Full wwPDB EM Validation Report

Nov 22, 2022 – 02:15 PM JST

PDB ID	:	7EGQ
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:

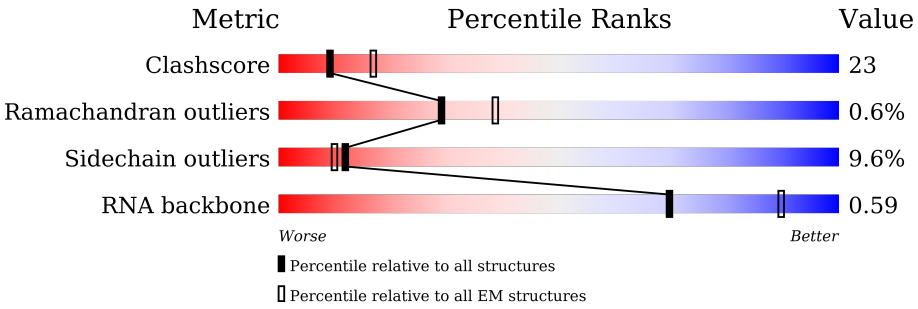
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	64% 26% 9%
1	N	932	62% 28% 8%
2	B	198	10% 56% 34% 6%
2	D	198	8% 56% 35% 6%
2	O	198	68% 24% 6%
2	Q	198	5% 55% 35% 6%
3	C	83	48% 31% 7% 13%

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Mol	Chain	Length	Quality of chain
3	P	83	52% 27% 8% 13%
4	E	601	18% 45% 51%
4	F	601	64% 50% 46%
4	R	601	6% 45% 49%
4	S	601	39% 46% 48% 5%
5	G	117	38% 44% 13%
5	T	117	41% 39% 15%
6	H	139	53% 37% 6%
6	U	139	45% 41% 7% 6%
7	K	527	61% 33% 5%
7	X	527	54% 38% 6%
8	I	25	36% 56% 8%
8	L	25	36% 56% 8%
9	J	33	39% 48% 9%
9	M	33	39% 45% 9% 6%

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 (three-letter code: 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 (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

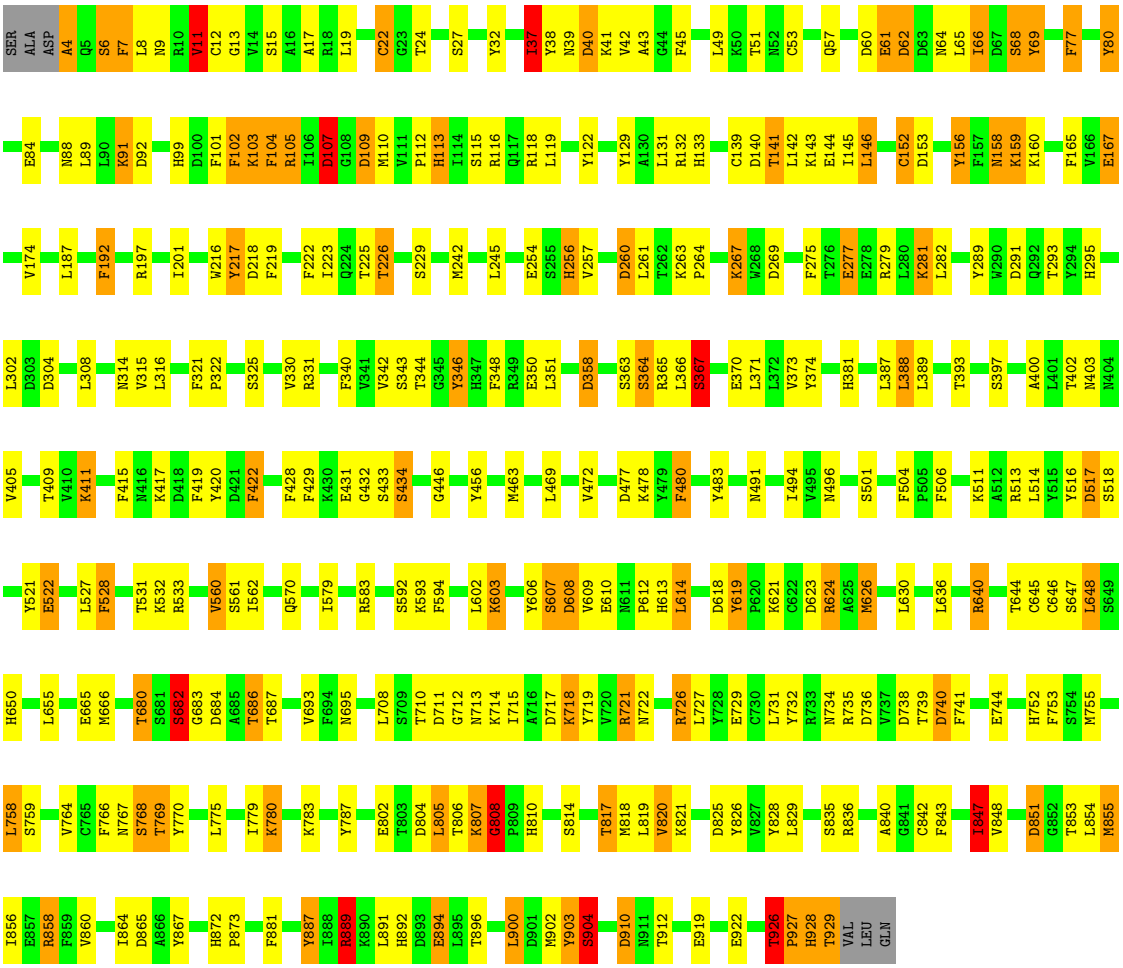
Mol	Chain	Residues	Atoms	AltConf
11	K	2	Total Mg 2 2	0
11	X	1	Total Mg 1 1	0

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.

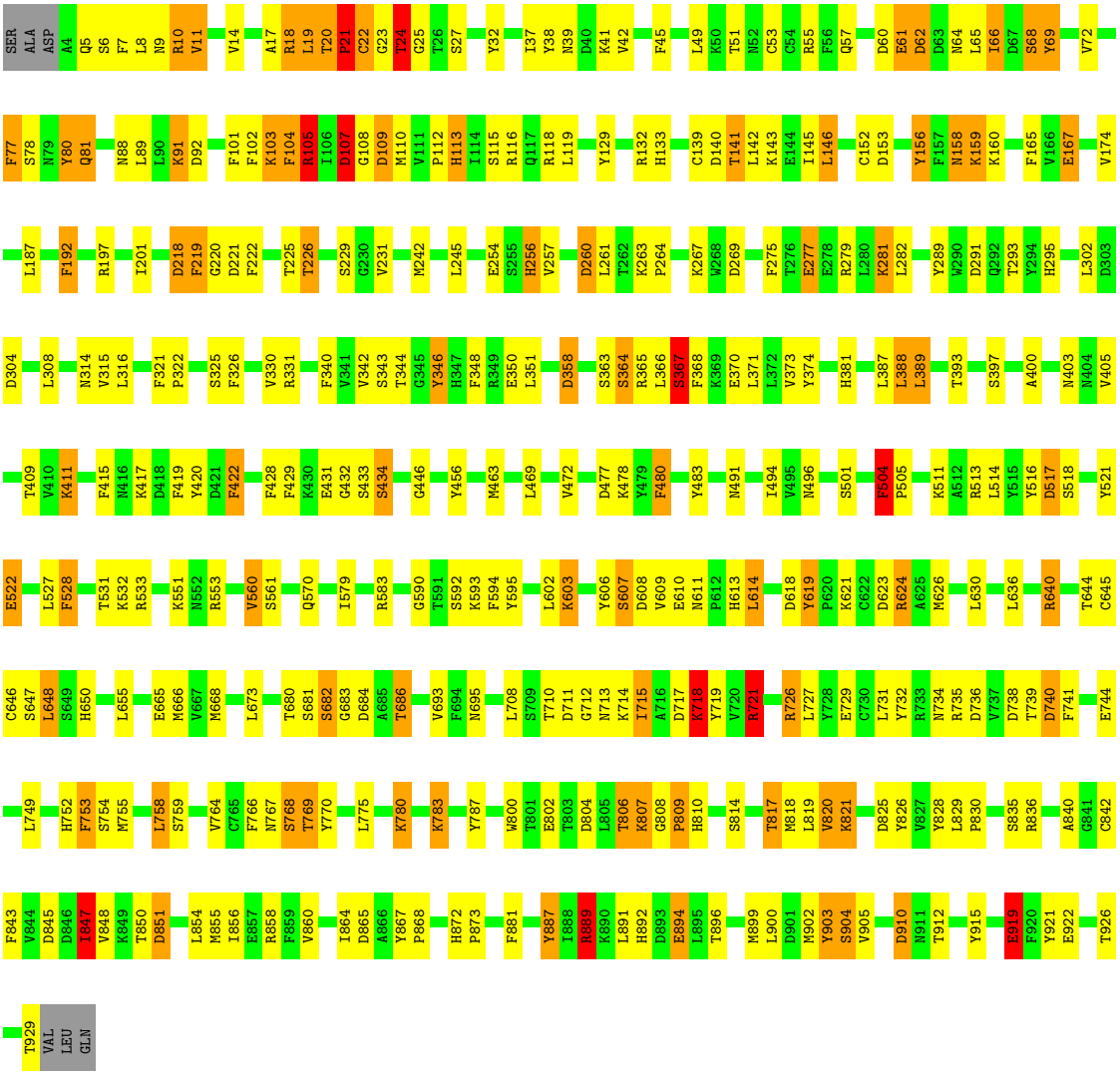
• Molecule 1: RNA-directed RNA polymerase

Chain A:



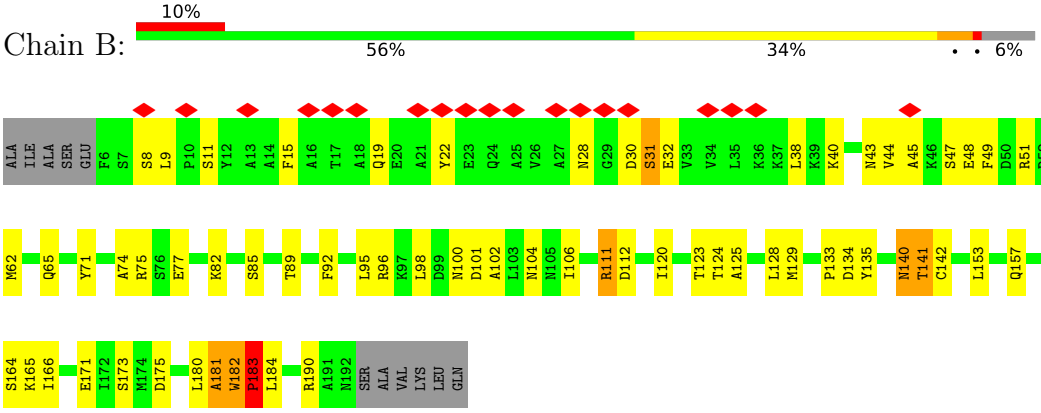
• Molecule 1: RNA-directed RNA polymerase

Chain N:



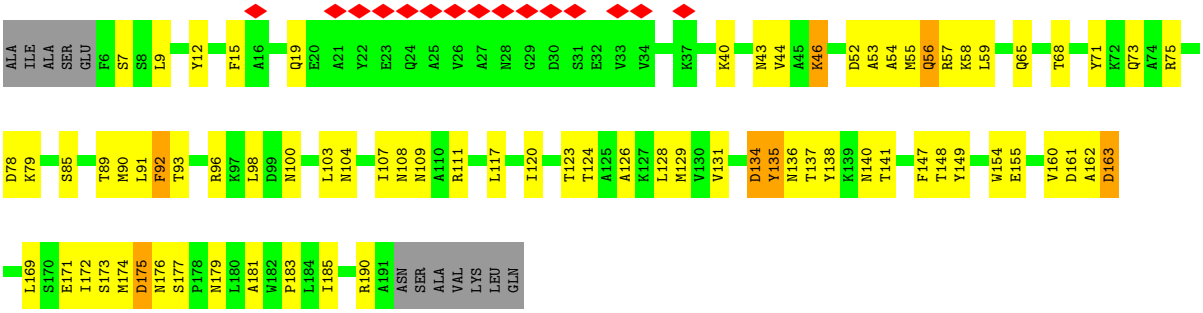
• Molecule 2: Non-structural protein 8

Chain B:



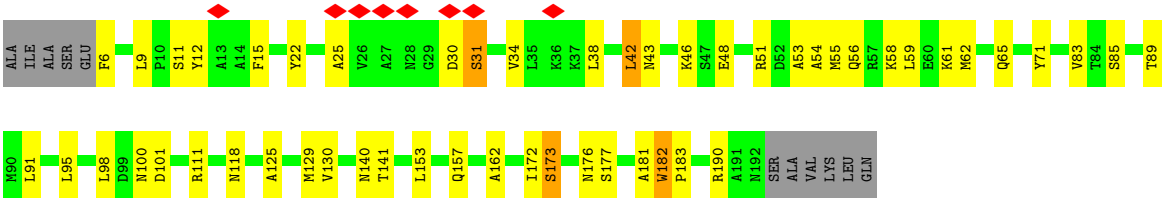
• Molecule 2: Non-structural protein 8

Chain D:



