.99	75.00	110.35
1	N	107	ASP	CB-CA-C	-25.46	75.08	111.23
2	B	141	THR	N-CA-C	25.33	144.66	113.50
4	F	536	SER	CB-CA-C	-24.49	70.96	110.14
6	H	39	THR	N-CA-C	24.20	144.13	111.71
1	N	23	GLY	N-CA-C	-22.96	71.62	111.57
1	N	855	MET	CB-CA-C	-22.88	72.79	111.23
4	F	337	ARG	N-CA-C	21.94	145.71	113.02
4	S	288	LYS	N-CA-C	21.92	137.25	111.82
7	K	469	LYS	CB-CA-C	-21.73	75.76	110.74
7	X	97	THR	N-CA-C	21.41	141.40	112.93
4	R	148	SER	N-CA-C	-20.85	84.20	110.88
1	A	855	MET	CB-CA-C	-20.84	77.58	111.13
4	R	147	LEU	N-CA-C	19.87	153.12	110.80
1	N	606	TYR	CB-CA-C	-19.68	82.59	112.12
1	A	607	SER	N-CA-C	19.00	137.13	111.30
1	N	19	LEU	CB-CA-C	-18.55	80.47	110.14
6	H	39	THR	CB-CA-C	-18.34	74.26	110.75
4	F	288	LYS	N-CA-C	18.01	130.60	110.97
2	Q	28	ASN	CB-CA-C	-17.65	83.97	110.62
4	S	456	VAL	N-CA-C	-17.03	98.10	111.90
4	F	578	ASP	N-CA-CB	-16.83	84.12	110.55
1	N	648	LEU	N-CA-C	16.74	131.59	111.33
6	U	88	GLY	N-CA-C	16.54	152.38	113.18
1	A	648	LEU	N-CA-C	15.70	129.95	111.11
2	D	135	TYR	N-CA-C	15.67	131.81	113.01
7	X	60	PHE	N-CA-C	-15.65	82.68	108.34
4	F	337	ARG	CB-CA-C	-15.56	84.29	110.44
4	E	150	GLY	N-CA-C	15.34	149.53	113.18
4	E	549	THR	N-CA-CB	-15.22	87.52	110.20
3	P	26	SER	N-CA-C	15.22	131.98	113.41
2	Q	126	ALA	N-CA-CB	-15.18	86.92	109.83
4	S	289	SER	N-CA-C	-15.15	92.42	114.39
2	O	141	THR	N-CA-C	15.13	132.61	113.55
4	E	548	GLN	N-CA-C	-15.06	84.16	108.41
7	X	384	PHE	N-CA-C	-14.90	85.09	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	904	SER	N-CA-C	14.83	133.84	113.37
7	K	424	HIS	N-CA-C	-14.75	85.35	109.40
1	A	926	THR	CB-CA-C	14.69	131.03	108.84
6	U	84	PRO	CB-CA-C	-14.69	86.09	111.21
4	F	455	LEU	N-CA-C	14.24	132.54	112.04
4	R	171	LYS	N-CA-CB	-14.19	85.12	110.37
7	K	31	THR	N-CA-C	14.18	130.04	113.02
7	X	460	VAL	CB-CA-C	-14.07	88.22	111.29
7	X	465	TYR	N-CA-C	-14.02	83.54	107.80
1	A	5	GLN	N-CA-C	-14.02	98.11	112.97
4	F	577	SER	CB-CA-C	-13.86	87.63	111.05
6	H	40	ASN	N-CA-CB	-13.74	88.63	111.17
1	N	753	PHE	N-CA-C	-13.61	87.91	108.46
4	R	549	THR	N-CA-CB	-13.57	89.72	109.94
4	S	350	SER	N-CA-C	13.57	139.70	110.80
2	Q	112	ASP	CB-CA-C	-13.56	89.29	111.13
5	T	24	THR	N-CA-C	-13.28	90.11	110.17
7	X	466	VAL	N-CA-CB	-13.10	96.66	111.20
7	X	209	LEU	N-CA-CB	-13.00	91.26	110.49
4	F	577	SER	N-CA-C	-12.96	85.93	108.23
7	X	61	LYS	N-CA-CB	-12.82	84.74	110.64
1	N	18	ARG	N-CA-C	-12.81	85.31	107.99
4	R	424	SER	N-CA-C	12.64	126.28	111.11
1	A	808	GLY	N-CA-C	12.54	137.92	112.34
1	A	855	MET	N-CA-C	12.46	128.70	112.26
1	A	904	SER	N-CA-C	12.43	128.21	112.92
1	N	856	ILE	N-CA-C	-12.39	98.92	113.42
1	A	903	TYR	N-CA-C	-12.36	91.97	110.14
4	S	349	ASN	N-CA-C	12.31	128.51	113.12
1	A	218	ASP	N-CA-CB	-12.31	89.50	110.17
1	A	504	PHE	C-N-CD	-12.19	93.77	120.60
1	A	11	VAL	CB-CA-C	-12.19	99.60	111.30
1	N	856	ILE	N-CA-CB	-12.13	95.61	112.35
4	F	258	ILE	N-CA-CB	12.03	128.39	111.90
1	N	754	SER	N-CA-C	-12.01	88.21	108.75
1	A	40	ASP	N-CA-C	11.97	127.07	111.75
4	F	338	ALA	N-CA-CB	-11.92	90.35	110.49
2	D	135	TYR	N-CA-CB	-11.84	89.67	110.39
1	N	607	SER	N-CA-CB	-11.84	90.49	110.49
1	N	68	SER	N-CA-C	-11.74	90.67	108.52
1	A	856	ILE	N-CA-CB	-11.74	92.11	110.54
1	N	69	TYR	N-CA-CB	11.70	131.20	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	239	THR	N-CA-C	11.66	128.19	112.68
4	R	548	GLN	CB-CA-C	-11.62	92.28	111.68
5	G	7	VAL	CB-CA-C	-11.57	93.58	110.83
4	R	149	TYR	N-CA-C	-11.53	90.80	108.67
6	U	85	ASN	CA-C-N	11.52	134.23	119.84
6	U	85	ASN	C-N-CA	11.52	134.23	119.84
7	K	62	MET	N-CA-C	11.51	129.90	107.57
1	A	403	ASN	N-CA-C	11.51	129.25	113.37
7	K	211	ASP	N-CA-CB	-11.48	93.77	110.65
4	R	341	GLU	N-CA-C	11.46	127.20	108.52
4	F	289	SER	N-CA-C	-11.35	99.43	113.38
1	A	504	PHE	CA-C-N	11.32	154.18	127.00
1	A	504	PHE	C-N-CA	11.32	154.18	127.00
1	A	22	CYS	N-CA-C	-11.26	96.72	113.61
2	Q	125	ALA	CB-CA-C	-11.23	90.15	110.70
2	D	134	ASP	N-CA-C	-11.12	92.36	108.60
7	X	58	MET	N-CA-C	11.12	128.58	111.56
7	K	31	THR	N-CA-CB	-11.09	94.39	110.47
7	X	208	CYS	CB-CA-C	-11.05	93.13	110.81
2	B	30	ASP	N-CA-C	11.04	127.61	112.93
4	S	66	GLY	N-CA-C	11.03	139.32	113.18
4	S	536	SER	CB-CA-C	-11.03	87.16	109.55
4	R	341	GLU	CB-CA-C	-10.97	92.20	110.19
7	K	470	SER	CB-CA-C	-10.96	86.60	109.94
1	A	904	SER	N-CA-CB	-10.91	94.63	110.56
1	N	903	TYR	N-CA-C	-10.83	92.39	109.72
4	E	484	VAL	N-CA-C	10.79	122.93	110.62
7	X	424	HIS	N-CA-C	-10.78	92.23	109.59
7	K	371	ALA	CB-CA-C	10.76	128.03	110.92
1	A	68	SER	N-CA-C	-10.75	92.23	108.46
3	C	26	SER	N-CA-C	10.63	127.34	112.04
4	R	169	VAL	N-CA-C	10.62	131.42	109.34
5	T	27	ASN	N-CA-CB	-10.62	94.20	110.44
4	F	537	GLN	N-CA-C	-10.59	98.49	114.16
2	B	28	ASN	CB-CA-C	-10.54	93.60	111.31
2	Q	99	ASP	N-CA-C	10.52	126.60	111.56
6	H	69	GLY	N-CA-C	-10.48	88.34	113.18
3	P	26	SER	CB-CA-C	-10.44	90.96	109.24
2	B	140	ASN	CB-CA-C	10.40	127.34	110.90
5	T	27	ASN	N-CA-C	10.40	126.05	113.16
1	N	20	THR	N-CA-CB	-10.34	92.93	110.10
1	N	218	ASP	N-CA-C	10.32	126.33	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	810	HIS	N-CA-C	-10.29	97.22	112.04
4	S	455	LEU	N-CA-C	10.26	127.25	111.56
7	X	461	SER	N-CA-CB	10.24	126.99	111.01
3	P	27	LYS	N-CA-C	-10.23	100.33	113.12
7	K	471	ALA	N-CA-CB	-9.97	96.00	110.56
1	A	69	TYR	N-CA-CB	9.95	129.01	111.69
1	A	109	ASP	N-CA-CB	-9.94	93.98	110.39
4	F	289	SER	N-CA-CB	-9.92	95.75	110.53
1	A	808	GLY	C-N-CD	-9.90	84.42	125.00
7	X	461	SER	N-CA-C	-9.89	98.76	114.09
6	U	90	CYS	N-CA-C	-9.82	98.01	110.19
7	X	505	GLY	N-CA-C	9.82	131.46	114.76
7	X	63	ASN	N-CA-C	-9.81	90.84	107.23
7	X	385	TRP	N-CA-C	-9.80	88.53	107.44
2	B	28	ASN	N-CA-C	-9.78	89.55	107.75
5	T	25	ASP	N-CA-CB	-9.78	95.63	109.91
4	S	537	GLN	N-CA-CB	-9.74	95.72	110.04
4	S	538	GLY	N-CA-C	9.68	128.18	115.40
7	X	267	ALA	N-CA-C	-9.66	95.58	110.17
7	X	423	LYS	CB-CA-C	9.63	129.59	110.42
5	G	7	VAL	N-CA-C	9.62	121.64	108.17
2	Q	113	GLY	N-CA-C	9.58	131.05	114.76
2	B	141	THR	CB-CA-C	-9.55	91.91	109.29
1	A	216	TRP	CB-CA-C	-9.54	93.45	109.48
7	X	504	ALA	CB-CA-C	-9.53	93.85	110.72
7	K	30	ASP	CB-CA-C	-9.51	94.11	109.80
7	X	177	LEU	N-CA-C	9.51	125.33	112.68
6	U	89	PHE	N-CA-CB	-9.50	95.63	110.55
1	A	926	THR	N-CA-C	-9.49	95.58	110.10
7	X	64	TYR	N-CA-C	-9.44	95.36	109.81
9	M	23	C	C2'-C3'-O3'	9.39	123.58	109.50
2	B	54	ALA	N-CA-CB	-9.37	96.82	110.40
4	F	257	ASN	N-CA-C	-9.34	90.90	110.80
4	F	259	SER	N-CA-C	-9.30	91.70	107.23
7	X	96	ALA	CB-CA-C	-9.28	94.72	109.84
7	K	234	ASP	N-CA-C	9.25	121.54	110.44
2	O	54	ALA	N-CA-CB	-9.22	98.33	110.59
6	U	89	PHE	N-CA-C	-9.11	93.67	108.52
4	F	348	VAL	N-CA-C	9.10	121.22	111.58
2	B	53	ALA	CB-CA-C	9.08	125.13	109.24
1	A	687	THR	N-CA-C	9.06	121.23	111.36
1	N	609	VAL	N-CA-C	-9.04	95.14	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	21	PRO	CB-CA-C	-9.04	95.88	110.25
7	K	372	THR	N-CA-C	9.04	124.71	111.96
7	X	250	THR	N-CA-C	8.97	124.61	111.96
1	N	754	SER	N-CA-CB	8.93	127.30	111.13
7	K	250	THR	N-CA-C	8.91	124.52	111.96
4	S	350	SER	N-CA-CB	-8.88	95.49	110.49
1	N	69	TYR	N-CA-C	-8.85	95.61	109.07
1	N	68	SER	CB-CA-C	8.83	124.21	109.99
1	N	753	PHE	CB-CA-C	8.82	123.92	109.72
1	A	647	SER	N-CA-C	-8.75	97.28	110.14
7	K	470	SER	N-CA-C	-8.74	95.27	108.99
4	R	470	GLN	N-CA-C	-8.70	100.56	113.61
4	F	258	ILE	N-CA-C	8.54	119.29	112.12
7	X	98	ARG	N-CA-C	-8.52	103.32	114.31
2	B	141	THR	N-CA-CB	-8.51	98.03	110.53
7	X	421	VAL	CB-CA-C	-8.50	101.03	111.32
2	B	112	ASP	N-CA-CB	-8.49	98.15	110.80
1	A	69	TYR	N-CA-C	-8.49	96.43	109.24
6	H	70	GLY	N-CA-C	8.45	122.87	112.64
5	T	26	ASP	N-CA-CB	8.40	125.06	111.20
1	A	109	ASP	N-CA-C	8.39	123.36	107.75
1	N	647	SER	N-CA-C	-8.37	97.83	110.14
4	F	537	GLN	CB-CA-C	8.37	123.25	110.37
7	X	98	ARG	N-CA-CB	8.36	122.02	110.90
7	K	457	LYS	CB-CA-C	-8.33	98.24	111.48
1	A	217	TYR	CB-CA-C	-8.30	94.38	109.15
4	E	230	HIS	N-CA-C	8.28	128.43	110.80
7	X	385	TRP	N-CA-CB	8.21	125.16	110.95
4	R	342	CYS	N-CA-CB	-8.17	96.69	110.49
7	K	198	PHE	N-CA-CB	-8.14	98.69	111.39
1	N	904	SER	N-CA-CB	-8.14	93.74	110.67
1	N	903	TYR	CB-CA-C	-8.13	93.31	109.33
4	F	337	ARG	N-CA-CB	-8.11	97.81	111.27
1	A	849	LYS	N-CA-C	-8.11	102.96	113.17
1	N	849	LYS	N-CA-C	-8.06	103.45	113.28
7	X	97	THR	N-CA-CB	-8.06	96.31	110.34
1	A	753	PHE	N-CA-CB	-8.05	98.91	111.23
7	K	30	ASP	N-CA-C	-8.05	97.94	110.42
4	E	240	LEU	N-CA-C	-8.02	93.74	108.02
4	S	537	GLN	CB-CA-C	8.01	123.95	109.62
4	F	580	ASP	N-CA-CB	-8.00	100.42	110.98
2	B	183	PRO	N-CA-C	-7.99	96.02	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	107	ASP	N-CA-C	7.98	127.80	110.80
4	R	150	GLY	N-CA-C	-7.94	94.36	113.18
4	R	483	ASP	CB-CA-C	-7.88	100.69	113.37
7	X	424	HIS	N-CA-CB	-7.85	98.05	110.69
7	K	423	LYS	CB-CA-C	7.85	125.70	111.03
1	A	20	THR	CA-C-N	-7.82	111.94	119.76
1	A	20	THR	C-N-CA	-7.82	111.94	119.76
4	E	239	THR	CB-CA-C	-7.80	97.21	110.24
4	F	456	VAL	N-CA-C	-7.78	93.16	109.34
1	N	403	ASN	N-CA-C	7.77	121.86	112.38
1	N	647	SER	CB-CA-C	-7.76	96.54	110.36
4	R	147	LEU	CB-CA-C	-7.76	94.97	110.42
1	N	15	SER	N-CA-C	-7.76	98.19	109.59
4	R	469	ALA	CB-CA-C	-7.75	95.00	110.42
1	N	17	ALA	CB-CA-C	-7.71	94.70	109.66
7	K	471	ALA	N-CA-C	7.63	122.31	112.92
1	A	68	SER	CB-CA-C	7.63	122.01	109.72
2	O	141	THR	N-CA-CB	-7.61	99.36	110.40
6	U	73	CYS	N-CA-C	7.59	122.84	112.90
4	R	189	LYS	CA-C-N	7.58	135.35	121.70
4	R	189	LYS	C-N-CA	7.58	135.35	121.70
4	E	189	LYS	CA-C-N	7.57	135.33	121.70
4	E	189	LYS	C-N-CA	7.57	135.33	121.70
7	X	417	GLY	N-CA-C	-7.57	98.40	111.57
4	S	289	SER	N-CA-CB	-7.56	101.00	110.98
2	B	142	CYS	N-CA-C	-7.52	92.92	107.44
4	F	536	SER	N-CA-C	7.50	120.64	108.34
7	K	372	THR	N-CA-CB	-7.49	96.87	110.27
1	A	647	SER	CB-CA-C	-7.48	97.04	110.36
7	K	32	LYS	N-CA-C	-7.43	102.55	111.69
4	S	189	LYS	CA-C-N	7.39	135.00	121.70
4	S	189	LYS	C-N-CA	7.39	135.00	121.70
1	A	402	THR	CB-CA-C	-7.34	96.44	110.24
2	Q	114	CYS	N-CA-C	-7.34	94.96	108.02
4	S	347	LYS	N-CA-C	7.33	119.79	110.33
2	Q	114	CYS	N-CA-CB	7.33	121.98	110.84
1	A	37	ILE	CB-CA-C	-7.32	101.48	110.99
4	S	348	VAL	N-CA-C	7.29	118.23	111.45
7	X	268	HIS	N-CA-C	7.28	121.69	107.57
1	N	687	THR	N-CA-C	7.26	118.98	111.14
1	N	24	THR	N-CA-C	7.25	126.24	110.80
4	F	189	LYS	CA-C-N	7.25	134.75	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	189	LYS	C-N-CA	7.25	134.75	121.70
7	X	60	PHE	CB-CA-C	-7.21	98.60	110.14
4	S	338	ALA	N-CA-C	7.21	119.34	110.91
1	N	758	LEU	CB-CA-C	7.20	123.17	110.36
3	C	26	SER	CB-CA-C	-7.17	97.44	110.56
1	A	928	HIS	N-CA-C	-7.15	95.58	110.80
7	K	198	PHE	N-CA-C	7.12	121.92	111.87
2	O	31	SER	N-CA-C	7.12	125.97	110.80
4	R	45	VAL	N-CA-C	-7.11	94.54	109.34
1	N	24	THR	N-CA-CB	-7.08	98.53	110.49
1	A	368	PHE	N-CA-C	7.02	122.96	111.37
2	B	31	SER	N-CA-CB	7.02	122.27	111.46
2	O	140	ASN	CB-CA-C	7.00	122.75	110.85
4	E	231	THR	N-CA-CB	6.99	121.52	110.55
4	R	484	VAL	N-CA-C	6.99	123.88	109.34
1	A	926	THR	C-N-CD	-6.99	96.35	125.00
4	R	168	GLU	N-CA-C	-6.98	100.40	110.24
4	S	190	ASN	CB-CA-C	-6.97	96.86	110.10
1	A	367	SER	CB-CA-C	-6.97	98.39	110.45
7	K	470	SER	N-CA-CB	-6.96	98.58	111.52
2	O	30	ASP	N-CA-C	-6.94	98.99	109.96
1	A	26	THR	N-CA-C	-6.92	102.70	113.02
2	B	30	ASP	CB-CA-C	-6.86	99.31	110.08
7	K	171	SER	CA-C-N	-6.85	111.23	122.54
7	K	171	SER	C-N-CA	-6.85	111.23	122.54
1	N	302	LEU	N-CA-C	6.84	122.03	111.56
7	X	177	LEU	CB-CA-C	-6.84	98.82	110.24
1	N	105	ARG	CG-CD-NE	6.80	126.96	112.00
4	S	190	ASN	N-CA-C	6.78	129.98	111.00
1	A	105	ARG	CG-CD-NE	6.78	126.91	112.00
4	S	441	CYS	CB-CA-C	-6.78	98.08	109.53
7	X	465	TYR	CA-C-N	6.76	127.19	122.60
7	X	465	TYR	C-N-CA	6.76	127.19	122.60
4	F	456	VAL	N-CA-CB	6.75	122.37	111.23
2	B	54	ALA	N-CA-C	6.75	122.05	113.55
5	T	25	ASP	CB-CA-C	-6.75	100.57	110.96
4	R	343	PHE	CB-CA-C	-6.73	98.86	109.70
1	A	153	ASP	N-CA-CB	-6.73	100.30	111.20
6	U	85	ASN	N-CA-C	-6.71	99.01	109.87
2	Q	100	ASN	N-CA-C	6.70	120.75	109.76
7	X	460	VAL	N-CA-C	6.70	123.27	109.34
1	A	683	GLY	N-CA-C	6.69	129.04	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	99	ASP	CB-CA-C	-6.63	103.33	111.82
1	N	368	PHE	N-CA-C	6.62	122.29	111.37
4	E	548	GLN	CB-CA-C	-6.62	99.89	110.81
7	K	211	ASP	N-CA-C	6.61	122.32	113.72
7	K	61	LYS	N-CA-C	6.60	120.19	111.28
1	A	807	LYS	N-CA-C	-6.58	99.26	108.54
2	O	30	ASP	CB-CA-C	-6.58	99.86	112.43
9	J	26	A	C1'-C2'-O2'	-6.54	98.59	108.40
7	K	63	ASN	N-CA-CB	-6.54	101.23	111.23
9	M	26	A	C1'-C2'-O2'	-6.53	98.61	108.40
1	N	24	THR	CB-CA-C	-6.52	97.45	110.42
6	U	85	ASN	CB-CA-C	6.52	123.73	110.31
1	N	851	ASP	N-CA-CB	-6.50	99.51	110.49
2	Q	28	ASN	N-CA-C	-6.48	96.48	108.02
7	X	421	VAL	N-CA-C	6.48	117.03	106.72
1	A	758	LEU	CB-CA-C	6.47	121.88	110.36
2	B	182	TRP	N-CA-C	6.46	124.10	109.81
1	A	721	ARG	N-CA-C	-6.46	104.17	111.14
1	N	446	GLY	N-CA-C	6.45	128.47	113.18
4	S	442	ARG	N-CA-CB	-6.45	101.67	110.95
1	A	851	ASP	N-CA-C	-6.43	97.11	110.80
4	F	436	MET	N-CA-CB	6.41	120.72	110.86
1	A	37	ILE	N-CA-C	6.37	117.41	107.28
1	A	4	ALA	CB-CA-C	-6.34	100.99	110.50
4	F	378	MET	N-CA-CB	-6.29	102.20	110.88
7	X	384	PHE	CB-CA-C	6.29	120.59	109.72
7	X	62	MET	N-CA-C	6.27	118.85	109.25
7	X	59	GLY	N-CA-C	-6.25	98.37	113.18
4	E	149	TYR	N-CA-C	6.24	124.09	110.80
4	R	548	GLN	N-CA-C	-6.24	95.46	107.57
1	N	807	LYS	N-CA-C	-6.24	100.81	110.10
1	A	752	HIS	CB-CA-C	6.21	119.51	109.07
1	N	758	LEU	N-CA-C	-6.21	101.01	110.14
2	O	53	ALA	CB-CA-C	6.20	120.56	109.29
2	B	142	CYS	N-CA-CB	6.18	121.64	110.95
7	X	386	ASN	CB-CA-C	-6.17	101.30	111.36
2	Q	126	ALA	N-CA-C	6.17	119.18	110.23
1	N	22	CYS	N-CA-CB	-6.17	100.80	110.98
4	S	410	THR	N-CA-C	6.17	119.64	111.75
4	R	343	PHE	N-CA-C	6.16	118.93	110.24
1	A	403	ASN	N-CA-CB	-6.14	97.89	110.67
7	K	22	GLN	N-CA-CB	-6.14	101.30	111.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	141	THR	CB-CA-C	-6.14	99.83	109.34
4	F	435	ASP	CB-CA-C	-6.10	98.29	110.42
4	R	423	ASN	CB-CA-C	-6.08	100.00	110.95
7	X	96	ALA	N-CA-C	6.08	119.42	109.76
1	A	446	GLY	N-CA-C	6.07	127.56	113.18
1	A	217	TYR	N-CA-CB	-6.06	101.84	110.81
2	O	54	ALA	N-CA-C	6.05	121.33	113.88
1	N	367	SER	CB-CA-C	-6.05	99.50	111.60
7	K	233	PHE	CB-CA-C	-6.05	99.55	109.53
7	K	62	MET	CB-CA-C	-6.04	101.60	111.68
7	X	178	SER	N-CA-C	-6.03	100.16	109.14
4	S	345	LYS	N-CA-C	6.01	120.69	112.04
1	N	303	ASP	N-CA-C	-6.00	100.65	109.18
6	U	83	HIS	CA-C-N	6.00	126.78	120.12
6	U	83	HIS	C-N-CA	6.00	126.78	120.12
4	F	290	HIS	N-CA-C	-5.99	104.33	111.69
3	C	27	LYS	N-CA-C	-5.97	104.35	111.69
4	S	67	GLY	N-CA-C	-5.94	99.10	113.18
1	A	753	PHE	N-CA-C	5.94	118.29	108.49
5	T	4	LEU	N-CA-C	5.93	121.44	113.72
4	R	344	ASP	N-CA-CB	-5.93	102.41	110.95
1	A	39	ASN	N-CA-C	-5.91	101.71	110.46
1	A	758	LEU	N-CA-C	-5.90	101.47	110.14
7	K	458	GLN	N-CA-C	-5.87	98.30	110.80
7	X	178	SER	N-CA-CB	5.87	121.13	111.62
4	R	44	SER	N-CA-C	5.86	123.28	110.80
1	A	720	VAL	CA-C-N	-5.85	112.49	120.44
1	A	720	VAL	C-N-CA	-5.85	112.49	120.44
1	N	718	LYS	CB-CG-CD	5.84	124.73	111.30
1	A	718	LYS	CB-CG-CD	5.83	124.72	111.30
1	N	153	ASP	N-CA-CB	-5.82	101.13	111.08
1	A	687	THR	CB-CA-C	-5.79	101.01	110.85
5	G	4	LEU	CA-C-N	-5.79	107.68	121.80
5	G	4	LEU	C-N-CA	-5.79	107.68	121.80
7	K	424	HIS	N-CA-CB	-5.78	100.78	110.83
4	F	455	LEU	CB-CA-C	-5.77	100.01	110.56
6	U	90	CYS	N-CA-CB	-5.76	102.42	110.25
5	G	68	GLU	CA-CB-CG	5.76	125.61	114.10
5	T	68	GLU	CA-CB-CG	5.75	125.61	114.10
7	K	251	GLY	N-CA-C	-5.74	104.70	112.57
1	N	919	GLU	CA-CB-CG	5.73	125.57	114.10
1	A	504	PHE	CB-CA-C	-5.73	100.71	108.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	919	GLU	CA-CB-CG	5.73	125.56	114.10
2	D	32	GLU	N-CA-C	5.72	119.44	112.23
4	F	44	SER	N-CA-C	-5.71	101.12	109.63
2	D	134	ASP	CB-CA-C	-5.68	100.03	111.17
7	K	97	THR	N-CA-CB	-5.68	100.89	110.49
5	G	8	ALA	N-CA-CB	-5.67	100.90	110.49
7	X	268	HIS	N-CA-CB	-5.63	101.18	110.53
4	F	336	ALA	CB-CA-C	5.63	118.51	109.27
1	A	688	ALA	N-CA-C	-5.61	104.79	111.69
4	R	168	GLU	CB-CA-C	5.58	118.69	109.70
7	K	197	TYR	CB-CA-C	5.56	119.69	110.90
1	A	682	SER	CB-CA-C	5.56	121.48	110.42
4	S	455	LEU	CB-CA-C	-5.53	100.69	111.03
1	N	847	ILE	CB-CA-C	-5.51	102.25	111.29
6	U	71	ALA	CA-C-N	-5.51	111.94	120.31
6	U	71	ALA	C-N-CA	-5.51	111.94	120.31
4	F	579	ARG	CB-CA-C	5.49	120.48	110.11
1	A	903	TYR	CB-CA-C	-5.47	100.62	110.36
7	K	423	LYS	N-CA-C	5.47	119.93	111.56
1	A	927	PRO	CA-N-CD	-5.47	104.34	112.00
1	N	302	LEU	CB-CA-C	-5.47	100.80	111.03
1	A	39	ASN	CB-CA-C	-5.45	101.02	110.45
7	X	250	THR	CB-CA-C	-5.45	101.23	110.88
4	E	240	LEU	N-CA-CB	5.44	119.11	110.84
2	B	111	ARG	CB-CA-C	5.42	120.66	110.63
1	N	721	ARG	CG-CD-NE	5.41	123.91	112.00
7	X	222	ASP	CB-CA-C	5.40	117.95	109.84
1	N	18	ARG	N-CA-CB	-5.40	101.50	110.47
4	E	146	LYS	N-CA-C	5.38	120.20	111.37
4	F	258	ILE	CB-CA-C	-5.38	105.64	110.91
7	X	97	THR	CB-CA-C	-5.37	101.65	110.08
1	A	402	THR	N-CA-C	-5.37	101.60	109.81
7	K	234	ASP	N-CA-CB	-5.37	99.62	111.69
1	A	152	CYS	CB-CA-C	-5.35	99.71	110.30
7	X	248	GLY	N-CA-C	5.34	125.84	113.18
1	N	220	GLY	N-CA-C	-5.33	100.54	113.18
7	X	249	PHE	N-CA-CB	-5.33	102.33	110.85
7	X	222	ASP	N-CA-C	-5.22	102.56	110.24
4	R	229	SER	N-CA-C	5.21	118.11	110.30
4	S	409	ARG	N-CA-C	5.21	118.31	111.28
1	N	608	ASP	N-CA-C	-5.17	99.79	110.80
2	Q	100	ASN	N-CA-CB	-5.16	102.01	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	289	SER	CB-CA-C	-5.12	100.73	109.65
7	X	474	ILE	CG1-CB-CG2	-5.07	95.49	110.70
4	R	172	PRO	CA-C-N	5.06	128.95	120.86
4	R	172	PRO	C-N-CA	5.06	128.95	120.86
7	X	387	CYS	N-CA-C	-5.05	99.56	108.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	926	THR	Peptide
4	E	230	HIS	Peptide
2	O	182	TRP	Peptide
4	R	147	LEU	Peptide
4	R	171	LYS	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	7462	0	7201	278	0
1	N	7462	0	7202	287	0
2	B	1400	0	1372	67	0
2	D	1418	0	1427	52	0
2	O	1400	0	1372	31	0
2	Q	1418	0	1427	63	0
3	C	553	0	585	28	0
3	P	553	0	585	21	0
4	E	4567	0	4508	314	0
4	F	4630	0	4584	258	0
4	R	4567	0	4508	297	0
4	S	4630	0	4584	257	0
5	G	868	0	880	64	0
5	T	868	0	880	60	0
6	H	955	0	910	41	0
6	U	947	0	906	59	0
7	K	4169	0	4051	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	4177	0	4058	186	0
8	I	545	0	272	22	0
8	L	545	0	272	19	0
9	J	692	0	355	37	0
9	M	692	0	355	57	0
10	A	2	0	0	0	0
10	E	3	0	0	0	0
10	F	3	0	0	0	0
10	H	2	0	0	0	0
10	K	3	0	0	0	0
10	N	2	0	0	0	0
10	R	3	0	0	0	0
10	S	3	0	0	0	0
10	U	2	0	0	0	0
10	X	3	0	0	2	0
11	K	2	0	0	0	0
11	X	1	0	0	0	0
All	All	54547	0	52294	2528	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 24.