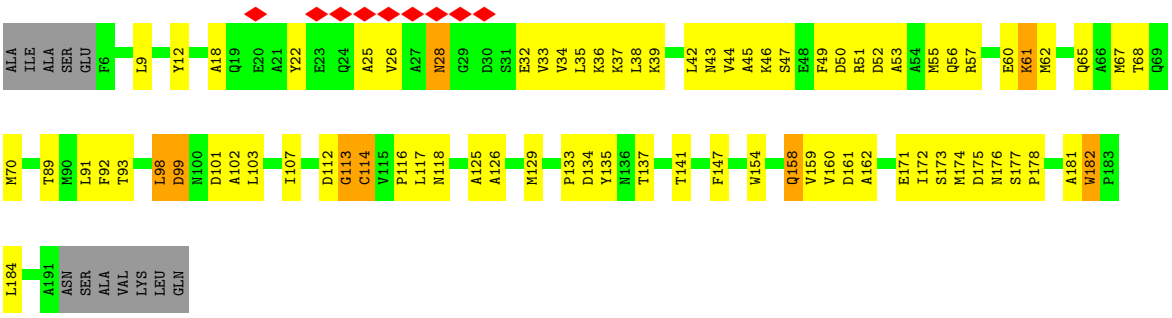
• Molecule 2: Non-structural protein 8

Chain O:



• Molecule 2: Non-structural protein 8

Chain Q:

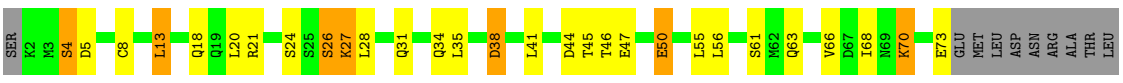


• Molecule 3: Non-structural protein 7

Chain C:

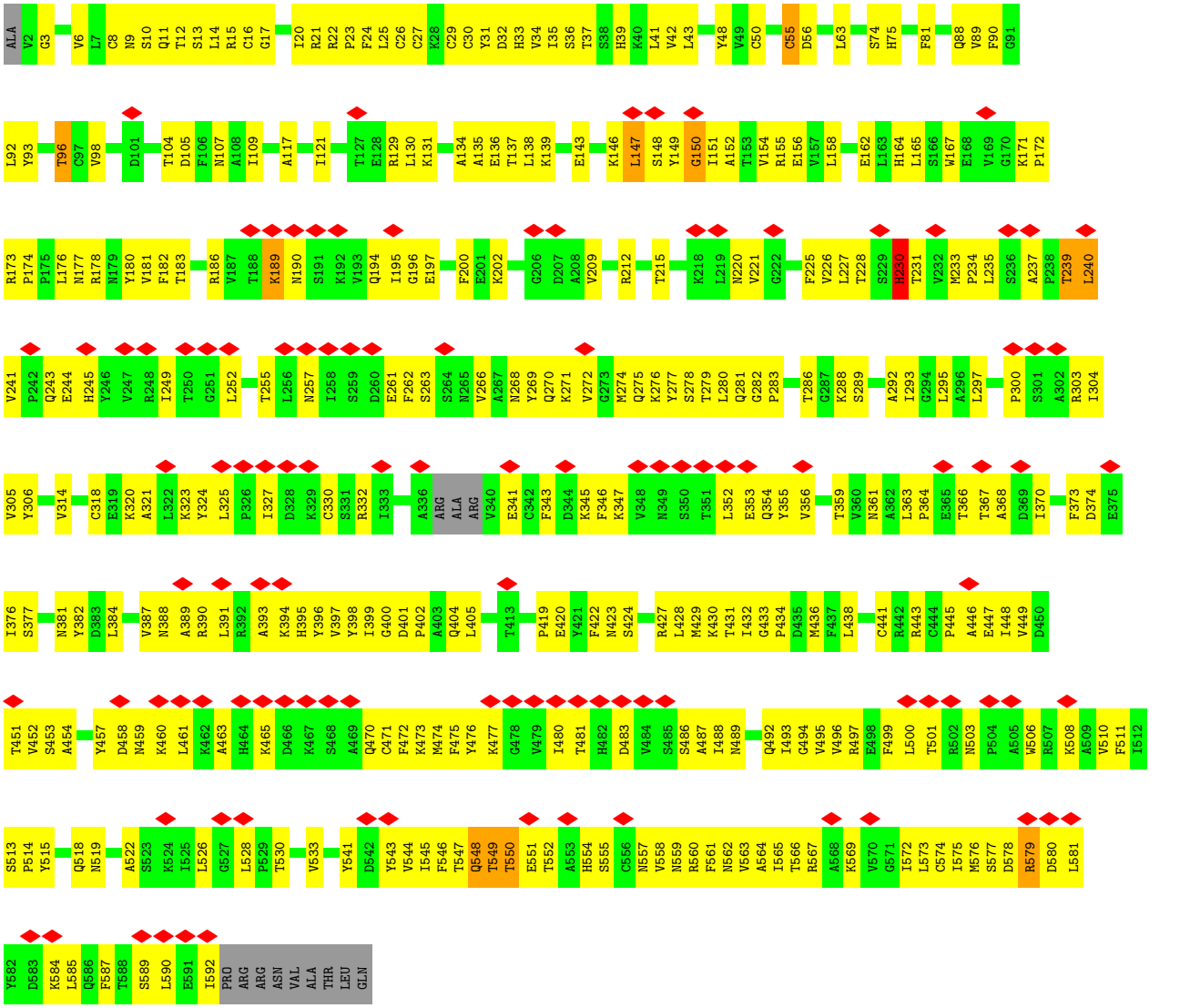
• Molecule 3: Non-structural protein 7

Chain P:



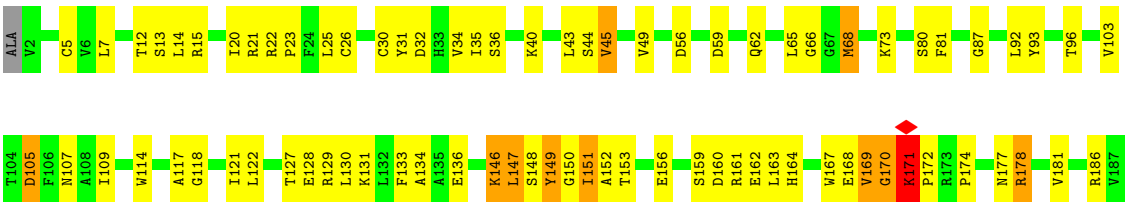
• Molecule 4: Helicase

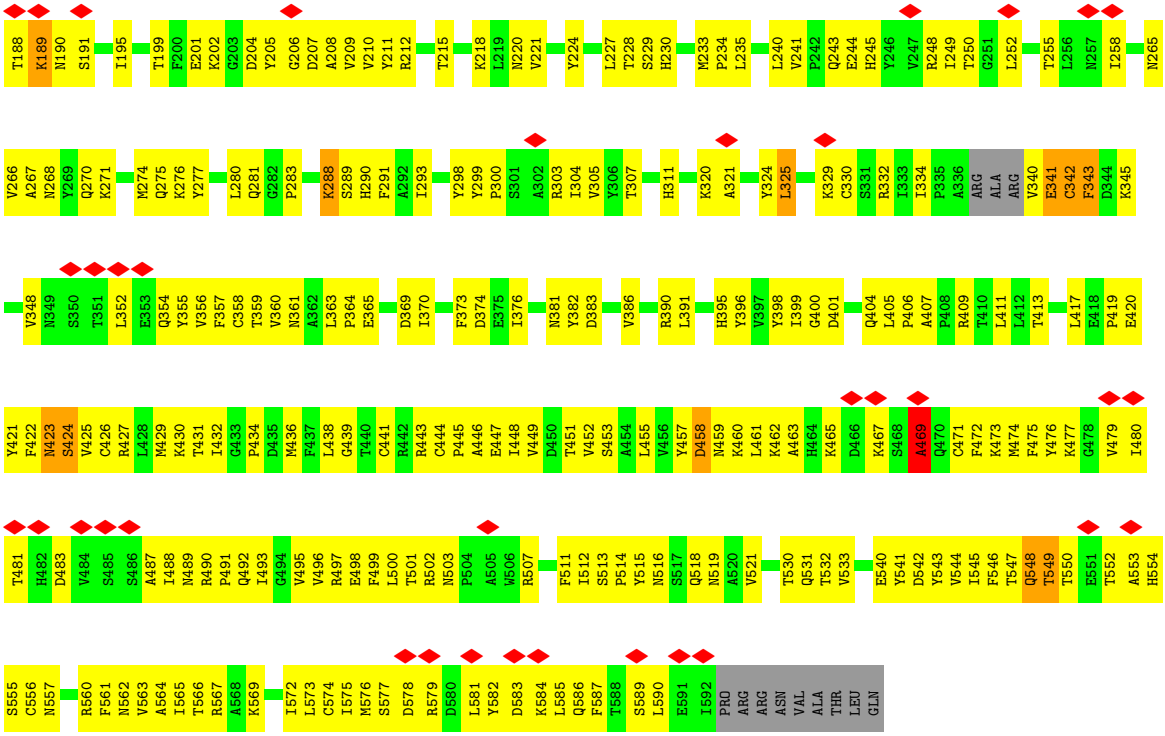
Chain E:



• Molecule 4: Helicase

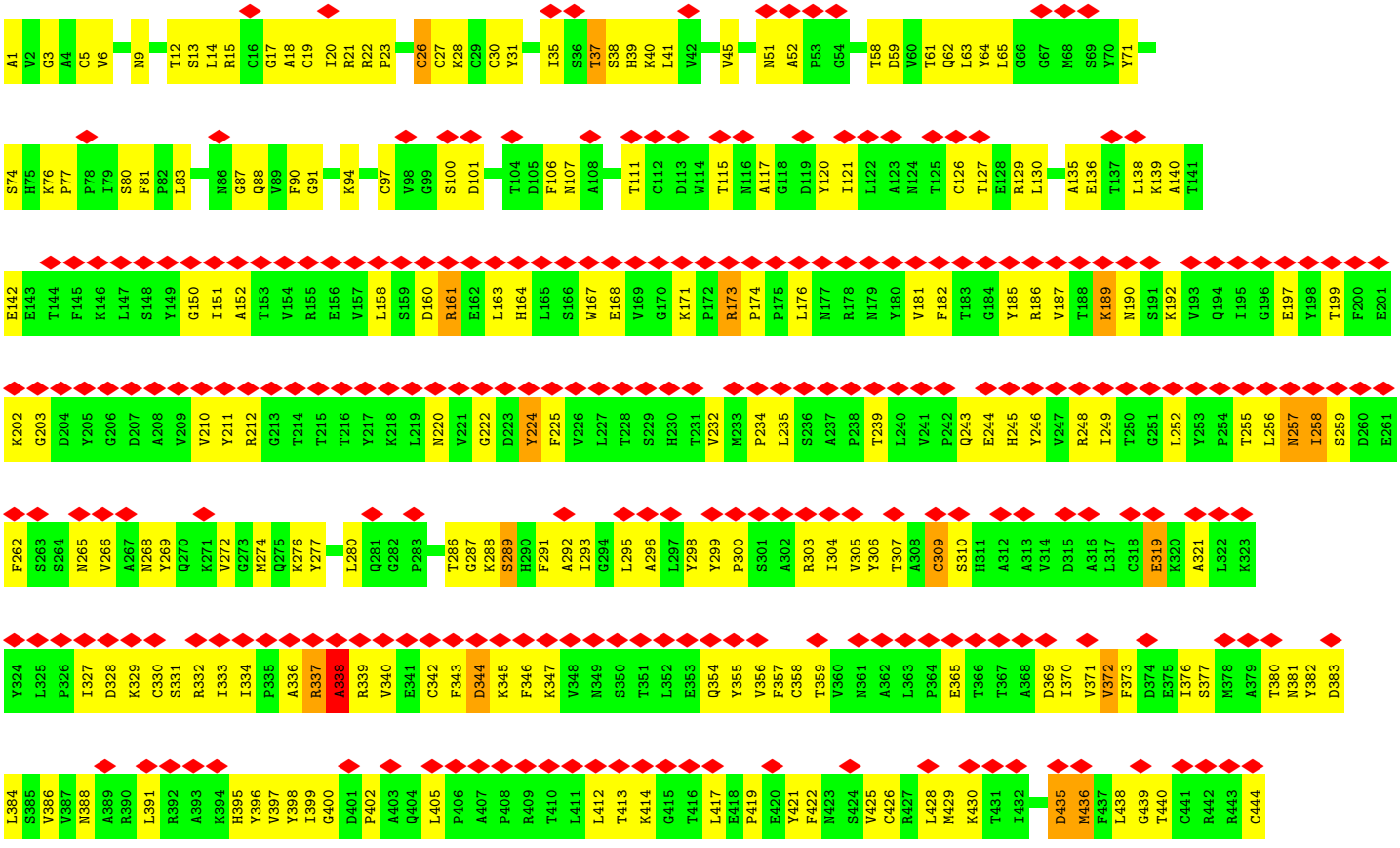
Chain R:

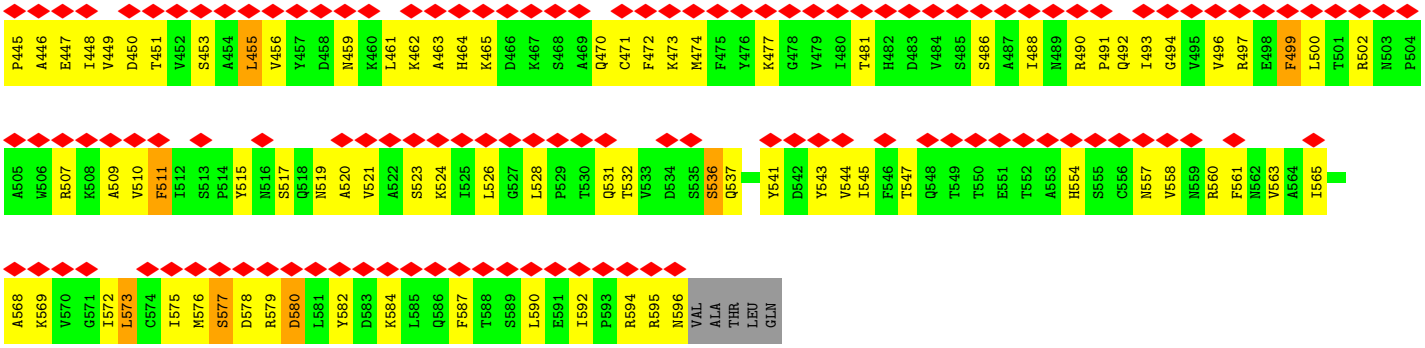




• Molecule 4: Helicase

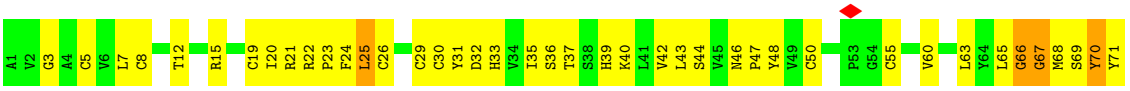
Chain F:

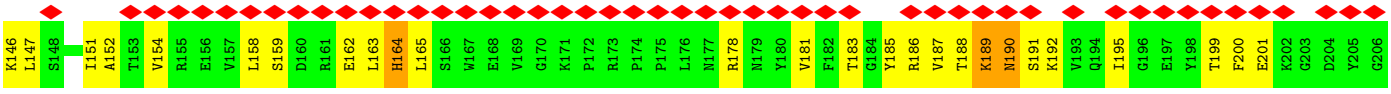


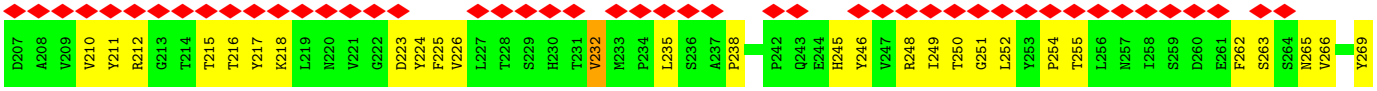


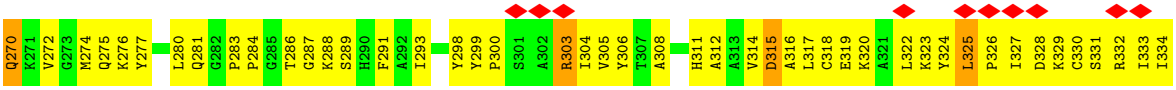
• Molecule 4: Helicase

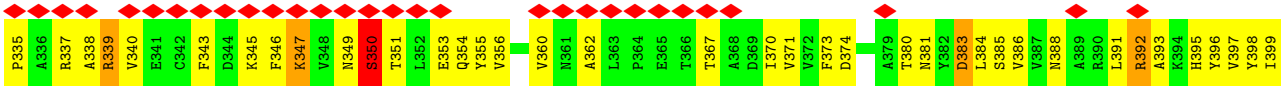
Chain S:

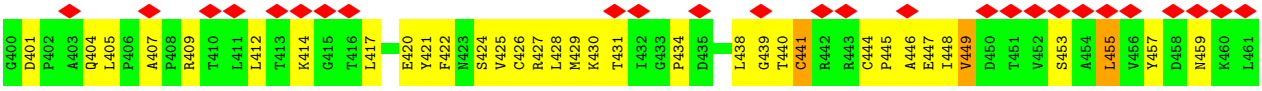


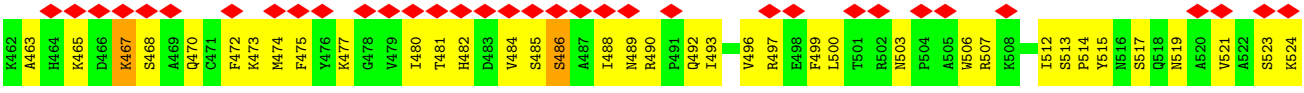


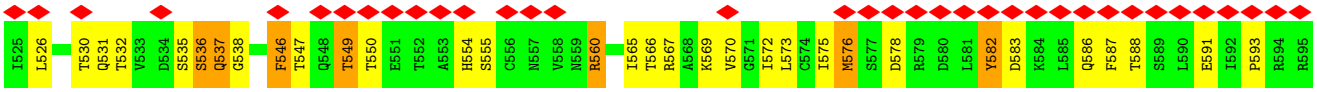


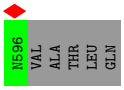






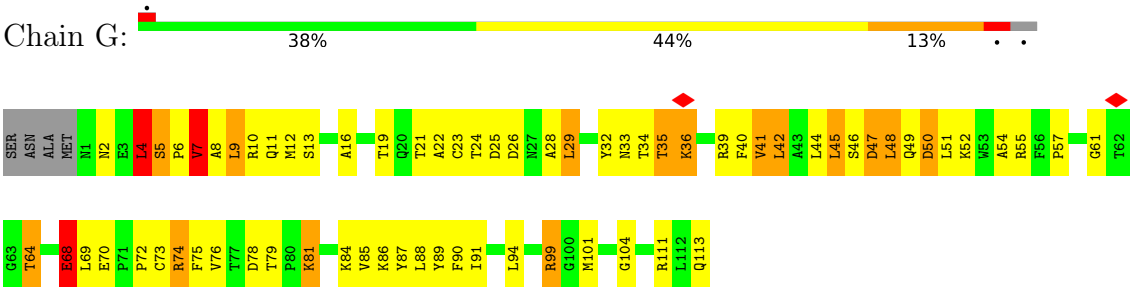






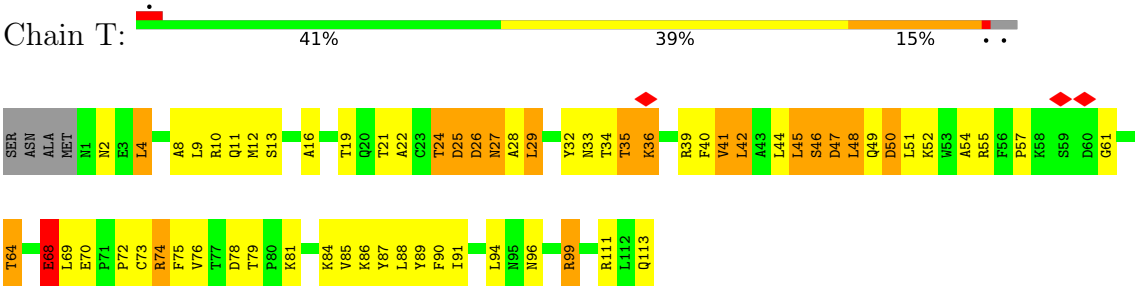
• Molecule 5: Non-structural protein 9

Chain G:



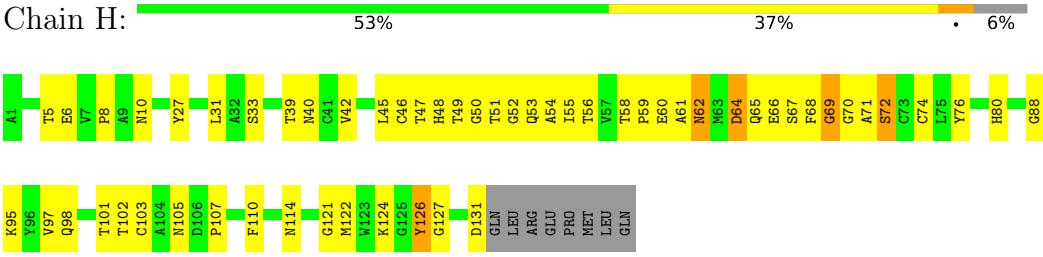
• Molecule 5: Non-structural protein 9

Chain T:



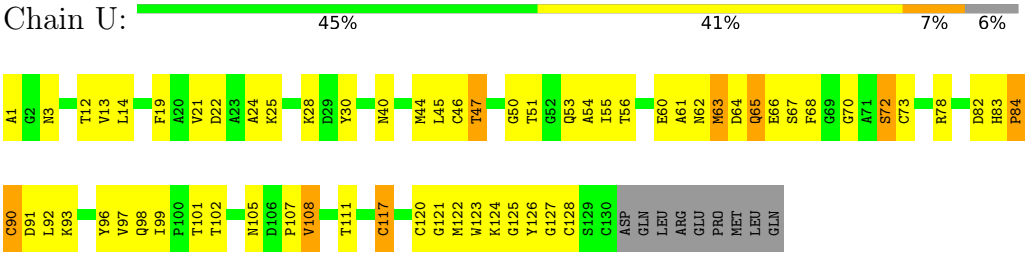
• Molecule 6: Non-structural protein 10

Chain H:



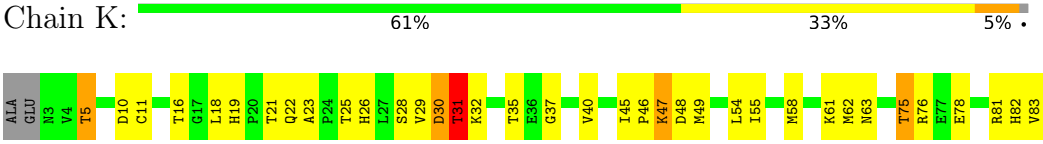
• Molecule 6: Non-structural protein 10

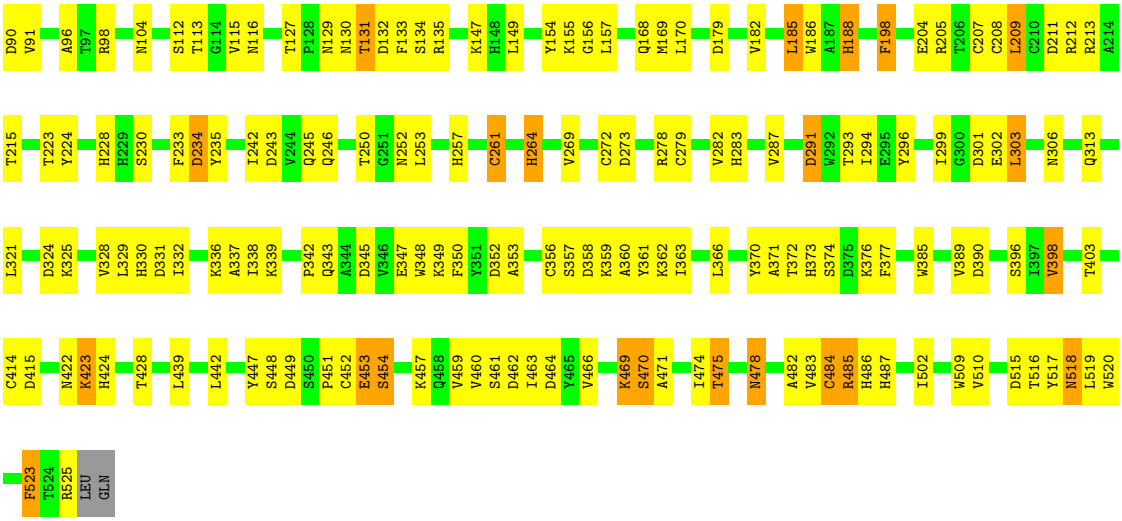
Chain U:



• Molecule 7: Proofreading exoribonuclease

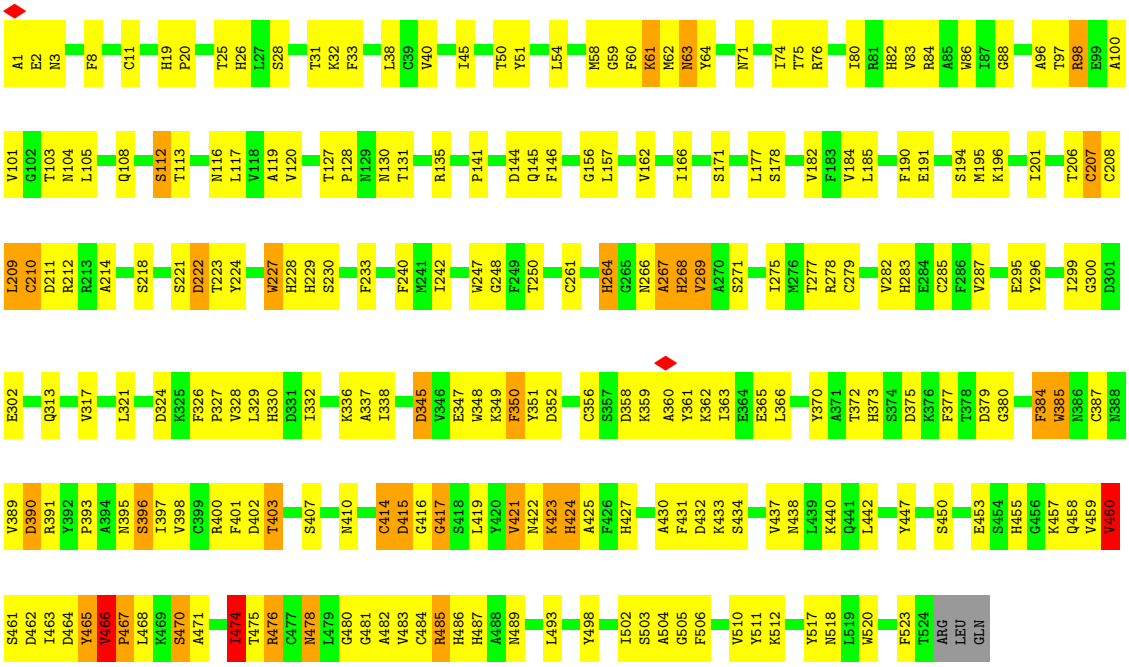
Chain K:





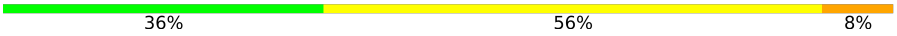
• Molecule 7: Proofreading exoribonuclease

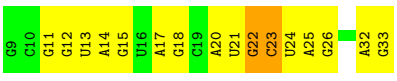
Chain X:



• Molecule 8: primer RNA

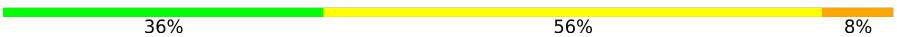
Chain I:





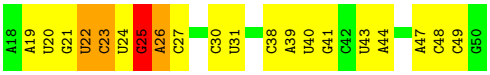
• Molecule 8: primer RNA

Chain L:



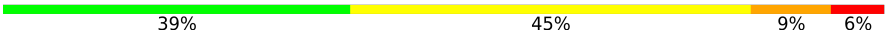
• Molecule 9: Template RNA

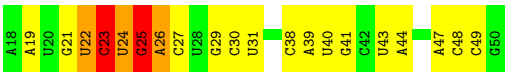
Chain J:



• 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: ZN, MG

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	0.60	1/7651 (0.0%)	0.84	57/10383 (0.5%)
1	N	0.52	0/7651	0.83	47/10383 (0.5%)
2	B	0.42	0/1418	0.92	16/1927 (0.8%)
2	D	0.30	0/1437	0.62	4/1948 (0.2%)
2	O	0.37	0/1418	0.69	7/1927 (0.4%)
2	Q	0.33	0/1437	0.91	10/1948 (0.5%)
3	C	0.39	0/556	0.63	2/749 (0.3%)
3	P	0.39	0/556	0.72	2/749 (0.3%)
4	E	0.29	0/4670	0.61	10/6358 (0.2%)
4	F	0.27	0/4734	0.79	24/6443 (0.4%)
4	R	0.30	0/4670	0.76	20/6358 (0.3%)
4	S	0.27	0/4734	0.71	20/6443 (0.3%)
5	G	0.40	0/884	0.79	5/1200 (0.4%)
5	T	0.37	0/884	1.00	7/1200 (0.6%)
6	H	0.39	0/976	0.84	4/1327 (0.3%)
6	U	0.48	0/968	0.89	5/1316 (0.4%)
7	K	0.44	0/4288	0.79	25/5831 (0.4%)
7	X	0.42	0/4297	0.88	37/5844 (0.6%)
8	I	0.89	1/611 (0.2%)	0.88	0/953
8	L	0.89	1/611 (0.2%)	0.88	0/953
9	J	0.91	2/770 (0.3%)	0.80	0/1195
9	M	1.02	4/770 (0.5%)	0.89	1/1195 (0.1%)
All	All	0.46	9/55991 (0.0%)	0.80	303/76630 (0.4%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	26	A	O3'-P	-7.94	1.51	1.61
9	M	26	A	O3'-P	-7.91	1.51	1.61
9	M	21	G	C1'-N9	-6.66	1.37	1.46
1	A	927	PRO	N-CD	6.60	1.57	1.47
8	I	32	A	N9-C4	-6.44	1.33	1.37
8	L	32	A	N9-C4	-6.24	1.34	1.37
9	M	19	A	C1'-N9	-5.30	1.39	1.46
9	M	25	G	O3'-P	-5.28	1.54	1.61
9	J	25	G	O3'-P	-5.14	1.54	1.61