All (2528) 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:A:7:PHE:HZ	1:A:113:HIS:CD2	1.45	1.32
9:M:22:U:H2'	9:M:23:C:N3	1.46	1.28
4:F:337:ARG:O	4:F:337:ARG:HD3	1.24	1.28
6:U:70:GLY:HA3	6:U:92:LEU:O	1.28	1.28
9:M:22:U:H2'	9:M:23:C:C2	1.68	1.26
4:F:337:ARG:O	4:F:337:ARG:CD	1.82	1.25
9:M:22:U:C6	9:M:23:C:N4	2.04	1.25
1:A:7:PHE:CZ	1:A:113:HIS:CD2	2.30	1.20
2:B:161:ASP:HA	2:B:184:LEU:HD23	1.22	1.16
1:A:682:SER:O	1:A:687:THR:HG21	1.48	1.12
1:N:24:THR:HG23	1:N:25:GLY:N	1.55	1.11
7:X:460:VAL:O	7:X:460:VAL:HG12	1.30	1.11
1:A:926:THR:CG2	1:A:927:PRO:HD2	1.81	1.10
7:X:465:TYR:CD1	7:X:465:TYR:O	2.03	1.09
1:A:602:LEU:O	1:A:606:TYR:HD2	1.37	1.08
1:N:24:THR:CG2	1:N:25:GLY:H	1.56	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:26:ASP:O	5:T:26:ASP:OD1	1.73	1.06
1:A:7:PHE:HZ	1:A:113:HIS:NE2	1.53	1.05
5:G:7:VAL:CG1	5:G:7:VAL:O	2.02	1.05
9:M:22:U:C5	9:M:23:C:N4	2.19	1.04
7:K:296:TYR:HD1	7:K:423:LYS:O	1.40	1.03
1:N:24:THR:HG23	1:N:25:GLY:H	0.90	1.03
1:N:105:ARG:HB2	1:N:105:ARG:HH11	1.21	1.02
1:A:926:THR:HG23	1:A:927:PRO:HD2	1.38	1.01
6:U:70:GLY:CA	6:U:92:LEU:O	2.08	1.01
5:G:7:VAL:O	5:G:7:VAL:HG13	1.57	1.00
9:M:22:U:C2'	9:M:23:C:C2	2.45	1.00
1:N:218:ASP:O	1:N:218:ASP:OD1	1.79	1.00
7:X:63:ASN:OD1	7:X:63:ASN:O	1.78	1.00
7:X:460:VAL:O	7:X:460:VAL:CG1	2.07	0.99
4:E:55:CYS:SG	4:E:75:HIS:HE1	1.84	0.99
4:E:239:THR:O	4:E:384:LEU:HD12	1.61	0.99
4:F:377:SER:O	4:F:422:PHE:HE2	1.46	0.97
1:A:602:LEU:O	1:A:606:TYR:CD2	2.18	0.96
4:R:341:GLU:O	4:R:341:GLU:CD	2.08	0.96
1:A:7:PHE:CZ	1:A:113:HIS:NE2	2.32	0.95
7:X:61:LYS:O	7:X:61:LYS:HG2	1.64	0.93
4:R:488:ILE:HG23	4:R:518:GLN:HA	1.52	0.92
1:A:721:ARG:HG2	1:A:721:ARG:HH11	1.34	0.92
1:A:37:ILE:HG22	1:A:37:ILE:O	1.70	0.90
4:E:453:SER:HA	4:E:457:TYR:HB2	1.54	0.90
1:A:612:PRO:HB2	1:A:805:LEU:CD1	2.01	0.90
4:E:149:TYR:HB2	4:E:172:PRO:HB2	1.52	0.90
4:F:377:SER:O	4:F:422:PHE:CE2	2.24	0.89
1:N:726:ARG:NH2	1:N:738:ASP:OD2	2.05	0.89
5:G:4:LEU:HD12	5:G:5:SER:HB3	1.55	0.89
1:A:726:ARG:NH2	1:A:738:ASP:OD2	2.05	0.88
9:M:22:U:C2'	9:M:23:C:N3	2.36	0.88
2:B:43:ASN:ND2	9:J:48:C:H5"	1.89	0.88
1:N:24:THR:CG2	1:N:25:GLY:N	2.24	0.88
3:C:71:LEU:HD23	2:D:96:ARG:HH22	1.39	0.87
9:M:25:G:N3	9:M:25:G:H2'	1.89	0.87
1:N:21:PRO:O	1:N:21:PRO:HG2	1.74	0.87
1:N:608:ASP:O	1:N:608:ASP:OD1	1.92	0.87
4:F:304:ILE:HD12	4:F:370:ILE:HG22	1.57	0.87
2:B:161:ASP:HA	2:B:184:LEU:CD2	2.05	0.87
2:D:147:PHE:HB3	2:D:154:TRP:HB2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:421:VAL:O	7:X:421:VAL:HG12	1.75	0.87
4:F:531:GLN:NE2	4:F:536:SER:OG	2.07	0.87
4:F:289:SER:O	4:F:293:ILE:HG13	1.75	0.87
4:S:503:ASN:HB2	4:S:506:TRP:HB2	1.57	0.86
7:X:210:CYS:HG	10:X:600:ZN:ZN	0.85	0.86
1:N:758:LEU:HD23	1:N:759:SER:H	1.41	0.86
9:J:25:G:N3	9:J:25:G:H2'	1.89	0.86
4:E:286:THR:H	4:E:288:LYS:HZ1	1.22	0.85
8:I:11:G:O6	9:J:49:C:N4	2.08	0.85
8:L:11:G:O6	9:M:49:C:N4	2.08	0.85
5:T:19:THR:H	5:T:22:ALA:HB3	1.41	0.85
1:A:7:PHE:CZ	1:A:113:HIS:HD2	1.90	0.85
4:R:228:THR:O	4:R:230:HIS:CD2	2.30	0.84
1:A:758:LEU:HD23	1:A:759:SER:H	1.42	0.84
1:A:6:SER:HB3	1:A:104:PHE:CZ	2.13	0.84
4:F:494:GLY:HA2	4:F:497:ARG:HE	1.42	0.84
4:S:591:GLU:HG3	4:S:593:PRO:HD2	1.58	0.84
2:Q:99:ASP:OD1	2:Q:99:ASP:O	1.96	0.83
4:F:332:ARG:HD3	4:F:347:LYS:O	1.78	0.83
5:G:19:THR:H	5:G:22:ALA:HB3	1.41	0.82
2:B:161:ASP:CA	2:B:184:LEU:HD23	2.07	0.82
4:F:303:ARG:HD3	4:F:354:GLN:HA	1.61	0.82
4:R:332:ARG:HG2	4:R:343:PHE:HB3	1.60	0.82
1:A:11:VAL:HG12	1:A:12:CYS:N	1.94	0.81
4:F:182:PHE:HD2	4:F:225:PHE:HB3	1.45	0.81
1:N:277:GLU:CD	1:N:277:GLU:H	1.89	0.81
1:N:501:SER:CB	9:M:25:G:OP1	2.29	0.81
1:N:105:ARG:HH11	1:N:105:ARG:CB	1.93	0.81
5:T:8:ALA:C	5:T:9:LEU:HD22	2.06	0.81
1:N:740:ASP:OD1	1:N:740:ASP:N	2.14	0.81
9:M:22:U:H2'	9:M:23:C:C4	2.16	0.81
1:A:740:ASP:OD1	1:A:740:ASP:N	2.14	0.81
4:F:332:ARG:HH22	4:F:345:LYS:HE3	1.44	0.81
4:E:12:THR:HG22	4:E:14:LEU:H	1.45	0.80
4:F:90:PHE:HA	4:F:94:LYS:HE2	1.63	0.80
1:A:277:GLU:H	1:A:277:GLU:CD	1.89	0.80
1:N:804:ASP:OD2	1:N:806:THR:OG1	2.00	0.80
4:R:228:THR:O	4:R:230:HIS:NE2	2.15	0.80
4:F:332:ARG:CD	4:F:347:LYS:O	2.30	0.79
4:E:16:CYS:HB3	4:E:23:PRO:HD2	1.63	0.79
7:K:484:CYS:SG	7:K:487:HIS:ND1	2.54	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:403:ASN:O	2:O:129:MET:HE1	1.83	0.79
1:N:511:LYS:NZ	9:M:25:G:H21	1.80	0.79
7:X:465:TYR:O	7:X:465:TYR:HD1	1.66	0.79
4:E:149:TYR:C	4:E:227:LEU:HD22	2.08	0.78
1:N:511:LYS:NZ	9:M:25:G:N2	2.32	0.78
2:Q:18:ALA:HB1	2:Q:42:LEU:HD22	1.64	0.78
1:A:808:GLY:HA3	1:A:817:THR:HG21	1.66	0.78
4:E:321:ALA:O	4:E:325:LEU:N	2.15	0.78
6:U:83:HIS:NE2	6:U:90:CYS:HB2	1.98	0.78
4:F:580:ASP:OD1	4:F:580:ASP:N	2.17	0.78
1:A:6:SER:HB3	1:A:104:PHE:HZ	1.48	0.77
1:A:607:SER:O	1:A:607:SER:OG	1.79	0.77
6:H:52:GLY:HA2	6:H:65:GLN:HE22	1.49	0.77
4:R:268:ASN:HA	4:R:271:LYS:HE3	1.65	0.77
4:R:189:LYS:HB2	4:R:190:ASN:HB2	1.66	0.77
1:A:513:ARG:O	1:A:517:ASP:HB2	1.85	0.77
1:N:513:ARG:O	1:N:517:ASP:HB2	1.85	0.77
4:S:474:MET:HE3	4:S:582:TYR:HB3	1.67	0.77
2:B:43:ASN:ND2	9:J:48:C:C5'	2.46	0.77
4:E:233:MET:HE3	4:E:234:PRO:HD2	1.67	0.77
4:S:407:ALA:HB3	4:S:409:ARG:HE	1.49	0.77
2:D:161:ASP:HB2	2:D:181:ALA:HB3	1.68	0.76
4:S:574:CYS:HB3	4:S:576:MET:HE1	1.65	0.76
7:X:88:GLY:H	7:X:112:SER:HB3	1.50	0.76
4:R:401:ASP:HB3	4:R:404:GLN:HG3	1.68	0.76
9:J:25:G:O2'	9:J:26:A:P	2.44	0.76
2:Q:99:ASP:O	2:Q:99:ASP:CG	2.28	0.76
9:M:25:G:O2'	9:M:26:A:P	2.44	0.76
2:B:141:THR:HG22	2:B:141:THR:O	1.86	0.75
4:E:22:ARG:HD2	4:E:43:LEU:HD12	1.68	0.75
4:R:533:VAL:HG21	4:R:560:ARG:HG2	1.68	0.75
4:E:493:ILE:HG22	4:E:497:ARG:HE	1.52	0.75
4:S:305:VAL:HB	4:S:371:VAL:HG22	1.69	0.75
4:R:128:GLU:HA	4:R:131:LYS:HD3	1.69	0.74
8:L:22:G:H1	9:M:38:C:H42	1.35	0.74
1:A:158:ASN:N	1:A:158:ASN:OD1	2.17	0.74
1:N:158:ASN:N	1:N:158:ASN:OD1	2.17	0.74
1:N:501:SER:OG	9:M:25:G:OP1	2.02	0.74
4:R:489:ASN:HB3	4:R:492:GLN:HB2	1.69	0.74
8:I:22:G:H1	9:J:38:C:H42	1.35	0.74
4:R:146:LYS:O	4:R:146:LYS:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:ARG:HB2	1:N:105:ARG:NH1	2.01	0.74
6:H:64:ASP:O	6:H:101:THR:OG1	2.05	0.74
7:X:156:GLY:HA3	7:X:157:LEU:HD23	1.68	0.74
1:A:612:PRO:HB2	1:A:805:LEU:HD12	1.69	0.73
5:T:44:LEU:HB3	5:T:89:TYR:HB2	1.69	0.73
5:G:44:LEU:HB3	5:G:89:TYR:HB2	1.69	0.73
5:T:73:CYS:HB3	5:T:88:LEU:HB3	1.70	0.73
4:F:19:CYS:SG	4:F:39:HIS:CE1	2.80	0.73
4:S:482:HIS:ND1	4:S:484:VAL:O	2.18	0.73
2:B:11:SER:HB3	2:B:48:GLU:HB3	1.70	0.73
4:R:156:GLU:HA	4:R:221:VAL:HG12	1.69	0.73
7:X:302:GLU:OE2	7:X:422:ASN:ND2	2.20	0.73
1:A:367:SER:N	1:A:370:GLU:OE2	2.21	0.73
7:K:296:TYR:CD1	7:K:423:LYS:O	2.32	0.73
7:X:296:TYR:HD2	7:X:423:LYS:O	1.70	0.73
4:E:15:ARG:HB3	4:E:22:ARG:HG3	1.68	0.73
4:E:330:CYS:HA	4:E:355:TYR:HB2	1.70	0.73
1:A:718:LYS:HA	1:A:721:ARG:HD3	1.69	0.73
7:K:264:HIS:HE1	7:K:279:CYS:SG	2.08	0.73
5:G:73:CYS:HB3	5:G:88:LEU:HB3	1.70	0.73
1:A:612:PRO:HB2	1:A:805:LEU:HD11	1.71	0.73
4:S:116:ASN:HB3	4:S:414:LYS:HE2	1.71	0.73
1:N:367:SER:N	1:N:370:GLU:OE2	2.21	0.73
4:F:337:ARG:CD	4:F:337:ARG:C	2.62	0.72
2:D:162:ALA:HB2	2:D:183:PRO:HG2	1.69	0.72
4:S:475:PHE:HB3	4:S:492:GLN:HE22	1.55	0.72
4:E:448:ILE:HG23	4:E:565:ILE:HG22	1.71	0.72
4:R:149:TYR:O	4:R:149:TYR:CD1	2.43	0.72
4:R:330:CYS:HB3	4:R:357:PHE:HE1	1.53	0.72
6:U:93:LYS:NZ	7:X:127:THR:O	2.22	0.72
2:B:161:ASP:HB3	2:B:184:LEU:HD21	1.69	0.72
4:R:406:PRO:HB2	4:R:409:ARG:HH12	1.55	0.72
1:A:11:VAL:CG1	1:A:12:CYS:N	2.48	0.72
4:R:114:TRP:O	4:R:411:LEU:HD21	1.90	0.72
4:S:576:MET:HG2	4:S:578:ASP:HB2	1.70	0.72
1:N:21:PRO:O	1:N:21:PRO:CG	2.36	0.72
6:U:19:PHE:HE1	7:X:196:LYS:HA	1.54	0.72
4:S:370:ILE:HG13	4:S:395:HIS:HB2	1.72	0.72
1:A:103:LYS:HZ2	1:A:103:LYS:HB3	1.54	0.72
2:Q:147:PHE:HB3	2:Q:154:TRP:HB2	1.71	0.72
1:A:522:GLU:OE1	1:A:522:GLU:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:174:PRO:HG3	4:R:227:LEU:HD11	1.72	0.71
2:B:95:LEU:HD12	2:B:98:LEU:HD21	1.73	0.71
4:E:401:ASP:HB3	4:E:404:GLN:HG2	1.72	0.71
1:N:103:LYS:HZ2	1:N:103:LYS:HB3	1.55	0.71
1:N:522:GLU:OE1	1:N:522:GLU:N	2.23	0.71
4:F:286:THR:HG22	4:F:287:GLY:H	1.56	0.71
4:F:337:ARG:O	4:F:337:ARG:CG	2.35	0.71
1:A:39:ASN:C	1:A:39:ASN:OD1	2.33	0.71
4:E:155:ARG:HB2	4:E:164:HIS:HB3	1.73	0.71
1:N:20:THR:CG2	1:N:21:PRO:HD2	2.20	0.71
4:R:441:CYS:HB3	4:R:461:LEU:HD11	1.73	0.71
1:N:594:PHE:HD2	9:M:31:U:H4'	1.55	0.71
1:N:501:SER:HB2	9:M:25:G:OP1	1.90	0.71
9:M:22:U:C6	9:M:23:C:C4	2.79	0.71
1:A:105:ARG:HD3	1:A:110:MET:HG3	1.72	0.71
4:S:536:SER:C	4:S:537:GLN:O	2.10	0.71
4:F:181:VAL:HG21	4:F:337:ARG:HH22	1.54	0.71
8:L:12:G:O6	9:M:48:C:N4	2.20	0.70
1:N:277:GLU:N	1:N:277:GLU:OE2	2.23	0.70
4:R:369:ASP:HB3	4:R:370:ILE:HD12	1.71	0.70
1:A:594:PHE:CD2	9:J:31:U:H4'	2.27	0.70
4:F:5:CYS:SG	4:F:26:CYS:N	2.64	0.70
7:K:483:VAL:HG12	7:K:485:ARG:H	1.55	0.70
2:Q:158:GLN:NE2	2:Q:159:VAL:O	2.23	0.70
4:E:429:MET:HG3	4:E:434:PRO:HD3	1.72	0.70
4:S:331:SER:H	4:S:332:ARG:CZ	2.05	0.70
7:X:210:CYS:SG	10:X:600:ZN:ZN	1.79	0.70
1:A:8:LEU:HD23	1:A:8:LEU:C	2.17	0.70
4:E:370:ILE:HG12	4:E:395:HIS:HB2	1.74	0.70
4:S:441:CYS:O	4:S:463:ALA:HA	1.91	0.70
1:A:37:ILE:O	1:A:43:ALA:HA	1.92	0.69
1:A:684:ASP:O	9:J:27:C:H4'	1.91	0.69
5:G:5:SER:HB2	5:G:101:MET:HG2	1.74	0.69
4:R:341:GLU:O	4:R:341:GLU:CG	2.32	0.69
7:X:485:ARG:O	7:X:489:ASN:ND2	2.25	0.69
4:R:12:THR:HG22	4:R:14:LEU:H	1.57	0.69
2:B:180:LEU:C	2:B:181:ALA:O	2.33	0.69
1:N:919:GLU:OE1	1:N:919:GLU:N	2.21	0.69
6:U:13:VAL:HG22	6:U:30:TYR:HE2	1.55	0.69
4:F:239:THR:O	4:F:388:ASN:ND2	2.26	0.69
4:E:150:GLY:HA2	4:E:174:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:302:GLU:OE2	7:K:422:ASN:ND2	2.25	0.69
5:T:48:LEU:HB3	5:T:51:LEU:HD11	1.75	0.69
2:O:25:ALA:HB3	2:O:38:LEU:HD11	1.75	0.69
4:R:36:SER:HB2	4:R:107:ASN:HD21	1.58	0.69
7:X:422:ASN:OD1	7:X:423:LYS:N	2.22	0.69
4:S:333:ILE:HB	4:S:334:ILE:HD12	1.75	0.69
1:N:592:SER:HB2	9:M:30:C:O3'	1.92	0.69
4:R:330:CYS:HB3	4:R:357:PHE:CE1	2.28	0.69
4:F:492:GLN:HE22	4:F:547:THR:HG22	1.58	0.69
1:A:277:GLU:N	1:A:277:GLU:OE2	2.23	0.69
5:G:48:LEU:HB3	5:G:51:LEU:HD11	1.75	0.69
4:R:265:ASN:HA	4:R:268:ASN:HD22	1.58	0.69
7:X:359:LYS:O	7:X:363:ILE:N	2.26	0.69
4:S:486:SER:OG	4:S:517:SER:OG	2.10	0.69
8:I:12:G:N1	9:J:48:C:N3	2.32	0.69
1:A:929:THR:O	1:A:929:THR:OG1	2.05	0.69
7:X:283:HIS:HA	7:X:287:VAL:HG23	1.75	0.69
4:S:76:LYS:NZ	4:S:77:PRO:O	2.25	0.69
4:E:151:ILE:HG12	4:E:226:VAL:HA	1.76	0.68
8:L:12:G:N1	9:M:48:C:N3	2.32	0.68
1:A:279:ARG:NH1	1:A:314:ASN:OD1	2.27	0.68
4:E:3:GLY:O	4:E:12:THR:N	2.23	0.68
4:E:27:CYS:HB3	4:E:88:GLN:HB2	1.73	0.68
2:Q:147:PHE:N	2:Q:154:TRP:O	2.27	0.68
2:Q:161:ASP:HB2	2:Q:181:ALA:HB3	1.74	0.68
6:U:68:PHE:CE2	6:U:99:ILE:HD12	2.28	0.68
1:A:105:ARG:HD3	1:A:110:MET:CG	2.23	0.68
4:R:291:PHE:HB2	4:R:438:LEU:HD11	1.75	0.68
1:N:197:ARG:NH1	1:N:289:TYR:OH	2.26	0.68
4:F:202:LYS:HE2	4:F:519:ASN:HB3	1.75	0.68
1:A:721:ARG:HG2	1:A:721:ARG:NH1	1.99	0.68
4:F:258:ILE:HG23	4:F:258:ILE:O	1.93	0.68
4:E:332:ARG:HG2	4:E:343:PHE:HB3	1.75	0.68
1:N:88:ASN:HA	1:N:91:LYS:HZ2	1.59	0.68
7:X:478:ASN:HA	7:X:482:ALA:HB1	1.76	0.68
4:S:189:LYS:HB2	4:S:190:ASN:HB2	1.74	0.68
1:A:197:ARG:NH1	1:A:289:TYR:OH	2.26	0.68
9:M:22:U:O2'	9:M:23:C:O2	2.10	0.68
4:E:286:THR:H	4:E:288:LYS:NZ	1.91	0.68
4:E:404:GLN:HE21	4:E:563:VAL:HG12	1.58	0.68
5:G:7:VAL:O	5:G:7:VAL:HG12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:463:ILE:HG23	7:X:465:TYR:CZ	2.28	0.68
6:U:45:LEU:HB2	7:X:38:LEU:HD23	1.76	0.68
4:E:473:LYS:NZ	4:E:589:SER:OG	2.21	0.67
1:N:279:ARG:NH1	1:N:314:ASN:OD1	2.27	0.67
4:R:549:THR:HG22	4:R:550:THR:HG23	1.75	0.67
4:F:334:ILE:H	4:F:343:PHE:HE1	1.41	0.67
8:I:12:G:O6	9:J:48:C:N4	2.20	0.67
1:A:167:GLU:OE2	1:A:167:GLU:HA	1.94	0.67
2:B:161:ASP:CA	2:B:184:LEU:CD2	2.71	0.67
4:E:563:VAL:O	4:E:567:ARG:NE	2.21	0.67
1:N:867:TYR:HA	1:N:881:PHE:CD2	2.29	0.67
1:A:112:PRO:O	1:A:113:HIS:ND1	2.23	0.67
4:F:333:ILE:HG12	4:F:358:CYS:HA	1.77	0.67
4:E:558:VAL:O	4:E:562:ASN:HB2	1.94	0.67
1:N:112:PRO:O	1:N:113:HIS:ND1	2.23	0.67
1:N:167:GLU:HA	1:N:167:GLU:OE2	1.94	0.67
4:R:423:ASN:C	4:R:423:ASN:OD1	2.37	0.67
1:A:867:TYR:HA	1:A:881:PHE:CD2	2.29	0.67
6:H:72:SER:O	6:H:72:SER:OG	2.11	0.67
1:N:810:HIS:ND1	1:N:810:HIS:O	2.27	0.67
1:A:560:VAL:HG21	1:A:684:ASP:HA	1.77	0.67
7:K:83:VAL:HG22	7:K:84:ARG:H	1.60	0.67
7:K:484:CYS:O	7:K:486:HIS:N	2.27	0.67
1:N:10:ARG:O	1:N:10:ARG:NH2	2.27	0.67
4:F:199:THR:HB	4:F:339:ARG:HD2	1.76	0.67
1:A:819:LEU:HD11	1:A:826:TYR:HB3	1.76	0.67
4:E:25:LEU:HD22	4:E:29:CYS:HB3	1.77	0.67
1:N:560:VAL:HG21	1:N:684:ASP:HA	1.77	0.67
4:R:407:ALA:O	4:R:409:ARG:NH1	2.28	0.67
5:T:32:TYR:HA	5:T:41:VAL:HA	1.75	0.67
4:S:536:SER:O	4:S:537:GLN:C	2.32	0.67
2:B:9:LEU:HD12	2:B:49:PHE:HE1	1.60	0.67
4:F:305:VAL:HB	4:F:371:VAL:HG22	1.75	0.67
4:F:519:ASN:ND2	4:F:532:THR:OG1	2.28	0.67
7:K:352:ASP:O	7:K:366:LEU:N	2.28	0.66
1:N:682:SER:O	1:N:682:SER:OG	2.10	0.66
1:N:819:LEU:HD11	1:N:826:TYR:HB3	1.76	0.66
5:G:32:TYR:HA	5:G:41:VAL:HA	1.75	0.66
7:X:447:TYR:HA	7:X:474:ILE:HG13	1.76	0.66
2:O:42:LEU:O	2:O:46:LYS:HG3	1.95	0.66
4:F:243:GLN:NE2	4:F:277:TYR:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:244:GLU:HB2	4:F:276:LYS:HB2	1.77	0.66
4:S:5:CYS:SG	4:S:26:CYS:N	2.64	0.66
1:A:291:ASP:OD1	1:A:735:ARG:NH2	2.29	0.66
1:N:291:ASP:OD1	1:N:735:ARG:NH2	2.29	0.66
4:S:185:TYR:HE2	4:S:226:VAL:HG22	1.60	0.66
2:D:174:MET:O	2:D:177:SER:OG	2.13	0.66
7:X:465:TYR:O	7:X:467:PRO:HD3	1.95	0.66
1:A:480:PHE:HE2	1:A:693:VAL:HG22	1.61	0.66
6:H:46:CYS:SG	6:H:47:THR:N	2.60	0.66
9:M:22:U:OP2	9:M:22:U:H6	1.78	0.66
6:H:122:MET:HE3	6:H:127:GLY:H	1.61	0.65
2:Q:39:LYS:O	2:Q:43:ASN:N	2.29	0.65
1:A:256:HIS:CD2	1:A:261:LEU:HA	2.32	0.65
4:E:283:PRO:O	4:E:288:LYS:NZ	2.28	0.65
4:F:384:LEU:O	4:F:388:ASN:ND2	2.29	0.65
1:A:612:PRO:CB	1:A:805:LEU:CD1	2.73	0.65
4:E:150:GLY:CA	4:E:174:PRO:HG3	2.27	0.65
4:E:481:THR:OG1	4:E:488:ILE:O	2.14	0.65
4:S:401:ASP:HB3	4:S:404:GLN:HE21	1.61	0.65
4:E:304:ILE:HD12	4:E:370:ILE:HB	1.78	0.65
1:N:20:THR:HG23	1:N:21:PRO:HD2	1.78	0.65
1:N:256:HIS:CD2	1:N:261:LEU:HA	2.32	0.65
1:N:594:PHE:CD2	9:M:31:U:H4'	2.30	0.65
2:O:9:LEU:HB2	2:O:12:TYR:H	1.62	0.65
4:S:138:LEU:O	4:S:142:GLU:HG2	1.96	0.65
1:A:594:PHE:HD2	9:J:31:U:H4'	1.59	0.65
7:K:88:GLY:H	7:K:112:SER:HB2	1.60	0.65
1:N:80:TYR:HD2	1:N:112:PRO:HB3	1.61	0.65
5:T:57:PRO:HB2	5:T:61:GLY:HA2	1.78	0.65
2:O:58:LYS:HA	2:O:61:LYS:HD2	1.79	0.65
5:T:29:LEU:HB2	5:T:45:LEU:O	1.97	0.65
2:Q:171:GLU:O	2:Q:176:ASN:ND2	2.29	0.65
4:F:419:PRO:HA	4:F:422:PHE:HB2	1.79	0.65
4:F:488:ILE:HG23	4:F:521:VAL:HG21	1.77	0.65
4:F:521:VAL:HA	4:F:524:LYS:HD3	1.76	0.65
4:S:481:THR:OG1	4:S:488:ILE:O	2.14	0.65
1:N:5:GLN:OE1	1:N:9:ASN:ND2	2.28	0.65
4:R:473:LYS:HG2	4:R:587:PHE:HB2	1.77	0.65
6:U:90:CYS:SG	6:U:91:ASP:N	2.70	0.65
1:A:80:TYR:HD2	1:A:112:PRO:HB3	1.61	0.64
5:G:29:LEU:HB2	5:G:45:LEU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:57:PRO:HB2	5:G:61:GLY:HA2	1.78	0.64
1:N:480:PHE:HE2	1:N:693:VAL:HG22	1.61	0.64
4:R:475:PHE:O	4:R:477:LYS:NZ	2.29	0.64
9:M:22:U:O2'	9:M:23:C:C2	2.50	0.64
4:E:533:VAL:HG13	4:E:564:ALA:HB2	1.79	0.64
4:S:306:TYR:HB3	4:S:317:LEU:HD21	1.80	0.64
1:N:872:HIS:HD2	1:N:873:PRO:HD2	1.63	0.64
4:F:372:VAL:HG12	4:F:397:VAL:HB	1.80	0.64
4:S:163:LEU:HD21	4:S:165:LEU:HD13	1.77	0.64
6:H:64:ASP:N	6:H:64:ASP:OD1	2.27	0.64
5:G:47:ASP:OD1	5:G:84:LYS:NZ	2.30	0.64
4:F:186:ARG:HH11	4:F:220:ASN:HD21	1.45	0.64
4:F:330:CYS:O	4:F:356:VAL:HA	1.98	0.64
4:E:150:GLY:HA3	4:E:174:PRO:HG3	1.79	0.64
7:K:398:VAL:HG22	7:K:509:TRP:HB2	1.78	0.64
1:N:759:SER:O	8:L:33:G:O3'	2.16	0.64
4:F:27:CYS:HB3	4:F:88:GLN:HB3	1.79	0.64
4:S:3:GLY:O	4:S:12:THR:N	2.29	0.64
1:A:364:SER:OG	1:A:365:ARG:N	2.31	0.64
4:E:249:ILE:HG22	4:E:252:LEU:HB2	1.78	0.64
4:F:377:SER:C	4:F:422:PHE:HE2	2.05	0.64
4:S:521:VAL:HA	4:S:524:LYS:HD2	1.79	0.64
4:E:303:ARG:HD3	4:E:368:ALA:HA	1.78	0.63
4:R:498:GLU:O	4:R:501:THR:OG1	2.13	0.63
5:T:47:ASP:OD1	5:T:84:LYS:NZ	2.30	0.63
1:A:88:ASN:HA	1:A:91:LYS:HZ2	1.63	0.63
1:A:889:ARG:HH11	1:A:889:ARG:HG3	1.63	0.63
4:E:548:GLN:HG2	4:E:576:MET:HA	1.79	0.63
1:N:364:SER:OG	1:N:365:ARG:N	2.31	0.63
4:R:152:ALA:HB2	4:R:167:TRP:HD1	1.62	0.63
4:R:152:ALA:HB2	4:R:167:TRP:CD1	2.33	0.63
1:A:926:THR:HG23	1:A:927:PRO:CD	2.24	0.63
4:S:547:THR:HG22	4:S:575:ILE:HD11	1.79	0.63
1:A:872:HIS:HD2	1:A:873:PRO:HD2	1.63	0.63
4:S:383:ASP:N	4:S:383:ASP:OD1	2.31	0.63
1:N:218:ASP:OD1	1:N:218:ASP:C	2.41	0.63
4:R:68:MET:N	4:R:68:MET:SD	2.68	0.63
4:R:358:CYS:SG	4:R:359:THR:N	2.71	0.63
4:R:473:LYS:HD3	4:R:585:LEU:HB2	1.81	0.63
4:E:151:ILE:HG13	4:E:171:LYS:HE3	1.80	0.63
6:H:62:ASN:H	6:H:65:GLN:HG2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:734:ASN:OD1	1:N:735:ARG:N	2.31	0.63
4:R:447:GLU:O	4:R:451:THR:HG23	1.98	0.63
6:U:50:GLY:O	6:U:62:ASN:ND2	2.30	0.63
4:F:280:LEU:HD21	4:F:438:LEU:HD12	1.80	0.63
4:F:435:ASP:O	4:F:436:MET:SD	2.56	0.63
1:A:614:LEU:HB2	1:A:802:GLU:HB3	1.80	0.63
1:A:734:ASN:OD1	1:A:735:ARG:N	2.31	0.63
1:N:614:LEU:HB2	1:N:802:GLU:HB3	1.80	0.63
4:R:178:ARG:HB2	4:R:212:ARG:HH22	1.64	0.63
1:A:8:LEU:HD23	1:A:8:LEU:O	1.97	0.63
2:B:58:LYS:HA	2:B:61:LYS:HG2	1.81	0.63
4:E:522:ALA:O	4:E:526:LEU:N	2.30	0.63
2:O:173:SER:HG	2:O:176:ASN:H	1.46	0.63
3:P:66:VAL:O	3:P:70:LYS:NZ	2.31	0.63
6:U:19:PHE:CE1	7:X:196:LYS:HA	2.34	0.63
7:X:266:ASN:OD1	7:X:267:ALA:O	2.16	0.63
4:S:337:ARG:HD2	4:S:338:ALA:H	1.63	0.63
4:S:467:LYS:HB2	4:S:468:SER:HB2	1.79	0.63
4:R:305:VAL:HG12	4:R:356:VAL:HB	1.80	0.62
7:X:350:PHE:HB3	7:X:363:ILE:HA	1.80	0.62
4:S:23:PRO:HB3	4:S:133:PHE:CE2	2.33	0.62
4:S:304:ILE:HD12	4:S:370:ILE:HB	1.81	0.62
4:S:320:LYS:H	4:S:323:LYS:HZ3	1.47	0.62
7:K:331:ASP:OD1	7:K:332:ILE:N	2.32	0.62
7:X:470:SER:OG	7:X:471:ALA:N	2.31	0.62
3:C:34:GLN:NE2	3:C:38:ASP:OD1	2.32	0.62
4:E:33:HIS:NE2	4:E:39:HIS:CG	2.66	0.62
2:D:67:MET:HG3	2:D:70:MET:HE2	1.81	0.62
4:E:293:ILE:HG13	4:E:320:LYS:HG3	1.80	0.62
1:N:511:LYS:HZ1	9:M:25:G:N2	1.96	0.62
3:P:34:GLN:NE2	3:P:38:ASP:OD1	2.33	0.62
4:R:513:SER:OG	4:R:547:THR:OG1	2.17	0.62
4:F:160:ASP:HB3	4:F:161:ARG:HH11	1.63	0.62
7:X:117:LEU:HD23	7:X:162:VAL:HG13	1.82	0.62
7:X:209:LEU:HD11	7:X:229:HIS:CG	2.35	0.62
3:C:66:VAL:O	3:C:70:LYS:NZ	2.31	0.62
5:G:44:LEU:O	5:G:89:TYR:N	2.25	0.62
1:A:804:ASP:HB2	1:A:807:LYS:HZ2	1.64	0.62
1:N:889:ARG:HG3	1:N:889:ARG:HH11	1.63	0.62
7:X:328:VAL:HA	7:X:347:GLU:HB3	1.81	0.62
4:R:311:HIS:CE1	4:R:359:THR:HG21	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:413:THR:HG23	4:F:414:LYS:HD2	1.82	0.62
2:Q:174:MET:O	2:Q:177:SER:OG	2.18	0.61
4:R:445:PRO:HD2	4:R:448:ILE:HD12	1.82	0.61
7:X:518:ASN:N	7:X:518:ASN:OD1	2.33	0.61
4:F:258:ILE:O	4:F:258:ILE:CG2	2.47	0.61
7:K:453:GLU:HG3	7:K:464:ASP:HB3	1.83	0.61
4:F:37:THR:OG1	4:F:38:SER:N	2.32	0.61
4:S:480:ILE:HG12	4:S:550:THR:HG21	1.81	0.61
1:N:415:PHE:HE1	1:N:417:LYS:HA	1.66	0.61
4:F:280:LEU:HD23	4:F:399:ILE:HG23	1.83	0.61
1:A:132:ARG:O	1:A:133:HIS:ND1	2.33	0.61
7:K:313:GLN:HE21	7:K:385:TRP:CG	2.17	0.61
2:Q:25:ALA:O	2:Q:28:ASN:O	2.18	0.61
7:X:230:SER:O	7:X:230:SER:OG	2.18	0.61
4:F:65:LEU:HB2	4:F:83:LEU:HD11	1.82	0.61
4:F:135:ALA:O	4:F:139:LYS:HG2	2.01	0.61
4:S:19:CYS:SG	4:S:39:HIS:HE1	2.13	0.61
2:O:22:TYR:HA	2:O:38:LEU:HD13	1.81	0.61
4:R:303:ARG:HA	4:R:354:GLN:HG2	1.83	0.61
5:T:4:LEU:HD12	5:T:4:LEU:O	2.01	0.61
4:F:187:VAL:HA	4:F:192:LYS:HA	1.82	0.61
2:B:182:TRP:H	2:B:183:PRO:HD3	1.65	0.61
4:E:33:HIS:O	4:E:37:THR:OG1	2.18	0.61
1:N:611:ASN:HD22	1:N:769:THR:HG23	1.65	0.61
1:N:867:TYR:HA	1:N:881:PHE:HD2	1.64	0.61
4:R:321:ALA:O	4:R:325:LEU:N	2.32	0.61
4:E:289:SER:HB2	4:E:320:LYS:HG2	1.83	0.61
4:E:445:PRO:HD2	4:E:448:ILE:HD12	1.82	0.61
4:R:258:ILE:HD11	4:R:298:TYR:HA	1.83	0.61
4:F:309:CYS:SG	4:F:310:SER:N	2.74	0.61
1:A:107:ASP:N	1:A:107:ASP:OD1	2.34	0.61
1:A:415:PHE:HE1	1:A:417:LYS:HA	1.66	0.61
4:E:474[B]:MET:HG2	4:E:590:LEU:HB2	1.82	0.61
1:N:380:MET:HB3	2:O:94:MET:HE3	1.82	0.61
1:N:899:MET:O	1:N:903:TYR:O	2.18	0.61
4:R:245:HIS:ND1	4:R:275:GLN:HB3	2.16	0.61
4:R:156:GLU:HB2	4:S:95:ASN:HD21	1.66	0.60
4:R:513:SER:HG	4:R:547:THR:HG1	1.48	0.60
7:X:419:LEU:HD11	7:X:425:ALA:HB1	1.82	0.60
4:F:494:GLY:HA2	4:F:497:ARG:NE	2.14	0.60
4:S:139:LYS:O	4:S:143:GLU:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:245:HIS:HE1	4:S:274:MET:HB3	1.66	0.60
4:S:277:TYR:HB2	4:S:396:TYR:HB2	1.83	0.60
4:E:150:GLY:HA2	4:E:174:PRO:CD	2.31	0.60
4:R:293:ILE:HD12	4:R:320:LYS:HE3	1.82	0.60
2:D:43:ASN:O	2:D:46:LYS:HG3	2.00	0.60
7:X:366:LEU:HD11	7:X:373:HIS:NE2	2.17	0.60
4:F:496:VAL:HA	4:F:499:PHE:HB2	1.83	0.60
4:S:347:LYS:HD2	4:S:347:LYS:C	2.26	0.60
1:A:7:PHE:O	1:A:11:VAL:HB	2.01	0.60
2:B:125:ALA:O	2:B:190:ARG:NH1	2.34	0.60
7:K:302:GLU:OE2	7:K:306:ASN:ND2	2.35	0.60
2:Q:99:ASP:OD1	2:Q:99:ASP:C	2.44	0.60
4:S:36:SER:OG	4:S:107:ASN:ND2	2.34	0.60
4:S:266:VAL:O	4:S:270:GLN:NE2	2.34	0.60
4:S:284:PRO:HB2	4:S:567:ARG:HH22	1.66	0.60
8:I:22:G:H2'	8:I:23:C:C6	2.37	0.60
1:A:867:TYR:HA	1:A:881:PHE:HD2	1.64	0.60
4:E:286:THR:HG22	4:E:441:CYS:HA	1.83	0.60
4:E:330:CYS:O	4:E:347:LYS:NZ	2.33	0.60
1:N:107:ASP:N	1:N:107:ASP:OD1	2.35	0.60
4:F:334:ILE:HG21	4:F:338:ALA:H	1.66	0.60
4:S:192:LYS:HD3	4:S:224:TYR:HE2	1.65	0.60
4:S:519:ASN:HD22	4:S:530:THR:HB	1.64	0.60
2:B:43:ASN:HD22	9:J:48:C:H5"	1.64	0.60
4:E:21:ARG:HD3	4:E:137:THR:HA	1.83	0.60
4:E:31:TYR:O	4:E:35:ILE:HG12	2.00	0.60
6:H:42:VAL:HG12	7:K:26:HIS:HA	1.83	0.60
5:T:74:ARG:HH11	5:T:74:ARG:HG3	1.67	0.60
4:F:369:ASP:O	4:F:395:HIS:N	2.34	0.60
1:A:57:GLN:HG2	1:A:69:TYR:CE1	2.37	0.60
6:U:51:THR:HG23	6:U:53:GLN:H	1.67	0.60
4:S:55:CYS:HB2	4:S:75:HIS:CE1	2.36	0.60
1:A:84:GLU:HG2	7:K:98:ARG:NH1	2.17	0.60
4:E:280:LEU:HG	4:E:436:MET:HB2	1.84	0.60
1:N:57:GLN:HG2	1:N:69:TYR:CE1	2.37	0.60
4:R:511:PHE:HB3	4:R:530:THR:HA	1.82	0.60
7:X:393:PRO:O	7:X:396:SER:OG	2.17	0.60
4:E:3:GLY:N	4:E:12:THR:O	2.32	0.60
4:E:420:GLU:HG3	4:E:427:ARG:HG2	1.82	0.60
1:N:731:LEU:HB3	1:N:732:TYR:CD1	2.37	0.60
9:J:40:U:H2'	9:J:41:G:H8	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:LEU:HB3	1:A:732:TYR:CD1	2.37	0.60
5:G:74:ARG:HG3	5:G:74:ARG:HH11	1.67	0.60
1:N:132:ARG:O	1:N:133:HIS:ND1	2.33	0.60
2:Q:57:ARG:HA	2:Q:60:GLU:HG3	1.84	0.60
4:F:203:GLY:HA2	4:F:210:VAL:HG23	1.83	0.60
4:F:523:SER:HA	4:F:526:LEU:HD22	1.84	0.60
8:L:22:G:H2'	8:L:23:C:C6	2.37	0.60
4:E:139:LYS:HZ1	4:E:382:TYR:HB2	1.66	0.59
4:R:457:TYR:HE1	4:R:562:ASN:HD21	1.48	0.59
7:X:457:LYS:HD2	7:X:458:GLN:H	1.65	0.59
4:F:376:ILE:HG21	4:F:398:TYR:HB3	1.83	0.59
4:S:486:SER:HB2	4:S:515:TYR:CD1	2.36	0.59
2:B:182:TRP:O	2:B:182:TRP:HE3	1.85	0.59
7:K:291:ASP:OD1	7:K:294:ILE:N	2.31	0.59
7:K:475:THR:O	7:K:475:THR:OG1	2.19	0.59
4:R:457:TYR:O	4:R:460:LYS:HG2	2.02	0.59
4:E:492:GLN:O	4:E:496:VAL:HG23	2.03	0.59
7:K:452:CYS:HB3	7:K:484:CYS:HB3	1.85	0.59
4:R:303:ARG:HG3	4:R:354:GLN:HA	1.84	0.59
5:T:44:LEU:O	5:T:89:TYR:N	2.25	0.59
4:E:131:LYS:HD3	4:E:239:THR:HG21	1.85	0.59
7:K:185:LEU:HD12	7:K:188:HIS:HA	1.82	0.59
2:D:137:THR:O	2:D:141:THR:OG1	2.16	0.59
2:D:147:PHE:N	2:D:154:TRP:O	2.36	0.59
1:N:504:PHE:CD1	1:N:504:PHE:C	2.80	0.59
7:X:403:THR:HG23	7:X:431:PHE:HB2	1.83	0.59
4:F:59:ASP:OD2	4:F:61:THR:OG1	2.20	0.59
4:S:69:SER:OG	4:S:70:TYR:N	2.35	0.59
3:C:13:LEU:HD12	2:D:91:LEU:HD11	1.84	0.59
4:E:92:LEU:HD12	4:E:93:TYR:H	1.66	0.59
4:E:240:LEU:HD11	4:E:424:SER:HB2	1.85	0.59
1:N:715:ILE:HB	1:N:721:ARG:NH1	2.17	0.59
4:R:178:ARG:HA	4:R:199:THR:HG21	1.85	0.59
4:R:341:GLU:O	4:R:341:GLU:OE2	2.19	0.59
4:R:343:PHE:HE1	4:R:345:LYS:HZ2	1.49	0.59
4:R:563:VAL:O	4:R:567:ARG:NE	2.36	0.59
1:A:805:LEU:O	1:A:805:LEU:HD23	2.03	0.59
5:G:94:LEU:HB3	5:G:99:ARG:NH1	2.18	0.59
1:N:256:HIS:HD2	1:N:261:LEU:HA	1.68	0.59
5:T:94:LEU:HB3	5:T:99:ARG:NH1	2.18	0.59
4:S:492:GLN:NE2	4:S:575:ILE:HB	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ASP:HA	2:B:104:ASN:HD22	1.67	0.59
4:F:449:VAL:HG22	4:F:461:LEU:HG	1.85	0.59
7:K:466:VAL:HG22	7:K:483:VAL:HG11	1.84	0.59
1:N:610:GLU:OE2	1:N:767:ASN:ND2	2.33	0.59
2:O:34:VAL:O	2:O:38:LEU:HG	2.02	0.59
4:F:561:PHE:O	4:F:565:ILE:HG12	2.02	0.59
1:A:57:GLN:HE22	1:A:66:ILE:H	1.50	0.59
4:E:15:ARG:N	4:E:43:LEU:O	2.34	0.59
4:E:171:LYS:HG2	4:E:172:PRO:HD2	1.83	0.59
4:R:451:THR:HA	4:R:586:GLN:HE22	1.68	0.59
4:F:447:GLU:O	4:F:451:THR:OG1	2.19	0.59
4:E:167:TRP:CG	4:E:173:ARG:HG2	2.38	0.58
4:E:405:LEU:HD11	4:E:560:ARG:HG2	1.85	0.58
7:K:330:HIS:ND1	7:K:377:PHE:HB3	2.18	0.58
2:Q:113:GLY:O	2:Q:133:PRO:HD3	2.03	0.58
4:F:337:ARG:O	4:F:337:ARG:HD2	1.96	0.58
4:F:477:LYS:HG2	4:F:577:SER:OG	2.02	0.58
4:S:60:VAL:HB	4:S:83:LEU:HD21	1.84	0.58
1:A:592:SER:HB2	9:J:30:C:O3'	2.03	0.58
7:K:352:ASP:OD1	7:K:353:ALA:N	2.36	0.58
1:N:57:GLN:HE22	1:N:66:ILE:H	1.50	0.58
9:M:22:U:H5"	9:M:23:C:OP2	2.03	0.58
1:A:682:SER:O	1:A:687:THR:CG2	2.38	0.58
2:B:161:ASP:CB	2:B:184:LEU:HD21	2.33	0.58
7:X:207:CYS:SG	7:X:229:HIS:HE1	2.26	0.58
4:S:245:HIS:CE1	4:S:274:MET:HB3	2.39	0.58
4:S:326:PRO:C	4:S:328:ASP:HB3	2.27	0.58
9:M:40:U:H2'	9:M:41:G:H8	1.67	0.58
4:E:268:ASN:O	4:E:272:VAL:HG23	2.04	0.58
5:T:49:GLN:OE1	5:T:50:ASP:HB3	2.04	0.58
7:X:31:THR:OG1	7:X:32:LYS:NZ	2.36	0.58
4:F:3:GLY:O	4:F:12:THR:N	2.35	0.58
1:N:767:ASN:OD1	1:N:768:SER:N	2.36	0.58
1:N:889:ARG:HH11	1:N:889:ARG:CG	2.17	0.58
2:O:43:ASN:HA	2:O:46:LYS:HE2	1.85	0.58
4:F:252:LEU:HB3	4:F:299:TYR:CE1	2.39	0.58
7:K:10:ASP:OD1	7:K:11:CYS:N	2.36	0.58
1:N:218:ASP:O	1:N:218:ASP:CG	2.40	0.58
1:N:684:ASP:O	9:M:27:C:H4'	2.03	0.58
4:R:447:GLU:CD	4:R:471:CYS:HB2	2.28	0.58
5:T:35:THR:OG1	5:T:36:LYS:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:64:TYR:CG	4:F:76:LYS:HD2	2.38	0.58
4:E:139:LYS:NZ	4:E:382:TYR:HB2	2.18	0.58
7:X:207:CYS:SG	7:X:229:HIS:CE1	2.97	0.58
4:E:134:ALA:HA	4:E:137:THR:HG22	1.86	0.58
4:S:186:ARG:NH2	4:S:218:LYS:O	2.36	0.58
4:S:262:PHE:HD1	4:S:265:ASN:HD22	1.52	0.58
4:E:515:TYR:O	4:E:519:ASN:ND2	2.36	0.58
1:A:7:PHE:CE1	1:A:113:HIS:CD2	2.89	0.58
1:A:726:ARG:HB3	1:A:741:PHE:HE2	1.69	0.58
4:E:181:VAL:HG22	4:E:230:HIS:CE1	2.39	0.58
7:K:469:LYS:HB3	1:N:905:VAL:HA	1.86	0.58
1:N:726:ARG:HB3	1:N:741:PHE:HE2	1.69	0.58
4:R:268:ASN:O	4:R:436:MET:HE1	2.03	0.58
4:R:365:GLU:HG3	4:R:390:ARG:HD3	1.86	0.58
7:X:453:GLU:HB2	7:X:486:HIS:HB2	1.84	0.58
4:S:320:LYS:N	4:S:323:LYS:HZ3	2.00	0.58
1:A:889:ARG:HH11	1:A:889:ARG:CG	2.17	0.57
4:E:451:THR:HG21	4:E:585:LEU:HD12	1.85	0.57
4:R:443:ARG:NH1	4:R:566:THR:O	2.29	0.57
6:U:51:THR:HG22	6:U:60:GLU:HG2	1.85	0.57
4:F:531:GLN:NE2	4:F:532:THR:O	2.33	0.57
1:A:713:ASN:HB2	1:A:714:LYS:NZ	2.19	0.57
5:G:35:THR:OG1	5:G:36:LYS:N	2.34	0.57
7:K:75:THR:OG1	7:K:76:ARG:N	2.36	0.57
1:N:24:THR:OG1	1:N:25:GLY:N	2.27	0.57
1:N:103:LYS:HB3	1:N:103:LYS:NZ	2.19	0.57
1:N:713:ASN:HB2	1:N:714:LYS:NZ	2.19	0.57
4:R:243:GLN:HE22	4:R:277:TYR:H	1.53	0.57
7:X:459:VAL:HG12	7:X:460:VAL:HG23	1.86	0.57
4:F:21:ARG:NH1	4:F:136:GLU:OE2	2.31	0.57
4:F:334:ILE:HG21	4:F:338:ALA:N	2.18	0.57
4:E:269:TYR:HD1	4:E:295:LEU:HD23	1.69	0.57
5:T:8:ALA:O	5:T:9:LEU:HD13	2.04	0.57
6:U:25:LYS:O	6:U:25:LYS:NZ	2.35	0.57
4:F:292:ALA:HB1	4:F:306:TYR:HE2	1.68	0.57
4:S:42:VAL:HG13	4:S:48:TYR:HD2	1.69	0.57
4:S:127:THR:O	4:S:131:LYS:N	2.34	0.57
1:A:767:ASN:OD1	1:A:768:SER:N	2.37	0.57
7:K:83:VAL:O	7:K:84:ARG:HB2	2.02	0.57
7:K:179:ASP:OD1	7:K:179:ASP:N	2.34	0.57
4:S:115:THR:OG1	4:S:414:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:49:GLN:OE1	5:G:50:ASP:HB3	2.04	0.57
4:R:340:VAL:HG23	4:R:340:VAL:O	2.03	0.57
4:S:293:ILE:HD11	4:S:325:LEU:HB2	1.85	0.57
1:A:4:ALA:C	1:A:6:SER:H	2.13	0.57
2:B:160:VAL:O	2:B:184:LEU:CD2	2.53	0.57
4:E:404:GLN:NE2	4:E:563:VAL:HG12	2.18	0.57
4:R:492:GLN:OE1	4:R:547:THR:HB	2.04	0.57
4:F:462:LYS:HG2	4:F:463:ALA:N	2.20	0.57
4:S:384:LEU:O	4:S:388:ASN:ND2	2.38	0.57
1:A:256:HIS:HD2	1:A:261:LEU:HA	1.68	0.57
4:E:279:THR:HG23	4:E:434:PRO:HA	1.86	0.57
4:E:286:THR:OG1	4:E:288:LYS:NZ	2.38	0.57
7:K:208:CYS:O	7:K:209:LEU:HG	2.05	0.57
4:R:181:VAL:O	4:R:230:HIS:NE2	2.38	0.57
7:X:2:GLU:OE1	7:X:3:ASN:N	2.38	0.57
4:S:66:GLY:N	4:S:69:SER:O	2.38	0.57
1:A:80:TYR:CE1	1:A:101:PHE:HB3	2.40	0.57
4:E:15:ARG:O	4:E:43:LEU:N	2.29	0.57
4:E:93:TYR:HB3	4:E:96:THR:HG23	1.87	0.57
2:O:101:ASP:N	2:O:101:ASP:OD1	2.33	0.57
4:R:498:GLU:O	4:R:502:ARG:HG3	2.05	0.57
1:A:142:LEU:O	1:A:146:LEU:HD12	2.05	0.57
4:E:480:ILE:HD13	4:E:550:THR:HG23	1.87	0.57
6:H:33:SER:O	6:H:33:SER:OG	2.21	0.57
6:H:61:ALA:HA	6:H:65:GLN:HE21	1.70	0.57
7:K:478:ASN:HA	7:K:482:ALA:HA	1.87	0.57
1:N:142:LEU:O	1:N:146:LEU:HD12	2.04	0.57
1:N:749:LEU:O	1:N:753:PHE:O	2.22	0.57
4:R:36:SER:HB2	4:R:107:ASN:ND2	2.20	0.57
1:N:315:VAL:HG23	1:N:350:GLU:HG3	1.85	0.57
1:A:612:PRO:CG	1:A:805:LEU:CD1	2.82	0.56
1:A:721:ARG:O	1:A:722:ASN:C	2.44	0.56
4:E:283:PRO:O	4:E:286:THR:OG1	2.17	0.56
4:R:496:VAL:O	4:R:500:LEU:HG	2.05	0.56
7:X:218:SER:HB2	7:X:233:PHE:CD1	2.40	0.56
7:X:465:TYR:O	7:X:465:TYR:CG	2.54	0.56
4:F:344:ASP:OD1	4:F:344:ASP:N	2.38	0.56
9:M:24:U:O2	9:M:24:U:H2'	2.04	0.56
1:A:387:LEU:HD12	1:A:388:LEU:H	1.70	0.56
1:A:686:THR:O	1:A:686:THR:OG1	2.21	0.56
1:A:759:SER:O	8:I:33:G:O3'	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:243:GLN:HE22	4:E:275:GLN:HB2	1.69	0.56
2:Q:32:GLU:O	2:Q:36:LYS:HG2	2.04	0.56
4:R:576:MET:HE1	4:R:581:LEU:HB3	1.87	0.56
7:X:83:VAL:HG22	7:X:84:ARG:H	1.70	0.56
4:F:333:ILE:HG21	4:F:359:THR:HG23	1.87	0.56
4:F:560:ARG:HA	4:F:563:VAL:HG12	1.86	0.56
6:H:52:GLY:HA2	6:H:65:GLN:NE2	2.18	0.56
7:K:466:VAL:HG22	7:K:483:VAL:HG21	1.86	0.56
1:N:80:TYR:CE1	1:N:101:PHE:HB3	2.39	0.56
2:Q:89:THR:O	2:Q:93:THR:HG23	2.05	0.56
9:J:38:C:H2'	9:J:39:A:C8	2.40	0.56
1:A:315:VAL:HG23	1:A:350:GLU:HG3	1.85	0.56
1:N:387:LEU:HD12	1:N:388:LEU:H	1.70	0.56
7:X:71:ASN:OD1	7:X:71:ASN:N	2.39	0.56
7:X:465:TYR:CD2	7:X:484:CYS:HA	2.40	0.56
4:S:270:GLN:O	4:S:274:MET:HG3	2.06	0.56
1:A:804:ASP:HB2	1:A:807:LYS:NZ	2.19	0.56
2:D:155:GLU:N	2:D:155:GLU:OE2	2.37	0.56
1:N:686:THR:O	1:N:686:THR:OG1	2.21	0.56
4:R:80:SER:OG	4:R:81:PHE:N	2.39	0.56
4:R:453:SER:HA	4:R:457:TYR:HB2	1.86	0.56
4:S:446:ALA:HA	4:S:449:VAL:HG12	1.87	0.56
4:S:453:SER:HB3	4:S:459:ASN:HA	1.85	0.56
4:R:290:HIS:HA	4:R:320:LYS:NZ	2.21	0.56
5:T:10:ARG:NH2	5:T:34:THR:OG1	2.39	0.56
7:X:54:LEU:HD23	7:X:100:ALA:HB3	1.87	0.56
4:F:455:LEU:HD22	4:F:558:VAL:HG13	1.88	0.56
1:A:527:LEU:O	1:A:531:THR:HG23	2.06	0.56
2:B:44:VAL:O	2:B:47:SER:OG	2.20	0.56
4:E:105:ASP:O	4:E:109:ILE:HG13	2.05	0.56
4:E:176:LEU:HD22	4:E:200:PHE:HB2	1.88	0.56
7:K:234:ASP:OD1	7:K:234:ASP:N	2.39	0.56
1:N:388:LEU:HD13	1:N:400:ALA:HB2	1.86	0.56
1:N:527:LEU:O	1:N:531:THR:HG23	2.06	0.56
7:X:414:CYS:O	7:X:427:HIS:NE2	2.38	0.56
4:S:120:TYR:CE2	4:S:412:LEU:HD21	2.41	0.56
1:A:88:ASN:HA	1:A:91:LYS:NZ	2.20	0.56
2:B:134:ASP:C	2:B:182:TRP:CZ3	2.83	0.56
3:C:63:GLN:N	3:C:63:GLN:OE1	2.39	0.56
5:G:10:ARG:NH2	5:G:34:THR:OG1	2.39	0.56
1:N:610:GLU:HG2	1:N:611:ASN:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:195:ILE:HG23	4:S:217:TYR:HD2	1.71	0.56
2:B:22:TYR:HA	2:B:38:LEU:HG	1.87	0.56
1:N:88:ASN:HA	1:N:91:LYS:NZ	2.20	0.56
4:R:189:LYS:HB2	4:R:190:ASN:CB	2.35	0.56
7:X:171:SER:OG	7:X:227:TRP:O	2.24	0.56
4:S:287:GLY:O	4:S:291:PHE:HB2	2.06	0.56
9:M:38:C:H2'	9:M:39:A:C8	2.40	0.56
1:A:388:LEU:HD13	1:A:400:ALA:HB2	1.86	0.56
5:G:90:PHE:HE2	5:G:99:ARG:HG2	1.71	0.56
1:N:348:PHE:HD2	1:N:351:LEU:HB2	1.71	0.56
4:S:25:LEU:HB3	4:S:30:CYS:HB2	1.88	0.56
4:S:178:ARG:HH12	4:S:535:SER:HA	1.70	0.56
4:S:201:GLU:HB3	4:S:210:VAL:HG13	1.88	0.56
8:I:23:C:H2'	8:I:24:U:C6	2.41	0.56
2:D:147:PHE:O	2:D:154:TRP:N	2.38	0.55
6:U:66:GLU:O	6:U:98:GLN:HA	2.06	0.55
7:X:84:ARG:HH21	7:X:421:VAL:HG12	1.71	0.55
7:X:115:VAL:HG11	7:X:169:MET:HE2	1.87	0.55
5:G:99:ARG:HH11	5:G:99:ARG:CG	2.18	0.55
7:K:523:PHE:HA	7:K:525:ARG:HH22	1.70	0.55
3:P:63:GLN:N	3:P:63:GLN:OE1	2.39	0.55
4:R:405:LEU:HD21	4:R:560:ARG:HA	1.87	0.55
5:T:99:ARG:HH11	5:T:99:ARG:CG	2.18	0.55
7:X:465:TYR:HE1	7:X:481:GLY:HA3	1.71	0.55
4:S:238:PRO:O	4:S:388:ASN:ND2	2.39	0.55
1:A:6:SER:HB3	1:A:104:PHE:CE2	2.40	0.55
4:E:27:CYS:HA	4:E:89:VAL:HG22	1.89	0.55
4:E:544:VAL:HB	4:E:572:ILE:HG13	1.86	0.55
1:N:624:ARG:HH11	1:N:624:ARG:HG3	1.72	0.55
2:O:59:LEU:HG	4:S:81:PHE:CD2	2.41	0.55
7:X:328:VAL:HG13	7:X:380:GLY:HA3	1.86	0.55
4:F:31:TYR:O	4:F:35:ILE:HG12	2.07	0.55
4:F:63:LEU:HB3	4:F:83:LEU:HD23	1.88	0.55
8:I:24:U:H2'	8:I:25:A:H8	1.69	0.55
4:R:360:VAL:HG11	4:R:383:ASP:HB3	1.88	0.55
6:U:68:PHE:CD2	6:U:99:ILE:HD12	2.42	0.55
4:S:332:ARG:HD2	4:S:347:LYS:O	2.06	0.55
1:A:103:LYS:HB3	1:A:103:LYS:NZ	2.19	0.55
1:A:156:TYR:CE1	1:A:159:LYS:HE3	2.42	0.55
2:D:169:LEU:O	2:D:172:ILE:HG22	2.07	0.55
7:K:212:ARG:HH12	7:K:228:HIS:CE1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:156:TYR:CE1	1:N:159:LYS:HE3	2.42	0.55
4:R:202:LYS:NZ	4:R:208:ALA:O	2.35	0.55
5:T:90:PHE:HE2	5:T:99:ARG:HG2	1.71	0.55
7:X:98:ARG:HG2	7:X:98:ARG:O	2.07	0.55
4:F:331:SER:H	4:F:332:ARG:CZ	2.19	0.55
4:S:548:GLN:HG2	4:S:576:MET:HE3	1.88	0.55
8:L:24:U:H2'	8:L:25:A:H8	1.69	0.55
1:A:39:ASN:OD1	1:A:39:ASN:O	2.24	0.55
4:E:20:ILE:HG12	4:E:21:ARG:HH11	1.70	0.55
7:K:442:LEU:HD12	7:K:510:VAL:HG21	1.88	0.55
2:Q:52:ASP:O	2:Q:55:MET:HG3	2.07	0.55
4:R:452:VAL:HA	4:R:455:LEU:HD12	1.87	0.55
7:X:283:HIS:CD2	7:X:287:VAL:HG21	2.40	0.55
7:X:372:THR:HG1	7:X:373:HIS:CE1	2.25	0.55
4:F:1:ALA:HB3	4:F:45:VAL:HG22	1.87	0.55
4:F:327:ILE:HG13	4:F:329:LYS:HB2	1.88	0.55
1:A:38:TYR:HB3	5:G:2:ASN:OD1	2.07	0.55
6:H:51:THR:HG22	6:H:60:GLU:CD	2.32	0.55
2:Q:103:LEU:O	2:Q:107:ILE:HG13	2.06	0.55
4:R:31:TYR:O	4:R:35:ILE:HG12	2.07	0.55
6:U:70:GLY:C	6:U:92:LEU:O	2.49	0.55
4:S:199:THR:HB	4:S:339:ARG:HD2	1.89	0.55
1:A:99:HIS:NE2	1:A:217:TYR:O	2.40	0.55
2:B:43:ASN:ND2	9:J:48:C:H5'	2.20	0.55
2:D:163:ASP:OD1	2:D:163:ASP:N	2.27	0.55
1:N:57:GLN:CD	1:N:65:LEU:HD23	2.32	0.55
4:R:178:ARG:HE	4:R:178:ARG:H	1.54	0.55
4:R:195:ILE:O	4:R:215:THR:OG1	2.25	0.55
4:R:277:TYR:HB3	4:R:396:TYR:HB2	1.89	0.55
4:R:363:LEU:HD12	4:R:364:PRO:HD2	1.87	0.55
4:F:171:LYS:NZ	4:F:174:PRO:HD3	2.22	0.55
4:F:332:ARG:NH1	4:F:346:PHE:HB2	2.22	0.55
8:I:22:G:H2'	8:I:23:C:H6	1.71	0.55
1:A:910:ASP:HB3	1:A:912:THR:HG23	1.89	0.55
4:R:23:PRO:HG2	4:R:25:LEU:HD21	1.88	0.55
4:F:462:LYS:HG2	4:F:463:ALA:H	1.72	0.55
1:A:348:PHE:HD2	1:A:351:LEU:HB2	1.71	0.55
1:A:624:ARG:HG3	1:A:624:ARG:HH11	1.72	0.55
4:E:476:TYR:N	4:E:576:MET:O	2.40	0.55
4:E:508:LYS:O	4:E:508:LYS:HD3	2.07	0.55
4:R:376:ILE:HG12	4:R:429:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:90:PHE:CE2	5:T:99:ARG:HG2	2.42	0.55
4:F:117:ALA:O	4:F:121:ILE:HG12	2.07	0.55
4:S:322:LEU:HB2	4:S:323:LYS:HZ2	1.71	0.55
4:S:465:LYS:NZ	4:S:569:LYS:O	2.32	0.55
4:E:262:PHE:CE2	4:E:297:LEU:HD12	2.42	0.54
5:G:90:PHE:CE2	5:G:99:ARG:HG2	2.43	0.54
2:O:98:LEU:O	2:O:100:ASN:N	2.39	0.54
6:U:120:CYS:HB2	6:U:122:MET:HE2	1.89	0.54
7:X:361:TYR:CE2	7:X:362:LYS:HE2	2.42	0.54
4:S:513:SER:OG	4:S:519:ASN:OD1	2.23	0.54
8:L:23:C:H2'	8:L:24:U:C6	2.41	0.54
1:A:57:GLN:CD	1:A:65:LEU:HD23	2.32	0.54
4:E:363:LEU:HD13	4:E:391:LEU:HD11	1.89	0.54
4:R:244:GLU:O	4:R:276:LYS:HG3	2.07	0.54
4:F:327:ILE:HA	4:F:328:ASP:C	2.33	0.54
4:S:43:LEU:HD22	4:S:47:PRO:HB3	1.90	0.54
2:B:180:LEU:O	2:B:181:ALA:O	2.25	0.54
6:H:54:ALA:HB1	6:H:98:GLN:H	1.70	0.54
7:K:356:CYS:O	7:K:360:ALA:HB2	2.08	0.54
1:N:910:ASP:HB3	1:N:912:THR:HG23	1.89	0.54
4:F:14:LEU:HD21	4:F:91:GLY:HA3	1.88	0.54
4:F:151:ILE:HB	4:F:224:TYR:CD1	2.43	0.54
4:F:471:CYS:HB2	4:F:590:LEU:HD13	1.89	0.54
2:B:160:VAL:O	2:B:184:LEU:HD22	2.07	0.54
4:E:486:SER:OG	4:E:487:ALA:N	2.41	0.54
7:K:81:ARG:NH1	7:K:81:ARG:HB2	2.23	0.54
7:K:204:GLU:OE1	7:K:213:ARG:NH2	2.39	0.54
1:N:7:PHE:HA	1:N:104:PHE:HE2	1.72	0.54
1:N:872:HIS:CD2	1:N:873:PRO:HD2	2.41	0.54
7:X:391:ARG:NH2	7:X:438:ASN:OD1	2.36	0.54
4:S:473:LYS:HZ1	4:S:573:LEU:HD13	1.72	0.54
1:A:6:SER:CB	1:A:104:PHE:HZ	2.18	0.54
1:A:872:HIS:CD2	1:A:873:PRO:HD2	2.41	0.54
2:D:124:THR:HA	2:D:190:ARG:HB3	1.89	0.54
4:E:3:GLY:HA3	4:E:24:PHE:CE2	2.42	0.54
1:N:105:ARG:HA	1:N:109:ASP:O	2.08	0.54
1:N:358:ASP:OD1	1:N:533:ARG:NH2	2.36	0.54
2:Q:53:ALA:O	2:Q:57:ARG:HG2	2.08	0.54
4:R:186:ARG:HD2	4:R:195:ILE:HG21	1.90	0.54
5:T:28:ALA:HB1	5:T:44:LEU:HD11	1.89	0.54
6:U:19:PHE:HB3	7:X:201:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:187:VAL:HA	4:S:192:LYS:HA	1.90	0.54
4:S:425:VAL:O	4:S:428:LEU:HG	2.08	0.54
1:A:302:LEU:O	1:A:648:LEU:HD21	2.07	0.54
1:A:684:ASP:O	9:J:27:C:C4'	2.56	0.54
1:A:926:THR:CB	1:A:927:PRO:HD2	2.05	0.54
3:C:71:LEU:HD23	2:D:96:ARG:NH2	2.16	0.54
4:E:499:PHE:O	4:E:503:ASN:N	2.38	0.54
7:X:328:VAL:HG11	7:X:379:ASP:OD2	2.07	0.54
7:X:337:ALA:HB2	7:X:363:ILE:HD11	1.90	0.54
4:F:496:VAL:HG11	4:F:511:PHE:HZ	1.72	0.54
4:S:21:ARG:NH1	4:S:136:GLU:HB3	2.23	0.54
8:I:25:A:H2'	8:I:26:G:C8	2.42	0.54
8:L:25:A:H2'	8:L:26:G:C8	2.42	0.54
1:A:420:TYR:OH	3:C:4:SER:OG	2.16	0.54
4:E:90:PHE:CZ	7:X:466:VAL:HA	2.43	0.54