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	536	SER	CB-CA-C	-20.60	70.96	110.10
1	N	855	MET	CB-CA-C	-18.80	72.79	110.40
4	R	170	GLY	N-CA-C	18.21	158.62	113.10
1	N	107	ASP	CB-CA-C	-17.66	75.08	110.40
7	K	469	LYS	CB-CA-C	-17.32	75.76	110.40
5	T	25	ASP	N-CA-C	17.21	157.46	111.00
1	N	23	GLY	N-CA-C	-16.59	71.62	113.10
2	Q	126	ALA	N-CA-CB	-16.56	86.92	110.10
1	A	808	GLY	C-N-CD	-16.45	84.42	120.60
1	A	855	MET	CB-CA-C	-16.41	77.58	110.40
1	A	217	TYR	N-CA-C	16.17	154.65	111.00
6	U	88	GLY	N-CA-C	15.71	152.38	113.10
1	N	19	LEU	CB-CA-C	-15.65	80.47	110.20
4	R	147	LEU	N-CA-C	15.60	153.12	111.00
7	X	208	CYS	N-CA-C	15.22	152.10	111.00
4	F	578	ASP	N-CA-CB	-14.71	84.12	110.60
4	E	150	GLY	N-CA-C	14.57	149.53	113.10
7	X	61	LYS	N-CA-CB	-14.36	84.74	110.60
4	R	171	LYS	N-CA-CB	-14.16	85.12	110.60
4	F	338	ALA	N-CA-CB	-14.11	90.35	110.10
1	N	606	TYR	CB-CA-C	-13.90	82.59	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	536	SER	N-CA-C	13.87	148.46	111.00
6	H	39	THR	CB-CA-C	-13.83	74.26	111.60
1	N	607	SER	N-CA-CB	-13.34	90.49	110.50
4	S	537	GLN	N-CA-C	-13.33	75.00	111.00
2	Q	125	ALA	CB-CA-C	-13.30	90.15	110.10
2	Q	28	ASN	CB-CA-C	-13.21	83.97	110.40
4	F	337	ARG	CB-CA-C	-13.05	84.29	110.40
4	F	337	ARG	N-CA-C	12.86	145.71	111.00
2	Q	125	ALA	N-CA-C	12.84	145.65	111.00
2	B	141	THR	N-CA-C	12.46	144.66	111.00
7	K	470	SER	CB-CA-C	-12.37	86.60	110.10
6	H	39	THR	N-CA-C	12.27	144.13	111.00
6	H	40	ASN	N-CA-CB	-12.21	88.63	110.60
7	X	460	VAL	CB-CA-C	-12.20	88.22	111.40
1	A	504	PHE	C-N-CD	-12.19	93.77	120.60
4	S	536	SER	CB-CA-C	-12.07	87.16	110.10
4	E	549	THR	N-CA-CB	-11.99	87.52	110.30
7	K	371	ALA	CB-CA-C	11.95	128.03	110.10
4	F	577	SER	CB-CA-C	-11.83	87.63	110.10
1	A	218	ASP	N-CA-CB	-11.72	89.50	110.60
2	D	135	TYR	N-CA-CB	-11.63	89.67	110.60
1	N	69	TYR	N-CA-CB	11.44	131.20	110.60
7	X	97	THR	N-CA-C	11.26	141.40	111.00
1	N	754	SER	N-CA-CB	11.20	127.30	110.50
1	N	904	SER	N-CA-CB	-11.17	93.74	110.50
1	A	926	THR	C-N-CD	-11.02	96.35	120.60
7	X	461	SER	N-CA-CB	10.99	126.99	110.50
7	X	504	ALA	CB-CA-C	-10.84	93.85	110.10
4	R	549	THR	N-CA-CB	-10.83	89.72	110.30
4	S	350	SER	N-CA-C	10.63	139.70	111.00
1	A	904	SER	N-CA-CB	-10.58	94.63	110.50
2	Q	112	ASP	CB-CA-C	-10.55	89.29	110.40
7	X	60	PHE	N-CA-C	-10.49	82.68	111.00
4	S	66	GLY	N-CA-C	10.49	139.32	113.10
6	U	84	PRO	CB-CA-C	-10.36	86.09	112.00
1	N	17	ALA	CB-CA-C	-10.27	94.70	110.10
7	X	96	ALA	CB-CA-C	-10.25	94.72	110.10
1	A	69	TYR	N-CA-CB	10.23	129.01	110.60
7	X	465	TYR	N-CA-C	-10.17	83.54	111.00
7	K	471	ALA	N-CA-CB	-10.07	96.00	110.10
3	P	26	SER	CB-CA-C	-10.07	90.96	110.10
4	R	469	ALA	CB-CA-C	-10.07	95.00	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	53	ALA	CB-CA-C	10.02	125.13	110.10
4	S	350	SER	N-CA-CB	-10.01	95.49	110.50
4	E	548	GLN	N-CA-C	-9.94	84.16	111.00
1	A	808	GLY	N-CA-C	9.93	137.92	113.10
4	R	148	SER	N-CA-C	-9.93	84.20	111.00
6	H	69	GLY	N-CA-C	-9.90	88.34	113.10
4	F	289	SER	N-CA-CB	-9.83	95.75	110.50
4	S	288	LYS	N-CA-C	9.72	137.25	111.00
1	A	607	SER	N-CA-C	9.68	137.13	111.00
7	X	384	PHE	N-CA-C	-9.60	85.09	111.00
7	X	423	LYS	CB-CA-C	9.60	129.59	110.40
7	X	209	LEU	N-CA-CB	-9.57	91.26	110.40
1	N	18	ARG	N-CA-C	-9.52	85.31	111.00
7	K	424	HIS	N-CA-C	-9.50	85.35	111.00
2	B	54	ALA	N-CA-CB	-9.49	96.82	110.10
5	G	7	VAL	CB-CA-C	-9.38	93.58	111.40
7	K	211	ASP	N-CA-CB	-9.35	93.77	110.60
4	F	577	SER	N-CA-C	-9.28	85.93	111.00
1	A	109	ASP	N-CA-CB	-9.23	93.98	110.60
1	N	20	THR	N-CA-CB	-9.14	92.93	110.30
5	T	27	ASN	N-CA-CB	-9.11	94.20	110.60
4	R	341	GLU	CB-CA-C	-9.10	92.20	110.40
4	R	548	GLN	CB-CA-C	-9.06	92.28	110.40
7	X	208	CYS	CB-CA-C	-8.64	93.13	110.40
1	N	753	PHE	N-CA-C	-8.55	87.91	111.00
1	N	903	TYR	CB-CA-C	-8.54	93.31	110.40
1	A	216	TRP	CB-CA-C	-8.48	93.45	110.40
2	B	140	ASN	CB-CA-C	8.47	127.34	110.40
1	N	904	SER	N-CA-C	8.46	133.84	111.00
1	N	754	SER	N-CA-C	-8.44	88.21	111.00
2	O	54	ALA	N-CA-CB	-8.41	98.33	110.10
2	B	28	ASN	CB-CA-C	-8.40	93.60	110.40
7	K	31	THR	N-CA-CB	-8.37	94.39	110.30
7	X	385	TRP	N-CA-C	-8.32	88.53	111.00
5	T	25	ASP	N-CA-CB	-8.32	95.63	110.60
6	U	89	PHE	N-CA-CB	-8.31	95.63	110.60
4	S	537	GLN	N-CA-CB	-8.27	95.72	110.60
7	K	30	ASP	CB-CA-C	-8.15	94.11	110.40
1	A	856	ILE	N-CA-CB	-8.13	92.11	110.80
7	X	385	TRP	N-CA-CB	8.09	125.16	110.60
5	T	26	ASP	N-CA-CB	8.03	125.06	110.60
4	R	147	LEU	CB-CA-C	-8.02	94.97	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	TYR	CB-CA-C	-8.01	94.38	110.40
2	O	141	THR	N-CA-C	8.00	132.61	111.00
4	F	455	LEU	N-CA-C	7.98	132.54	111.00
7	K	470	SER	N-CA-CB	-7.95	98.58	110.50
2	B	28	ASN	N-CA-C	-7.94	89.55	111.00
2	B	31	SER	N-CA-CB	7.85	122.27	110.50
3	P	26	SER	N-CA-C	7.77	131.98	111.00
5	T	24	THR	N-CA-C	-7.74	90.11	111.00
4	R	342	CYS	N-CA-CB	-7.73	96.69	110.60
2	D	135	TYR	N-CA-C	7.71	131.81	111.00
1	A	808	GLY	C-N-CA	7.67	154.19	122.00
1	A	504	PHE	C-N-CA	7.66	154.18	122.00
7	K	423	LYS	CB-CA-C	7.65	125.70	110.40
1	A	926	THR	C-N-CA	7.65	154.14	122.00
4	F	258	ILE	N-CA-CB	7.65	128.39	110.80
1	N	648	LEU	N-CA-C	7.62	131.59	111.00
4	R	169	VAL	N-CA-C	7.56	131.42	111.00
1	N	68	SER	N-CA-C	-7.53	90.67	111.00
4	R	150	GLY	N-CA-C	-7.49	94.36	113.10
4	R	149	TYR	N-CA-C	-7.48	90.80	111.00
7	X	63	ASN	N-CA-C	-7.47	90.84	111.00
4	F	257	ASN	N-CA-C	-7.44	90.90	111.00
1	N	68	SER	CB-CA-C	7.43	124.21	110.10
7	X	97	THR	N-CA-CB	-7.36	96.31	110.30
7	X	505	GLY	N-CA-C	7.34	131.46	113.10
2	B	141	THR	CB-CA-C	-7.29	91.91	111.60
4	F	288	LYS	N-CA-C	7.26	130.60	111.00
7	X	474	ILE	CG1-CB-CG2	-7.23	95.49	111.40
1	N	105	ARG	CG-CD-NE	7.22	126.96	111.80
1	A	105	ARG	CG-CD-NE	7.20	126.91	111.80
1	A	926	THR	CB-CA-C	7.20	131.03	111.60
2	Q	113	GLY	N-CA-C	7.18	131.05	113.10
4	F	259	SER	N-CA-C	-7.15	91.70	111.00
1	N	647	SER	CB-CA-C	-7.14	96.54	110.10
4	F	337	ARG	N-CA-CB	-7.11	97.81	110.60
7	X	178	SER	N-CA-CB	7.08	121.13	110.50
7	K	372	THR	N-CA-CB	-7.07	96.87	110.30
1	A	403	ASN	N-CA-CB	-7.06	97.89	110.60
7	K	31	THR	N-CA-C	7.05	130.04	111.00
1	A	903	TYR	N-CA-C	-7.05	91.97	111.00
4	S	190	ASN	N-CA-C	7.03	129.98	111.00
1	A	648	LEU	N-CA-C	7.02	129.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	62	MET	N-CA-C	7.00	129.90	111.00
2	O	53	ALA	CB-CA-C	6.98	120.56	110.10
7	X	424	HIS	N-CA-CB	-6.97	98.05	110.60
1	A	68	SER	N-CA-C	-6.95	92.23	111.00
7	X	424	HIS	N-CA-C	-6.95	92.23	111.00
1	N	105	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	B	112	ASP	N-CA-CB	-6.92	98.15	110.60
2	D	134	ASP	N-CA-C	-6.90	92.36	111.00
1	N	903	TYR	N-CA-C	-6.89	92.39	111.00
4	S	289	SER	N-CA-C	-6.88	92.42	111.00
1	A	647	SER	CB-CA-C	-6.87	97.04	110.10
1	N	758	LEU	CB-CA-C	6.83	123.17	110.20
4	S	537	GLN	CB-CA-C	6.78	123.95	110.40
4	S	190	ASN	CB-CA-C	-6.77	96.86	110.40
1	A	105	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	403	ASN	N-CA-C	6.76	129.25	111.00
1	N	753	PHE	CB-CA-C	6.76	123.92	110.40
7	X	466	VAL	N-CA-CB	-6.75	96.66	111.50
2	B	142	CYS	N-CA-C	-6.70	92.92	111.00
6	U	85	ASN	CB-CA-C	6.67	123.73	110.40
3	C	26	SER	CB-CA-C	-6.66	97.44	110.10
7	K	198	PHE	N-CA-CB	-6.61	98.69	110.60
4	F	456	VAL	N-CA-C	-6.61	93.16	111.00
1	N	856	ILE	N-CA-CB	-6.60	95.61	110.80
5	G	8	ALA	N-CA-CB	-6.57	100.90	110.10
1	A	855	MET	N-CA-C	6.56	128.70	111.00
7	X	58	MET	N-CA-C	6.51	128.58	111.00
1	A	753	PHE	N-CA-CB	-6.49	98.91	110.60
4	S	349	ASN	N-CA-C	6.48	128.51	111.00
2	B	141	THR	N-CA-CB	-6.46	98.03	110.30
4	E	230	HIS	N-CA-C	6.45	128.43	111.00
1	N	21	PRO	CB-CA-C	-6.45	95.88	112.00
4	F	537	GLN	CB-CA-C	6.43	123.25	110.40
6	U	89	PHE	N-CA-C	-6.42	93.67	111.00
4	E	240	LEU	N-CA-C	-6.39	93.74	111.00
1	A	683	GLY	N-CA-C	6.38	129.04	113.10
1	A	904	SER	N-CA-C	6.37	128.21	111.00
4	E	239	THR	N-CA-C	6.37	128.19	111.00
7	X	98	ARG	N-CA-CB	6.34	122.02	110.60
4	S	289	SER	N-CA-CB	-6.33	101.00	110.50
2	Q	114	CYS	N-CA-CB	6.32	121.98	110.60
1	A	68	SER	CB-CA-C	6.27	122.01	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	107	ASP	N-CA-C	6.22	127.80	111.00
1	A	11	VAL	CB-CA-C	-6.21	99.60	111.40
1	N	24	THR	N-CA-CB	-6.20	98.53	110.30
2	B	183	PRO	N-CA-C	-6.18	96.02	112.10
9	M	23	C	C2'-C3'-O3'	6.18	123.58	113.70
2	O	140	ASN	CB-CA-C	6.17	122.75	110.40
1	N	851	ASP	N-CA-CB	-6.16	99.51	110.60
1	A	367	SER	CB-CA-C	-6.16	98.39	110.10
4	S	441	CYS	CB-CA-C	-6.16	98.08	110.40
2	B	30	ASP	N-CA-C	6.15	127.61	111.00
1	A	758	LEU	CB-CA-C	6.15	121.88	110.20
1	N	446	GLY	N-CA-C	6.15	128.47	113.10
2	B	142	CYS	N-CA-CB	6.13	121.64	110.60
7	K	234	ASP	N-CA-CB	-6.10	99.62	110.60
4	R	45	VAL	N-CA-C	-6.09	94.54	111.00
7	K	457	LYS	CB-CA-C	-6.08	98.24	110.40
1	A	4	ALA	CB-CA-C	-6.07	100.99	110.10
4	F	435	ASP	CB-CA-C	-6.05	98.29	110.40
3	C	26	SER	N-CA-C	6.05	127.34	111.00
4	S	538	GLY	N-CA-C	6.03	128.18	113.10
4	S	455	LEU	N-CA-C	6.02	127.25	111.00
4	R	341	GLU	N-CA-C	6.00	127.20	111.00
1	A	682	SER	CB-CA-C	5.99	121.48	110.10
7	X	177	LEU	CB-CA-C	-5.99	98.82	110.20
1	A	40	ASP	N-CA-C	5.95	127.07	111.00
2	Q	114	CYS	N-CA-C	-5.94	94.96	111.00
7	K	96	ALA	CB-CA-C	-5.94	101.19	110.10
4	E	231	THR	N-CA-CB	5.91	121.52	110.30
7	X	60	PHE	CB-CA-C	-5.90	98.60	110.40
7	X	59	GLY	N-CA-C	-5.89	98.37	113.10
7	X	417	GLY	N-CA-C	-5.88	98.40	113.10
1	N	609	VAL	N-CA-C	-5.87	95.14	111.00
7	K	470	SER	N-CA-C	-5.83	95.27	111.00
7	X	64	TYR	N-CA-C	-5.79	95.36	111.00
1	A	446	GLY	N-CA-C	5.78	127.56	113.10
2	Q	99	ASP	N-CA-C	5.78	126.60	111.00
4	R	343	PHE	CB-CA-C	-5.77	98.86	110.40
1	N	721	ARG	CG-CD-NE	5.77	123.91	111.80
2	O	141	THR	N-CA-CB	-5.75	99.36	110.30
4	R	548	GLN	N-CA-C	-5.75	95.46	111.00
1	A	153	ASP	N-CA-CB	-5.72	100.30	110.60
1	A	928	HIS	N-CA-C	-5.71	95.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	267	ALA	N-CA-C	-5.71	95.58	111.00
1	A	926	THR	N-CA-C	-5.71	95.58	111.00
1	N	69	TYR	N-CA-C	-5.70	95.61	111.00
1	N	218	ASP	N-CA-C	5.68	126.33	111.00
4	R	424	SER	N-CA-C	5.66	126.28	111.00
4	F	580	ASP	N-CA-CB	-5.66	100.42	110.60
1	A	889	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	N	24	THR	N-CA-C	5.65	126.24	111.00
4	F	436	MET	N-CA-CB	5.62	120.72	110.60
1	A	402	THR	CB-CA-C	-5.62	96.44	111.60
5	G	4	LEU	C-N-CA	-5.61	107.68	121.70
4	F	336	ALA	CB-CA-C	5.60	118.51	110.10
4	S	67	GLY	N-CA-C	-5.60	99.10	113.10
1	N	367	SER	CB-CA-C	-5.58	99.50	110.10
5	T	27	ASN	N-CA-C	5.57	126.05	111.00
5	G	68	GLU	CA-CB-CG	5.55	125.61	113.40
5	T	68	GLU	CA-CB-CG	5.55	125.61	113.40
2	O	31	SER	N-CA-C	5.55	125.97	111.00
2	B	30	ASP	CB-CA-C	-5.54	99.31	110.40
1	N	919	GLU	CA-CB-CG	5.53	125.57	113.40
1	A	919	GLU	CA-CB-CG	5.53	125.56	113.40
1	N	889	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	N	504	PHE	CB-CG-CD1	5.49	124.64	120.80
7	K	209	LEU	CA-CB-CG	5.49	127.92	115.30
4	R	189	LYS	C-N-CA	5.46	135.35	121.70
7	X	421	VAL	CB-CA-C	-5.46	101.03	111.40
7	K	424	HIS	N-CA-CB	-5.46	100.78	110.60
4	E	189	LYS	C-N-CA	5.45	135.33	121.70
1	N	22	CYS	N-CA-CB	-5.44	100.80	110.60
7	K	233	PHE	CB-CA-C	-5.43	99.55	110.40
1	A	69	TYR	N-CA-C	-5.40	96.43	111.00
2	Q	28	ASN	N-CA-C	-5.38	96.48	111.00
4	F	455	LEU	CB-CA-C	-5.36	100.01	110.20
1	A	152	CYS	CB-CA-C	-5.34	99.71	110.40
4	F	455	LEU	CA-CB-CG	5.34	127.57	115.30
4	E	239	THR	CB-CA-C	-5.33	97.21	111.60
4	S	189	LYS	C-N-CA	5.32	135.00	121.70
7	X	177	LEU	N-CA-C	5.31	125.33	111.00
1	A	22	CYS	N-CA-C	-5.29	96.72	111.00
2	O	30	ASP	CB-CA-C	-5.27	99.86	110.40
1	N	153	ASP	N-CA-CB	-5.26	101.13	110.60
4	E	548	GLN	CB-CA-C	-5.25	99.89	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	105	ARG	CD-NE-CZ	5.25	130.95	123.60
1	N	24	THR	CB-CA-C	-5.24	97.45	111.60
7	X	268	HIS	N-CA-CB	-5.23	101.18	110.60
4	F	189	LYS	C-N-CA	5.22	134.75	121.70
1	N	910	ASP	CB-CG-OD2	5.21	122.99	118.30
7	K	63	ASN	N-CA-CB	-5.21	101.23	110.60
5	G	25	ASP	CB-CG-OD2	5.21	122.98	118.30
4	R	423	ASN	CB-CA-C	-5.20	100.00	110.40
1	N	105	ARG	CD-NE-CZ	5.20	130.87	123.60
2	D	134	ASP	CB-CA-C	-5.19	100.03	110.40
7	K	22	GLN	N-CA-CB	-5.17	101.30	110.60
1	A	608	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	851	ASP	N-CA-C	-5.14	97.11	111.00
1	A	910	ASP	CB-CG-OD2	5.13	122.92	118.30
2	B	111	ARG	CB-CA-C	5.13	120.66	110.40
1	A	927	PRO	CA-N-CD	-5.11	104.34	111.50
1	A	810	HIS	N-CA-C	-5.11	97.22	111.00
7	X	384	PHE	CB-CA-C	5.10	120.59	110.40
7	X	248	GLY	N-CA-C	5.10	125.84	113.10
1	A	647	SER	N-CA-C	-5.08	97.28	111.00
7	K	372	THR	N-CA-C	5.08	124.71	111.00
1	A	37	ILE	CB-CA-C	-5.06	101.48	111.60
1	N	18	ARG	N-CA-CB	-5.05	101.50	110.60
1	N	718	LYS	CB-CG-CD	5.05	124.73	111.60
1	A	718	LYS	CB-CG-CD	5.04	124.72	111.60
7	X	250	THR	N-CA-C	5.04	124.61	111.00
4	F	579	ARG	CB-CA-C	5.04	120.48	110.40
1	N	220	GLY	N-CA-C	-5.03	100.54	113.10
7	K	250	THR	N-CA-C	5.01	124.52	111.00
4	S	455	LEU	CB-CA-C	-5.01	100.69	110.20

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	262	0
1	N	7462	0	7202	271	0
2	B	1400	0	1372	64	0
2	D	1418	0	1427	51	0
2	O	1400	0	1372	27	0
2	Q	1418	0	1427	59	0
3	C	553	0	585	27	0
3	P	553	0	585	20	0
4	E	4567	0	4508	308	0
4	F	4630	0	4584	252	0
4	R	4567	0	4508	283	0
4	S	4630	0	4584	247	0
5	G	868	0	880	62	0
5	T	868	0	880	57	0
6	H	955	0	910	40	0
6	U	947	0	906	56	0
7	K	4169	0	4051	136	0
7	X	4177	0	4058	180	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	56	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	2430	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 23.