5:G:11:GLN:NE2	5:G:12:MET:O	2.41	0.54
4:R:44:SER:OG	4:R:45:VAL:N	2.40	0.54
8:L:22:G:H2'	8:L:23:C:H6	1.70	0.54
1:A:105:ARG:HA	1:A:109:ASP:O	2.08	0.54
7:K:324:ASP:O	7:K:325:LYS:NZ	2.39	0.54
1:N:105:ARG:HH12	1:N:108:GLY:H	1.55	0.54
4:R:514:PRO:O	4:R:554:HIS:NE2	2.27	0.54
6:U:89:PHE:C	6:U:90:CYS:O	2.47	0.54
6:U:123:TRP:HB2	6:U:126:TYR:HB2	1.89	0.54
4:S:315:ASP:HA	4:S:318:CYS:SG	2.48	0.54
1:N:755:MET:HG2	1:N:764:VAL:HG22	1.90	0.54
2:Q:117:LEU:HD12	2:Q:129:MET:HE2	1.88	0.54
4:R:545:ILE:HG23	4:R:573:LEU:HB3	1.89	0.54
5:T:11:GLN:NE2	5:T:12:MET:O	2.41	0.54
1:A:358:ASP:OD1	1:A:533:ARG:NH2	2.36	0.54
4:E:9:ASN:O	4:E:11:GLN:NE2	2.39	0.54
4:E:325:LEU:HD22	4:E:355:TYR:CE2	2.43	0.54
7:K:72:MET:SD	7:K:241:MET:HE3	2.48	0.54
1:N:683:GLY:O	9:M:26:A:O2'	2.18	0.54
4:R:458:ASP:HB2	4:R:460:LYS:HZ2	1.73	0.54
7:X:130:ASN:ND2	7:X:131:THR:O	2.40	0.54
4:S:120:TYR:HD2	4:S:417:LEU:HD11	1.73	0.54
1:A:855:MET:O	1:A:858:ARG:HG2	2.08	0.53
4:R:114:TRP:C	4:R:411:LEU:HD21	2.32	0.53
4:F:171:LYS:HZ1	4:F:174:PRO:HD3	1.71	0.53
4:S:383:ASP:HA	4:S:386:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:MET:HG2	1:A:764:VAL:HG22	1.90	0.53
4:E:81:PHE:HZ	4:E:90:PHE:CD1	2.26	0.53
4:E:447:GLU:OE2	4:E:587:PHE:HA	2.09	0.53
2:O:6:PHE:HA	2:O:9:LEU:HD21	1.90	0.53
4:R:169:VAL:O	4:R:169:VAL:CG2	2.55	0.53
4:F:287:GLY:O	4:F:291:PHE:HB2	2.08	0.53
4:F:509:ALA:HA	4:F:543:TYR:HB2	1.88	0.53
4:F:576:MET:HG2	4:F:577:SER:O	2.08	0.53
2:B:164:SER:C	2:B:165:LYS:HD2	2.33	0.53
4:E:194:GLN:NE2	4:E:196:GLY:O	2.41	0.53
7:K:291:ASP:OD2	7:K:293:THR:OG1	2.25	0.53
4:R:153:THR:HA	4:R:224:TYR:HA	1.89	0.53
4:R:186:ARG:NH2	4:R:220:ASN:HB2	2.24	0.53
4:R:476:TYR:CE2	4:R:495:VAL:HG21	2.43	0.53
4:S:66:GLY:HA3	4:S:71:TYR:CE2	2.43	0.53
1:A:814:SER:O	1:A:814:SER:OG	2.24	0.53
4:E:271:LYS:O	4:E:275:GLN:NE2	2.42	0.53
6:U:19:PHE:CD2	7:X:62:MET:HE1	2.43	0.53
7:X:330:HIS:CG	7:X:377:PHE:HD2	2.27	0.53
4:S:90:PHE:HA	4:S:94:LYS:NZ	2.22	0.53
4:S:402:PRO:HD3	4:S:429:MET:HE2	1.91	0.53
4:S:453:SER:HA	4:S:457:TYR:HB2	1.90	0.53
1:A:11:VAL:C	1:A:13:GLY:N	2.65	0.53
1:N:814:SER:O	1:N:814:SER:OG	2.24	0.53
4:R:267:ALA:HA	4:R:270:GLN:OE1	2.09	0.53
6:U:83:HIS:NE2	6:U:90:CYS:CB	2.71	0.53
4:S:37:THR:O	4:S:40:LYS:NZ	2.41	0.53
4:S:152:ALA:HB3	4:S:225:PHE:HB2	1.90	0.53
9:M:22:U:C5'	9:M:23:C:OP2	2.55	0.53
2:B:31:SER:OG	2:B:32:GLU:N	2.40	0.53
4:E:292:ALA:O	4:E:306:TYR:OH	2.18	0.53
4:E:488:ILE:HD12	4:E:518:GLN:HG2	1.90	0.53
4:R:550:THR:HB	4:R:552:THR:HG23	1.91	0.53
4:R:556:CYS:HA	4:R:561:PHE:CE2	2.43	0.53
7:X:33:PHE:CE1	7:X:45:ILE:HD11	2.43	0.53
4:F:163:LEU:HB2	4:F:211:TYR:CD1	2.43	0.53
4:F:426:CYS:HA	4:F:429:MET:HG2	1.90	0.53
4:S:124:ASN:ND2	4:S:422:PHE:O	2.42	0.53
4:S:565:ILE:HG13	4:S:572:ILE:HG12	1.90	0.53
1:A:370:GLU:HA	1:A:373:VAL:HG22	1.91	0.53
1:A:665:GLU:OE1	1:A:665:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:SER:N	2:D:176:ASN:OD1	2.42	0.53
4:E:293:ILE:HG21	4:E:324:TYR:HB2	1.90	0.53
1:N:8:LEU:HD11	1:N:19:LEU:O	2.08	0.53
7:X:278:ARG:O	7:X:282:VAL:HG23	2.08	0.53
7:X:510:VAL:HG12	7:X:511:TYR:N	2.23	0.53
1:A:511:LYS:NZ	9:J:25:G:H21	2.06	0.53
1:A:836:ARG:NH2	1:A:840:ALA:HB2	2.24	0.53
4:E:402:PRO:HG3	4:E:429:MET:HG2	1.91	0.53
1:N:836:ARG:NH2	1:N:840:ALA:HB2	2.24	0.53
7:X:25:THR:OG1	7:X:26:HIS:N	2.40	0.53
4:F:15:ARG:NH1	4:F:15:ARG:HB2	2.24	0.53
4:F:473:LYS:HG2	4:F:590:LEU:HB2	1.90	0.53
4:S:19:CYS:SG	4:S:33:HIS:HE1	2.31	0.53
4:E:15:ARG:HE	4:E:24:PHE:HE1	1.57	0.53
4:R:453:SER:O	4:R:458:ASP:N	2.42	0.53
4:F:453:SER:HB2	4:F:459:ASN:HA	1.91	0.53
4:S:21:ARG:NH1	4:S:136:GLU:OE1	2.36	0.53
1:A:717:ASP:OD2	1:A:719:TYR:HB3	2.09	0.53
4:E:510:VAL:HG13	4:E:544:VAL:HG13	1.90	0.53
5:G:9:LEU:HD12	5:G:32:TYR:O	2.09	0.53
5:G:28:ALA:HB1	5:G:44:LEU:HD11	1.89	0.53
5:T:52:LYS:O	5:T:68:GLU:HA	2.09	0.53
6:U:125:GLY:N	6:U:128:CYS:SG	2.82	0.53
7:X:261:CYS:SG	7:X:415:ASP:HB2	2.49	0.53
7:X:463:ILE:O	7:X:465:TYR:CD2	2.62	0.53
1:A:731:LEU:HB3	1:A:732:TYR:HD1	1.74	0.52
1:A:904:SER:HB3	7:X:468:LEU:H	1.74	0.52
4:E:494:GLY:HA2	4:E:497:ARG:HD2	1.91	0.52
4:E:511:PHE:HD2	4:E:526:LEU:HD22	1.74	0.52
4:E:557:ASN:HB3	4:E:560:ARG:HB2	1.91	0.52
7:K:313:GLN:NE2	7:K:385:TRP:CD1	2.77	0.52
1:N:504:PHE:C	1:N:504:PHE:HD1	2.17	0.52
5:T:76:VAL:HG12	5:T:85:VAL:HG22	1.91	0.52
7:X:416:GLY:O	7:X:430:ALA:HB2	2.09	0.52
4:F:176:LEU:HD22	4:F:202:LYS:HA	1.91	0.52
4:F:402:PRO:HD3	4:F:429:MET:HE2	1.91	0.52
4:S:3:GLY:HA3	4:S:24:PHE:CD2	2.43	0.52
1:A:528:PHE:HD2	1:A:570:GLN:HE21	1.56	0.52
1:A:731:LEU:HD23	1:A:732:TYR:HE1	1.74	0.52
2:B:15:PHE:HA	2:B:45:ALA:HB1	1.91	0.52
4:E:474[B]:MET:O	4:E:576:MET:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:496:VAL:O	4:E:500:LEU:HG	2.09	0.52
4:E:514:PRO:O	4:E:554:HIS:NE2	2.31	0.52
1:N:511:LYS:HZ3	9:M:25:G:N2	2.06	0.52
1:N:665:GLU:OE1	1:N:665:GLU:N	2.41	0.52
1:N:717:ASP:OD2	1:N:719:TYR:HB3	2.09	0.52
1:N:780:LYS:NZ	1:N:780:LYS:HB2	2.25	0.52
3:P:27:LYS:O	3:P:31:GLN:HG3	2.09	0.52
4:R:15:ARG:N	4:R:43:LEU:O	2.40	0.52
4:F:296:ALA:O	4:F:355:TYR:OH	2.22	0.52
4:S:489:ASN:ND2	4:S:549:THR:HA	2.24	0.52
4:E:492:GLN:OE1	4:E:548:GLN:O	2.27	0.52
1:N:275:PHE:HE2	1:N:321:PHE:HB3	1.74	0.52
2:Q:182:TRP:O	2:Q:184:LEU:N	2.42	0.52
4:R:363:LEU:HD11	4:R:391:LEU:HD21	1.91	0.52
4:R:548:GLN:NE2	4:R:577:SER:H	2.07	0.52
4:F:20:ILE:O	4:F:22:ARG:NH1	2.42	0.52
8:L:24:U:H2'	8:L:25:A:C8	2.44	0.52
1:A:7:PHE:CE1	1:A:113:HIS:HD2	2.26	0.52
4:E:181:VAL:O	4:E:228:THR:OG1	2.27	0.52
4:E:449:VAL:HG13	4:E:461:LEU:HG	1.91	0.52
5:G:69:LEU:HD23	5:G:89:TYR:CD2	2.44	0.52
1:N:528:PHE:HD2	1:N:570:GLN:HE21	1.56	0.52
1:N:718:LYS:HZ3	1:N:718:LYS:HA	1.75	0.52
4:F:573:LEU:HD12	4:F:575:ILE:HD11	1.92	0.52
4:S:7:LEU:HD13	4:S:29:CYS:HB3	1.92	0.52
4:E:42:VAL:HB	4:E:48:TYR:HD2	1.75	0.52
5:G:5:SER:CB	5:G:101:MET:HG2	2.39	0.52
5:G:52:LYS:O	5:G:68:GLU:HA	2.09	0.52
1:A:260:ASP:HB3	1:A:263:LYS:HG3	1.91	0.52
4:E:445:PRO:O	4:E:449:VAL:HG23	2.10	0.52
4:E:497:ARG:O	4:E:501:THR:HG23	2.10	0.52
5:G:76:VAL:HG12	5:G:85:VAL:HG22	1.92	0.52
2:O:71:TYR:CE1	4:S:92:LEU:HD22	2.45	0.52
2:Q:33:VAL:O	2:Q:37:LYS:HG3	2.10	0.52
4:R:15:ARG:HD2	4:R:22:ARG:O	2.09	0.52
4:R:475:PHE:HB2	4:R:582:TYR:CE2	2.45	0.52
4:E:376:ILE:HG22	4:E:400:GLY:HA3	1.90	0.52
7:K:342:PRO:HB2	7:K:343:GLN:OE1	2.09	0.52
1:N:731:LEU:HB3	1:N:732:TYR:HD1	1.74	0.52
1:N:731:LEU:HD23	1:N:732:TYR:HE1	1.74	0.52
1:N:808:GLY:HA3	1:N:817:THR:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:13:LEU:HD12	2:Q:91:LEU:HD11	1.92	0.52
4:R:159:SER:OG	4:R:162:GLU:HG2	2.10	0.52
4:R:376:ILE:HG22	4:R:400:GLY:HA3	1.91	0.52
4:R:546:PHE:HB3	4:R:574:CYS:HA	1.92	0.52
7:X:127:THR:OG1	7:X:130:ASN:O	2.23	0.52
7:X:359:LYS:HA	7:X:362:LYS:HD2	1.92	0.52
8:I:24:U:H2'	8:I:25:A:C8	2.44	0.52
1:A:501:SER:OG	9:J:25:G:OP1	2.23	0.52
2:B:8:SER:O	2:B:9:LEU:HD23	2.09	0.52
3:C:27:LYS:O	3:C:31:GLN:HG3	2.09	0.52
4:E:167:TRP:HB2	4:E:173:ARG:CZ	2.40	0.52
5:G:12:MET:HG3	5:G:13:SER:N	2.23	0.52
1:N:22:CYS:HB3	1:N:55:ARG:O	2.10	0.52
4:R:5:CYS:SG	4:R:26:CYS:HB3	2.49	0.52
4:R:266:VAL:HG22	4:R:270:GLN:NE2	2.24	0.52
6:U:13:VAL:HG22	6:U:30:TYR:CE2	2.41	0.52
4:F:20:ILE:HG13	4:F:21:ARG:HD2	1.92	0.52
4:S:90:PHE:HA	4:S:94:LYS:HZ1	1.75	0.52
8:L:21:U:C2	8:L:22:G:C8	2.98	0.52
1:A:415:PHE:HE2	3:C:8:CYS:SG	2.33	0.52
1:A:780:LYS:HB2	1:A:780:LYS:NZ	2.25	0.52
3:P:46:THR:O	3:P:50:GLU:HG2	2.10	0.52
1:A:904:SER:C	7:X:468:LEU:HB2	2.35	0.52
2:B:59:LEU:HD22	4:F:81:PHE:HD2	1.75	0.52
2:B:123:THR:O	2:B:190:ARG:NH1	2.43	0.52
4:E:394:LYS:HB2	4:E:395:HIS:CE1	2.45	0.52
4:E:473:LYS:HE3	4:E:587:PHE:O	2.09	0.52
1:N:415:PHE:CE1	1:N:417:LYS:HA	2.45	0.52
4:R:283:PRO:HG3	4:R:457:TYR:CE2	2.44	0.52
4:R:290:HIS:HA	4:R:320:LYS:HZ3	1.75	0.52
7:X:384:PHE:O	7:X:398:VAL:HA	2.10	0.52
7:X:476:ARG:HD3	7:X:476:ARG:N	2.25	0.52
4:S:246:TYR:N	4:S:274:MET:O	2.43	0.52
4:S:477:LYS:NZ	4:S:492:GLN:OE1	2.42	0.52
4:S:532:THR:O	4:S:535:SER:OG	2.24	0.52
1:A:304:ASP:OD2	1:A:640:ARG:NH1	2.43	0.51
2:B:141:THR:O	2:B:141:THR:CG2	2.53	0.51
4:E:473:LYS:HD3	4:E:585:LEU:HD23	1.92	0.51
4:E:493:ILE:HG22	4:E:497:ARG:NE	2.24	0.51
7:K:474:ILE:O	7:K:474:ILE:HG13	2.10	0.51
1:N:20:THR:HG22	1:N:21:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:304:ASP:OD2	1:N:640:ARG:NH1	2.43	0.51
1:N:370:GLU:HA	1:N:373:VAL:HG22	1.91	0.51
1:N:420:TYR:OH	3:P:4:SER:OG	2.21	0.51
5:T:69:LEU:HD23	5:T:89:TYR:CD2	2.44	0.51
4:F:304:ILE:HG23	4:F:370:ILE:HG23	1.92	0.51
4:F:565:ILE:HG23	4:F:572:ILE:HD13	1.92	0.51
4:S:248:ARG:HE	4:S:249:ILE:HG12	1.74	0.51
4:E:11:GLN:HB2	4:E:93:TYR:CD2	2.45	0.51
1:N:260:ASP:HB3	1:N:263:LYS:HG3	1.90	0.51
5:T:12:MET:HG3	5:T:13:SER:N	2.23	0.51
4:F:59:ASP:O	4:F:62:GLN:NE2	2.44	0.51
4:S:72:CYS:SG	4:S:75:HIS:N	2.75	0.51
4:S:124:ASN:ND2	4:S:421:TYR:O	2.43	0.51
8:I:21:U:C2	8:I:22:G:C8	2.98	0.51
3:C:46:THR:O	3:C:50:GLU:HG2	2.10	0.51
4:E:20:ILE:O	4:E:21:ARG:NH1	2.44	0.51
4:R:163:LEU:HG	4:R:211:TYR:CE1	2.45	0.51
4:R:488:ILE:HD13	4:R:521:VAL:HG21	1.93	0.51
4:R:553:ALA:HA	4:R:556:CYS:HB3	1.92	0.51
7:X:358:ASP:CG	7:X:359:LYS:HD2	2.35	0.51
4:S:151:ILE:HB	4:S:224:TYR:HD1	1.76	0.51
1:A:275:PHE:HE2	1:A:321:PHE:HB3	1.74	0.51
1:A:415:PHE:CE1	1:A:417:LYS:HA	2.45	0.51
2:B:85:SER:O	2:B:89:THR:HG23	2.09	0.51
4:R:563:VAL:HA	4:R:567:ARG:HH21	1.76	0.51
6:U:56:THR:HG23	6:U:96:TYR:HB2	1.92	0.51
7:X:483:VAL:O	7:X:484:CYS:C	2.52	0.51
4:F:257:ASN:O	4:F:258:ILE:HD13	2.11	0.51
4:S:66:GLY:HA3	4:S:71:TYR:HE2	1.75	0.51
1:A:156:TYR:HE2	1:A:174:VAL:HG21	1.76	0.51
2:D:15:PHE:O	2:D:19:GLN:HG2	2.11	0.51
4:E:470:GLN:HA	4:E:472:PHE:HE1	1.73	0.51
1:N:156:TYR:HE2	1:N:174:VAL:HG21	1.76	0.51
1:N:419:PHE:CD1	1:N:887:TYR:CE2	2.98	0.51
1:N:713:ASN:HB2	1:N:714:LYS:HZ2	1.74	0.51
4:R:281:GLN:HB2	4:R:434:PRO:HG3	1.93	0.51
7:X:352:ASP:O	7:X:365:GLU:HA	2.11	0.51
1:A:419:PHE:CD1	1:A:887:TYR:CE2	2.99	0.51
6:H:126:TYR:N	6:H:127:GLY:HA2	2.25	0.51
7:K:474:ILE:HG22	7:K:520:TRP:CZ2	2.46	0.51
2:Q:147:PHE:O	2:Q:154:TRP:N	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:483:ASP:OD2	4:R:488:ILE:HD11	2.10	0.51
5:T:68:GLU:C	5:T:68:GLU:CD	2.79	0.51
7:X:185:LEU:HB2	7:X:191:GLU:OE2	2.11	0.51
4:E:282:GLY:HA2	4:E:438:LEU:HB2	1.91	0.51
6:H:70:GLY:HA2	6:H:97:VAL:HG23	1.92	0.51
1:N:62:ASP:OD1	1:N:62:ASP:N	2.44	0.51
1:N:342:VAL:HG11	1:N:374:TYR:CE2	2.46	0.51
1:N:726:ARG:HE	1:N:741:PHE:HD2	1.58	0.51
4:R:73:LYS:H	4:R:73:LYS:HZ3	1.58	0.51
1:A:726:ARG:HE	1:A:741:PHE:HD2	1.58	0.51
4:E:375:GLU:HB3	4:E:378:MET:HE2	1.91	0.51
5:G:68:GLU:C	5:G:68:GLU:CD	2.79	0.51
7:K:29:VAL:HG13	7:K:30:ASP:O	2.11	0.51
7:K:389:VAL:HG23	7:K:390:ASP:O	2.11	0.51
4:R:474[B]:MET:O	4:R:576:MET:N	2.42	0.51
5:T:113:GLN:HB3	6:U:1:ALA:H1	1.76	0.51
4:S:151:ILE:HB	4:S:224:TYR:CD1	2.46	0.51
4:S:549:THR:OG1	4:S:550:THR:N	2.43	0.51
1:A:321:PHE:HB3	1:A:322:PRO:HD2	1.93	0.51
1:A:683:GLY:O	9:J:26:A:O2'	2.23	0.51
3:C:70:LYS:HD2	2:D:92:PHE:HD2	1.76	0.51
4:R:448:ILE:O	4:R:452:VAL:HG22	2.11	0.51
4:R:519:ASN:OD1	4:R:532:THR:OG1	2.28	0.51
4:F:268:ASN:O	4:F:272:VAL:HG23	2.11	0.51
4:F:545:ILE:HG23	4:F:573:LEU:HD21	1.92	0.51
4:E:152:ALA:HA	4:E:167:TRP:HA	1.92	0.51
3:P:13:LEU:HD11	3:P:56:LEU:HD13	1.93	0.51
4:R:127:THR:HG23	4:R:130:LEU:H	1.75	0.51
4:R:228:THR:O	4:R:230:HIS:CE1	2.64	0.51
4:R:490:ARG:HA	4:R:493:ILE:HD12	1.93	0.51
6:U:25:LYS:HZ3	6:U:28:LYS:HB2	1.75	0.51
7:X:222:ASP:OD1	7:X:222:ASP:N	2.39	0.51
7:X:465:TYR:CE1	7:X:481:GLY:HA3	2.45	0.51
4:S:311:HIS:HA	4:S:314:VAL:HG22	1.93	0.51
1:A:477:ASP:OD2	1:A:640:ARG:NE	2.28	0.50
1:A:532:LYS:HD3	1:A:650:HIS:HD2	1.76	0.50
4:E:576:MET:HG3	4:E:578:ASP:OD1	2.11	0.50
1:N:477:ASP:OD2	1:N:640:ARG:NE	2.28	0.50
1:N:718:LYS:HA	1:N:718:LYS:NZ	2.26	0.50
2:D:171:GLU:O	2:D:176:ASN:ND2	2.43	0.50
4:E:139:LYS:HE3	4:E:382:TYR:CD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:202:LYS:HA	4:E:209:VAL:HG12	1.92	0.50
7:K:154:TYR:HB2	7:K:155:LYS:NZ	2.25	0.50
7:K:345:ASP:OD1	7:K:345:ASP:N	2.43	0.50
1:N:269:ASP:OD1	1:N:269:ASP:N	2.42	0.50
2:O:11:SER:HA	2:O:48:GLU:CD	2.37	0.50
4:R:540:GLU:HB2	4:R:569:LYS:HE3	1.93	0.50
7:X:210:CYS:SG	7:X:211:ASP:N	2.85	0.50
7:X:391:ARG:HH12	7:X:438:ASN:HD21	1.58	0.50
7:X:474:ILE:HG22	7:X:520:TRP:CE2	2.46	0.50
1:A:342:VAL:HG11	1:A:374:TYR:CE2	2.46	0.50
2:B:51:ARG:O	2:B:55:MET:HG2	2.12	0.50
3:C:13:LEU:HD11	3:C:56:LEU:HD13	1.93	0.50
4:E:354:GLN:HG2	4:E:355:TYR:CE1	2.45	0.50
1:N:915:TYR:O	1:N:921:TYR:OH	2.21	0.50
2:Q:53:ALA:O	2:Q:56:GLN:HG3	2.10	0.50
4:R:62:GLN:HB3	4:R:73:LYS:NZ	2.26	0.50
4:R:73:LYS:H	4:R:73:LYS:NZ	2.09	0.50
4:R:447:GLU:OE1	4:R:471:CYS:HB2	2.12	0.50
4:R:480:ILE:HG21	4:R:550:THR:HG22	1.93	0.50
6:U:54:ALA:HB1	6:U:98:GLN:H	1.76	0.50
4:F:212:ARG:HD3	4:F:340:VAL:HA	1.92	0.50
4:F:376:ILE:HG12	4:F:400:GLY:HA3	1.93	0.50
2:B:161:ASP:CB	2:B:184:LEU:CD2	2.90	0.50
4:E:453:SER:HB3	4:E:461:LEU:HB3	1.93	0.50
2:Q:162:ALA:HB3	2:Q:181:ALA:HB1	1.93	0.50
6:U:82:ASP:OD1	6:U:83:HIS:N	2.45	0.50
7:X:61:LYS:O	7:X:61:LYS:CG	2.42	0.50
4:E:272:VAL:HA	4:E:275:GLN:HE21	1.76	0.50
7:K:48:ASP:OD1	7:K:49:MET:N	2.45	0.50
7:K:361:TYR:CD1	7:K:362:LYS:HG3	2.46	0.50
7:K:447:TYR:CD2	7:K:519:LEU:HD22	2.46	0.50
4:R:21:ARG:HH22	4:R:229:SER:HB2	1.77	0.50
2:D:7:SER:O	2:D:9:LEU:N	2.42	0.50
4:E:56:ASP:OD1	4:E:56:ASP:N	2.30	0.50
4:E:262:PHE:HB3	4:E:269:TYR:OH	2.12	0.50
6:H:66:GLU:O	6:H:98:GLN:HA	2.12	0.50
7:K:31:THR:OG1	7:K:32:LYS:NZ	2.45	0.50
1:N:532:LYS:HD3	1:N:650:HIS:HD2	1.76	0.50
4:R:496:VAL:HG13	4:R:545:ILE:HG21	1.93	0.50
7:X:328:VAL:HG23	7:X:347:GLU:OE2	2.12	0.50
4:F:370:ILE:HD12	4:F:395:HIS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:HIS:CE1	1:A:217:TYR:O	2.65	0.50
1:A:225:THR:HG22	1:A:226:THR:H	1.76	0.50
2:B:45:ALA:HA	2:B:48:GLU:CD	2.36	0.50
4:E:249:ILE:CG2	4:E:252:LEU:HB2	2.42	0.50
5:G:28:ALA:O	5:G:29:LEU:HD13	2.12	0.50
7:K:291:ASP:OD1	7:K:293:THR:N	2.44	0.50
1:N:611:ASN:HD22	1:N:769:THR:CG2	2.25	0.50
4:R:451:THR:HG21	4:R:587:PHE:CE1	2.47	0.50
4:R:516:ASN:HA	4:R:519:ASN:OD1	2.11	0.50
7:X:302:GLU:HG3	7:X:422:ASN:HB2	1.94	0.50
4:F:17:GLY:HA2	4:F:22:ARG:HG2	1.93	0.50
4:S:424:SER:HA	4:S:427:ARG:HD3	1.93	0.50
9:J:39:A:H2'	9:J:40:U:O4'	2.11	0.50
9:J:47:A:H2'	9:J:48:C:C6	2.47	0.50
9:M:39:A:H2'	9:M:40:U:O4'	2.11	0.50
1:A:428:PHE:HB3	1:A:429:PHE:CD1	2.47	0.50
1:A:624:ARG:HH11	1:A:624:ARG:CG	2.25	0.50
5:G:113:GLN:OE1	5:G:113:GLN:HA	2.12	0.50
7:K:147:LYS:C	7:K:149:LEU:H	2.20	0.50
1:N:225:THR:HG22	1:N:226:THR:H	1.76	0.50
4:R:151:ILE:HB	4:R:168:GLU:OE2	2.12	0.50
4:R:171:LYS:HB3	4:R:172:PRO:CD	2.42	0.50
4:R:446:ALA:HA	4:R:449:VAL:HB	1.94	0.50
4:R:581:LEU:HA	4:R:584:LYS:HB2	1.94	0.50
4:S:303:ARG:HA	4:S:354:GLN:HB2	1.94	0.50
9:M:47:A:H2'	9:M:48:C:C6	2.47	0.50
1:A:103:LYS:NZ	1:A:110:MET:O	2.44	0.50
1:A:269:ASP:OD1	1:A:269:ASP:N	2.42	0.50
6:H:48:HIS:HA	6:H:61:ALA:HB3	1.93	0.50
7:K:154:TYR:HB2	7:K:155:LYS:HZ2	1.77	0.50
1:N:129:TYR:CE2	1:N:133:HIS:HD2	2.30	0.50
1:N:321:PHE:HB3	1:N:322:PRO:HD2	1.93	0.50
2:Q:47:SER:O	2:Q:51:ARG:HG3	2.11	0.50
4:R:7:LEU:C	4:R:129:ARG:HH12	2.20	0.50
4:R:424:SER:O	4:R:427:ARG:HB3	2.12	0.50
4:S:337:ARG:HH22	4:S:362:ALA:HB2	1.76	0.50
1:A:9:ASN:C	1:A:11:VAL:H	2.19	0.49
4:E:443:ARG:NH1	4:E:566:THR:O	2.42	0.49
4:E:447:GLU:OE2	4:E:471:CYS:HB2	2.12	0.49
6:H:55:ILE:HD11	6:H:95:LYS:HG3	1.92	0.49
4:R:557:ASN:OD1	4:R:560:ARG:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:566:THR:OG1	4:R:567:ARG:NH2	2.41	0.49
4:E:452:VAL:HG11	4:E:566:THR:HG23	1.94	0.49
7:K:358:ASP:OD1	7:K:358:ASP:N	2.44	0.49
7:K:373:HIS:HA	7:K:376:LYS:HD3	1.94	0.49
1:N:636:LEU:HD21	1:N:655:LEU:HD22	1.93	0.49
2:Q:137:THR:O	2:Q:141:THR:OG1	2.25	0.49
4:R:472:PHE:N	4:R:572:ILE:O	2.25	0.49
4:R:474[A]:MET:O	4:R:576:MET:N	2.43	0.49
7:X:370:TYR:HE1	7:X:393:PRO:HA	1.76	0.49
4:S:181:VAL:HB	4:S:339:ARG:HD3	1.93	0.49
4:S:549:THR:HG23	4:S:555:SER:HB2	1.94	0.49
1:A:12:CYS:SG	1:A:17:ALA:HA	2.53	0.49
1:A:860:VAL:O	1:A:864:ILE:HG13	2.12	0.49
4:E:32:ASP:O	4:E:36:SER:HB3	2.12	0.49
1:N:105:ARG:HB3	1:N:110:MET:SD	2.52	0.49
4:R:21:ARG:NE	4:R:21:ARG:HA	2.27	0.49
4:R:32:ASP:HB3	4:R:103:VAL:HG21	1.94	0.49
4:R:548:GLN:HE22	4:R:578:ASP:H	1.60	0.49
6:U:54:ALA:HA	6:U:98:GLN:HB2	1.93	0.49
6:U:62:ASN:HB2	6:U:65:GLN:HG2	1.93	0.49
7:X:474:ILE:HG22	7:X:520:TRP:CZ2	2.47	0.49
4:F:100:SER:OG	4:F:101:ASP:N	2.43	0.49
4:S:235:LEU:HD23	4:S:385:SER:OG	2.13	0.49
1:A:129:TYR:CE2	1:A:133:HIS:HD2	2.30	0.49
1:A:612:PRO:CB	1:A:805:LEU:HD12	2.38	0.49
5:G:51:LEU:H	5:G:89:TYR:HE2	1.60	0.49
1:N:431:GLU:OE1	1:N:432:GLY:N	2.46	0.49
1:N:624:ARG:HH11	1:N:624:ARG:CG	2.25	0.49
1:N:860:VAL:O	1:N:864:ILE:HG13	2.12	0.49
4:R:277:TYR:HB2	4:R:398:TYR:HE1	1.77	0.49
4:R:544:VAL:O	4:R:572:ILE:HA	2.12	0.49
7:X:242:ILE:HD11	7:X:247:TRP:HE1	1.78	0.49
1:A:388:LEU:HD23	1:A:397:SER:OG	2.12	0.49
1:A:431:GLU:OE1	1:A:432:GLY:N	2.46	0.49
1:A:636:LEU:HD21	1:A:655:LEU:HD22	1.93	0.49
4:E:477:LYS:HE2	4:E:579:ARG:NH2	2.27	0.49
7:K:131:THR:OG1	7:K:132:ASP:N	2.44	0.49
7:K:515:ASP:OD1	7:K:516:THR:N	2.46	0.49
1:N:809:PRO:HD2	1:N:817:THR:HG21	1.94	0.49
4:R:40:LYS:HE2	4:R:59:ASP:OD1	2.12	0.49
4:R:66:GLY:HA2	4:R:80:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:561:PHE:CE2	4:R:581:LEU:HG	2.48	0.49
7:X:366:LEU:HD11	7:X:373:HIS:HE2	1.76	0.49
4:F:117:ALA:HA	4:F:412:LEU:HD11	1.94	0.49
4:F:235:LEU:HD11	4:F:382:TYR:CZ	2.47	0.49
4:S:44:SER:OG	4:S:46:ASN:O	2.28	0.49
5:G:33:ASN:N	5:G:40:PHE:O	2.46	0.49
7:K:339:LYS:HG2	7:K:348:TRP:CE3	2.47	0.49
1:N:225:THR:HG22	1:N:226:THR:N	2.27	0.49
4:R:228:THR:HG22	4:R:229:SER:H	1.78	0.49
5:T:113:GLN:OE1	5:T:113:GLN:HA	2.12	0.49
4:S:66:GLY:HA2	4:S:80:SER:HB2	1.94	0.49
4:S:192:LYS:HD3	4:S:224:TYR:CE2	2.47	0.49
9:M:25:G:HO2'	9:M:26:A:P	2.35	0.49
1:A:225:THR:HG22	1:A:226:THR:N	2.26	0.49
3:C:71:LEU:HD13	2:D:111:ARG:HE	1.78	0.49
4:E:16:CYS:O	4:E:22:ARG:HD3	2.13	0.49
4:E:377:SER:OG	4:E:401:ASP:O	2.31	0.49
4:E:580:ASP:O	4:E:584:LYS:HG3	2.13	0.49
6:H:50:GLY:HA3	6:H:60:GLU:HG2	1.94	0.49
7:X:330:HIS:CD2	7:X:349:LYS:HD2	2.48	0.49
4:F:306:TYR:HB2	4:F:357:PHE:HD1	1.77	0.49
4:S:293:ILE:HG21	4:S:324:TYR:CD1	2.48	0.49
4:S:311:HIS:CE1	4:S:338:ALA:HA	2.48	0.49
4:E:492:GLN:CD	4:E:547:THR:HB	2.37	0.49
7:K:207:CYS:SG	7:K:208:CYS:N	2.86	0.49
1:N:428:PHE:HB3	1:N:429:PHE:CD1	2.47	0.49
5:T:51:LEU:H	5:T:89:TYR:HE2	1.59	0.49
6:U:19:PHE:HD2	7:X:62:MET:HE1	1.78	0.49
6:U:64:ASP:O	6:U:101:THR:HG23	2.13	0.49
7:X:465:TYR:HD1	7:X:467:PRO:HD3	1.78	0.49
4:F:152:ALA:O	4:F:225:PHE:N	2.43	0.49
4:F:327:ILE:HA	4:F:329:LYS:HG2	1.93	0.49
4:F:445:PRO:HB3	4:F:465:LYS:NZ	2.27	0.49
4:S:332:ARG:NE	4:S:346:PHE:HB2	2.27	0.49
1:A:619:TYR:OH	1:A:695:ASN:OD1	2.28	0.49
2:B:15:PHE:O	2:B:19:GLN:HG2	2.13	0.49
4:E:182:PHE:CD1	4:E:227:LEU:HA	2.48	0.49
1:N:388:LEU:HD23	1:N:397:SER:OG	2.12	0.49
1:N:809:PRO:O	1:N:809:PRO:HG2	2.11	0.49
4:R:189:LYS:N	4:R:190:ASN:O	2.41	0.49
4:R:240:LEU:HD23	4:R:240:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:426:CYS:HA	4:R:429:MET:HG2	1.93	0.49
5:T:8:ALA:O	5:T:9:LEU:HD22	2.12	0.49
5:T:28:ALA:O	5:T:29:LEU:HD13	2.12	0.49
5:T:33:ASN:N	5:T:40:PHE:O	2.46	0.49
4:F:450:ASP:O	4:F:453:SER:OG	2.27	0.49
4:S:39:HIS:CE1	4:S:110:ALA:HB1	2.48	0.49
4:S:481:THR:O	4:S:488:ILE:HB	2.13	0.49
1:A:626:MET:HE3	1:A:680:THR:HG22	1.95	0.49
4:E:135:ALA:HB2	4:E:381:ASN:ND2	2.28	0.49
5:G:69:LEU:HD23	5:G:89:TYR:HD2	1.77	0.49
6:H:47:THR:OG1	6:H:49:THR:OG1	2.17	0.49
6:H:56:THR:O	6:H:95:LYS:HB3	2.13	0.49
7:K:283:HIS:O	7:K:287:VAL:HG22	2.13	0.49
2:Q:9:LEU:HB2	2:Q:12:TYR:HB2	1.95	0.49
7:X:467:PRO:HD2	7:X:481:GLY:O	2.13	0.49
4:F:13:SER:O	4:F:13:SER:OG	2.30	0.49
4:S:212:ARG:HH11	4:S:340:VAL:HB	1.78	0.49
4:S:523:SER:HA	4:S:526:LEU:HD22	1.95	0.49
1:A:842:CYS:C	1:A:843:PHE:HD1	2.20	0.48
2:B:120:ILE:O	2:B:124:THR:HG22	2.12	0.48
7:K:54:LEU:HD12	7:K:55:ILE:H	1.78	0.48
1:N:107:ASP:O	1:N:109:ASP:OD2	2.29	0.48
1:N:428:PHE:HB3	1:N:429:PHE:HD1	1.78	0.48
1:N:590:GLY:HA2	9:M:29:G:O2'	2.13	0.48
1:N:610:GLU:HG2	1:N:611:ASN:N	2.27	0.48
4:R:511:PHE:O	4:R:531:GLN:N	2.44	0.48
4:S:426:CYS:HA	4:S:429:MET:HG2	1.95	0.48
2:B:71:TYR:O	2:B:75:ARG:HG2	2.13	0.48
4:E:42:VAL:HB	4:E:48:TYR:CD2	2.47	0.48
4:E:158:LEU:HD21	4:E:164:HIS:HD2	1.78	0.48
5:T:113:GLN:HB3	6:U:1:ALA:N	2.28	0.48
6:U:117:CYS:HB3	6:U:120:CYS:SG	2.53	0.48
7:X:119:ALA:HA	7:X:157:LEU:H	1.78	0.48
4:F:5:CYS:HB3	4:F:9:ASN:H	1.78	0.48
4:F:402:PRO:HB3	4:F:426:CYS:SG	2.53	0.48
8:I:25:A:H2'	8:I:26:G:H8	1.77	0.48
1:A:358:ASP:CG	1:A:533:ARG:HH21	2.21	0.48
2:D:40:LYS:O	2:D:44:VAL:HG23	2.13	0.48
4:E:275:GLN:NE2	4:E:278:SER:HB2	2.28	0.48
1:N:358:ASP:CG	1:N:533:ARG:HH21	2.21	0.48
1:N:842:CYS:C	1:N:843:PHE:HD1	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:127:THR:O	4:R:131:LYS:HG3	2.13	0.48
4:F:332:ARG:HH11	4:F:346:PHE:HB2	1.77	0.48
4:S:263:SER:HA	4:S:266:VAL:HG22	1.94	0.48
4:E:318:CYS:HB3	4:E:343:PHE:CD2	2.48	0.48
5:G:113:GLN:C	6:H:1:ALA:H1	2.21	0.48
6:H:6:GLU:OE2	6:H:10:ASN:ND2	2.45	0.48
7:K:134:SER:OG	7:K:135:ARG:N	2.46	0.48
1:N:595:TYR:CD2	1:N:929:THR:HB	2.48	0.48
2:O:56:GLN:HA	2:O:59:LEU:HD22	1.95	0.48
4:R:490:ARG:HD2	4:R:521:VAL:HG11	1.95	0.48
4:S:322:LEU:HB2	4:S:323:LYS:NZ	2.28	0.48
4:S:332:ARG:CZ	4:S:346:PHE:HB2	2.44	0.48
1:A:420:TYR:OH	3:C:5:ASP:OD1	2.32	0.48
4:E:167:TRP:CD2	4:E:173:ARG:HG2	2.48	0.48
4:E:189:LYS:HB2	4:E:190:ASN:HB3	1.94	0.48
7:K:359:LYS:HG2	7:K:362:LYS:HD3	1.95	0.48
7:K:366:LEU:HD11	7:K:377:PHE:HZ	1.76	0.48
1:N:619:TYR:OH	1:N:695:ASN:OD1	2.27	0.48
4:F:370:ILE:HB	4:F:395:HIS:HB2	1.94	0.48
4:F:510:VAL:HG22	4:F:544:VAL:HA	1.94	0.48
4:S:117:ALA:O	4:S:121:ILE:HG12	2.13	0.48
4:S:426:CYS:O	4:S:430:LYS:HG2	2.13	0.48
1:A:607:SER:O	1:A:608:ASP:HB2	2.14	0.48
4:E:92:LEU:HA	7:X:466:VAL:HG11	1.95	0.48
4:E:156:GLU:HA	4:E:221:VAL:HG22	1.95	0.48
1:N:403:ASN:O	2:O:129:MET:CE	2.59	0.48
2:Q:38:LEU:C	2:Q:42:LEU:HG	2.39	0.48
7:X:271:SER:O	7:X:275:ILE:HG13	2.14	0.48
8:L:25:A:H2'	8:L:26:G:H8	1.77	0.48
1:A:411:LYS:HB2	1:A:411:LYS:HE2	1.57	0.48
1:A:713:ASN:HB2	1:A:714:LYS:HZ2	1.79	0.48
2:D:56:GLN:O	2:D:59:LEU:HG	2.14	0.48
4:E:177:ASN:HB2	4:E:180:TYR:HD2	1.78	0.48
4:E:483:ASP:C	4:E:483:ASP:OD1	2.57	0.48
7:K:29:VAL:HG22	7:K:30:ASP:H	1.79	0.48
1:N:103:LYS:NZ	1:N:110:MET:O	2.44	0.48
1:N:626:MET:HE3	1:N:680:THR:HG22	1.95	0.48
4:S:15:ARG:HB2	4:S:22:ARG:HB3	1.95	0.48
4:S:316:ALA:HA	4:S:319:GLU:OE1	2.13	0.48
4:E:195:ILE:O	4:E:198:TYR:OH	2.25	0.48
1:N:682:SER:O	9:M:26:A:C2	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:810:HIS:ND1	1:N:810:HIS:C	2.71	0.48
4:R:181:VAL:H	4:R:230:HIS:CD2	2.32	0.48
4:R:458:ASP:HB2	4:R:460:LYS:NZ	2.29	0.48
4:R:476:TYR:N	4:R:576:MET:O	2.46	0.48
5:T:57:PRO:HA	5:T:64:THR:HA	1.96	0.48
7:X:80:ILE:HD11	7:X:285:CYS:HB3	1.96	0.48
7:X:336:LYS:O	7:X:338:ILE:N	2.47	0.48
7:X:463:ILE:HG23	7:X:465:TYR:CE2	2.49	0.48
1:A:501:SER:CB	9:J:25:G:OP1	2.62	0.48
1:A:752:HIS:CE1	1:A:770:TYR:HE2	2.32	0.48
1:N:619:TYR:N	1:N:619:TYR:CD1	2.82	0.48
6:U:68:PHE:HB2	6:U:97:VAL:HG13	1.96	0.48
7:X:416:GLY:O	7:X:430:ALA:CB	2.62	0.48
7:X:465:TYR:CD1	7:X:465:TYR:C	2.85	0.48
1:A:223:ILE:HD12	5:G:104:GLY:HA2	1.95	0.48
1:A:511:LYS:NZ	9:J:25:G:N2	2.61	0.48
4:E:3:GLY:HA3	4:E:24:PHE:CD2	2.49	0.48
1:N:415:PHE:HE2	3:P:8:CYS:SG	2.36	0.48
1:N:752:HIS:CE1	1:N:770:TYR:HE2	2.32	0.48
4:R:381:ASN:ND2	4:R:424:SER:OG	2.46	0.48
6:U:90:CYS:SG	6:U:92:LEU:N	2.87	0.48
7:X:221:SER:O	7:X:222:ASP:C	2.57	0.48
4:F:139:LYS:HA	4:F:142:GLU:HG2	1.95	0.48
4:F:445:PRO:HB3	4:F:465:LYS:HZ1	1.79	0.48
4:S:496:VAL:HG23	4:S:497:ARG:HH12	1.78	0.48
1:A:8:LEU:C	1:A:8:LEU:CD2	2.84	0.47
1:A:39:ASN:HD21	1:A:42:VAL:HG22	1.79	0.47
1:A:62:ASP:OD1	1:A:62:ASP:N	2.44	0.47
1:A:428:PHE:HB3	1:A:429:PHE:HD1	1.78	0.47
2:B:82:LYS:HB2	2:B:82:LYS:HE3	1.57	0.47
1:N:491:ASN:HB3	1:N:521:TYR:CE2	2.49	0.47
4:R:562:ASN:O	4:R:566:THR:OG1	2.31	0.47
7:X:330:HIS:HD2	7:X:349:LYS:HD2	1.79	0.47
4:S:405:LEU:HD11	4:S:560:ARG:HA	1.96	0.47
1:A:192:PHE:O	1:A:192:PHE:HD1	1.97	0.47
7:K:18:LEU:HB2	7:K:23:ALA:HB2	1.95	0.47
7:K:366:LEU:HD11	7:K:377:PHE:CZ	2.49	0.47
7:K:469:LYS:HG2	1:N:905:VAL:HG23	1.95	0.47
4:R:40:LYS:HE2	4:R:59:ASP:CG	2.39	0.47
4:R:149:TYR:O	4:R:149:TYR:CG	2.65	0.47
6:U:24:ALA:O	6:U:28:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:434:SER:O	7:X:434:SER:OG	2.31	0.47
7:X:442:LEU:HB2	7:X:510:VAL:HG23	1.96	0.47
4:S:300:PRO:O	4:S:354:GLN:NE2	2.41	0.47
4:S:308:ALA:O	4:S:360:VAL:HG23	2.14	0.47
4:E:189:LYS:HB2	4:E:190:ASN:CB	2.44	0.47
4:E:431:THR:OG1	4:E:432:ILE:N	2.46	0.47
4:E:546:PHE:O	4:E:574:CYS:HA	2.15	0.47
7:K:478:ASN:O	7:K:478:ASN:ND2	2.47	0.47
2:Q:67:MET:HE3	2:Q:67:MET:HB2	1.73	0.47
5:T:69:LEU:HD23	5:T:89:TYR:HD2	1.77	0.47
6:U:92:LEU:HD11	6:U:111:THR:HG21	1.95	0.47
7:X:104:ASN:O	7:X:105:LEU:HD23	2.14	0.47
4:F:548:GLN:HE21	4:F:576:MET:HE2	1.79	0.47
4:F:576:MET:HE1	4:F:581:LEU:HD13	1.95	0.47
4:S:63:LEU:HD12	4:S:70:TYR:HB2	1.96	0.47
8:L:13:U:H2'	8:L:14:A:O4'	2.14	0.47
1:A:122:TYR:OH	1:A:144:GLU:OE1	2.13	0.47
4:E:158:LEU:HD21	4:E:164:HIS:CD2	2.48	0.47
5:G:57:PRO:HA	5:G:64:THR:HA	1.96	0.47
1:N:681:SER:O	1:N:683:GLY:N	2.44	0.47
4:R:114:TRP:O	4:R:411:LEU:CD2	2.61	0.47
4:F:115:THR:HG22	4:F:413:THR:HG22	1.95	0.47
4:E:341:GLU:N	4:E:341:GLU:OE1	2.48	0.47
7:K:26:HIS:NE2	7:K:37:GLY:O	2.30	0.47
7:K:313:GLN:NE2	7:K:385:TRP:CG	2.83	0.47
4:R:304:ILE:N	4:R:354:GLN:O	2.29	0.47
4:R:332:ARG:NE	4:R:342:CYS:SG	2.74	0.47
7:X:144:ASP:OD1	7:X:145:GLN:N	2.47	0.47
4:F:472:PHE:HB2	4:F:474:MET:SD	2.54	0.47
4:S:330:CYS:O	4:S:356:VAL:HA	2.13	0.47
4:E:181:VAL:HB	4:E:197:GLU:HG3	1.95	0.47
4:E:364:PRO:O	4:E:390:ARG:HB3	2.14	0.47
4:E:424:SER:HA	4:E:427:ARG:HB2	1.96	0.47
2:Q:42:LEU:HA	2:Q:45:ALA:HB3	1.97	0.47
4:R:289:SER:HB2	4:R:320:LYS:HE2	1.97	0.47
7:X:116:ASN:HD21	7:X:269:VAL:HG13	1.79	0.47
4:F:449:VAL:HG11	4:F:463:ALA:N	2.30	0.47
4:S:514:PRO:HG2	4:S:549:THR:HG22	1.96	0.47
1:A:254:GLU:OE1	1:A:254:GLU:HA	2.15	0.47
1:A:330:VAL:HA	1:A:343:SER:HA	1.96	0.47
1:A:491:ASN:HB3	1:A:521:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:VAL:HG12	1:A:610:GLU:H	1.80	0.47
1:A:619:TYR:N	1:A:619:TYR:CD1	2.82	0.47
1:A:711:ASP:OD1	1:A:712:GLY:N	2.48	0.47
1:A:806:THR:HG22	1:A:806:THR:O	2.14	0.47
2:B:182:TRP:N	2:B:183:PRO:HD3	2.29	0.47
4:E:446:ALA:HA	4:E:463:ALA:HB1	1.96	0.47
4:E:573:LEU:HD21	4:E:575:ILE:HD11	1.97	0.47
1:N:10:ARG:C	1:N:10:ARG:HH21	2.22	0.47
1:N:105:ARG:HH12	1:N:108:GLY:N	2.12	0.47
4:R:561:PHE:O	4:R:565:ILE:HG12	2.15	0.47
7:X:33:PHE:HE1	7:X:45:ILE:HD11	1.80	0.47
4:F:27:CYS:HB2	4:F:97:CYS:SG	2.55	0.47
4:F:136:GLU:OE1	4:F:234:PRO:HA	2.15	0.47
4:F:337:ARG:HH12	4:F:339:ARG:HD3	1.78	0.47
4:F:446:ALA:HA	4:F:449:VAL:HG12	1.97	0.47
4:S:165:LEU:HD22	4:S:200:PHE:CZ	2.50	0.47
4:S:376:ILE:HD11	4:S:429:MET:HE1	1.96	0.47
4:S:420:GLU:HA	4:S:430:LYS:HG3	1.97	0.47
4:S:445:PRO:HG2	4:S:448:ILE:HG13	1.95	0.47
8:I:13:U:H2'	8:I:14:A:O4'	2.15	0.47
4:E:259:SER:O	4:E:263:SER:OG	2.30	0.47
4:E:441:CYS:HB2	4:E:461:LEU:HD11	1.97	0.47
4:E:513:SER:HB2	4:E:519:ASN:ND2	2.29	0.47
1:N:77:PHE:HD1	1:N:77:PHE:O	1.98	0.47
1:N:192:PHE:O	1:N:192:PHE:HD1	1.97	0.47
1:N:711:ASP:OD1	1:N:712:GLY:N	2.48	0.47
1:N:905:VAL:HG11	2:Q:67:MET:SD	2.55	0.47
2:Q:135:TYR:HB2	2:Q:182:TRP:HH2	1.79	0.47
4:R:252:LEU:HB3	4:R:299:TYR:CD1	2.49	0.47
5:T:13:SER:HA	5:T:28:ALA:O	2.15	0.47
7:X:433:LYS:HA	7:X:433:LYS:HD2	1.68	0.47
4:F:41:LEU:HD21	4:F:58:THR:HB	1.96	0.47
4:S:15:ARG:HA	4:S:23:PRO:O	2.14	0.47
4:S:187:VAL:HB	4:S:192:LYS:HG3	1.97	0.47
4:S:401:ASP:O	4:S:404:GLN:HG2	2.15	0.47
1:A:41:LYS:HZ3	1:A:42:VAL:HG13	1.79	0.47
2:D:175:ASP:OD1	2:D:175:ASP:N	2.42	0.47
4:E:366:THR:OG1	4:E:367:THR:N	2.48	0.47
1:N:107:ASP:N	1:N:109:ASP:OD1	2.48	0.47
7:X:389:VAL:HG23	7:X:390:ASP:O	2.14	0.47
7:X:442:LEU:HD13	7:X:510:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:187:VAL:HB	4:F:192:LYS:HE2	1.97	0.47
4:F:306:TYR:HB2	4:F:357:PHE:HA	1.96	0.47
4:F:474:MET:HE3	4:F:576:MET:H	1.78	0.47
4:F:517:SER:O	4:F:521:VAL:HG22	2.15	0.47
4:F:554:HIS:CE1	4:F:560:ARG:HH12	2.33	0.47
1:N:330:VAL:HA	1:N:343:SER:HA	1.97	0.47
1:N:496:ASN:OD1	1:N:496:ASN:N	2.35	0.47
2:Q:172:ILE:H	2:Q:172:ILE:HD12	1.80	0.47
4:R:109:ILE:HD13	4:R:134:ALA:HB2	1.97	0.47
4:R:270:GLN:C	4:R:274:MET:HE3	2.40	0.47
4:R:512:ILE:HD12	4:R:564:ALA:HB1	1.96	0.47
4:R:514:PRO:HG3	4:R:560:ARG:CZ	2.45	0.47
4:F:426:CYS:SG	4:F:430:LYS:HD2	2.55	0.47
1:A:105:ARG:HG2	1:A:109:ASP:C	2.40	0.46
3:C:50:GLU:HG2	3:C:50:GLU:H	1.47	0.46
1:N:89:LEU:HD13	1:N:201:ILE:HD11	1.96	0.46
2:Q:116:PRO:O	2:Q:117:LEU:HD23	2.15	0.46
4:R:169:VAL:O	4:R:169:VAL:HG22	2.15	0.46
7:X:500:MET:HE3	7:X:500:MET:HB2	1.70	0.46
1:A:139:CYS:O	1:A:143:LYS:HG3	2.15	0.46
1:A:603:LYS:HD2	1:A:603:LYS:HA	1.72	0.46
2:D:123:THR:O	2:D:190:ARG:HD2	2.15	0.46
4:E:447:GLU:CD	4:E:467:LYS:HZ3	2.23	0.46
4:E:448:ILE:O	4:E:452:VAL:HG22	2.16	0.46
7:K:336:LYS:O	7:K:338:ILE:N	2.46	0.46
7:K:448:SER:HB3	7:K:475:THR:HB	1.96	0.46
7:K:466:VAL:H	7:K:483:VAL:HG11	1.80	0.46
1:N:39:ASN:HD21	1:N:42:VAL:HG22	1.79	0.46
4:R:265:ASN:HA	4:R:268:ASN:ND2	2.27	0.46
4:E:15:ARG:HA	4:E:23:PRO:O	2.15	0.46
4:E:374:ASP:OD1	4:E:399:ILE:HB	2.16	0.46
4:E:511:PHE:CD2	4:E:526:LEU:HD22	2.50	0.46
7:K:45:ILE:HD12	7:K:46:PRO:HD2	1.96	0.46
1:N:736:ASP:OD1	1:N:736:ASP:N	2.47	0.46
4:R:467:LYS:HE3	4:R:469:ALA:HA	1.97	0.46
4:F:51:ASN:HB2	4:F:71:TYR:CE1	2.51	0.46
4:F:140:ALA:HA	4:F:232:VAL:HG21	1.97	0.46
4:S:36:SER:OG	4:S:37:THR:N	2.49	0.46
4:S:116:ASN:OD1	4:S:116:ASN:N	2.48	0.46
4:S:143:GLU:O	4:S:147:LEU:HG	2.15	0.46
1:A:267:LYS:HB2	1:A:267:LYS:HE2	1.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ASP:OD1	1:A:736:ASP:N	2.47	0.46
3:C:66:VAL:HG22	3:C:68:ILE:HG22	1.98	0.46
4:E:283:PRO:HG2	4:E:461:LEU:HD13	1.98	0.46
4:E:320:LYS:HA	4:E:323:LYS:HD3	1.98	0.46
4:E:347:LYS:HD2	4:E:353:GLU:OE1	2.15	0.46
5:G:13:SER:HA	5:G:28:ALA:O	2.15	0.46
7:K:212:ARG:HH12	7:K:228:HIS:CG	2.33	0.46
4:R:266:VAL:HG22	4:R:270:GLN:HE21	1.79	0.46
4:S:252:LEU:HB3	4:S:299:TYR:CE1	2.50	0.46
1:A:77:PHE:O	1:A:77:PHE:HD1	1.98	0.46
1:A:806:THR:HG22	1:A:819:LEU:CD2	2.46	0.46
4:E:448:ILE:HG12	4:E:587:PHE:CZ	2.51	0.46
7:X:440:LYS:HG2	7:X:512:LYS:HA	1.97	0.46
4:F:77:PRO:HG2	4:F:80:SER:HB2	1.97	0.46
4:F:447:GLU:HG3	4:F:587:PHE:CE1	2.50	0.46
4:S:91:GLY:C	4:S:94:LYS:HD3	2.40	0.46
4:S:477:LYS:HZ3	4:S:576:MET:HA	1.79	0.46
4:S:561:PHE:HE2	4:S:576:MET:HE2	1.80	0.46
9:M:43:U:H2'	9:M:44:A:H8	1.80	0.46
1:A:11:VAL:O	1:A:13:GLY:N	2.48	0.46
1:A:102:PHE:CD1	1:A:102:PHE:C	2.94	0.46
2:B:163:ASP:O	2:B:164:SER:OG	2.29	0.46
4:E:173:ARG:HG3	4:E:173:ARG:HH11	1.80	0.46
7:K:453:GLU:HB3	7:K:454:SER:H	1.53	0.46
3:P:66:VAL:HG22	3:P:68:ILE:HG22	1.98	0.46
2:Q:34:VAL:HA	2:Q:37:LYS:HE2	1.96	0.46
2:Q:65:GLN:O	2:Q:68:THR:HG22	2.16	0.46
7:X:115:VAL:CG1	7:X:169:MET:HE2	2.46	0.46
4:S:140:ALA:HB2	4:S:232:VAL:HG21	1.98	0.46
4:S:303:ARG:HG3	4:S:354:GLN:HA	1.97	0.46
9:J:43:U:H2'	9:J:44:A:H8	1.80	0.46
1:A:89:LEU:HD13	1:A:201:ILE:HD11	1.96	0.46
1:A:415:PHE:CE2	3:C:8:CYS:HB3	2.50	0.46
2:D:117:LEU:HD11	2:D:131:VAL:HG23	1.97	0.46
4:E:269:TYR:CD1	4:E:295:LEU:HD23	2.49	0.46
4:E:423:ASN:CG	4:E:424:SER:H	2.24	0.46
7:K:291:ASP:CG	7:K:293:THR:H	2.23	0.46
7:K:315:MET:HE2	7:K:315:MET:HB2	1.77	0.46
1:N:41:LYS:HZ3	1:N:42:VAL:HG13	1.79	0.46
1:N:102:PHE:CD1	1:N:102:PHE:C	2.94	0.46
1:N:139:CYS:O	1:N:143:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:204:ASP:OD1	4:R:205:TYR:HD1	1.99	0.46
4:F:83:LEU:HD12	4:F:90:PHE:HB2	1.98	0.46
4:S:101:ASP:OD1	4:S:101:ASP:N	2.41	0.46
2:D:103:LEU:O	2:D:107:ILE:HG13	2.16	0.46
4:E:363:LEU:O	4:E:390:ARG:HD2	2.16	0.46
7:K:325:LYS:HE2	7:K:325:LYS:HB2	1.82	0.46
7:K:517:TYR:HA	7:K:520:TRP:HD1	1.81	0.46
4:R:92:LEU:HB3	4:R:93:TYR:CD1	2.51	0.46
4:R:320:LYS:O	4:R:324:TYR:HD1	1.99	0.46
4:F:303:ARG:O	4:F:304:ILE:HD13	2.15	0.46
4:F:496:VAL:HG11	4:F:511:PHE:CZ	2.51	0.46
4:S:120:TYR:CD2	4:S:417:LEU:HD11	2.50	0.46
4:S:199:THR:O	4:S:211:TYR:HB2	2.15	0.46
4:S:266:VAL:HA	4:S:269:TYR:CD2	2.51	0.46
4:S:281:GLN:HG2	4:S:434:PRO:HB3	1.98	0.46
7:K:518:ASN:OD1	7:K:518:ASN:N	2.48	0.46
1:N:808:GLY:H	1:N:817:THR:CG2	2.29	0.46
1:N:819:LEU:HD13	1:N:828:TYR:CE1	2.51	0.46
4:R:248:ARG:HE	4:R:250:THR:HA	1.81	0.46
5:T:24:THR:OG1	5:T:27:ASN:ND2	2.49	0.46
5:T:25:ASP:OD1	5:T:25:ASP:C	2.57	0.46
6:U:44:MET:HB2	6:U:67:SER:O	2.16	0.46
7:X:227:TRP:HA	7:X:227:TRP:CE3	2.50	0.46
4:S:189:LYS:CB	4:S:190:ASN:HB2	2.45	0.46
1:A:80:TYR:CZ	1:A:101:PHE:HB3	2.50	0.46
1:A:456:TYR:CE1	1:A:624:ARG:HG2	2.52	0.46
4:E:117:ALA:O	4:E:121:ILE:HG12	2.15	0.46
4:E:473:LYS:HE2	4:E:585:LEU:O	2.15	0.46
7:K:204:GLU:CD	7:K:213:ARG:HH21	2.22	0.46
2:Q:22:TYR:HB2	2:Q:42:LEU:HD11	1.98	0.46
2:Q:38:LEU:HA	2:Q:42:LEU:HG	1.98	0.46
2:Q:177:SER:OG	2:Q:178:PRO:HD3	2.16	0.46
7:X:141:PRO:HB2	7:X:146:PHE:CD2	2.51	0.46
7:X:384:PHE:O	7:X:397:ILE:O	2.34	0.46
7:X:415:ASP:C	7:X:417:GLY:H	2.24	0.46
7:X:455:HIS:N	7:X:462:ASP:OD2	2.49	0.46
4:F:6:VAL:HG11	4:F:23:PRO:HB2	1.98	0.46
4:F:265:ASN:HB3	4:F:269:TYR:CZ	2.51	0.46
4:F:380:THR:OG1	4:F:381:ASN:N	2.49	0.46
4:F:473:LYS:HB3	4:F:473:LYS:HE2	1.79	0.46
4:S:280:LEU:HD21	4:S:438:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:488:ILE:HG23	4:S:521:VAL:HG11	1.98	0.46
1:A:11:VAL:O	1:A:12:CYS:C	2.57	0.45
2:B:98:LEU:O	2:B:100:ASN:N	2.39	0.45
4:E:171:LYS:HG2	4:E:172:PRO:CD	2.46	0.45
6:H:53:GLN:CD	6:H:121:GLY:HA3	2.40	0.45
7:K:35:THR:O	7:K:35:THR:OG1	2.33	0.45
1:N:371:LEU:HA	1:N:371:LEU:HD23	1.63	0.45
1:N:891:LEU:O	1:N:894:GLU:HG3	2.17	0.45
7:X:480:GLY:C	7:X:482:ALA:HB2	2.41	0.45
4:F:121:ILE:HG23	4:F:421:TYR:CE2	2.51	0.45
4:F:383:ASP:HA	4:F:386:VAL:HG22	1.98	0.45
4:S:68:MET:N	4:S:68:MET:SD	2.89	0.45
8:L:11:G:N1	9:M:49:C:N3	2.54	0.45
1:A:105:ARG:HD3	1:A:110:MET:HG2	1.94	0.45
1:A:242:MET:HG2	1:A:463:MET:HE2	1.98	0.45
1:A:506:PHE:CE2	1:A:562:ILE:HG22	2.52	0.45
4:E:154:VAL:HG12	4:E:165:LEU:HD23	1.98	0.45
4:E:541:TYR:O	4:E:569:LYS:N	2.45	0.45
7:K:243:ASP:HB3	7:K:246:GLN:HB2	1.99	0.45
1:N:80:TYR:CZ	1:N:101:PHE:HB3	2.50	0.45
1:N:219:PHE:HA	1:N:222:PHE:CE1	2.51	0.45
1:N:602:LEU:HD11	1:N:809:PRO:HD3	1.99	0.45
4:R:164:HIS:CD2	4:R:207:ASP:HB2	2.51	0.45
4:R:186:ARG:NH1	4:R:218:LYS:O	2.45	0.45
4:R:249:ILE:HG22	4:R:252:LEU:HB2	1.97	0.45
7:X:184:VAL:HG12	7:X:277:THR:HG22	1.98	0.45
4:F:500:LEU:HD13	4:F:507:ARG:HH12	1.80	0.45
4:S:334:ILE:HG21	4:S:338:ALA:HB2	1.98	0.45
7:K:154:TYR:C	7:K:155:LYS:HD3	2.41	0.45
4:R:118:GLY:O	4:R:122:LEU:HG	2.16	0.45
4:R:121:ILE:O	4:R:125:THR:OG1	2.22	0.45
4:R:259:SER:OG	4:R:261:GLU:OE2	2.33	0.45
4:R:406:PRO:HB3	4:R:422:PHE:CD2	2.50	0.45
4:F:557:ASN:OD1	4:F:560:ARG:HB3	2.16	0.45
4:S:371:VAL:HG21	4:S:391:LEU:HD23	1.98	0.45
8:I:22:G:H1	9:J:38:C:N4	2.11	0.45
1:A:819:LEU:HD13	1:A:828:TYR:CE1	2.51	0.45
1:A:891:LEU:O	1:A:894:GLU:HG3	2.16	0.45
2:D:9:LEU:HB3	2:D:12:TYR:H	1.82	0.45
2:D:136:ASN:O	2:D:140:ASN:ND2	2.49	0.45
4:E:17:GLY:HA3	4:E:41:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:158:LEU:HB3	4:E:162:GLU:OE2	2.16	0.45
4:E:495:VAL:HG21	4:E:592:ILE:HD12	1.98	0.45
4:E:566:THR:OG1	4:E:567:ARG:NH2	2.45	0.45
5:G:73:CYS:O	5:G:87:TYR:HA	2.16	0.45
1:N:721:ARG:NH1	1:N:721:ARG:HB2	2.32	0.45
1:N:810:HIS:O	1:N:810:HIS:CG	2.69	0.45
4:R:30:CYS:O	4:R:34:VAL:HG13	2.17	0.45
7:X:1:ALA:HA	7:X:2:GLU:HA	1.62	0.45
7:X:162:VAL:O	7:X:166:ILE:HG13	2.15	0.45
7:X:391:ARG:HH21	7:X:437:VAL:HB	1.81	0.45
9:M:24:U:C6	9:M:24:U:OP1	2.69	0.45
9:M:24:U:C6	9:M:24:U:O5'	2.70	0.45
1:A:4:ALA:C	1:A:6:SER:N	2.75	0.45
1:A:900:LEU:O	1:A:903:TYR:O	2.35	0.45
4:E:6:VAL:O	4:E:129:ARG:NH2	2.42	0.45
4:E:150:GLY:N	4:E:227:LEU:CD2	2.79	0.45
4:E:443:ARG:HA	4:E:569:LYS:NZ	2.32	0.45
5:G:41:VAL:HG22	5:G:91:ILE:HD11	1.98	0.45
7:K:61:LYS:HE2	7:K:61:LYS:HB3	1.80	0.45
1:N:39:ASN:C	1:N:39:ASN:OD1	2.59	0.45
1:N:57:GLN:NE2	1:N:66:ILE:O	2.49	0.45
1:N:326:PHE:O	2:O:118:ASN:ND2	2.50	0.45
1:N:419:PHE:HA	1:N:887:TYR:HE2	1.81	0.45
4:R:136:GLU:OE2	4:R:235:LEU:N	2.50	0.45
4:R:431:THR:OG1	4:R:432:ILE:N	2.50	0.45
5:T:41:VAL:HG22	5:T:91:ILE:HD11	1.98	0.45
7:X:247:TRP:N	7:X:247:TRP:CD1	2.83	0.45
7:X:358:ASP:C	7:X:360:ALA:H	2.25	0.45
4:F:150:GLY:HA3	4:F:168:GLU:OE1	2.17	0.45
4:F:255:THR:HG22	4:F:256:LEU:H	1.82	0.45
4:F:292:ALA:HB1	4:F:306:TYR:CE2	2.48	0.45
4:F:592:ILE:O	4:F:595:ARG:NH1	2.49	0.45
4:S:142:GLU:O	4:S:146:LYS:HG2	2.16	0.45
4:S:370:ILE:HA	4:S:395:HIS:O	2.16	0.45
1:A:847:ILE:H	1:A:847:ILE:HG13	1.26	0.45
2:B:134:ASP:HA	2:B:182:TRP:CE3	2.52	0.45
3:C:21:ARG:NE	3:C:21:ARG:HA	2.32	0.45
4:E:178:ARG:HD2	4:E:212:ARG:NH2	2.31	0.45
4:E:419:PRO:HB2	4:E:430:LYS:HE3	1.97	0.45
7:K:132:ASP:OD1	7:K:133:PHE:N	2.49	0.45
1:N:107:ASP:O	1:N:107:ASP:CG	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:254:GLU:OE1	1:N:254:GLU:HA	2.15	0.45
1:N:281:LYS:HE2	1:N:281:LYS:HB3	1.53	0.45
1:N:456:TYR:CE1	1:N:624:ARG:HG2	2.51	0.45
2:O:70:MET:HE2	4:S:92:LEU:HD11	1.99	0.45
3:P:63:GLN:HB2	4:R:352:LEU:HD11	1.97	0.45
4:R:202:LYS:HZ1	4:R:206:GLY:HA2	1.81	0.45
4:R:363:LEU:O	4:R:390:ARG:NH1	2.49	0.45
5:T:73:CYS:O	5:T:87:TYR:HA	2.16	0.45
7:X:351:TYR:HB3	7:X:366:LEU:HB3	1.98	0.45
4:F:370:ILE:HD11	4:F:397:VAL:HG23	1.99	0.45
4:F:576:MET:HG2	4:F:577:SER:C	2.42	0.45
1:A:57:GLN:NE2	1:A:66:ILE:O	2.49	0.45
2:B:166:ILE:HD12	2:B:166:ILE:H	1.82	0.45
3:C:70:LYS:HD2	2:D:92:PHE:CD2	2.52	0.45
4:E:150:GLY:N	4:E:227:LEU:HD22	2.32	0.45
4:E:576:MET:HE1	4:E:585:LEU:HD22	1.98	0.45
7:K:90:ASP:OD1	7:K:91:VAL:N	2.49	0.45
7:K:257:HIS:CE1	7:K:261:CYS:HB3	2.52	0.45
7:K:328:VAL:HG23	7:K:347:GLU:HB3	1.98	0.45
7:K:483:VAL:CG1	7:K:485:ARG:H	2.27	0.45
4:R:498:GLU:HB3	4:R:502:ARG:HH21	1.82	0.45
7:X:330:HIS:ND1	7:X:377:PHE:HB3	2.32	0.45
7:X:510:VAL:CG1	7:X:511:TYR:N	2.80	0.45
4:S:586:GLN:O	4:S:586:GLN:HG2	2.16	0.45
1:A:419:PHE:HA	1:A:887:TYR:HE2	1.81	0.45
1:A:928:HIS:O	1:A:929:THR:C	2.59	0.45
2:B:92:PHE:O	2:B:96:ARG:HG3	2.16	0.45
2:B:180:LEU:O	2:B:181:ALA:C	2.60	0.45
4:E:343:PHE:CZ	4:E:345:LYS:HB2	2.52	0.45
6:H:110:PHE:CE2	6:H:114:ASN:ND2	2.84	0.45
3:P:21:ARG:NE	3:P:21:ARG:HA	2.32	0.45
4:R:579:ARG:HH12	4:R:583:ASP:N	2.15	0.45
4:R:581:LEU:O	4:R:585:LEU:HG	2.16	0.45
5:T:50:ASP:C	5:T:51:LEU:HD12	2.42	0.45
4:F:447:GLU:HB3	4:F:470:GLN:OE1	2.16	0.45
4:S:20:ILE:HG13	4:S:21:ARG:HG2	1.98	0.45
4:S:50:CYS:HA	4:S:71:TYR:HA	1.99	0.45
4:S:102:ASN:OD1	4:S:130:LEU:HD11	2.16	0.45
3:C:70:LYS:HZ2	3:C:70:LYS:HG3	1.71	0.45
2:D:75:ARG:HH11	2:D:75:ARG:HG2	1.82	0.45
4:E:149:TYR:HB3	4:E:227:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:154:VAL:HA	4:E:165:LEU:HA	1.99	0.45
4:E:405:LEU:HD11	4:E:560:ARG:HA	1.98	0.45
5:G:4:LEU:O	5:G:5:SER:CB	2.60	0.45
1:N:242:MET:HG2	1:N:463:MET:HE2	1.98	0.45
3:P:70:LYS:HD2	2:Q:92:PHE:CD2	2.52	0.45
4:R:307:THR:HG23	4:R:373:PHE:HD1	1.82	0.45
4:R:457:TYR:HE1	4:R:562:ASN:ND2	2.14	0.45
4:R:481:THR:N	4:R:488:ILE:O	2.45	0.45
6:U:105:ASN:O	6:U:107:PRO:HD3	2.17	0.45
4:F:120:TYR:CD2	4:F:417:LEU:HD21	2.52	0.45
4:F:255:THR:N	4:F:298:TYR:O	2.50	0.45
8:L:22:G:O2'	8:L:23:C:OP1	2.32	0.45
9:M:24:U:OP1	9:M:24:U:C5	2.70	0.45
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.85	0.45
1:A:371:LEU:HA	1:A:371:LEU:HD23	1.63	0.45
2:B:61:LYS:HG3	2:B:62:MET:N	2.31	0.45
2:D:100:ASN:O	2:D:104:ASN:ND2	2.48	0.45
4:E:500:LEU:HD11	4:E:526:LEU:HG	1.98	0.45
7:K:337:ALA:HA	7:K:350:PHE:CE1	2.52	0.45
1:N:850:THR:O	1:N:851:ASP:C	2.60	0.45
4:R:170:GLY:O	4:R:171:LYS:HG2	2.17	0.45
4:R:474[B]:MET:SD	4:R:590:LEU:HD23	2.56	0.45
4:F:173:ARG:HG2	4:F:174:PRO:HD2	1.99	0.45
4:F:185:TYR:HB3	4:F:192:LYS:HD3	1.99	0.45
4:S:312:ALA:HA	4:S:315:ASP:OD2	2.17	0.45
1:A:39:ASN:OD1	1:A:41:LYS:N	2.49	0.44
1:A:281:LYS:HE2	1:A:281:LYS:HB3	1.53	0.44
1:N:81:GLN:HB3	7:X:98:ARG:HH12	1.82	0.44
4:R:31:TYR:CE2	4:R:87:GLY:HA2	2.52	0.44
4:F:121:ILE:HD12	4:F:421:TYR:HD2	1.81	0.44
4:F:304:ILE:HB	4:F:355:TYR:HD1	1.80	0.44
4:S:500:LEU:HD22	4:S:507:ARG:HH22	1.82	0.44
8:L:17:A:H2'	8:L:18:G:H8	1.82	0.44
2:B:102:ALA:O	2:B:106:ILE:HG23	2.17	0.44
4:E:453:SER:O	4:E:458:ASP:N	2.50	0.44
5:G:11:GLN:C	5:G:32:TYR:HE1	2.26	0.44
7:K:415:ASP:OD1	7:K:415:ASP:N	2.49	0.44
1:N:39:ASN:OD1	1:N:41:LYS:N	2.49	0.44
2:O:67:MET:HE3	2:O:67:MET:HB2	1.81	0.44
2:O:85:SER:O	2:O:89:THR:HG22	2.17	0.44
5:T:70:GLU:HB2	5:T:90:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:44:MET:HG3	6:U:96:TYR:HE2	1.82	0.44
7:X:414:CYS:HA	7:X:415:ASP:HA	1.70	0.44
4:F:90:PHE:HA	4:F:94:LYS:CE	2.43	0.44
4:F:120:TYR:HD2	4:F:417:LEU:HD21	1.81	0.44
4:F:158:LEU:HD11	4:F:164:HIS:HB2	1.98	0.44
4:S:72:CYS:O	4:S:76:LYS:HB3	2.18	0.44
4:S:278:SER:HB3	4:S:436:MET:HE1	1.99	0.44
4:S:334:ILE:H	4:S:343:PHE:HE1	1.65	0.44
4:S:393:ALA:N	4:S:396:TYR:OH	2.35	0.44
2:B:182:TRP:O	2:B:182:TRP:CE3	2.68	0.44
4:E:17:GLY:N	4:E:41:LEU:O	2.43	0.44
4:E:492:GLN:O	4:E:495:VAL:HG12	2.17	0.44
7:K:116:ASN:HD21	7:K:269:VAL:HB	1.82	0.44
7:K:198:PHE:HA	7:K:235:TYR:CE1	2.52	0.44
7:K:447:TYR:CE2	7:K:519:LEU:HD22	2.52	0.44
1:N:275:PHE:CE2	1:N:321:PHE:HB3	2.52	0.44
1:N:420:TYR:OH	3:P:5:ASP:OD1	2.36	0.44
4:R:288:LYS:HE2	4:R:288:LYS:HB2	1.67	0.44
4:R:499:PHE:O	4:R:503:ASN:N	2.48	0.44
6:U:83:HIS:HA	6:U:84:PRO:HD3	1.82	0.44
4:E:477:LYS:HA	4:E:577:SER:HA	1.98	0.44
7:K:156:GLY:O	7:K:157:LEU:HD23	2.17	0.44
1:N:10:ARG:HA	1:N:10:ARG:HD2	1.56	0.44
1:N:684:ASP:O	9:M:27:C:C4'	2.65	0.44
2:Q:22:TYR:HA	2:Q:38:LEU:HD13	1.99	0.44
4:R:487:ALA:HB3	4:R:515:TYR:CD2	2.53	0.44
5:T:34:THR:HA	5:T:39:ARG:HA	1.99	0.44
7:X:32:LYS:HA	7:X:32:LYS:HD3	1.86	0.44
4:S:212:ARG:NH1	4:S:340:VAL:HB	2.32	0.44
4:S:373:PHE:HB3	4:S:398:TYR:HD1	1.83	0.44
4:S:477:LYS:HE2	4:S:549:THR:O	2.17	0.44
1:A:316:LEU:HD22	1:A:463:MET:SD	2.58	0.44
1:A:807:LYS:HZ2	1:A:807:LYS:HG3	1.63	0.44
1:A:821:LYS:HZ2	1:A:821:LYS:HG2	1.68	0.44
4:E:143:GLU:HA	4:E:147:LEU:HB3	1.98	0.44
4:E:327:ILE:HD12	4:E:346:PHE:HE1	1.82	0.44
5:G:50:ASP:C	5:G:51:LEU:HD12	2.42	0.44
5:G:70:GLU:HB2	5:G:90:PHE:O	2.17	0.44
7:K:313:GLN:NE2	7:K:385:TRP:CE2	2.82	0.44
1:N:708:LEU:HD21	1:N:727:LEU:HD23	1.99	0.44
4:R:271:LYS:HA	4:R:274:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:479:VAL:HB	4:R:491:PRO:HG2	2.00	0.44
7:X:108:GLN:HE21	7:X:116:ASN:HB3	1.83	0.44
7:X:356:CYS:O	7:X:360:ALA:HB2	2.17	0.44
7:X:484:CYS:O	7:X:487:HIS:N	2.51	0.44
8:I:17:A:H2'	8:I:18:G:H8	1.82	0.44
9:J:48:C:H2'	9:J:49:C:C6	2.53	0.44
5:G:34:THR:HA	5:G:39:ARG:HA	1.99	0.44
1:N:6:SER:HA	1:N:9:ASN:HD22	1.82	0.44
4:R:471:CYS:SG	4:R:572:ILE:HG22	2.58	0.44
4:R:488:ILE:HB	4:R:490:ARG:HE	1.83	0.44
7:X:214:ALA:HB1	7:X:224:TYR:HB3	2.00	0.44
7:X:498:TYR:O	7:X:502:ILE:HG12	2.17	0.44
4:S:325:LEU:HD11	4:S:355:TYR:CD2	2.53	0.44
1:A:61:GLU:OE1	1:A:61:GLU:N	2.51	0.44
1:A:257:VAL:HG23	1:A:264:PRO:O	2.17	0.44
1:A:483:TYR:CD2	1:A:579:ILE:HG12	2.53	0.44
1:A:612:PRO:HG2	1:A:805:LEU:CD1	2.47	0.44
4:E:135:ALA:O	4:E:138:LEU:HG	2.18	0.44
7:K:454:SER:C	7:K:456:GLY:N	2.76	0.44
1:N:257:VAL:HG23	1:N:264:PRO:O	2.17	0.44
3:P:70:LYS:HZ2	3:P:70:LYS:HG3	1.64	0.44
4:R:473:LYS:NZ	4:R:582:TYR:O	2.46	0.44
5:T:11:GLN:C	5:T:32:TYR:HE1	2.26	0.44
9:J:39:A:C6	9:J:40:U:C4	3.06	0.44
1:A:602:LEU:HD12	1:A:606:TYR:HE2	1.83	0.44
4:E:92:LEU:HD12	4:E:93:TYR:N	2.32	0.44
5:G:10:ARG:NH2	5:G:32:TYR:HE2	2.16	0.44
6:H:8:PRO:HG3	7:K:5:THR:HG22	1.99	0.44
7:K:186:TRP:O	7:K:188:HIS:N	2.50	0.44
1:N:61:GLU:OE1	1:N:61:GLU:N	2.51	0.44
1:N:316:LEU:HD22	1:N:463:MET:SD	2.58	0.44
2:Q:44:VAL:HA	2:Q:47:SER:HG	1.83	0.44
2:Q:174:MET:O	2:Q:174:MET:HE3	2.18	0.44
4:R:56:ASP:OD1	4:R:56:ASP:N	2.50	0.44
7:X:86:TRP:HA	7:X:182:VAL:HG22	1.99	0.44
7:X:402:ASP:OD1	7:X:403:THR:N	2.51	0.44
4:F:121:ILE:HG23	4:F:421:TYR:CD2	2.53	0.44
4:F:365:GLU:OE1	4:F:365:GLU:N	2.51	0.44
4:S:322:LEU:HA	4:S:327:ILE:HD11	1.99	0.44
1:A:380:MET:HE1	2:B:95:LEU:HD13	1.99	0.44
2:B:74:ALA:O	2:B:77:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:8:CYS:C	4:E:10:SER:H	2.26	0.44
4:E:43:LEU:HD23	4:E:43:LEU:HA	1.79	0.44
4:E:263:SER:HA	4:E:266:VAL:HG13	1.99	0.44
4:E:487:ALA:O	4:E:518:GLN:HB2	2.18	0.44
4:E:511:PHE:HB3	4:E:530:THR:HG22	2.00	0.44
4:E:514:PRO:HB3	4:E:560:ARG:HH12	1.83	0.44
7:K:198:PHE:HA	7:K:235:TYR:HE1	1.83	0.44
7:K:303:LEU:HD23	7:K:303:LEU:H	1.83	0.44
1:N:483:TYR:CD2	1:N:579:ILE:HG12	2.53	0.44
2:Q:162:ALA:H	2:Q:181:ALA:HB3	1.82	0.44
4:F:197:GLU:OE1	4:F:197:GLU:N	2.50	0.44
4:F:246:TYR:N	4:F:274:MET:O	2.33	0.44
4:F:370:ILE:HA	4:F:395:HIS:O	2.18	0.44
4:F:425:VAL:O	4:F:428:LEU:HG	2.17	0.44
4:F:492:GLN:HE21	4:F:575:ILE:HB	1.83	0.44
9:M:25:G:H5'	9:M:25:G:C4	2.53	0.44
1:A:9:ASN:C	1:A:11:VAL:N	2.76	0.43
1:A:275:PHE:CE2	1:A:321:PHE:HB3	2.52	0.43
4:E:561:PHE:CG	4:E:581:LEU:HD23	2.52	0.43
6:H:102:THR:OG1	6:H:103:CYS:N	2.51	0.43
1:N:429:PHE:HD1	1:N:429:PHE:N	2.16	0.43
1:N:504:PHE:CD2	1:N:668:MET:HE2	2.52	0.43
1:N:683:GLY:HA2	9:M:26:A:N3	2.33	0.43
2:O:59:LEU:O	2:O:62:MET:HG3	2.19	0.43
4:F:27:CYS:SG	4:F:94:LYS:HD3	2.57	0.43
4:S:306:TYR:HE1	4:S:355:TYR:HB3	1.83	0.43
4:S:472:PHE:CD1	4:S:474:MET:HE2	2.53	0.43
4:S:512:ILE:HG22	4:S:531:GLN:O	2.17	0.43
4:E:237:ALA:CB	4:E:389:ALA:HB2	2.48	0.43
4:E:472:PHE:N	4:E:572:ILE:O	2.33	0.43
5:G:47:ASP:OD1	5:G:86:LYS:HG2	2.18	0.43
7:K:28:SER:O	7:K:28:SER:OG	2.26	0.43
7:K:83:VAL:C	7:K:85:ALA:H	2.26	0.43
1:N:38:TYR:HB3	5:T:2:ASN:OD1	2.19	0.43
4:R:241:VAL:HG23	4:R:277:TYR:CE1	2.52	0.43
4:R:444:CYS:O	4:R:465:LYS:HD3	2.17	0.43
4:R:447:GLU:HG2	4:R:587:PHE:CD1	2.53	0.43
4:F:64:TYR:HB3	4:F:80:SER:OG	2.19	0.43
4:F:305:VAL:HG13	4:F:356:VAL:HG23	2.00	0.43
4:F:371:VAL:HB	4:F:396:TYR:CE1	2.53	0.43
4:S:15:ARG:HG2	4:S:43:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:272:VAL:HG22	4:S:397:VAL:HG21	1.99	0.43
4:S:367:THR:HB	4:S:392:ARG:HH22	1.83	0.43
1:A:419:PHE:CD1	1:A:887:TYR:HE2	2.36	0.43
2:D:128:LEU:HD12	2:D:129:MET:N	2.33	0.43
5:G:72:PRO:HB2	5:G:87:TYR:HB3	1.99	0.43
6:H:62:ASN:HB2	6:H:64:ASP:OD1	2.19	0.43
1:N:433:SER:OG	1:N:434:SER:N	2.51	0.43
3:P:66:VAL:O	3:P:66:VAL:HG13	2.18	0.43
4:R:220:ASN:OD1	4:R:221:VAL:N	2.51	0.43
4:R:248:ARG:NH2	4:R:249:ILE:O	2.50	0.43
4:R:382:TYR:O	4:R:386:VAL:HG23	2.19	0.43
5:T:47:ASP:OD1	5:T:86:LYS:HG2	2.18	0.43
6:U:63:MET:HG2	6:U:64:ASP:OD1	2.19	0.43
4:S:329:LYS:HA	4:S:353:GLU:HG2	2.00	0.43
9:M:48:C:H2'	9:M:49:C:C6	2.53	0.43
1:A:57:GLN:HG2	1:A:69:TYR:CD1	2.53	0.43
1:A:102:PHE:C	1:A:102:PHE:HD1	2.26	0.43
1:A:156:TYR:O	1:A:156:TYR:HD1	2.02	0.43
2:D:108:ASN:O	2:D:111:ARG:HG2	2.18	0.43
4:E:104:THR:HA	4:E:107:ASN:HB2	2.00	0.43
4:E:314:VAL:HG21	4:E:359:THR:HG22	2.01	0.43
4:E:443:ARG:HG2	4:E:569:LYS:HD2	2.00	0.43
4:E:557:ASN:OD1	4:E:559:ASN:HB2	2.19	0.43
1:N:57:GLN:HG2	1:N:69:TYR:CD1	2.53	0.43
1:N:242:MET:HA	1:N:245:LEU:HD12	2.01	0.43
1:N:302:LEU:O	1:N:648:LEU:HD21	2.17	0.43
1:N:881:PHE:CD1	1:N:881:PHE:C	2.97	0.43
2:Q:174:MET:C	2:Q:177:SER:HG	2.22	0.43
4:R:62:GLN:HB3	4:R:73:LYS:HZ2	1.84	0.43
4:R:117:ALA:O	4:R:121:ILE:HG12	2.18	0.43
6:U:52:GLY:C	6:U:122:MET:HG2	2.42	0.43
7:X:80:ILE:HA	7:X:80:ILE:HD13	1.69	0.43
7:X:415:ASP:C	7:X:417:GLY:N	2.77	0.43
4:F:121:ILE:HD12	4:F:421:TYR:CD2	2.53	0.43
4:F:510:VAL:HG21	4:F:541:TYR:CD2	2.53	0.43
8:L:21:U:N3	8:L:22:G:N7	2.66	0.43
9:M:40:U:C2	9:M:41:G:C8	3.06	0.43
1:A:429:PHE:CD1	1:A:429:PHE:N	2.86	0.43
1:A:429:PHE:HD1	1:A:429:PHE:N	2.16	0.43
2:B:160:VAL:O	2:B:184:LEU:HD23	2.17	0.43
4:E:30:CYS:O	4:E:34:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:239:THR:OG1	4:E:240:LEU:N	2.51	0.43
4:E:293:ILE:O	4:E:297:LEU:HG	2.18	0.43
4:E:384:LEU:O	4:E:388:ASN:ND2	2.46	0.43
7:K:414:CYS:HA	7:K:415:ASP:HA	1.69	0.43
1:N:102:PHE:C	1:N:102:PHE:HD1	2.26	0.43
1:N:105:ARG:NH1	1:N:108:GLY:H	2.16	0.43
1:N:156:TYR:O	1:N:156:TYR:HD1	2.02	0.43
4:R:15:ARG:HA	4:R:23:PRO:O	2.18	0.43
4:R:233:MET:SD	4:R:234:PRO:HD2	2.59	0.43
4:R:244:GLU:HB3	4:R:276:LYS:HD2	2.00	0.43
5:T:72:PRO:HB2	5:T:87:TYR:HB3	1.99	0.43
4:F:18:ALA:HB2	4:F:41:LEU:HB2	2.00	0.43
4:F:189:LYS:CB	4:F:190:ASN:HB2	2.49	0.43
4:S:548:GLN:CG	4:S:576:MET:HE3	2.47	0.43
9:M:39:A:C6	9:M:40:U:C4	3.06	0.43
1:A:242:MET:HA	1:A:245:LEU:HD12	2.01	0.43
1:N:429:PHE:CD1	1:N:429:PHE:N	2.86	0.43
1:N:553:ARG:HE	1:N:553:ARG:HB2	1.70	0.43
2:Q:175:ASP:OD1	2:Q:176:ASN:N	2.43	0.43
4:R:218:LYS:O	4:R:218:LYS:HD3	2.19	0.43
4:R:280:LEU:HA	4:R:436:MET:HB2	1.99	0.43
4:F:303:ARG:C	4:F:304:ILE:HD13	2.43	0.43
4:F:327:ILE:HD11	4:F:345:LYS:HD3	2.00	0.43
4:F:450:ASP:OD1	4:F:451:THR:N	2.51	0.43
4:S:276:LYS:O	4:S:395:HIS:HA	2.19	0.43
2:B:140:ASN:OD1	2:B:140:ASN:N	2.52	0.43
4:E:152:ALA:HB2	4:E:167:TRP:CD1	2.54	0.43
4:E:373:PHE:N	4:E:397:VAL:O	2.50	0.43
2:Q:135:TYR:HB2	2:Q:182:TRP:CH2	2.53	0.43
4:R:15:ARG:HH11	4:R:15:ARG:HG3	1.82	0.43
6:U:53:GLN:HG3	6:U:121:GLY:O	2.19	0.43
7:X:345:ASP:OD1	7:X:345:ASP:N	2.51	0.43
4:F:173:ARG:HD3	4:F:174:PRO:O	2.18	0.43
4:F:249:ILE:HG13	4:F:249:ILE:O	2.19	0.43
4:S:188:THR:HB	4:S:190:ASN:O	2.19	0.43
4:S:347:LYS:NZ	4:S:351:THR:H	2.16	0.43
4:S:477:LYS:NZ	4:S:576:MET:HA	2.33	0.43
8:I:11:G:N1	9:J:49:C:N3	2.54	0.43
9:M:25:G:O2'	9:M:26:A:OP2	2.35	0.43
1:A:708:LEU:HD21	1:A:727:LEU:HD23	1.99	0.43
1:A:770:TYR:CD1	1:A:775:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:278:ARG:O	7:K:282:VAL:HG23	2.18	0.43
1:N:847:ILE:H	1:N:847:ILE:HG12	1.30	0.43
4:R:105:ASP:OD1	4:R:105:ASP:N	2.51	0.43
4:R:202:LYS:HA	4:R:209:VAL:HG12	2.01	0.43
4:R:329:LYS:O	4:R:355:TYR:HD1	2.01	0.43
4:R:334:ILE:HD12	4:R:348:VAL:HG23	2.00	0.43
5:T:10:ARG:NH2	5:T:32:TYR:HE2	2.16	0.43
4:F:138:LEU:HD12	4:F:139:LYS:HD3	2.00	0.43
4:F:445:PRO:HG2	4:F:448:ILE:HG12	2.00	0.43
4:S:329:LYS:HE3	4:S:329:LYS:HB3	1.70	0.43
8:I:21:U:N3	8:I:22:G:N7	2.66	0.43
9:M:24:U:H2'	9:M:25:G:H5"	2.00	0.43
1:A:720:VAL:O	1:A:721:ARG:C	2.59	0.43
1:A:881:PHE:CD1	1:A:881:PHE:C	2.97	0.43
4:E:92:LEU:N	7:X:466:VAL:HG21	2.34	0.43
4:E:129:ARG:HG3	4:E:130:LEU:N	2.33	0.43
4:E:200:PHE:HZ	4:E:225:PHE:CD2	2.36	0.43
4:E:237:ALA:HB2	4:E:389:ALA:HB2	2.01	0.43
4:E:550:THR:HG22	4:E:551:GLU:H	1.83	0.43
5:G:7:VAL:HG22	5:G:9:LEU:HD22	2.00	0.43
5:G:74:ARG:HH11	5:G:74:ARG:CG	2.32	0.43
7:K:321:LEU:HD23	7:K:321:LEU:HA	1.84	0.43
1:N:140:ASP:N	1:N:140:ASP:OD1	2.51	0.43
1:N:770:TYR:CD1	1:N:775:LEU:HD12	2.53	0.43
2:O:22:TYR:HA	2:O:38:LEU:HD22	2.01	0.43
3:P:27:LYS:HE2	3:P:27:LYS:HB2	1.78	0.43
6:U:122:MET:HE3	6:U:122:MET:HB2	1.89	0.43
7:X:489:ASN:O	7:X:493:LEU:HG	2.19	0.43
4:S:500:LEU:HD22	4:S:507:ARG:HH12	1.84	0.43
9:J:25:G:H5'	9:J:25:G:C4	2.53	0.43
9:J:40:U:C2	9:J:41:G:C8	3.06	0.43
9:M:40:U:H2'	9:M:41:G:C8	2.51	0.43
4:E:20:ILE:HG23	4:E:21:ARG:HD2	2.01	0.43
4:E:21:ARG:NE	4:E:136:GLU:OE2	2.44	0.43
4:E:404:GLN:O	4:E:559:ASN:ND2	2.50	0.43
6:H:45:LEU:HB3	7:K:40:VAL:HG22	2.00	0.43
7:K:452:CYS:O	7:K:453:GLU:C	2.61	0.43
2:Q:101:ASP:OD1	2:Q:102:ALA:N	2.52	0.43
5:T:87:TYR:HB2	5:T:89:TYR:HE1	1.84	0.43
7:X:211:ASP:N	7:X:211:ASP:OD1	2.52	0.43
4:S:135:ALA:HB2	4:S:381:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:447:GLU:OE2	4:S:470:GLN:HB2	2.19	0.43
9:J:40:U:H2'	9:J:41:G:C8	2.51	0.43
9:M:38:C:H2'	9:M:39:A:O4'	2.19	0.43
1:A:346:TYR:CD2	1:A:348:PHE:CE1	3.07	0.42
1:A:623:ASP:OD1	1:A:624:ARG:HG3	2.19	0.42
3:C:66:VAL:O	3:C:66:VAL:HG13	2.18	0.42
2:D:54:ALA:O	2:D:58:LYS:HG2	2.18	0.42
4:E:8:CYS:SG	4:E:98:VAL:HB	2.59	0.42
4:E:475:PHE:CZ	4:E:579:ARG:HB3	2.54	0.42
6:H:71:ALA:HB2	6:H:93:LYS:HA	2.01	0.42
1:N:346:TYR:CD2	1:N:348:PHE:CE1	3.07	0.42
1:N:415:PHE:CE2	3:P:8:CYS:HB3	2.54	0.42
1:N:718:LYS:HZ2	1:N:721:ARG:NH2	2.18	0.42
2:O:162:ALA:HB3	2:O:181:ALA:HB1	2.00	0.42
4:R:7:LEU:HA	4:R:129:ARG:HH22	1.84	0.42
4:R:405:LEU:HD23	4:R:563:VAL:HG11	2.01	0.42
4:R:429:MET:O	4:R:430:LYS:HE2	2.19	0.42
7:X:299:ILE:HA	7:X:300:GLY:HA2	1.81	0.42
4:F:371:VAL:HG21	4:F:391:LEU:HG	2.01	0.42
4:S:326:PRO:O	4:S:327:ILE:HD13	2.19	0.42
1:A:851:ASP:HB2	2:D:79:LYS:HE3	2.01	0.42
2:D:85:SER:O	2:D:89:THR:HG22	2.19	0.42
4:E:460:LYS:HA	4:E:460:LYS:HE3	2.01	0.42
7:K:36:GLU:C	7:K:38:LEU:H	2.27	0.42
1:N:370:GLU:O	1:N:374:TYR:HD1	2.02	0.42
1:N:800:TRP:CD2	1:N:810:HIS:HB3	2.54	0.42
4:R:556:CYS:HA	4:R:561:PHE:CZ	2.54	0.42
7:X:476:ARG:HA	7:X:523:PHE:CZ	2.54	0.42
4:F:307:THR:HA	4:F:358:CYS:O	2.19	0.42
4:F:339:ARG:HG2	4:F:339:ARG:HH11	1.83	0.42
4:F:490:ARG:HD3	4:F:493:ILE:HB	2.01	0.42
1:A:156:TYR:CE2	1:A:174:VAL:HG21	2.54	0.42
1:A:367:SER:O	1:A:370:GLU:OE2	2.37	0.42
2:B:62:MET:HA	2:B:65:GLN:HG3	2.00	0.42
2:D:56:GLN:HG3	2:D:57:ARG:N	2.33	0.42
4:E:139:LYS:HE3	4:E:382:TYR:HD2	1.83	0.42
4:E:189:LYS:N	4:E:190:ASN:O	2.52	0.42
4:E:245:HIS:HA	4:E:275:GLN:HA	2.01	0.42
4:E:445:PRO:HA	4:E:465:LYS:HG3	2.01	0.42
4:E:552:THR:HG23	4:E:555:SER:H	1.83	0.42
5:G:48:LEU:CB	5:G:51:LEU:HD11	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:87:TYR:HB2	5:G:89:TYR:HE1	1.84	0.42
7:K:78:GLU:OE1	7:K:82:HIS:ND1	2.52	0.42
1:N:156:TYR:CE2	1:N:174:VAL:HG21	2.54	0.42
3:P:44:ASP:OD1	3:P:44:ASP:N	2.49	0.42
2:Q:67:MET:O	2:Q:70:MET:HG2	2.19	0.42
4:R:130:LEU:HD12	4:R:133:PHE:HB3	2.02	0.42
4:R:178:ARG:HB2	4:R:212:ARG:NH2	2.31	0.42
4:R:227:LEU:CG	4:R:230:HIS:HE1	2.32	0.42
4:R:557:ASN:HB3	4:R:560:ARG:HB2	2.00	0.42
7:X:103:THR:OG1	7:X:104:ASN:N	2.52	0.42
4:S:496:VAL:HG23	4:S:497:ARG:NH1	2.35	0.42
1:A:141:THR:O	1:A:145:ILE:HG13	2.18	0.42
2:B:135:TYR:HA	2:B:182:TRP:CH2	2.54	0.42
3:C:44:ASP:OD1	3:C:44:ASP:N	2.49	0.42
4:E:472:PHE:CD2	4:E:590:LEU:HD21	2.54	0.42
6:H:54:ALA:O	6:H:56:THR:HG22	2.20	0.42
6:H:89:PHE:HD1	7:K:130:ASN:ND2	2.17	0.42
7:K:81:ARG:HB2	7:K:81:ARG:CZ	2.50	0.42
7:K:390:ASP:O	7:K:391:ARG:C	2.63	0.42
1:N:389:LEU:HD23	2:O:130:VAL:HG13	2.01	0.42
1:N:623:ASP:OD1	1:N:624:ARG:HG3	2.19	0.42
4:R:43:LEU:HD23	4:R:43:LEU:HA	1.84	0.42
4:R:283:PRO:HD2	4:R:438:LEU:O	2.19	0.42
4:R:419:PRO:HA	4:R:422:PHE:CD1	2.55	0.42
4:F:126:CYS:SG	4:F:130:LEU:HB3	2.60	0.42
4:F:439:GLY:HA2	4:F:440:THR:HA	1.68	0.42
9:J:38:C:H2'	9:J:39:A:O4'	2.19	0.42
1:A:80:TYR:C	1:A:80:TYR:CD1	2.98	0.42
2:D:65:GLN:O	2:D:68:THR:HG22	2.20	0.42
4:E:6:VAL:HG23	4:E:24:PHE:O	2.20	0.42
4:E:405:LEU:HA	4:E:405:LEU:HD12	1.83	0.42
4:E:428:LEU:O	4:E:433:GLY:N	2.51	0.42
4:E:480:ILE:HA	4:E:489:ASN:OD1	2.19	0.42
6:H:42:VAL:CG2	6:H:69:GLY:HA3	2.49	0.42
7:K:145:GLN:CD	7:K:145:GLN:H	2.27	0.42
1:N:480:PHE:CE2	1:N:693:VAL:HG22	2.48	0.42
2:O:95:LEU:O	2:O:98:LEU:HG	2.20	0.42
4:R:145:PHE:C	4:R:147:LEU:H	2.27	0.42
4:R:363:LEU:HD11	4:R:391:LEU:HD11	2.02	0.42
4:R:490:ARG:HB2	4:R:491:PRO:HD3	2.01	0.42
4:R:514:PRO:HG2	4:R:555:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:519:ASN:O	4:R:530:THR:HG21	2.20	0.42
6:U:14:LEU:HD13	7:X:8:PHE:HE2	1.84	0.42
4:F:167:TRP:CD1	4:F:174:PRO:HD2	2.55	0.42
4:F:256:LEU:HD23	4:F:257:ASN:HB2	2.01	0.42
4:F:474:MET:SD	4:F:474:MET:N	2.92	0.42
4:S:374:ASP:HA	4:S:399:ILE:O	2.19	0.42
4:S:576:MET:N	4:S:576:MET:SD	2.92	0.42
2:B:128:LEU:HD12	2:B:129:MET:H	1.85	0.42
2:B:133:PRO:O	2:B:182:TRP:O	2.38	0.42
4:E:182:PHE:HB2	4:E:225:PHE:HB3	2.01	0.42
4:E:241:VAL:HG21	4:E:396:TYR:CE2	2.54	0.42
4:E:305:VAL:HG13	4:E:356:VAL:HB	2.00	0.42
4:E:353:GLU:HG3	4:E:354:GLN:N	2.35	0.42
7:K:272:CYS:SG	7:K:273:ASP:N	2.93	0.42
1:N:141:THR:O	1:N:145:ILE:HG13	2.18	0.42
2:Q:32:GLU:O	2:Q:35:LEU:HG	2.18	0.42
4:R:542:ASP:HA	4:R:569:LYS:HB2	2.02	0.42
4:F:194:GLN:CD	4:F:194:GLN:H	2.28	0.42
4:F:303:ARG:HH11	4:F:354:GLN:HA	1.84	0.42
4:F:334:ILE:HG21	4:F:338:ALA:HB2	2.01	0.42
4:F:554:HIS:O	4:F:557:ASN:ND2	2.52	0.42
4:S:249:ILE:O	4:S:251:GLY:N	2.49	0.42
4:S:439:GLY:HA2	4:S:440:THR:HA	1.59	0.42
4:S:448:ILE:HG22	4:S:566:THR:HG22	2.00	0.42
4:S:468:SER:H	4:S:570:VAL:HG13	1.84	0.42
4:S:496:VAL:HA	4:S:499:PHE:HB3	2.01	0.42
4:E:235:LEU:HD21	4:E:382:TYR:CD2	2.55	0.42
4:E:280:LEU:HD23	4:E:281:GLN:N	2.34	0.42
6:H:67:SER:HA	6:H:98:GLN:HG3	2.02	0.42
6:H:105:ASN:O	6:H:107:PRO:HD3	2.20	0.42
7:K:447:TYR:CE1	7:K:449:ASP:HB2	2.54	0.42
7:K:474:ILE:O	7:K:523:PHE:HE2	2.02	0.42
4:R:160:ASP:OD1	4:R:161:ARG:HG2	2.19	0.42
4:R:438:LEU:HD23	4:R:438:LEU:HA	1.85	0.42
4:R:473:LYS:HD2	4:R:582:TYR:CD1	2.54	0.42
4:R:473:LYS:HE3	4:R:589:SER:HB2	2.00	0.42
4:R:507:ARG:HG2	4:R:507:ARG:HH21	1.84	0.42
7:X:76:ARG:HE	7:X:76:ARG:HB3	1.71	0.42
4:F:51:ASN:HB2	4:F:71:TYR:HE1	1.84	0.42
4:F:187:VAL:HB	4:F:192:LYS:CE	2.50	0.42
4:S:277:TYR:HA	4:S:396:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:472:PHE:HD1	4:S:474:MET:HG2	1.84	0.42
1:A:219:PHE:HA	1:A:222:PHE:CE1	2.55	0.42
1:A:304:ASP:OD1	1:A:304:ASP:N	2.52	0.42
4:E:257:ASN:OD1	4:E:257:ASN:N	2.51	0.42
4:E:384:LEU:HA	4:E:387:VAL:HG12	2.00	0.42
4:E:561:PHE:O	4:E:565:ILE:HG12	2.20	0.42
1:N:80:TYR:CD1	1:N:80:TYR:C	2.98	0.42
4:R:248:ARG:HH21	4:R:250:THR:HA	1.85	0.42
6:U:61:ALA:HA	6:U:98:GLN:HG2	2.01	0.42
6:U:73:CYS:O	6:U:108:VAL:HG12	2.19	0.42
4:F:186:ARG:HH12	4:F:222:GLY:HA3	1.85	0.42
4:S:158:LEU:HD11	4:S:164:HIS:CG	2.55	0.42
4:S:512:ILE:HG13	4:S:546:PHE:HA	2.02	0.42
8:I:22:G:HO2'	8:I:23:C:P	2.43	0.42
1:A:370:GLU:O	1:A:374:TYR:HD1	2.02	0.42
2:B:59:LEU:HB3	4:F:81:PHE:CE2	2.54	0.42
3:C:66:VAL:C	3:C:70:LYS:HZ1	2.24	0.42
4:E:270:GLN:O	4:E:274:MET:HG2	2.20	0.42
4:E:321:ALA:HB1	4:E:325:LEU:HB2	2.02	0.42
6:H:68:PHE:N	6:H:97:VAL:O	2.51	0.42
6:H:74:CYS:SG	6:H:76:TYR:HB2	2.60	0.42
7:K:329:LEU:HD23	7:K:348:TRP:CE2	2.55	0.42
7:K:485:ARG:O	7:K:486:HIS:C	2.63	0.42
1:N:603:LYS:HD2	1:N:603:LYS:HA	1.72	0.42
1:N:808:GLY:O	1:N:809:PRO:C	2.60	0.42
3:P:66:VAL:C	3:P:70:LYS:HZ1	2.26	0.42
4:R:342:CYS:SG	4:R:343:PHE:N	2.93	0.42
4:R:405:LEU:HD21	4:R:560:ARG:CA	2.49	0.42
7:X:330:HIS:O	7:X:332:ILE:N	2.52	0.42
4:F:269:TYR:CE1	4:F:295:LEU:HB2	2.55	0.42
4:S:15:ARG:HE	4:S:22:ARG:HB3	1.84	0.42
4:S:332:ARG:HH22	4:S:345:LYS:HB2	1.85	0.42
1:A:422:PHE:HE2	1:A:887:TYR:HA	1.85	0.42
1:A:496:ASN:OD1	1:A:496:ASN:N	2.35	0.42
4:E:9:ASN:OD1	4:E:129:ARG:NH2	2.53	0.42
4:E:454:ALA:HA	4:E:459:ASN:OD1	2.20	0.42
5:G:72:PRO:HB3	5:G:89:TYR:CE1	2.55	0.42
6:H:5:THR:O	7:K:25:THR:HG21	2.18	0.42
7:K:370:TYR:O	7:K:374:SER:HB3	2.20	0.42
7:K:447:TYR:HE1	7:K:449:ASP:HB2	1.83	0.42
1:N:528:PHE:HD2	1:N:570:GLN:NE2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:731:LEU:HD23	1:N:732:TYR:CE1	2.55	0.42
5:T:72:PRO:HB3	5:T:89:TYR:CE1	2.55	0.42
7:X:11:CYS:HB2	7:X:101:VAL:O	2.20	0.42
7:X:62:MET:HB3	7:X:62:MET:HE2	1.67	0.42
4:F:76:LYS:NZ	4:F:80:SER:HB3	2.35	0.42
4:F:202:LYS:HG3	4:F:202:LYS:O	2.20	0.42
4:F:544:VAL:HG11	4:F:568:ALA:HB2	2.02	0.42
4:S:280:LEU:N	4:S:398:TYR:O	2.48	0.42
4:S:472:PHE:CD2	4:S:587:PHE:HB2	2.54	0.42
8:I:12:G:N2	9:J:48:C:O2	2.34	0.42
8:I:20:A:C6	9:J:41:G:C6	3.08	0.42
9:M:24:U:C6	9:M:24:U:P	3.13	0.42
2:D:90:MET:O	2:D:93:THR:HG22	2.20	0.41
1:N:304:ASP:OD1	1:N:304:ASP:N	2.53	0.41
1:N:919:GLU:N	1:N:919:GLU:CD	2.78	0.41
4:R:309:CYS:SG	4:R:378:MET:HE3	2.60	0.41
5:T:48:LEU:CB	5:T:51:LEU:HD11	2.46	0.41
4:F:266:VAL:HA	4:F:269:TYR:CD2	2.55	0.41
4:S:325:LEU:HD23	4:S:326:PRO:HD2	2.02	0.41
1:A:80:TYR:C	1:A:80:TYR:HD1	2.29	0.41
2:B:40:LYS:O	2:B:44:VAL:HG13	2.20	0.41
4:E:13:SER:OG	4:E:92:LEU:HB3	2.20	0.41
4:E:276:LYS:HG3	4:E:277:TYR:HD1	1.85	0.41
5:G:9:LEU:HD12	5:G:9:LEU:HA	1.87	0.41
1:N:783:LYS:HB3	1:N:783:LYS:HE3	1.79	0.41
4:R:93:TYR:HB3	4:R:96:THR:OG1	2.20	0.41
4:R:276:LYS:O	4:R:395:HIS:HA	2.20	0.41
4:R:519:ASN:HB3	4:R:530:THR:CG2	2.49	0.41
7:X:33:PHE:HD2	7:X:40:VAL:O	2.04	0.41
7:X:191:GLU:O	7:X:195:MET:HG3	2.20	0.41
4:F:74:SER:C	4:F:76:LYS:H	2.27	0.41
4:F:129:ARG:HB2	4:F:129:ARG:NH1	2.35	0.41
4:F:248:ARG:HG2	4:F:249:ILE:N	2.36	0.41
4:F:346:PHE:HB3	4:F:347:LYS:H	1.70	0.41
4:S:338:ALA:O	4:S:340:VAL:O	2.37	0.41
8:L:20:A:C6	9:M:41:G:C6	3.08	0.41
1:A:433:SER:OG	1:A:434:SER:N	2.51	0.41
1:A:619:TYR:N	1:A:619:TYR:HD1	2.17	0.41
2:B:59:LEU:HD22	4:F:81:PHE:CD2	2.55	0.41
2:B:171:GLU:OE1	2:B:171:GLU:N	2.49	0.41
3:C:28:LEU:HD12	3:C:28:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:ASP:HA	2:D:55:MET:HG3	2.01	0.41
2:D:135:TYR:O	2:D:138:TYR:HB3	2.21	0.41
4:E:419:PRO:HA	4:E:422:PHE:CD2	2.55	0.41
4:E:452:VAL:HG11	4:E:566:THR:CG2	2.50	0.41
5:G:11:GLN:HE22	5:G:29:LEU:CA	2.33	0.41
7:K:168:GLN:HB3	1:N:431:GLU:HG2	2.02	0.41
1:N:11:VAL:HG21	1:N:72:VAL:HG21	2.01	0.41
1:N:331:ARG:HE	1:N:344:THR:HG21	1.85	0.41
1:N:422:PHE:HE2	1:N:887:TYR:HA	1.85	0.41
1:N:551:LYS:HE2	1:N:551:LYS:HB2	1.71	0.41
2:Q:118:ASN:OD1	2:Q:118:ASN:N	2.53	0.41
4:R:13:SER:OG	4:R:92:LEU:HD13	2.20	0.41
4:R:194:GLN:CD	4:R:196:GLY:H	2.28	0.41
4:R:476:TYR:HB3	4:R:575:ILE:HG23	2.02	0.41
4:R:541:TYR:HD2	4:R:543:TYR:O	2.04	0.41
5:T:11:GLN:HE22	5:T:29:LEU:CA	2.33	0.41
5:T:12:MET:HE2	5:T:39:ARG:NE	2.36	0.41
7:X:321:LEU:HD23	7:X:321:LEU:HA	1.78	0.41
4:F:150:GLY:H	4:F:171:LYS:HE3	1.85	0.41
4:F:244:GLU:O	4:F:276:LYS:N	2.53	0.41
4:F:499:PHE:CD1	4:F:502:ARG:HD3	2.55	0.41
4:S:371:VAL:HB	4:S:396:TYR:CD1	2.55	0.41
1:A:60:ASP:HB3	1:A:64:ASN:OD1	2.20	0.41
1:A:331:ARG:HE	1:A:344:THR:HG21	1.85	0.41
1:A:605:VAL:O	1:A:606:TYR:C	2.64	0.41
1:A:731:LEU:HD23	1:A:732:TYR:CE1	2.55	0.41
1:A:853:THR:OG1	1:A:894:GLU:OE2	2.26	0.41
2:D:52:ASP:OD1	2:D:53:ALA:N	2.53	0.41
4:E:39:HIS:CD2	4:E:39:HIS:N	2.89	0.41
7:K:359:LYS:O	7:K:363:ILE:N	2.41	0.41
1:N:78:SER:O	1:N:81:GLN:HG3	2.21	0.41
1:N:80:TYR:C	1:N:80:TYR:HD1	2.28	0.41
1:N:231:VAL:HB	5:T:96:ASN:HD22	1.85	0.41
1:N:821:LYS:HZ2	1:N:821:LYS:HG2	1.74	0.41
1:N:892:HIS:O	1:N:896:THR:HG23	2.20	0.41
4:R:374:ASP:HA	4:R:399:ILE:HB	2.02	0.41
4:R:417:LEU:HG	4:R:421:TYR:HB2	2.01	0.41
4:F:369:ASP:C	4:F:393:ALA:HB1	2.46	0.41
4:F:486:SER:HB3	4:F:515:TYR:CD1	2.56	0.41
4:S:281:GLN:OE1	4:S:401:ASP:HA	2.19	0.41
4:S:283:PRO:HD2	4:S:286:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:244:GLU:H	4:E:276:LYS:CB	2.33	0.41
4:E:503:ASN:HB3	4:E:506:TRP:CD1	2.55	0.41
1:N:367:SER:OG	1:N:368:PHE:N	2.48	0.41
1:N:419:PHE:CD1	1:N:887:TYR:HE2	2.36	0.41
2:O:125:ALA:O	2:O:190:ARG:NH1	2.53	0.41
2:Q:173:SER:HB2	2:Q:175:ASP:OD1	2.20	0.41
4:R:170:GLY:O	4:R:171:LYS:CG	2.69	0.41
4:R:455:LEU:HD21	4:R:584:LYS:HB3	2.03	0.41
5:T:46:SER:O	5:T:87:TYR:N	2.43	0.41
4:S:31:TYR:O	4:S:35:ILE:HG12	2.20	0.41
4:S:154:VAL:HG13	4:S:165:LEU:HD12	2.02	0.41
4:S:159:SER:OG	4:S:162:GLU:HB3	2.20	0.41
4:S:178:ARG:HB3	4:S:339:ARG:NH2	2.35	0.41
1:A:615:MET:HE2	1:A:615:MET:HB3	1.84	0.41
7:K:460:VAL:HA	7:K:461:SER:HA	1.71	0.41
2:Q:12:TYR:HD1	2:Q:49:PHE:CE1	2.39	0.41
4:R:20:ILE:HB	4:R:21:ARG:HH12	1.85	0.41
4:R:167:TRP:O	4:R:168:GLU:C	2.64	0.41
4:R:255:THR:HB	4:R:300:PRO:HD3	2.02	0.41
4:R:449:VAL:HG11	4:R:463:ALA:HA	2.03	0.41
7:X:74:ILE:HD13	7:X:240:PHE:HD2	1.84	0.41
7:X:120:VAL:HG21	7:X:135:ARG:HE	1.85	0.41
7:X:264:HIS:CD2	7:X:264:HIS:H	2.35	0.41
7:X:324:ASP:HB3	7:X:326:PHE:CZ	2.56	0.41
7:X:327:PRO:HD2	7:X:380:GLY:HA2	2.02	0.41
7:X:432:ASP:OD1	7:X:433:LYS:N	2.53	0.41
4:S:21:ARG:HH11	4:S:136:GLU:HB3	1.85	0.41
4:S:83:LEU:HD23	4:S:83:LEU:H	1.86	0.41
1:A:140:ASP:OD1	1:A:140:ASP:N	2.51	0.41
1:A:480:PHE:CE2	1:A:693:VAL:HG22	2.48	0.41
3:C:57:SER:HB2	2:D:120:ILE:HG13	2.02	0.41
4:E:384:LEU:HD11	4:E:398:TYR:CE2	2.56	0.41
4:E:419:PRO:HA	4:E:422:PHE:CE2	2.56	0.41
4:E:476:TYR:HB3	4:E:575:ILE:HG22	2.02	0.41
6:H:58:THR:HG23	6:H:59:PRO:HD2	2.03	0.41
7:K:115:VAL:HG21	7:K:169:MET:SD	2.59	0.41
7:K:349:LYS:HB3	7:K:349:LYS:HE2	1.80	0.41
4:R:21:ARG:HG2	4:R:21:ARG:HH11	1.86	0.41
4:R:425:VAL:HG12	4:R:429:MET:CE	2.50	0.41
4:R:533:VAL:HG11	4:R:560:ARG:HD2	2.01	0.41
7:X:11:CYS:O	7:X:100:ALA:HB1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:51:TYR:CD1	7:X:128:PRO:HD3	2.55	0.41
4:F:40:LYS:N	4:F:40:LYS:HD2	2.34	0.41
4:S:154:VAL:HG21	4:S:223:ASP:HB2	2.03	0.41
4:S:327:ILE:HA	4:S:328:ASP:C	2.46	0.41
1:A:612:PRO:HG2	1:A:805:LEU:HD12	2.03	0.41
3:C:27:LYS:HB2	3:C:27:LYS:HE2	1.78	0.41
4:E:186:ARG:HB3	4:E:220:ASN:HD21	1.86	0.41
5:G:12:MET:HE2	5:G:39:ARG:NE	2.36	0.41
7:K:342:PRO:HG2	7:K:343:GLN:NE2	2.36	0.41
1:N:45:PHE:CE1	1:N:129:TYR:HD2	2.38	0.41
1:N:60:ASP:HB3	1:N:64:ASN:OD1	2.20	0.41
1:N:619:TYR:N	1:N:619:TYR:HD1	2.17	0.41
2:Q:62:MET:HE3	2:Q:62:MET:HB2	1.85	0.41
2:Q:158:GLN:HE22	2:Q:160:VAL:HB	1.85	0.41
4:R:443:ARG:HH12	4:R:567:ARG:CZ	2.33	0.41
4:R:458:ASP:N	4:R:458:ASP:OD1	2.53	0.41
4:R:475:PHE:CE1	4:R:477:LYS:HE3	2.56	0.41
4:R:499:PHE:CE2	4:R:573:LEU:HD13	2.55	0.41
4:S:338:ALA:O	4:S:340:VAL:N	2.54	0.41
4:S:346:PHE:HB3	4:S:347:LYS:H	1.74	0.41
4:S:493:ILE:O	4:S:497:ARG:NH1	2.54	0.41
1:A:11:VAL:C	1:A:13:GLY:H	2.26	0.41
1:A:105:ARG:HG2	1:A:110:MET:N	2.36	0.41
1:A:380:MET:HE1	2:B:95:LEU:CD1	2.51	0.41
1:A:718:LYS:HA	1:A:721:ARG:CD	2.46	0.41
1:A:926:THR:CG2	1:A:927:PRO:CD	2.73	0.41
4:E:9:ASN:OD1	4:E:129:ARG:NH1	2.54	0.41
4:E:50:CYS:N	4:E:63:LEU:HD11	2.35	0.41
4:E:474[A]:MET:O	4:E:576:MET:N	2.32	0.41
4:E:476:TYR:HD2	4:E:495:VAL:HG11	1.86	0.41
4:E:542:ASP:CG	4:E:543:TYR:H	2.29	0.41
7:K:205:ARG:NH2	7:K:224:TYR:OH	2.54	0.41
7:K:329:LEU:N	7:K:347:GLU:O	2.33	0.41
1:N:715:ILE:HB	1:N:721:ARG:HH12	1.86	0.41
1:N:726:ARG:NE	1:N:741:PHE:HD2	2.18	0.41
4:R:21:ARG:NH2	4:R:229:SER:HB2	2.36	0.41
4:R:177:ASN:OD1	4:R:178:ARG:NH1	2.47	0.41
4:R:293:ILE:HD13	4:R:321:ALA:HA	2.01	0.41
4:R:423:ASN:OD1	4:R:423:ASN:O	2.39	0.41
4:R:439:GLY:HA3	4:R:462:LYS:HE2	2.02	0.41
6:U:67:SER:OG	6:U:98:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:72:SER:O	6:U:78:ARG:NH2	2.50	0.41
7:X:25:THR:HG23	7:X:28:SER:H	1.86	0.41
7:X:283:HIS:HA	7:X:287:VAL:CG2	2.48	0.41
7:X:457:LYS:HD2	7:X:458:GLN:N	2.34	0.41
7:X:487:HIS:N	7:X:487:HIS:CD2	2.89	0.41
4:F:342:CYS:SG	4:F:343:PHE:N	2.93	0.41
4:F:369:ASP:O	4:F:395:HIS:ND1	2.53	0.41
4:F:510:VAL:HG11	4:F:541:TYR:CD2	2.56	0.41
4:F:594:ARG:NH2	4:F:596:ASN:HD21	2.18	0.41
4:S:332:ARG:HG3	4:S:347:LYS:HZ2	1.85	0.41
4:S:428:LEU:HA	4:S:431:THR:HG22	2.02	0.41
4:S:477:LYS:HE3	4:S:489:ASN:HD22	1.86	0.41
4:S:484:VAL:HG12	4:S:485:SER:H	1.86	0.41
1:A:45:PHE:CE1	1:A:129:TYR:HD2	2.38	0.41
1:A:68:SER:HA	1:A:119:LEU:O	2.20	0.41
1:A:767:ASN:OD1	1:A:769:THR:N	2.54	0.41
1:A:892:HIS:O	1:A:896:THR:HG23	2.20	0.41
2:B:56:GLN:O	2:B:60:GLU:HG2	2.21	0.41
2:B:95:LEU:C	2:B:97:LYS:H	2.29	0.41
4:E:21:ARG:CZ	4:E:21:ARG:HA	2.51	0.41
4:E:135:ALA:O	4:E:139:LYS:HE2	2.21	0.41
4:E:151:ILE:CG1	4:E:171:LYS:HE3	2.51	0.41
4:E:325:LEU:HD23	4:E:325:LEU:HA	1.90	0.41
4:E:514:PRO:HB3	4:E:560:ARG:NH1	2.36	0.41
4:E:579:ARG:H	4:E:579:ARG:HG2	1.74	0.41
5:G:44:LEU:HD23	5:G:69:LEU:HD21	2.03	0.41
7:K:127:THR:OG1	7:K:130:ASN:O	2.25	0.41
7:K:129:ASN:OD1	7:K:130:ASN:N	2.54	0.41
7:K:396:SER:OG	7:K:439:LEU:HD21	2.21	0.41
1:N:22:CYS:CB	1:N:55:ARG:O	2.69	0.41
1:N:68:SER:HA	1:N:119:LEU:O	2.21	0.41
1:N:105:ARG:HH12	1:N:108:GLY:CA	2.34	0.41
1:N:504:PHE:CD1	1:N:505:PRO:N	2.89	0.41
1:N:645:CYS:SG	1:N:646:CYS:N	2.94	0.41
1:N:767:ASN:OD1	1:N:769:THR:N	2.54	0.41
2:Q:22:TYR:O	2:Q:26:VAL:HG22	2.21	0.41
7:X:329:LEU:HD22	7:X:348:TRP:CE3	2.56	0.41
7:X:401:PHE:HB2	7:X:506:PHE:CE1	2.56	0.41
4:F:31:TYR:CD1	4:F:87:GLY:HA2	2.56	0.41
4:F:548:GLN:NE2	4:F:576:MET:HE2	2.36	0.41
4:S:154:VAL:HG22	4:S:165:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:380:THR:O	4:S:384:LEU:HG	2.21	0.41
4:S:519:ASN:ND2	4:S:530:THR:HB	2.33	0.41
4:S:561:PHE:CE2	4:S:576:MET:HE2	2.55	0.41
9:J:22:U:H2'	9:J:23:C:C2	2.56	0.41
1:A:820:VAL:HG11	1:A:829:LEU:HD12	2.03	0.40
2:B:123:THR:OG1	2:B:124:THR:N	2.54	0.40
3:C:63:GLN:HB2	4:E:352:LEU:HD11	2.04	0.40
4:E:195:ILE:O	4:E:215:THR:OG1	2.21	0.40
4:E:514:PRO:HG2	4:E:555:SER:OG	2.21	0.40
4:E:545:ILE:HG23	4:E:573:LEU:HD22	2.03	0.40
1:N:152:CYS:HB2	1:N:156:TYR:HD2	1.86	0.40
1:N:192:PHE:C	1:N:192:PHE:CD1	3.00	0.40
1:N:820:VAL:HG11	1:N:829:LEU:HD12	2.03	0.40
2:Q:18:ALA:CB	2:Q:42:LEU:HD22	2.44	0.40
4:R:118:GLY:HA2	4:R:121:ILE:HG12	2.02	0.40
4:R:243:GLN:HB2	4:R:277:TYR:CZ	2.57	0.40
4:R:361:ASN:OD1	4:R:361:ASN:N	2.54	0.40
4:R:579:ARG:HA	4:R:579:ARG:HD2	1.92	0.40
6:U:46:CYS:SG	6:U:47:THR:N	2.91	0.40
6:U:85:ASN:CB	6:U:86:PRO:HD2	2.50	0.40
7:X:313:GLN:HG3	7:X:385:TRP:CH2	2.56	0.40
4:S:65:LEU:N	4:S:81:PHE:O	2.49	0.40
4:S:332:ARG:NH2	4:S:345:LYS:HB2	2.36	0.40
4:S:338:ALA:HB1	4:S:340:VAL:O	2.22	0.40
1:A:192:PHE:C	1:A:192:PHE:CD1	2.99	0.40
1:A:609:VAL:HG12	1:A:610:GLU:N	2.36	0.40
1:A:726:ARG:NE	1:A:741:PHE:HD2	2.18	0.40
2:D:160:VAL:HG13	2:D:185:ILE:HB	2.02	0.40
4:E:155:ARG:HA	4:E:155:ARG:NE	2.37	0.40
4:E:158:LEU:HB2	4:E:162:GLU:HG2	2.04	0.40
4:E:176:LEU:CD2	4:E:200:PHE:HB2	2.51	0.40
4:E:515:TYR:HE2	4:E:549:THR:HB	1.87	0.40
4:E:533:VAL:HB	4:E:560:ARG:NH2	2.37	0.40
6:H:27:TYR:CE2	6:H:31:LEU:HD11	2.56	0.40
7:K:357:SER:OG	7:K:358:ASP:N	2.48	0.40
1:N:807:LYS:O	1:N:807:LYS:CG	2.69	0.40
2:Q:98:LEU:HD23	2:Q:98:LEU:HA	1.73	0.40
4:R:65:LEU:HD23	4:R:81:PHE:CE1	2.56	0.40
5:T:33:ASN:HB2	5:T:42:LEU:HD11	2.04	0.40
7:X:295:GLU:OE2	7:X:424:HIS:NE2	2.54	0.40
4:F:127:THR:OG1	4:F:130:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:151:ILE:HB	4:F:224:TYR:HD1	1.82	0.40
4:F:262:PHE:O	4:F:266:VAL:HG23	2.21	0.40
4:S:88:GLN:OE1	4:S:94:LYS:HE2	2.22	0.40
8:I:20:A:H2'	8:I:21:U:C6	2.57	0.40
9:J:25:G:OP2	9:J:25:G:C2	2.74	0.40
1:A:152:CYS:HB2	1:A:156:TYR:HD2	1.86	0.40
1:A:779:ILE:HD13	1:A:779:ILE:HA	1.98	0.40
3:C:60:LEU:HD23	3:C:60:LEU:HA	1.85	0.40
2:D:57:ARG:HG3	2:D:58:LYS:HD3	2.03	0.40
2:D:162:ALA:H	2:D:181:ALA:HB3	1.85	0.40
4:E:149:TYR:HB2	4:E:172:PRO:CB	2.38	0.40
4:E:229:SER:O	4:E:229:SER:OG	2.33	0.40
4:E:272:VAL:HG22	4:E:436:MET:HE1	2.04	0.40
4:E:405:LEU:HD13	4:E:563:VAL:HG21	2.04	0.40
4:E:470:GLN:HA	4:E:472:PHE:CE1	2.55	0.40
4:E:510:VAL:HG12	4:E:543:TYR:O	2.21	0.40
4:E:526:LEU:HB3	4:E:528:LEU:HG	2.03	0.40
6:H:124:LYS:HB2	6:H:124:LYS:HE2	1.83	0.40
1:N:20:THR:CG2	1:N:21:PRO:CD	2.97	0.40
1:N:411:LYS:HE2	1:N:411:LYS:HB2	1.56	0.40
1:N:469:LEU:HA	1:N:472:VAL:HG22	2.03	0.40
1:N:595:TYR:N	1:N:595:TYR:CD1	2.89	0.40
2:Q:37:LYS:HB2	2:Q:37:LYS:HE3	1.59	0.40
2:Q:61:LYS:HG3	2:Q:62:MET:N	2.36	0.40
4:R:188:THR:OG1	4:R:191:SER:HB3	2.21	0.40
4:R:201:GLU:HB2	4:R:210:VAL:CG2	2.51	0.40
4:R:453:SER:HB2	4:R:459:ASN:HA	2.04	0.40
6:U:117:CYS:HB2	6:U:124:LYS:NZ	2.36	0.40
6:U:126:TYR:N	6:U:127:GLY:HA2	2.36	0.40
7:X:467:PRO:HG2	7:X:482:ALA:N	2.36	0.40
4:F:152:ALA:HB2	4:F:167:TRP:CD1	2.56	0.40
4:F:286:THR:HG23	4:F:440:THR:C	2.46	0.40
4:F:419:PRO:HB2	4:F:430:LYS:CE	2.52	0.40
4:F:595:ARG:HA	4:F:595:ARG:HD3	1.87	0.40
4:S:127:THR:O	4:S:131:LYS:HG3	2.20	0.40
4:S:254:PRO:HB3	4:S:298:TYR:CZ	2.56	0.40
9:M:25:G:OP2	9:M:25:G:C2	2.74	0.40
1:A:7:PHE:HD1	1:A:7:PHE:HA	1.55	0.40
1:A:19:LEU:HA	1:A:19:LEU:HD23	1.75	0.40
1:A:645:CYS:SG	1:A:646:CYS:N	2.94	0.40
2:D:71:TYR:HE1	2:D:75:ARG:NH2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:LEU:HD23	2:D:98:LEU:HA	1.76	0.40
2:D:109:ASN:HD22	2:D:149:TYR:HE1	1.69	0.40
4:E:10:SER:OG	4:E:26:CYS:HB3	2.22	0.40
4:E:74:SER:O	4:E:74:SER:OG	2.37	0.40
4:E:261:GLU:HG3	4:E:262:PHE:CE1	2.56	0.40
4:E:544:VAL:O	4:E:572:ILE:HA	2.21	0.40
5:G:9:LEU:HD11	5:G:33:ASN:HA	2.04	0.40
5:G:16:ALA:HA	5:G:54:ALA:HA	2.04	0.40
5:G:44:LEU:HD12	5:G:44:LEU:HA	1.89	0.40
7:K:502:ILE:HD13	1:N:889:ARG:NH2	2.35	0.40
1:N:129:TYR:CZ	1:N:133:HIS:HD2	2.39	0.40
1:N:221:ASP:OD1	1:N:221:ASP:N	2.55	0.40
1:N:718:LYS:HA	1:N:718:LYS:CE	2.52	0.40
3:P:28:LEU:HD12	3:P:28:LEU:HA	1.92	0.40
2:Q:57:ARG:O	2:Q:60:GLU:HG3	2.21	0.40
5:T:16:ALA:HA	5:T:54:ALA:HA	2.04	0.40
7:X:363:ILE:H	7:X:363:ILE:HG13	1.73	0.40
4:F:52:ALA:HB2	4:F:71:TYR:CE2	2.57	0.40
4:F:293:ILE:HD13	4:F:321:ALA:HA	2.02	0.40
4:F:300:PRO:HA	4:F:355:TYR:OH	2.21	0.40
4:F:446:ALA:N	4:F:464:HIS:O	2.55	0.40
4:F:520:ALA:O	4:F:524:LYS:HD2	2.22	0.40
4:S:490:ARG:HA	4:S:493:ILE:HB	2.03	0.40
1:A:422:PHE:HD2	1:A:887:TYR:CD2	2.40	0.40
1:A:469:LEU:HA	1:A:472:VAL:HG22	2.03	0.40
2:D:108:ASN:HA	2:D:111:ARG:HG2	2.03	0.40
4:E:255:THR:HB	4:E:300:PRO:HD3	2.03	0.40
4:E:359:THR:OG1	4:E:361:ASN:OD1	2.37	0.40
4:E:393:ALA:HB3	4:E:396:TYR:CE1	2.56	0.40
5:G:33:ASN:HB2	5:G:42:LEU:HD11	2.04	0.40
7:K:19:HIS:ND1	7:K:47:LYS:HB3	2.36	0.40
7:K:252:ASN:OD1	7:K:252:ASN:N	2.54	0.40
1:N:381:HIS:CE1	2:O:94:MET:HE1	2.57	0.40
1:N:668:MET:HG2	1:N:673:LEU:HD23	2.04	0.40
1:N:830:PRO:O	1:N:868:PRO:HG2	2.21	0.40
2:O:55:MET:HA	2:O:58:LYS:HG3	2.01	0.40
2:O:91:LEU:HD23	2:O:91:LEU:HA	1.86	0.40
4:R:420:GLU:HB2	4:R:427:ARG:HE	1.87	0.40
4:R:455:LEU:HD23	4:R:584:LYS:HD3	2.03	0.40
5:T:16:ALA:C	5:T:23:CYS:HA	2.46	0.40
6:U:40:ASN:OD1	7:X:26:HIS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:55:ILE:HD12	6:U:55:ILE:HA	1.92	0.40
7:X:19:HIS:CE1	7:X:20:PRO:HG2	2.56	0.40
7:X:372:THR:HG1	7:X:373:HIS:H	1.70	0.40
4:F:248:ARG:HG2	4:F:249:ILE:H	1.87	0.40
4:F:307:THR:HG23	4:F:373:PHE:CD1	2.57	0.40
4:F:405:LEU:HD23	4:F:405:LEU:HA	1.89	0.40
4:F:440:THR:HG21	4:F:462:LYS:HB3	2.04	0.40
4:F:490:ARG:N	4:F:491:PRO:HD2	2.37	0.40
4:S:8:CYS:HB2	4:S:98:VAL:HG13	2.03	0.40
4:S:32:ASP:HB2	4:S:103:VAL:HG21	2.04	0.40
4:S:212:ARG:HD2	4:S:340:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	924/932 (99%)	825 (89%)	97 (10%)	2 (0%)	43 70
1	N	924/932 (99%)	831 (90%)	88 (10%)	5 (0%)	24 52
2	B	185/198 (93%)	175 (95%)	7 (4%)	3 (2%)	7 28
2	D	184/198 (93%)	172 (94%)	11 (6%)	1 (0%)	24 52
2	O	185/198 (93%)	172 (93%)	10 (5%)	3 (2%)	7 28
2	Q	184/198 (93%)	171 (93%)	13 (7%)	0	100 100
3	C	70/83 (84%)	69 (99%)	1 (1%)	0	100 100
3	P	70/83 (84%)	69 (99%)	1 (1%)	0	100 100
4	E	585/601 (97%)	530 (91%)	55 (9%)	0	100 100
4	F	594/601 (99%)	515 (87%)	77 (13%)	2 (0%)	36 63
4	R	585/601 (97%)	530 (91%)	52 (9%)	3 (0%)	24 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	S	594/601 (99%)	516 (87%)	73 (12%)	5 (1%)	16 44
5	G	111/117 (95%)	97 (87%)	12 (11%)	2 (2%)	6 26
5	T	111/117 (95%)	100 (90%)	11 (10%)	0	100 100
6	H	129/139 (93%)	113 (88%)	15 (12%)	1 (1%)	16 44
6	U	128/139 (92%)	111 (87%)	17 (13%)	0	100 100
7	K	521/527 (99%)	445 (85%)	70 (13%)	6 (1%)	10 33
7	X	522/527 (99%)	434 (83%)	83 (16%)	5 (1%)	12 38
All	All	6606/6792 (97%)	5875 (89%)	693 (10%)	38 (1%)	23 49