All (2430) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:210:CYS:HG	10:X:600:ZN:ZN	0.82	0.91
4:R:341:GLU:O	4:R:341:GLU:CD	2.08	0.91
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:501:SER:CB	9:M:25:G:OP1	2.29	0.81
4:E:286:THR:H	4:E:288:LYS:HZ1	1.27	0.81
1:N:105:ARG:HH11	1:N:105:ARG:CB	1.93	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: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
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
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
2:B:43:ASN:ND2	9:J:48:C:C5'	2.46	0.77
4:S:407:ALA:HB3	4:S:409:ARG:HE	1.49	0.77
1:A:11:VAL:CG1	1:A:12:CYS:N	2.48	0.77
2:D:161:ASP:HB2	2:D:181:ALA:HB3	1.68	0.76
1:N:277:GLU:CD	1:N:277:GLU:H	1.89	0.76
5:T:8:ALA:C	5:T:9:LEU:HD22	2.06	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
9:M:25:G:O2'	9:M:26:A:P	2.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:277:GLU:H	1:A:277:GLU:CD	1.89	0.75
4:E:493:ILE:HG22	4:E:497:ARG:HE	1.52	0.75
6:H:122:MET:HE3	6:H:127:GLY:H	1.51	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
1:A:929:THR:OG1	1:A:929:THR:O	2.05	0.74
4:R:146:LYS:O	4:R:146:LYS:HG2	1.87	0.74
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
4:E:149:TYR:C	4:E:227:LEU:HD22	2.08	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
4:E:473:LYS:NZ	4:E:589:SER:OG	2.21	0.73
1:N:367:SER:N	1:N:370:GLU:OE2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
2:Q:99:ASP:O	2:Q:99:ASP:CG	2.28	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
6:H:46:CYS:SG	6:H:47:THR:N	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
4:S:320:LYS:H	4:S:323:LYS:HZ3	1.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:536:SER:C	4:S:537:GLN:O	2.10	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
1:A:39:ASN:C	1:A:39:ASN:OD1	2.33	0.66
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
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
9:M:22:U:OP2	9:M:22:U:H6	1.78	0.66
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:8:LEU:HD23	1:A:8:LEU:C	2.17	0.65
1:A:594:PHE:HD2	9:J:31:U:H4'	1.59	0.65
1:A:804:ASP:HB2	1:A:807:LYS:HZ2	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:180:LEU:C	2:B:181:ALA:O	2.33	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
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: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
1:N:24:THR:OG1	1:N:25:GLY:N	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:R:358:CYS:SG	4:R:359:THR:N	2.71	0.63
7:X:470:SER:OG	7:X:471:ALA:N	2.31	0.63
4:F:337:ARG:CD	4:F:337:ARG:C	2.62	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
4:R:68:MET:N	4:R:68:MET:SD	2.68	0.63
4:R:473:LYS:HD3	4:R:585:LEU:HB2	1.81	0.63
1:A:8:LEU:HD23	1:A:8:LEU:O	1.97	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
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
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
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
5:G:5:SER:O	5:G:5:SER:OG	2.17	0.62
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:477:LYS:HZ3	4:S:576:MET:HA	1.63	0.62
7:K:331:ASP:OD1	7:K:332:ILE:N	2.32	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
4:R:423:ASN:C	4:R:423:ASN:OD1	2.37	0.62
4:F:37:THR:OG1	4:F:38:SER:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:S:536:SER:O	4:S:537:GLN:C	2.32	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
7:X:393:PRO:O	7:X:396:SER:OG	2.17	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
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
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
2:Q:117:LEU:HD12	2:Q:129:MET:HE2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:K:83:VAL:O	7:K:84:ARG:HB2	2.02	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
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:377:SER:C	4:F:422:PHE:HE2	2.05	0.59
4:F:561:PHE:O	4:F:565:ILE:HG12	2.02	0.59
4:S:320:LYS:N	4:S:323:LYS:HZ3	2.01	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
4:E:33:HIS:O	4:E:37:THR:OG1	2.18	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
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
1:N:218:ASP:OD1	1:N:218:ASP:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:684:ASP:O	9:M:27:C:H4'	2.03	0.58
5:T:35:THR:OG1	5:T:36:LYS:N	2.34	0.58
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: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
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: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:296:ALA:O	4:F:355:TYR:OH	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:ASN:OD1	1:A:768:SER:N	2.37	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
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
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
7:K:230:SER:O	7:K:230:SER:OG	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:SER:O	8:I:33:G:O3'	2.24	0.56
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:S:347:LYS:HD2	4:S:347:LYS:C	2.26	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
2:Q:99:ASP:OD1	2:Q:99:ASP:C	2.44	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
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
1:N:504:PHE:CD1	1:N:504:PHE:C	2.80	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
9:J:25:G:HO2'	9:J:26:A:P	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:212:ARG:HH12	7:K:228:HIS:CE1	2.25	0.55
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
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
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
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
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:171:LYS:HZ1	4:F:174:PRO:HD3	1.70	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
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:465:LYS:NZ	4:S:569:LYS:O	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:88:ASN:HA	1:N:91:LYS:HZ2	1.73	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:X:510:VAL:HG12	7:X:511:TYR:N	2.23	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
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: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
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
4:S:326:PRO:C	4:S:328:ASP:HB3	2.27	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: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
7:K:154:TYR:HB2	7:K:155:LYS:HZ2	1.74	0.53
4:S:383:ASP:HA	4:S:386:VAL:HG22	1.90	0.53
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
6:U:25:LYS:HZ3	6:U:28:LYS:HB2	1.73	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
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
1:N:218:ASP:O	1:N:218:ASP:CG	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:453:SER:HA	4:S:457:TYR:HB2	1.90	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
4:R:447:GLU:CD	4:R:471:CYS:HB2	2.28	0.53
6:U:83:HIS:NE2	6:U:90:CYS:CB	2.71	0.53
7:X:25:THR:OG1	7:X:26:HIS:N	2.40	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
7:K:28:SER:O	7:K:28:SER:OG	2.26	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:4:ALA:C	1:A:6:SER:H	2.13	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
1:A:721:ARG:O	1:A:722:ASN:C	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:134:ASP:C	2:B:182:TRP:CZ3	2.83	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
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
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
4:R:483:ASP:OD2	4:R:488:ILE:HD11	2.10	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
1:A:726:ARG:HE	1:A:741:PHE:HD2	1.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:U:25:LYS:O	6:U:25:LYS:NZ	2.35	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
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
1:N:809:PRO:O	1:N:809:PRO:HG2	2.11	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:O:173:SER:HG	2:O:176:ASN:H	1.56	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:NZ	4:R:73:LYS:H	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
6:H:51:THR:HG22	6:H:60:GLU:CD	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:162:ALA:HB3	2:Q:181:ALA:HB1	1.93	0.50
6:U:70:GLY:C	6:U:92:LEU:O	2.49	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
1:N:57:GLN:CD	1:N:65:LEU:HD23	2.32	0.50
1:N:403:ASN:O	2:O:129:MET:CE	2.59	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:GLN:CD	1:A:65:LEU:HD23	2.32	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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:R:114:TRP:C	4:R:411:LEU:HD21	2.32	0.49
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
6:U:89:PHE:C	6:U:90:CYS:O	2.47	0.49
4:F:327:ILE:HA	4:F:328:ASP:C	2.33	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:11:VAL:C	1:A:13:GLY:N	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:311:HIS:CE1	4:S:338:ALA:HA	2.48	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: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
7:K:134:SER:OG	7:K:135:ARG:N	2.46	0.49
1:N:388:LEU:HD23	1:N:397:SER:OG	2.12	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
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
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
2:B:120:ILE:O	2:B:124:THR:HG22	2.12	0.48
2:B:164:SER:C	2:B:165:LYS:HD2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:686:THR:O	1:A:686:THR:OG1	2.21	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
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
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
1:A:415:PHE:HE2	3:C:8:CYS:HG	1.60	0.48
4:E:318:CYS:HB3	4:E:343:PHE:CD2	2.48	0.48
6:H:6:GLU:OE2	6:H:10:ASN:ND2	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:139:LYS:HZ1	4:E:382:TYR:HB2	1.77	0.48
1:N:682:SER:O	9:M:26:A:C2	2.67	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
4:S:90:PHE:HA	4:S:94:LYS:HZ1	1.78	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:504:PHE:C	1:N:504:PHE:HD1	2.17	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
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
4:F:139:LYS:HA	4:F:142:GLU:HG2	1.95	0.48
4:S:496:VAL:HG23	4:S:497:ARG:HH12	1.78	0.48
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:469:LYS:HG2	1:N:905:VAL:HG23	1.95	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
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
1:A:806:THR:HG22	1:A:806:THR:O	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
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: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
1:N:686:THR:O	1:N:686:THR:OG1	2.21	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:116:ASN:OD1	4:S:116:ASN:N	2.48	0.47
4:S:514:PRO:HG2	4:S:549:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:O	1:A:37:ILE:CG2	2.42	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
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:904:SER:C	7:X:468:LEU:HB2	2.35	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:105:ARG:HH12	1:N:108:GLY:N	2.12	0.47
1:N:254:GLU:OE1	1:N:254:GLU:HA	2.15	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: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
4:S:473:LYS:HZ1	4:S:573:LEU:HD13	1.80	0.47
8:I:13:U:H2'	8:I:14:A:O4'	2.15	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
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
7:K:324:ASP:O	7:K:325:LYS:NZ	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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
4:R:511:PHE:HZ	4:R:547:THR:HG1	1.62	0.46
7:X:483:VAL:O	7:X:484:CYS:C	2.52	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: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: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
1:A:736:ASP:OD1	1:A:736:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:X:358:ASP:CG	7:X:359:LYS:HD2	2.35	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:F:576:MET:HB3	4:F:576:MET:HE2	1.79	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
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
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:576:MET:HE1	4:E:585:LEU:HD22	1.97	0.46
1:N:139:CYS:O	1:N:143:LYS:HG3	2.15	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:415:ASP:N	7:K:415:ASP:OD1	2.49	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
2:O:11:SER:HA	2:O:48:GLU:CD	2.37	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
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:357:SER:OG	7:K:358:ASP:N	2.48	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: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
4:S:488:ILE:HG23	4:S:521:VAL:HG11	1.98	0.46
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:R:118:GLY:O	4:R:122:LEU:HG	2.16	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:K:147:LYS:C	7:K:149:LEU:H	2.20	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
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: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
3:P:63:GLN:HB2	4:R:352:LEU:HD11	1.97	0.45
4:R:7:LEU:C	4:R:129:ARG:HH12	2.20	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:S:474:MET:HE3	4:S:582:TYR:HB3	1.98	0.45
1:A:9:ASN:C	1:A:11:VAL:H	2.19	0.45
1:A:57:GLN:NE2	1:A:66:ILE:O	2.49	0.45
2:B:45:ALA:HA	2:B:48:GLU:CD	2.36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Q:44:VAL:HA	2:Q:47:SER:HG	1.82	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
2:B:92:PHE:O	2:B:96:ARG:HG3	2.16	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
3:P:26:SER:O	3:P:26:SER:OG	2.28	0.45
4:R:73:LYS:H	4:R:73:LYS:HZ3	1.64	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
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
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
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
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
4:R:170:GLY:O	4:R:171:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:S:347:LYS:HZ3	4:S:351:THR:H	1.65	0.45
4:S:473:LYS:HZ2	4:S:573:LEU:HD22	1.81	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
1:N:39:ASN:OD1	1:N:41:LYS:N	2.49	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
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:322:LEU:HB2	4:S:323:LYS:HZ1	1.80	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
4:E:492:GLN:CD	4:E:547:THR:HB	2.37	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:105:ASP:OD1	4:R:105:ASP:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
4:S:474:MET:HE1	4:S:578:ASP:OD2	2.17	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
1:A:842:CYS:C	1:A:843:PHE:HD1	2.20	0.44
4:E:135:ALA:O	4:E:138:LEU:HG	2.18	0.44
1:N:257:VAL:HG23	1:N:264:PRO:O	2.17	0.44
1:N:842:CYS:C	1:N:843:PHE:HD1	2.20	0.44
9:J:39:A:C6	9:J:40:U:C4	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:445:PRO:HB3	4:F:465:LYS:HZ1	1.83	0.44
4:S:322:LEU:HA	4:S:327:ILE:HD11	1.99	0.44
1:A:358:ASP:CG	1:A:533:ARG:HH21	2.21	0.44
2:B:74:ALA:O	2:B:77:GLU:HG3	2.18	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:358:ASP:CG	1:N:533:ARG:HH21	2.21	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
6:U:19:PHE:CE2	7:X:62:MET:HE1	2.53	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: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:41:LYS:HZ3	1:N:42:VAL:HG13	1.83	0.43
1:N:429:PHE:HD1	1:N:429:PHE:N	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:306:TYR:HE1	4:S:355:TYR:HB3	1.83	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
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
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
2:Q:137:THR:O	2:Q:141:THR:OG1	2.25	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:F:477:LYS:HZ3	4:F:492:GLN:HG3	1.83	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: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:483:ASP:OD1	4:E:483:ASP:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:117:ALA:O	4:R:121:ILE:HG12	2.18	0.43
7:X:80:ILE:HA	7:X:80:ILE:HD13	1.69	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
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: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
1:N:810:HIS:ND1	1:N:810:HIS:C	2.71	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
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
7:X:465:TYR:CD1	7:X:465:TYR:C	2.85	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:221:SER:O	7:X:222:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:K:58:MET:HE1	7:K:104:ASN:H	1.83	0.43
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: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
4:S:477:LYS:NZ	4:S:576:MET:HA	2.33	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:626:MET:HE3	1:A:680:THR:HG22	2.01	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:107:ASP:O	1:N:107:ASP:CG	2.36	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
4:R:40:LYS:HE2	4:R:59:ASP:CG	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:N:10:ARG:HH21	1:N:10:ARG:C	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:403:ASN:O	2:O:129:MET:HE3	2.19	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: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
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
2:Q:38:LEU:C	2:Q:42:LEU:HG	2.39	0.42
4:R:542:ASP:HA	4:R:569:LYS:HB2	2.02	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:444:CYS:HA	4:F:569:LYS:HZ1	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:105:ARG:HG2	1:A:109:ASP:C	2.40	0.42
1:A:370:GLU:O	1:A:374:TYR:HD1	2.02	0.42
1:A:433:SER:OG	1:A:434:SER:N	2.51	0.42
2:B:59:LEU:HB3	4:F:81:PHE:CE2	2.54	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
5:G:68:GLU:C	5:G:68:GLU:CD	2.79	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
1:N:603:LYS:HD2	1:N:603:LYS:HA	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:731:LEU:HD23	1:N:732:TYR:CE1	2.55	0.42
5:T:68:GLU:C	5:T:68:GLU:CD	2.79	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
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
4:E:233:MET:CE	4:E:234:PRO:HD2	2.50	0.41
1:N:304:ASP:N	1:N:304:ASP:OD1	2.53	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
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:290:HIS:HA	4:R:320:LYS:HZ1	1.83	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: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:91:GLY:C	4:S:94:LYS:HD3	2.40	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:619:TYR:N	1:A:619:TYR:HD1	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
6:U:120:CYS:HB2	6:U:122:MET:HE2	2.02	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:41:LYS:HZ3	1:A:42:VAL:HG13	1.86	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: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: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: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:423:ASN:CG	4:E:424:SER:H	2.24	0.41
4:E:503:ASN:HB3	4:E:506:TRP:CD1	2.55	0.41
7:K:291:ASP:CG	7:K:293:THR:H	2.23	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:37:THR:O	4:S:40:LYS:NZ	2.41	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
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: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
1:N:39:ASN:OD1	1:N:39:ASN:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:8:LEU:C	1:A:8:LEU:CD2	2.84	0.41
1:A:102:PHE:C	1:A:102:PHE:CD1	2.94	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
7:K:204:GLU:CD	7:K:213:ARG:HH21	2.22	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: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
5:T:25:ASP:OD1	5:T:25:ASP:C	2.57	0.41
7:X:415:ASP:C	7:X:417:GLY:H	2.24	0.41
4:F:107:ASN:O	4:F:111:THR:OG1	2.29	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:O	1:A:12:CYS:C	2.57	0.41
1:A:105:ARG:HG2	1:A:110:MET:N	2.36	0.41
1:A:718:LYS:HA	1:A:721:ARG:CD	2.46	0.41
1:A:807:LYS:HZ2	1:A:807:LYS:HG3	1.68	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:131:LYS:HZ1	4:E:424:SER:CB	2.33	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
5:G:81:LYS:HZ3	5:G:81:LYS:HG3	1.64	0.41
6:H:53:GLN:CD	6:H:121:GLY:HA3	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:480:GLY:C	7:X:482:ALA:HB2	2.41	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: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
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:154:TYR:C	7:K:155:LYS:HD3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:154:VAL:HG22	4:S:165:LEU:HD11	2.03	0.41
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
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:295:GLU:OE2	7:X:424:HIS:NE2	2.54	0.40
7:X:358:ASP:C	7:X:360:ALA:H	2.25	0.40
4:F:127:THR:OG1	4:F:130:LEU:HB2	2.21	0.40
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: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:419:PRO:HB2	4:F:430:LYS:CE	2.52	0.40
4:F:576:MET:HG2	4:F:577:SER:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:928:HIS:O	1:A:929:THR:C	2.59	0.40
2:B:180:LEU:O	2:B:181:ALA:C	2.60	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:455:LEU:HD23	4:R:584:LYS:HD3	2.03	0.40
5:T:50:ASP:C	5:T:51:LEU:HD12	2.42	0.40
6:U:40:ASN:OD1	7:X:26:HIS:HB3	2.21	0.40
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%)	47 78
1	N	924/932 (99%)	831 (90%)	88 (10%)	5 (0%)	29 63
2	B	185/198 (93%)	175 (95%)	7 (4%)	3 (2%)	9 38
2	D	184/198 (93%)	172 (94%)	11 (6%)	1 (0%)	29 63
2	O	185/198 (93%)	172 (93%)	10 (5%)	3 (2%)	9 38
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	F	594/601 (99%)	515 (87%)	77 (13%)	2 (0%)	41 73
4	R	585/601 (97%)	530 (91%)	52 (9%)	3 (0%)	29 63
4	S	594/601 (99%)	516 (87%)	73 (12%)	5 (1%)	19 53
5	G	111/117 (95%)	97 (87%)	12 (11%)	2 (2%)	8 35
5	T	111/117 (95%)	100 (90%)	11 (10%)	0	100 100
6	H	129/139 (93%)	113 (88%)	15 (12%)	1 (1%)	19 53
6	U	128/139 (92%)	111 (87%)	17 (13%)	0	100 100
7	K	521/527 (99%)	445 (85%)	70 (13%)	6 (1%)	13 44
7	X	522/527 (99%)	434 (83%)	83 (16%)	5 (1%)	15 49
All	All	6606/6792 (97%)	5875 (89%)	693 (10%)	38 (1%)	29 59