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	181	ALA
7	K	454	SER
7	K	485	ARG
1	N	850	THR
2	O	183	PRO
7	X	464	ASP
7	X	467	PRO
4	S	191	SER
1	A	808	GLY
7	K	453	GLU
1	N	851	ASP
4	F	319	GLU
4	S	339	ARG
5	G	6	PRO
1	N	24	THR
4	S	350	SER
2	B	182	TRP
5	G	23	CYS
1	N	607	SER
2	O	31	SER
4	R	171	LYS
4	R	469	ALA
7	X	228	HIS
4	F	338	ALA
4	R	146	LYS
7	X	460	VAL
7	X	475	THR
2	B	183	PRO

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Mol	Chain	Res	Type
2	D	126	ALA
1	A	847	ILE
1	N	847	ILE
7	K	451	PRO
7	K	459	VAL
2	O	172	ILE
4	S	67	GLY
4	S	335	PRO
6	H	88	GLY
7	K	299	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	818/823 (99%)	696 (85%)	122 (15%)	3 12
1	N	818/823 (99%)	690 (84%)	128 (16%)	2 10
2	B	146/167 (87%)	138 (94%)	8 (6%)	19 47
2	D	150/167 (90%)	142 (95%)	8 (5%)	20 48
2	O	146/167 (87%)	134 (92%)	12 (8%)	10 35
2	Q	150/167 (90%)	141 (94%)	9 (6%)	17 44
3	C	67/77 (87%)	51 (76%)	16 (24%)	1 2
3	P	67/77 (87%)	51 (76%)	16 (24%)	1 2
4	E	507/523 (97%)	496 (98%)	11 (2%)	45 63
4	F	514/523 (98%)	494 (96%)	20 (4%)	28 54
4	R	507/523 (97%)	490 (97%)	17 (3%)	32 58
4	S	514/523 (98%)	474 (92%)	40 (8%)	11 37
5	G	94/97 (97%)	68 (72%)	26 (28%)	0 1
5	T	94/97 (97%)	72 (77%)	22 (23%)	1 2
6	H	105/113 (93%)	95 (90%)	10 (10%)	8 29
6	U	104/113 (92%)	92 (88%)	12 (12%)	5 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	K	458/462 (99%)	410 (90%)	48 (10%)	6 24
7	X	459/462 (99%)	413 (90%)	46 (10%)	7 26
All	All	5718/5904 (97%)	5147 (90%)	571 (10%)	9 26

All (571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	7	PHE
1	A	11	VAL
1	A	15	SER
1	A	24	THR
1	A	27	SER
1	A	32	TYR
1	A	37	ILE
1	A	40	ASP
1	A	49	LEU
1	A	51	THR
1	A	53	CYS
1	A	61	GLU
1	A	62	ASP
1	A	65	LEU
1	A	66	ILE
1	A	92	ASP
1	A	98	LYS
1	A	102	PHE
1	A	103	LYS
1	A	107	ASP
1	A	113	HIS
1	A	114	ILE
1	A	115	SER
1	A	116	ARG
1	A	118	ARG
1	A	141	THR
1	A	158	ASN
1	A	159	LYS
1	A	160	LYS
1	A	165	PHE
1	A	167	GLU
1	A	180	GLU
1	A	187	LEU

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Mol	Chain	Res	Type
1	A	204	VAL
1	A	226	THR
1	A	229	SER
1	A	260	ASP
1	A	262	THR
1	A	267	LYS
1	A	277	GLU
1	A	281	LYS
1	A	282	LEU
1	A	293	THR
1	A	295	HIS
1	A	299	VAL
1	A	308	LEU
1	A	315	VAL
1	A	325	SER
1	A	335	VAL
1	A	363	SER
1	A	366	LEU
1	A	367	SER
1	A	388	LEU
1	A	389	LEU
1	A	391	LYS
1	A	393	THR
1	A	405	VAL
1	A	409	THR
1	A	411	LYS
1	A	434	SER
1	A	435	VAL
1	A	478	LYS
1	A	480	PHE
1	A	494	ILE
1	A	496	ASN
1	A	514	LEU
1	A	517	ASP
1	A	518	SER
1	A	522	GLU
1	A	560	VAL
1	A	561	SER
1	A	583	ARG
1	A	593	LYS
1	A	609	VAL
1	A	614	LEU