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

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Mol	Chain	Res	Type
7	X	460	VAL
7	X	475	THR
2	B	183	PRO
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%)	689 (84%)	129 (16%)	2 11
1	N	818/823 (99%)	682 (83%)	136 (17%)	2 9
2	B	146/167 (87%)	140 (96%)	6 (4%)	30 61
2	D	150/167 (90%)	140 (93%)	10 (7%)	16 47
2	O	146/167 (87%)	135 (92%)	11 (8%)	13 42
2	Q	150/167 (90%)	142 (95%)	8 (5%)	22 54
3	C	67/77 (87%)	51 (76%)	16 (24%)	0 2
3	P	67/77 (87%)	51 (76%)	16 (24%)	0 2
4	E	507/523 (97%)	499 (98%)	8 (2%)	62 81
4	F	514/523 (98%)	493 (96%)	21 (4%)	30 61
4	R	507/523 (97%)	497 (98%)	10 (2%)	55 78
4	S	514/523 (98%)	479 (93%)	35 (7%)	16 46
5	G	94/97 (97%)	67 (71%)	27 (29%)	0 1
5	T	94/97 (97%)	72 (77%)	22 (23%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	H	105/113 (93%)	98 (93%)	7 (7%)	16 47
6	U	104/113 (92%)	92 (88%)	12 (12%)	5 22
7	K	458/462 (99%)	425 (93%)	33 (7%)	14 44
7	X	459/462 (99%)	418 (91%)	41 (9%)	9 34
All	All	5718/5904 (97%)	5170 (90%)	548 (10%)	12 30

All (548) 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	22	CYS
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	66	ILE
1	A	77	PHE
1	A	80	TYR
1	A	91	LYS
1	A	92	ASP
1	A	102	PHE
1	A	103	LYS
1	A	104	PHE
1	A	107	ASP
1	A	113	HIS
1	A	115	SER
1	A	116	ARG
1	A	118	ARG
1	A	141	THR
1	A	146	LEU
1	A	156	TYR
1	A	158	ASN

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Mol	Chain	Res	Type
1	A	159	LYS
1	A	160	LYS
1	A	165	PHE
1	A	167	GLU
1	A	187	LEU
1	A	192	PHE
1	A	226	THR
1	A	229	SER
1	A	256	HIS
1	A	260	ASP
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	308	LEU
1	A	325	SER
1	A	340	PHE
1	A	346	TYR
1	A	358	ASP
1	A	363	SER
1	A	364	SER
1	A	366	LEU
1	A	367	SER
1	A	381	HIS
1	A	388	LEU
1	A	389	LEU
1	A	393	THR
1	A	405	VAL
1	A	409	THR
1	A	411	LYS
1	A	422	PHE
1	A	434	SER
1	A	478	LYS
1	A	480	PHE
1	A	494	ILE
1	A	514	LEU
1	A	516	TYR
1	A	517	ASP
1	A	518	SER
1	A	522	GLU

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Mol	Chain	Res	Type
1	A	528	PHE
1	A	560	VAL
1	A	561	SER
1	A	583	ARG
1	A	593	LYS
1	A	603	LYS
1	A	613	HIS
1	A	614	LEU
1	A	618	ASP
1	A	619	TYR
1	A	621	LYS
1	A	624	ARG
1	A	626	MET
1	A	630	LEU
1	A	640	ARG
1	A	644	THR
1	A	666	MET
1	A	680	THR
1	A	682	SER
1	A	686	THR
1	A	710	THR
1	A	715	ILE
1	A	721	ARG
1	A	726	ARG
1	A	729	GLU
1	A	739	THR
1	A	740	ASP
1	A	744	GLU
1	A	766	PHE
1	A	768	SER
1	A	769	THR
1	A	780	LYS
1	A	783	LYS
1	A	787	TYR
1	A	805	LEU
1	A	807	LYS
1	A	817	THR
1	A	818	MET
1	A	820	VAL
1	A	821	LYS
1	A	825	ASP
1	A	835	SER

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Mol	Chain	Res	Type
1	A	847	ILE
1	A	848	VAL
1	A	854	LEU
1	A	858	ARG
1	A	865	ASP
1	A	887	TYR
1	A	889	ARG
1	A	894	GLU
1	A	900	LEU
1	A	902	MET
1	A	904	SER
1	A	922	GLU
1	A	929	THR
2	B	111	ARG
2	B	153	LEU
2	B	157	GLN
2	B	160	VAL
2	B	173	SER
2	B	175	ASP
3	C	4	SER
3	C	13	LEU
3	C	18	GLN
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	70	LYS
3	C	73	GLU
2	D	46	LYS
2	D	56	GLN
2	D	73	GLN
2	D	78	ASP
2	D	92	PHE
2	D	134	ASP
2	D	148	THR

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Mol	Chain	Res	Type
2	D	163	ASP
2	D	175	ASP
2	D	179	ASN
4	E	55	CYS
4	E	96	THR
4	E	146	LYS
4	E	147	LEU
4	E	148	SER
4	E	183	THR
4	E	550	THR
4	E	579	ARG
5	G	4	LEU
5	G	5	SER
5	G	7	VAL
5	G	9	LEU
5	G	21	THR
5	G	24	THR
5	G	26	ASP
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	46	SER
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	74	ARG
5	G	75	PHE
5	G	78	ASP
5	G	79	THR
5	G	81	LYS
5	G	99	ARG
5	G	111	ARG
6	H	62	ASN
6	H	64	ASP
6	H	72	SER
6	H	80	HIS