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Mol	Chain	Res	Type
1	A	618	ASP
1	A	619	TYR
1	A	621	LYS
1	A	624	ARG
1	A	630	LEU
1	A	640	ARG
1	A	644	THR
1	A	666	MET
1	A	667	VAL
1	A	680	THR
1	A	682	SER
1	A	686	THR
1	A	708	LEU
1	A	710	THR
1	A	715	ILE
1	A	721	ARG
1	A	729	GLU
1	A	731	LEU
1	A	737	VAL
1	A	739	THR
1	A	740	ASP
1	A	744	GLU
1	A	768	SER
1	A	769	THR
1	A	780	LYS
1	A	783	LYS
1	A	805	LEU
1	A	806	THR
1	A	807	LYS
1	A	817	THR
1	A	818	MET
1	A	820	VAL
1	A	821	LYS
1	A	835	SER
1	A	847	ILE
1	A	848	VAL
1	A	854	LEU
1	A	865	ASP
1	A	889	ARG
1	A	894	GLU
1	A	899	MET
1	A	900	LEU

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Mol	Chain	Res	Type
1	A	902	MET
1	A	904	SER
1	A	922	GLU
1	A	929	THR
2	B	107	ILE
2	B	111	ARG
2	B	115	VAL
2	B	140	ASN
2	B	153	LEU
2	B	157	GLN
2	B	160	VAL
2	B	175	ASP
3	C	4	SER
3	C	13	LEU
3	C	20	LEU
3	C	24	SER
3	C	27	LYS
3	C	35	LEU
3	C	38	ASP
3	C	41	LEU
3	C	45	THR
3	C	47	GLU
3	C	50	GLU
3	C	55	LEU
3	C	61	SER
3	C	62	MET
3	C	70	LYS
3	C	73	GLU
2	D	34	VAL
2	D	56	GLN
2	D	78	ASP
2	D	145	THR
2	D	148	THR
2	D	163	ASP
2	D	175	ASP
2	D	179	ASN
4	E	2	VAL
4	E	55	CYS
4	E	56	ASP
4	E	96	THR
4	E	146	LYS
4	E	147	LEU

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Mol	Chain	Res	Type
4	E	183	THR
4	E	228	THR
4	E	405	LEU
4	E	481	THR
4	E	550	THR
5	G	4	LEU
5	G	5	SER
5	G	7	VAL
5	G	9	LEU
5	G	12	MET
5	G	21	THR
5	G	24	THR
5	G	29	LEU
5	G	35	THR
5	G	36	LYS
5	G	41	VAL
5	G	42	LEU
5	G	45	LEU
5	G	47	ASP
5	G	48	LEU
5	G	50	ASP
5	G	55	ARG
5	G	64	THR
5	G	68	GLU
5	G	69	LEU
5	G	74	ARG
5	G	75	PHE
5	G	78	ASP
5	G	79	THR
5	G	81	LYS
5	G	99	ARG
6	H	12	THR
6	H	62	ASN
6	H	64	ASP
6	H	72	SER
6	H	89	PHE
6	H	108	VAL
6	H	115	THR
6	H	118	THR
6	H	130	CYS
6	H	131	ASP
7	K	5	THR

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Mol	Chain	Res	Type
7	K	16	THR
7	K	21	THR
7	K	31	THR
7	K	35	THR
7	K	62	MET
7	K	74	ILE
7	K	75	THR
7	K	113	THR
7	K	115	VAL
7	K	131	THR
7	K	170	LEU
7	K	178	SER
7	K	182	VAL
7	K	185	LEU
7	K	188	HIS
7	K	215	THR
7	K	221	SER
7	K	223	THR
7	K	242	ILE
7	K	253	LEU
7	K	261	CYS
7	K	269	VAL
7	K	290	VAL
7	K	291	ASP
7	K	301	ASP
7	K	303	LEU
7	K	325	LYS
7	K	332	ILE
7	K	346	VAL
7	K	396	SER
7	K	398	VAL
7	K	403	THR
7	K	411	LEU
7	K	428	THR
7	K	462	ASP
7	K	463	ILE
7	K	466	VAL
7	K	468	LEU
7	K	470	SER
7	K	475	THR
7	K	478	ASN
7	K	483	VAL

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Mol	Chain	Res	Type
7	K	484	CYS
7	K	493	LEU
7	K	501	MET
7	K	518	ASN
7	K	523	PHE
1	N	10	ARG
1	N	11	VAL
1	N	14	VAL
1	N	18	ARG
1	N	21	PRO
1	N	27	SER
1	N	32	TYR
1	N	37	ILE
1	N	49	LEU
1	N	51	THR
1	N	53	CYS
1	N	61	GLU
1	N	62	ASP
1	N	65	LEU
1	N	66	ILE
1	N	81	GLN
1	N	92	ASP
1	N	98	LYS
1	N	102	PHE
1	N	103	LYS
1	N	105	ARG
1	N	107	ASP
1	N	109	ASP
1	N	113	HIS
1	N	114	ILE
1	N	115	SER
1	N	116	ARG
1	N	118	ARG
1	N	141	THR
1	N	158	ASN
1	N	159	LYS
1	N	160	LYS
1	N	165	PHE
1	N	167	GLU
1	N	180	GLU
1	N	187	LEU
1	N	204	VAL

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Mol	Chain	Res	Type
1	N	219	PHE
1	N	226	THR
1	N	229	SER
1	N	260	ASP
1	N	262	THR
1	N	267	LYS
1	N	277	GLU
1	N	281	LYS
1	N	282	LEU
1	N	293	THR
1	N	295	HIS
1	N	299	VAL
1	N	308	LEU
1	N	315	VAL
1	N	325	SER
1	N	335	VAL
1	N	363	SER
1	N	366	LEU
1	N	367	SER
1	N	388	LEU
1	N	389	LEU
1	N	391	LYS
1	N	393	THR
1	N	405	VAL
1	N	409	THR
1	N	411	LYS
1	N	434	SER
1	N	435	VAL
1	N	478	LYS
1	N	480	PHE
1	N	494	ILE
1	N	496	ASN
1	N	504	PHE
1	N	514	LEU
1	N	517	ASP
1	N	518	SER
1	N	522	GLU
1	N	560	VAL
1	N	561	SER
1	N	583	ARG
1	N	593	LYS
1	N	614	LEU

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Mol	Chain	Res	Type
1	N	618	ASP
1	N	619	TYR
1	N	621	LYS
1	N	624	ARG
1	N	630	LEU
1	N	640	ARG
1	N	644	THR
1	N	666	MET
1	N	667	VAL
1	N	680	THR
1	N	682	SER
1	N	686	THR
1	N	708	LEU
1	N	710	THR
1	N	715	ILE
1	N	718	LYS
1	N	721	ARG
1	N	729	GLU
1	N	731	LEU
1	N	737	VAL
1	N	739	THR
1	N	740	ASP
1	N	744	GLU
1	N	768	SER
1	N	769	THR
1	N	780	LYS
1	N	783	LYS
1	N	805	LEU
1	N	806	THR
1	N	807	LYS
1	N	809	PRO
1	N	817	THR
1	N	818	MET
1	N	820	VAL
1	N	821	LYS
1	N	835	SER
1	N	847	ILE
1	N	848	VAL
1	N	854	LEU
1	N	865	ASP
1	N	889	ARG
1	N	894	GLU

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Mol	Chain	Res	Type
1	N	899	MET
1	N	900	LEU
1	N	902	MET
1	N	904	SER
1	N	919	GLU
1	N	922	GLU
1	N	926	THR
2	O	33	VAL
2	O	42	LEU
2	O	51	ARG
2	O	59	LEU
2	O	67	MET
2	O	83	VAL
2	O	107	ILE
2	O	153	LEU
2	O	157	GLN
2	O	173	SER
2	O	177	SER
2	O	180	LEU
3	P	4	SER
3	P	13	LEU
3	P	20	LEU
3	P	24	SER
3	P	27	LYS
3	P	35	LEU
3	P	38	ASP
3	P	41	LEU
3	P	45	THR
3	P	47	GLU
3	P	50	GLU
3	P	55	LEU
3	P	61	SER
3	P	62	MET
3	P	70	LYS
3	P	73	GLU
2	Q	50	ASP
2	Q	89	THR
2	Q	98	LEU
2	Q	114	CYS
2	Q	115	VAL
2	Q	123	THR
2	Q	153	LEU

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Mol	Chain	Res	Type
2	Q	159	VAL
2	Q	180	LEU
4	R	7	LEU
4	R	49	VAL
4	R	79	ILE
4	R	105	ASP
4	R	116	ASN
4	R	151	ILE
4	R	178	ARG
4	R	181	VAL
4	R	195	ILE
4	R	228	THR
4	R	288	LYS
4	R	325	LEU
4	R	383	ASP
4	R	413	THR
4	R	458	ASP
4	R	488	ILE
4	R	495	VAL
5	T	4	LEU
5	T	12	MET
5	T	21	THR
5	T	29	LEU
5	T	35	THR
5	T	36	LYS
5	T	41	VAL
5	T	42	LEU
5	T	45	LEU
5	T	47	ASP
5	T	48	LEU
5	T	50	ASP
5	T	55	ARG
5	T	64	THR
5	T	68	GLU
5	T	69	LEU
5	T	74	ARG
5	T	75	PHE
5	T	78	ASP
5	T	79	THR
5	T	81	LYS
5	T	99	ARG
6	U	3	ASN

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Mol	Chain	Res	Type
6	U	12	THR
6	U	21	VAL
6	U	31	LEU
6	U	47	THR
6	U	57	VAL
6	U	72	SER
6	U	90	CYS
6	U	97	VAL
6	U	102	THR
6	U	108	VAL
6	U	119	VAL
7	X	5	THR
7	X	14	VAL
7	X	50	THR
7	X	74	ILE
7	X	75	THR
7	X	80	ILE
7	X	82	HIS
7	X	87	ILE
7	X	112	SER
7	X	113	THR
7	X	118	VAL
7	X	127	THR
7	X	182	VAL
7	X	193	THR
7	X	194	SER
7	X	206	THR
7	X	207	CYS
7	X	212	ARG
7	X	222	ASP
7	X	223	THR
7	X	264	HIS
7	X	268	HIS
7	X	269	VAL
7	X	279	CYS
7	X	317	VAL
7	X	328	VAL
7	X	345	ASP
7	X	387	CYS
7	X	395	ASN
7	X	396	SER
7	X	398	VAL

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Mol	Chain	Res	Type
7	X	400	ARG
7	X	403	THR
7	X	407	SER
7	X	410	ASN
7	X	414	CYS
7	X	415	ASP
7	X	437	VAL
7	X	466	VAL
7	X	470	SER
7	X	474	ILE
7	X	476	ARG
7	X	478	ASN
7	X	487	HIS
7	X	503	SER
7	X	518	ASN
4	F	25	LEU
4	F	37	THR
4	F	74	SER
4	F	83	LEU
4	F	151	ILE
4	F	193	VAL
4	F	216	THR
4	F	247	VAL
4	F	250	THR
4	F	255	THR
4	F	258	ILE
4	F	309	CYS
4	F	319	GLU
4	F	372	VAL
4	F	481	THR
4	F	495	VAL
4	F	496	VAL
4	F	528	LEU
4	F	544	VAL
4	F	582	TYR
4	S	25	LEU
4	S	58	THR
4	S	70	TYR
4	S	74	SER
4	S	96	THR
4	S	98	VAL
4	S	157	VAL

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Mol	Chain	Res	Type
4	S	164	HIS
4	S	183	THR
4	S	215	THR
4	S	216	THR
4	S	232	VAL
4	S	241	VAL
4	S	249	ILE
4	S	250	THR
4	S	252	LEU
4	S	255	THR
4	S	270	GLN
4	S	275	GLN
4	S	286	THR
4	S	315	ASP
4	S	325	LEU
4	S	333	ILE
4	S	350	SER
4	S	351	THR
4	S	383	ASP
4	S	387	VAL
4	S	392	ARG
4	S	449	VAL
4	S	455	LEU
4	S	484	VAL
4	S	495	VAL
4	S	528	LEU
4	S	549	THR
4	S	554	HIS
4	S	572	ILE
4	S	575	ILE
4	S	582	TYR
4	S	583	ASP
4	S	588	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	198	ASN
1	A	256	HIS
1	A	295	HIS
1	A	541	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	A	725	HIS
1	A	789	GLN
1	A	791	ASN
1	A	822	GLN
1	A	928	HIS
2	B	43	ASN
2	B	104	ASN
2	D	108	ASN
2	D	140	ASN
4	E	51	ASN
4	E	164	HIS
4	E	190	ASN
4	E	245	HIS
4	E	275	GLN
4	E	489	ASN
4	E	492	GLN
5	G	11	GLN
6	H	65	GLN
6	H	80	HIS
7	K	65	GLN
7	K	254	GLN
7	K	257	HIS
1	N	57	GLN
1	N	81	GLN
1	N	150	ASN
1	N	198	ASN
1	N	256	HIS
1	N	295	HIS
1	N	381	HIS
1	N	611	ASN
1	N	789	GLN
1	N	791	ASN
2	O	65	GLN
2	O	118	ASN
2	O	158	GLN
2	Q	108	ASN
4	R	9	ASN
4	R	86	ASN
4	R	107	ASN
4	R	243	GLN
4	R	548	GLN
5	T	11	GLN

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Mol	Chain	Res	Type
6	U	36	GLN
7	X	63	ASN
7	X	82	HIS
7	X	104	ASN
7	X	108	GLN
7	X	176	ASN
7	X	257	HIS
7	X	283	HIS
7	X	441	GLN
7	X	487	HIS
4	F	33	HIS
4	F	102	ASN
4	F	220	ASN
4	F	492	GLN
4	F	519	ASN
4	F	531	GLN
4	S	33	HIS
4	S	95	ASN
4	S	107	ASN
4	S	388	ASN
4	S	404	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	24/25 (96%)	2 (8%)	1 (4%)
8	L	24/25 (96%)	2 (8%)	1 (4%)
9	J	32/33 (96%)	7 (21%)	0
9	M	32/33 (96%)	4 (12%)	2 (6%)
All	All	112/116 (96%)	15 (13%)	4 (3%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	15	G
8	I	23	C
9	J	19	A
9	J	20	U
9	J	21	G
9	J	22	U
9	J	23	C

Continued on next page...

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Mol	Chain	Res	Type
9	J	24	U
9	J	25	G
8	L	15	G
8	L	23	C
9	M	22	U
9	M	23	C
9	M	24	U
9	M	25	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	22	G
8	L	22	G
9	M	22	U
9	M	23	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 29 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

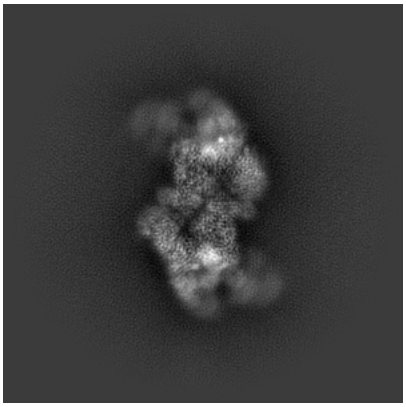
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31138. These allow visual inspection of the internal detail of the map and identification of artifacts.

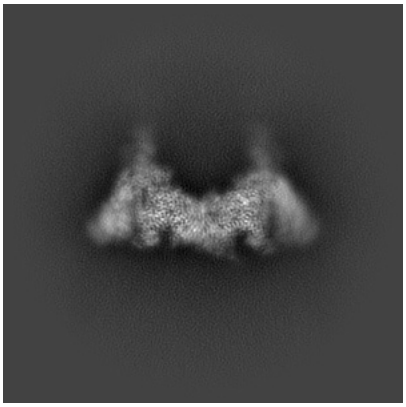
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

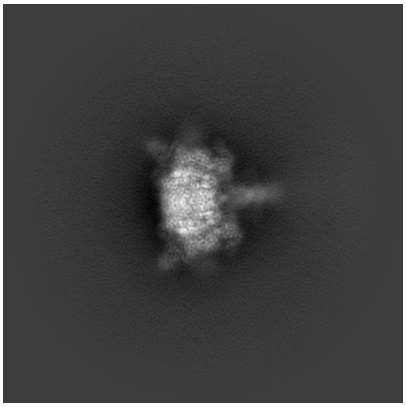
6.1.1 Primary map



X



Y

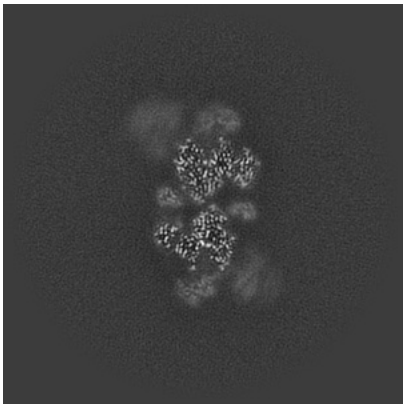


Z

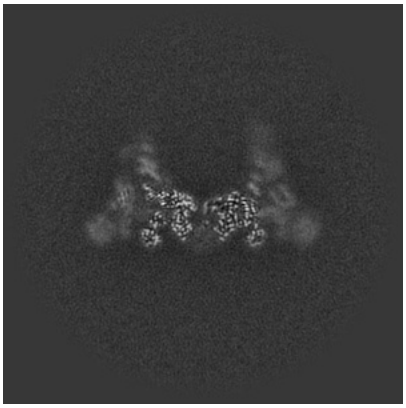
The images above show the map projected in three orthogonal directions.

6.2 Central slices

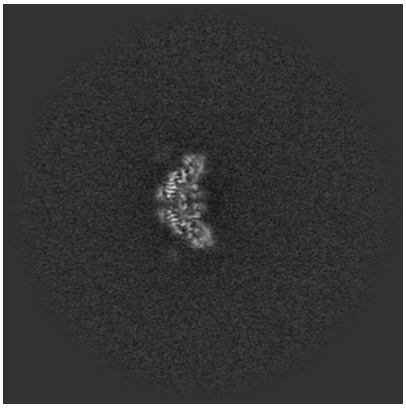
6.2.1 Primary map



X Index: 224



Y Index: 224

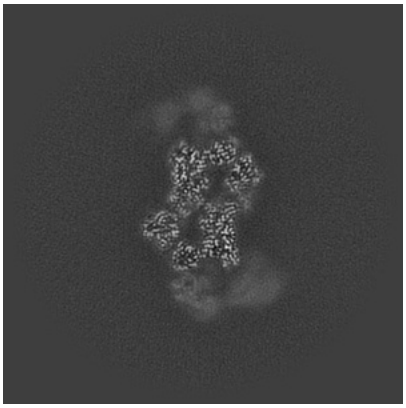


Z Index: 224

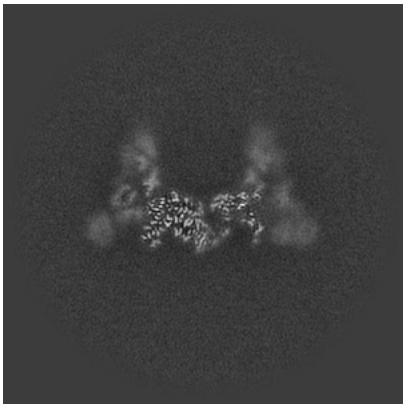
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

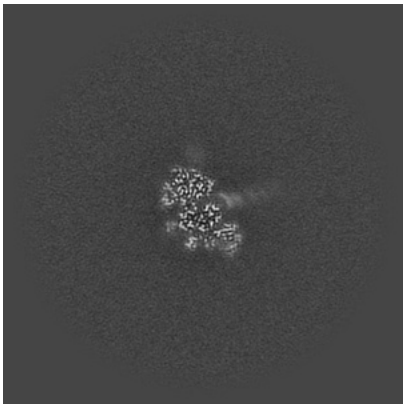
6.3.1 Primary map



X Index: 203



Y Index: 232

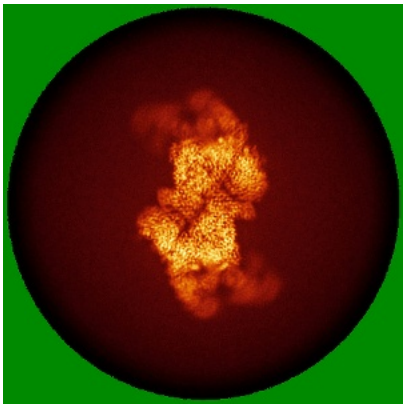


Z Index: 172

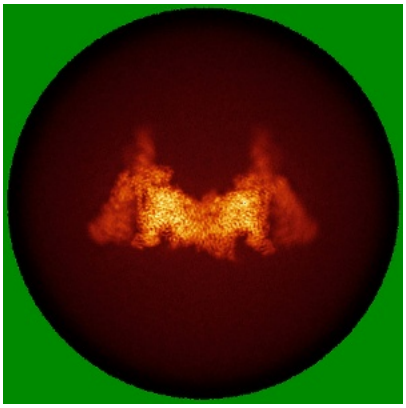
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

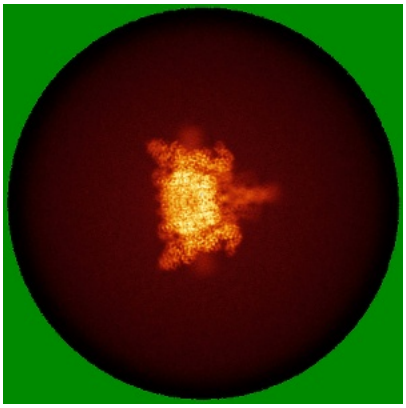
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

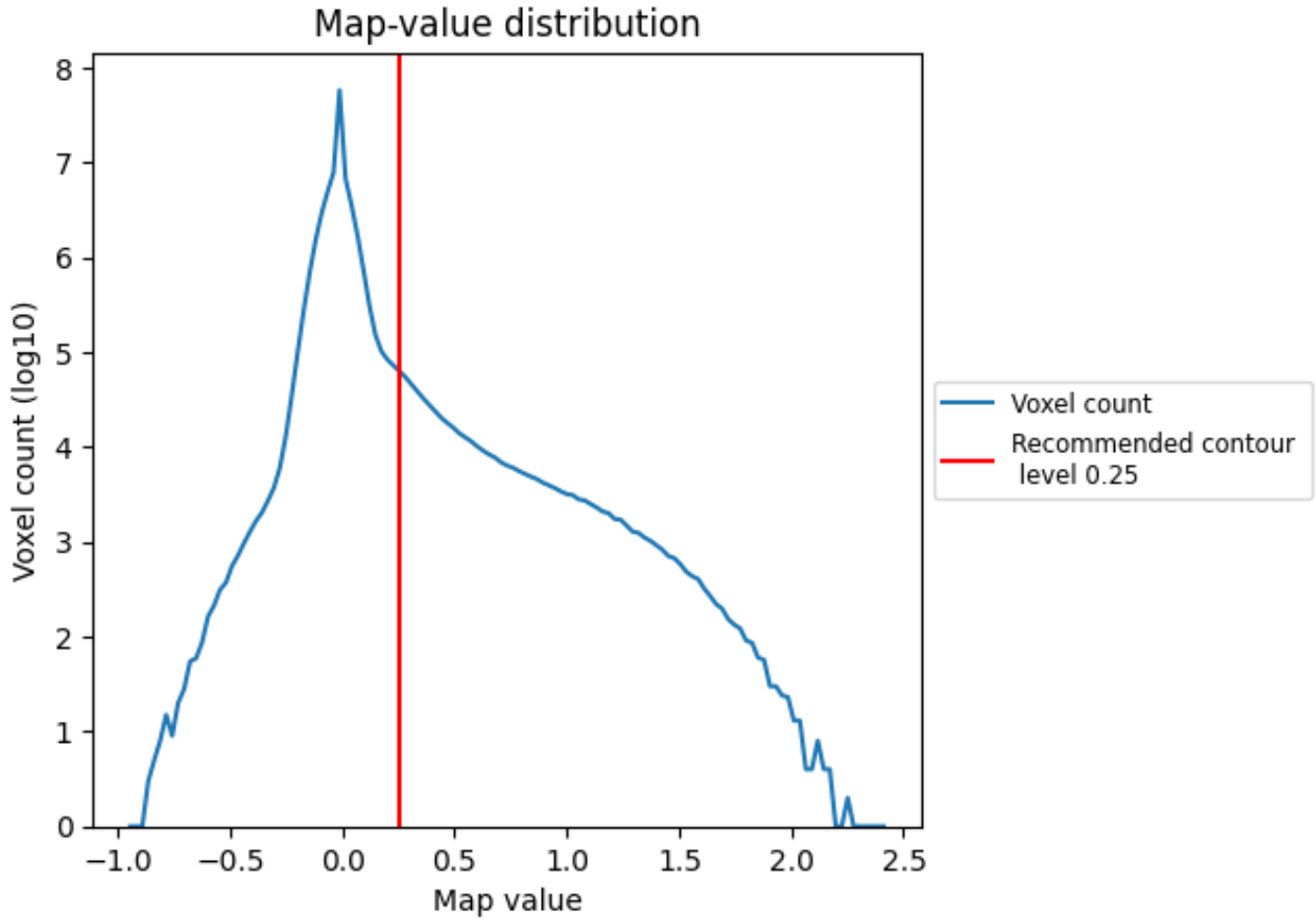
6.6 Mask visualisation (i)

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

7 Map analysis

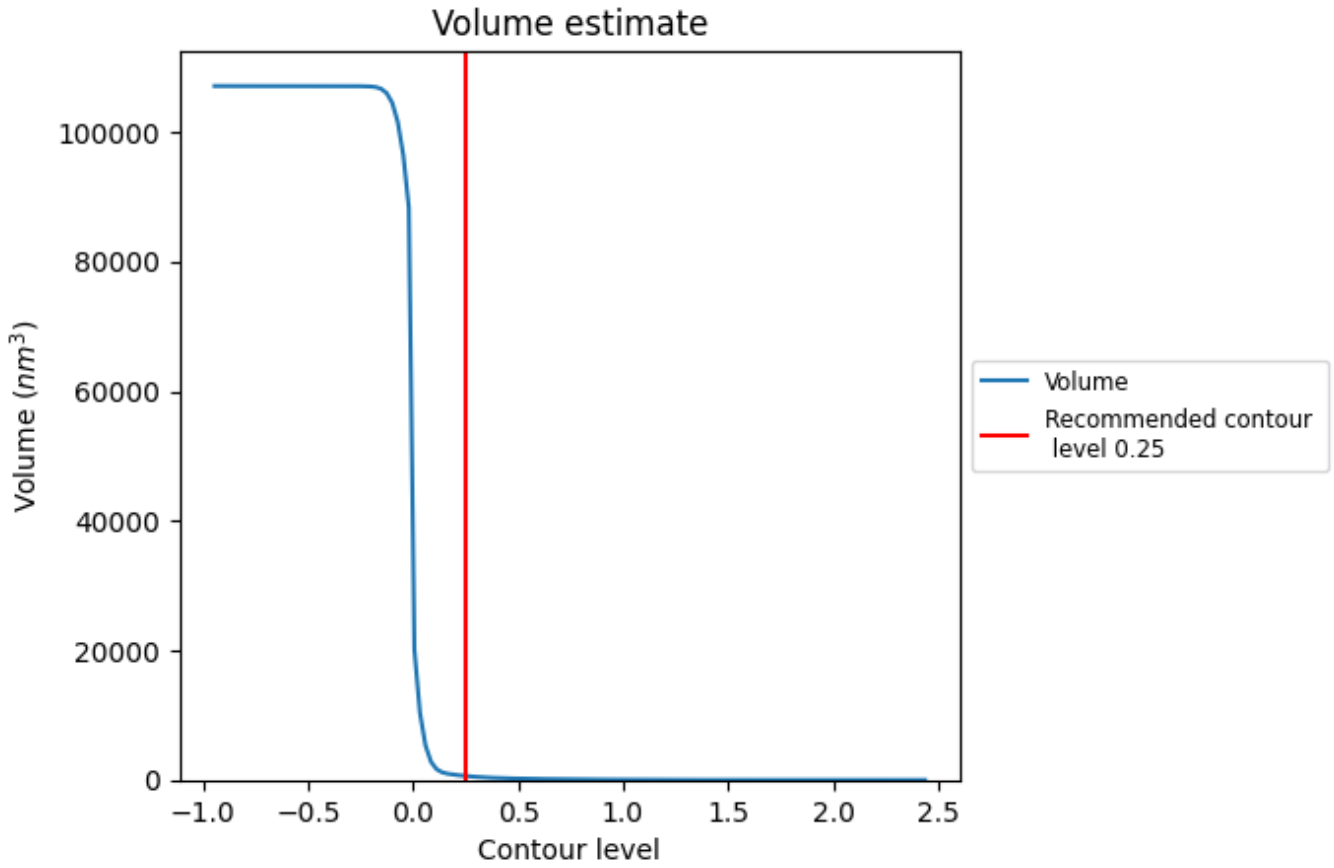
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

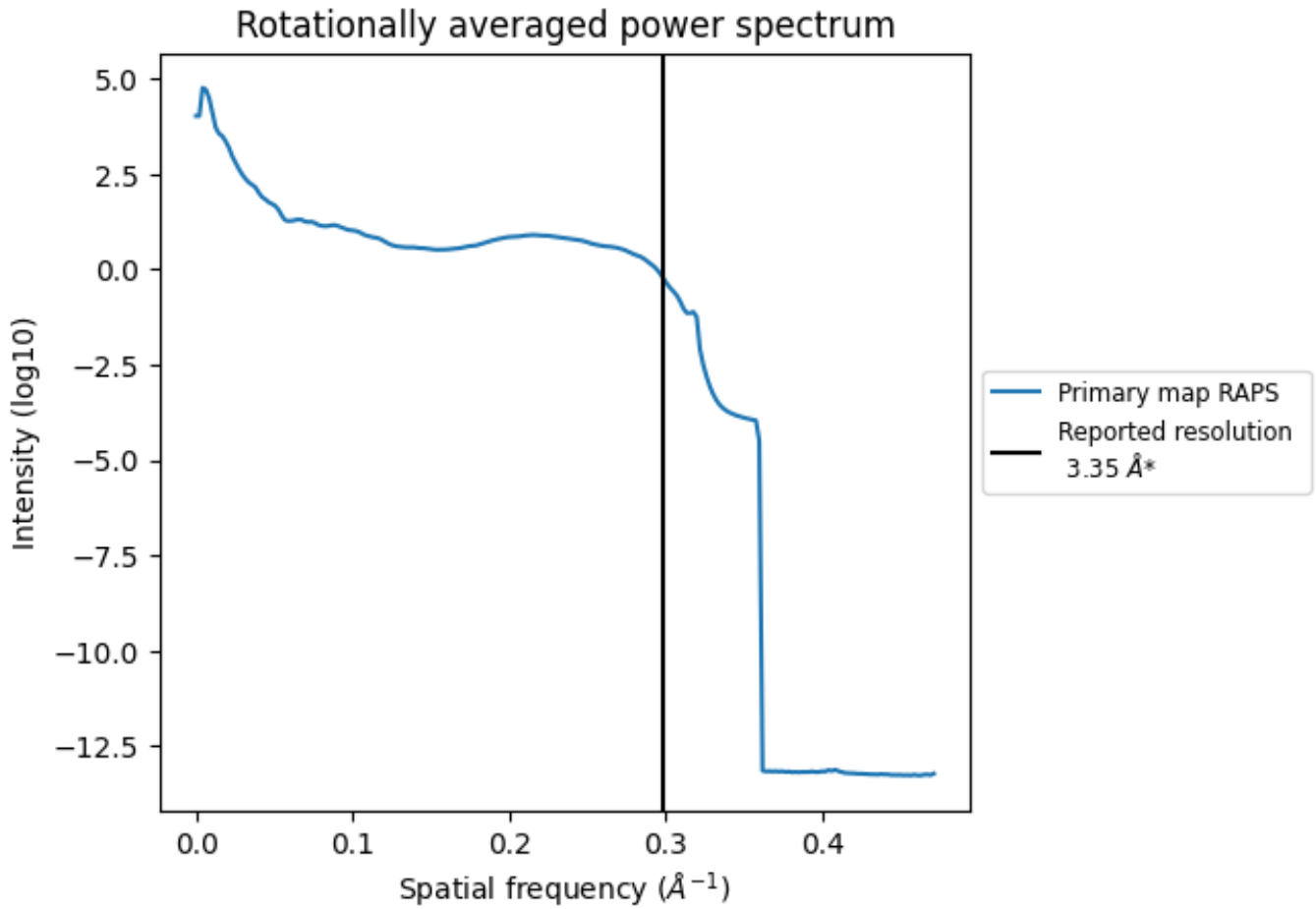
7.2 Volume estimate



The volume at the recommended contour level is 614 nm^3; this corresponds to an approximate mass of 555 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.299 $Å^{-1}$

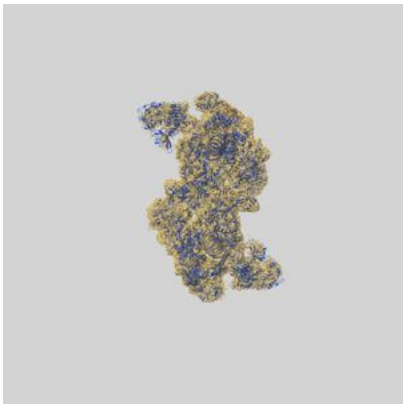
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

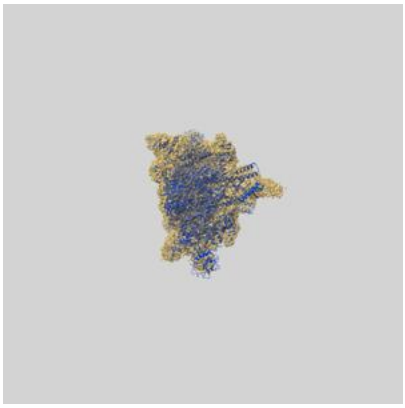
This section contains information regarding the fit between EMDB map EMD-31138 and PDB model 7EGQ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay



X

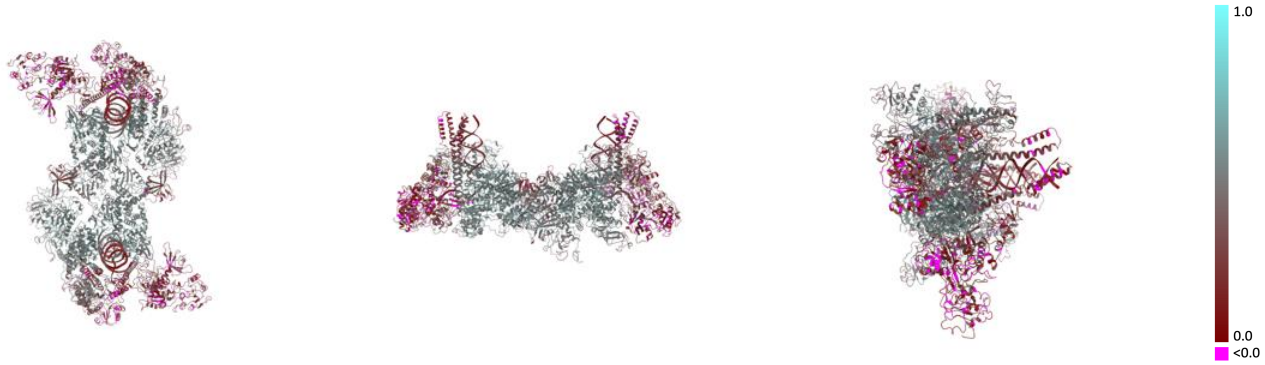
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

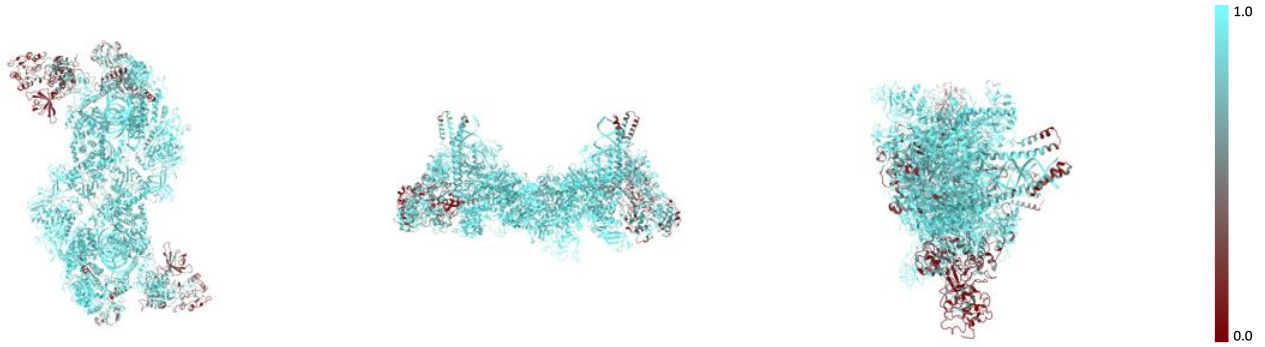
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

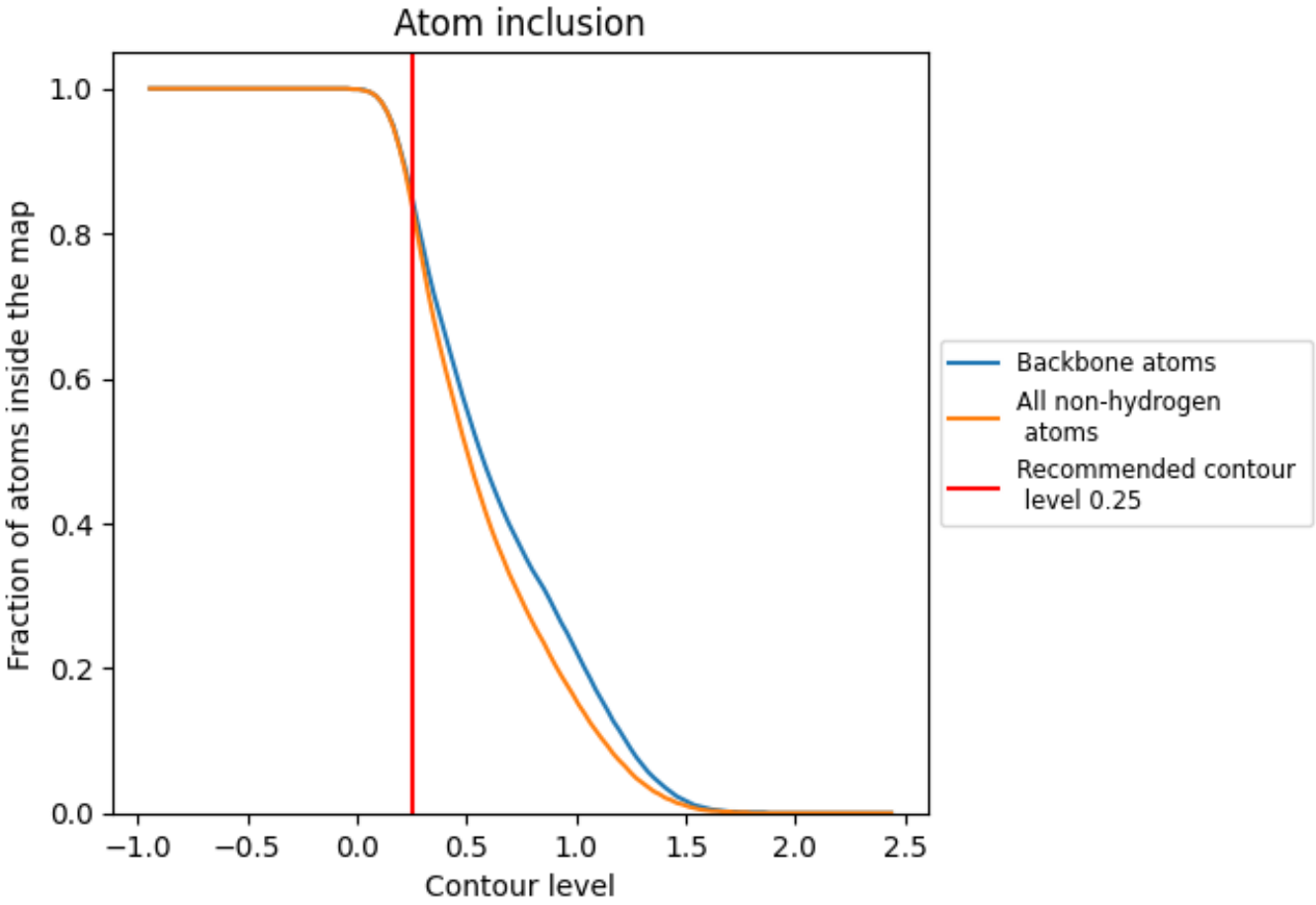
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.3840
A	0.9720	0.5200
B	0.8540	0.3890
C	0.9550	0.5070
D	0.8710	0.3790
E	0.6990	0.2140
F	0.3210	0.1710
G	0.9480	0.3630
H	0.9930	0.4660
I	0.9060	0.2680
J	0.9710	0.2770
K	0.9850	0.5130
L	0.8940	0.2740
M	0.9650	0.2800
N	0.9780	0.5320
O	0.9270	0.4190
P	0.9580	0.5070
Q	0.9200	0.4000
R	0.8710	0.3000
S	0.5360	0.1800
T	0.9320	0.3380
U	0.9920	0.4590
X	0.9670	0.4760