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Mol	Chain	Res	Type
6	H	89	PHE
6	H	126	TYR
6	H	131	ASP
7	K	5	THR
7	K	16	THR
7	K	21	THR
7	K	31	THR
7	K	47	LYS
7	K	75	THR
7	K	113	THR
7	K	131	THR
7	K	170	LEU
7	K	182	VAL
7	K	185	LEU
7	K	188	HIS
7	K	215	THR
7	K	223	THR
7	K	242	ILE
7	K	245	GLN
7	K	253	LEU
7	K	261	CYS
7	K	264	HIS
7	K	291	ASP
7	K	301	ASP
7	K	303	LEU
7	K	398	VAL
7	K	403	THR
7	K	428	THR
7	K	462	ASP
7	K	463	ILE
7	K	470	SER
7	K	475	THR
7	K	478	ASN
7	K	484	CYS
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

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Mol	Chain	Res	Type
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	66	ILE
1	N	77	PHE
1	N	80	TYR
1	N	81	GLN
1	N	91	LYS
1	N	92	ASP
1	N	102	PHE
1	N	103	LYS
1	N	104	PHE
1	N	105	ARG
1	N	107	ASP
1	N	109	ASP
1	N	113	HIS
1	N	115	SER
1	N	116	ARG
1	N	118	ARG
1	N	141	THR
1	N	146	LEU
1	N	156	TYR
1	N	158	ASN
1	N	159	LYS
1	N	160	LYS
1	N	165	PHE
1	N	167	GLU
1	N	187	LEU
1	N	192	PHE
1	N	219	PHE
1	N	226	THR
1	N	229	SER
1	N	256	HIS
1	N	260	ASP
1	N	267	LYS
1	N	277	GLU
1	N	281	LYS
1	N	282	LEU

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Mol	Chain	Res	Type
1	N	293	THR
1	N	295	HIS
1	N	308	LEU
1	N	325	SER
1	N	340	PHE
1	N	346	TYR
1	N	358	ASP
1	N	363	SER
1	N	364	SER
1	N	366	LEU
1	N	367	SER
1	N	381	HIS
1	N	388	LEU
1	N	389	LEU
1	N	393	THR
1	N	405	VAL
1	N	409	THR
1	N	411	LYS
1	N	422	PHE
1	N	434	SER
1	N	478	LYS
1	N	480	PHE
1	N	494	ILE
1	N	504	PHE
1	N	514	LEU
1	N	516	TYR
1	N	517	ASP
1	N	518	SER
1	N	522	GLU
1	N	528	PHE
1	N	560	VAL
1	N	561	SER
1	N	583	ARG
1	N	593	LYS
1	N	603	LYS
1	N	613	HIS
1	N	614	LEU
1	N	618	ASP
1	N	619	TYR
1	N	621	LYS
1	N	624	ARG
1	N	626	MET

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Mol	Chain	Res	Type
1	N	630	LEU
1	N	640	ARG
1	N	644	THR
1	N	666	MET
1	N	680	THR
1	N	682	SER
1	N	686	THR
1	N	710	THR
1	N	715	ILE
1	N	718	LYS
1	N	721	ARG
1	N	726	ARG
1	N	729	GLU
1	N	739	THR
1	N	740	ASP
1	N	744	GLU
1	N	766	PHE
1	N	768	SER
1	N	769	THR
1	N	780	LYS
1	N	783	LYS
1	N	787	TYR
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	825	ASP
1	N	835	SER
1	N	845	ASP
1	N	847	ILE
1	N	848	VAL
1	N	854	LEU
1	N	858	ARG
1	N	865	ASP
1	N	887	TYR
1	N	889	ARG
1	N	894	GLU
1	N	900	LEU
1	N	902	MET

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Mol	Chain	Res	Type
1	N	904	SER
1	N	919	GLU
1	N	922	GLU
1	N	926	THR
2	O	15	PHE
2	O	42	LEU
2	O	51	ARG
2	O	65	GLN
2	O	83	VAL
2	O	111	ARG
2	O	153	LEU
2	O	157	GLN
2	O	173	SER
2	O	177	SER
2	O	182	TRP
3	P	4	SER
3	P	13	LEU
3	P	18	GLN
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	70	LYS
3	P	73	GLU
2	Q	46	LYS
2	Q	50	ASP
2	Q	61	LYS
2	Q	98	LEU
2	Q	114	CYS
2	Q	134	ASP
2	Q	158	GLN
2	Q	182	TRP
4	R	49	VAL
4	R	68	MET
4	R	105	ASP

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Mol	Chain	Res	Type
4	R	151	ILE
4	R	178	ARG
4	R	288	LYS
4	R	325	LEU
4	R	413	THR
4	R	458	ASP
4	R	497	ARG
5	T	4	LEU
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	46	SER
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	74	ARG
5	T	75	PHE
5	T	78	ASP
5	T	79	THR
5	T	81	LYS
5	T	99	ARG
5	T	111	ARG
6	U	3	ASN
6	U	12	THR
6	U	21	VAL
6	U	22	ASP
6	U	47	THR
6	U	63	MET
6	U	65	GLN
6	U	72	SER
6	U	90	CYS
6	U	102	THR
6	U	108	VAL
6	U	117	CYS
7	X	50	THR

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Mol	Chain	Res	Type
7	X	75	THR
7	X	82	HIS
7	X	112	SER
7	X	113	THR
7	X	190	PHE
7	X	194	SER
7	X	206	THR
7	X	207	CYS
7	X	210	CYS
7	X	212	ARG
7	X	222	ASP
7	X	223	THR
7	X	227	TRP
7	X	264	HIS
7	X	268	HIS
7	X	269	VAL
7	X	279	CYS
7	X	317	VAL
7	X	345	ASP
7	X	350	PHE
7	X	375	ASP
7	X	387	CYS
7	X	390	ASP
7	X	395	ASN
7	X	396	SER
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	450	SER
7	X	466	VAL
7	X	470	SER
7	X	474	ILE
7	X	476	ARG
7	X	478	ASN
7	X	485	ARG
7	X	503	SER
7	X	517	TYR
4	F	26	CYS
4	F	28	LYS

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Mol	Chain	Res	Type
4	F	30	CYS
4	F	37	THR
4	F	74	SER
4	F	106	PHE
4	F	161	ARG
4	F	173	ARG
4	F	224	TYR
4	F	245	HIS
4	F	309	CYS
4	F	319	GLU
4	F	344	ASP
4	F	372	VAL
4	F	481	THR
4	F	499	PHE
4	F	511	PHE
4	F	528	LEU
4	F	573	LEU
4	F	582	TYR
4	F	584	LYS
4	S	25	LEU
4	S	70	TYR
4	S	74	SER
4	S	76	LYS
4	S	96	THR
4	S	145	PHE
4	S	164	HIS
4	S	183	THR
4	S	215	THR
4	S	216	THR
4	S	232	VAL
4	S	250	THR
4	S	255	THR
4	S	270	GLN
4	S	275	GLN
4	S	303	ARG
4	S	315	ASP
4	S	325	LEU
4	S	347	LYS
4	S	350	SER
4	S	383	ASP
4	S	392	ARG
4	S	444	CYS

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Mol	Chain	Res	Type
4	S	449	VAL
4	S	455	LEU
4	S	467	LYS
4	S	486	SER
4	S	546	PHE
4	S	549	THR
4	S	554	HIS
4	S	560	ARG
4	S	576	MET
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 (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	256	HIS
1	A	295	HIS
1	A	356	ASN
1	A	822	GLN
2	B	43	ASN
2	B	65	GLN
2	B	104	ASN
4	E	164	HIS
4	E	194	GLN
4	E	230	HIS
4	E	275	GLN
4	E	492	GLN
5	G	11	GLN
6	H	65	GLN
7	K	257	HIS
1	N	57	GLN
1	N	256	HIS
1	N	295	HIS
1	N	356	ASN
1	N	611	ASN
2	O	158	GLN
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	98	GLN
7	X	63	ASN
7	X	104	ASN
7	X	257	HIS
7	X	478	ASN
7	X	487	HIS
7	X	489	ASN
4	F	33	HIS
4	F	220	ASN
4	F	492	GLN
4	F	519	ASN
4	F	531	GLN
4	S	33	HIS
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
9	J	24	U
9	J	25	G
8	L	15	G
8	L	23	C
9	M	22	U

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Mol	Chain	Res	Type
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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

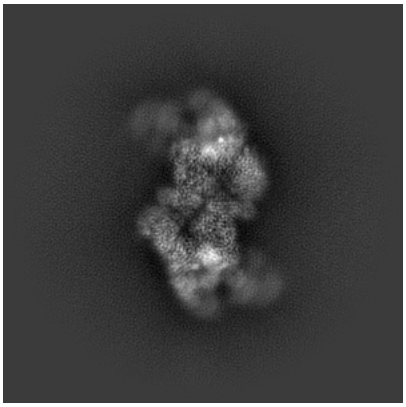
6 Map visualisation

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.

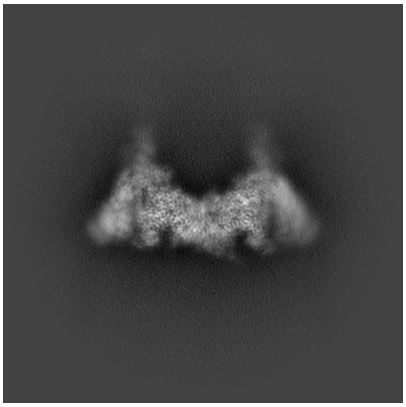
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

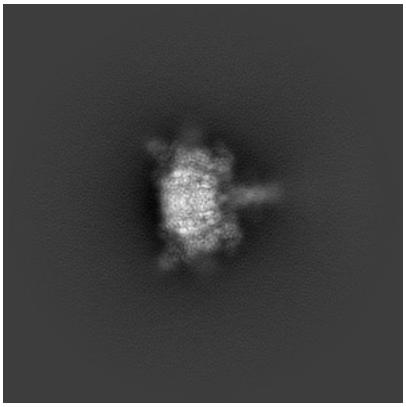
6.1.1 Primary map



X



Y

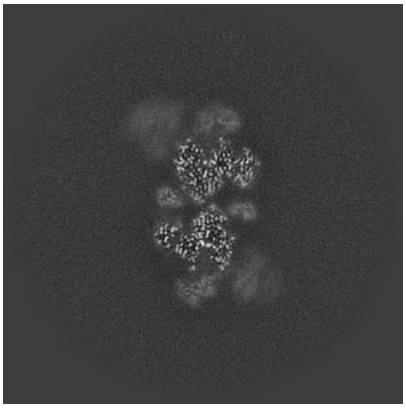


Z

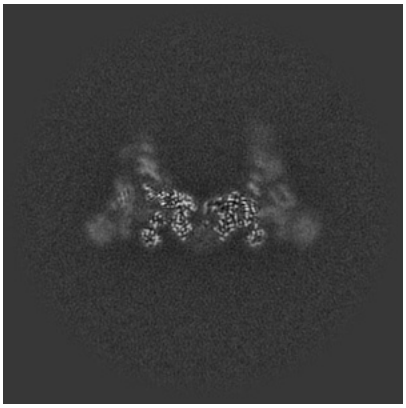
The images above show the map projected in three orthogonal directions.

6.2 Central slices

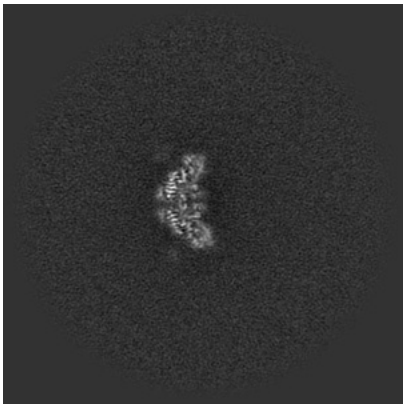
6.2.1 Primary map



X Index: 224



Y Index: 224

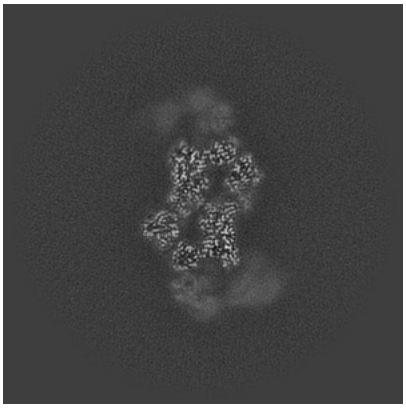


Z Index: 224

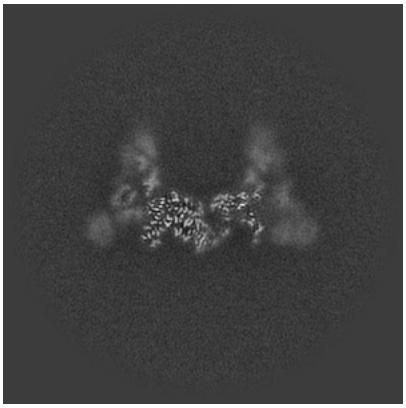
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

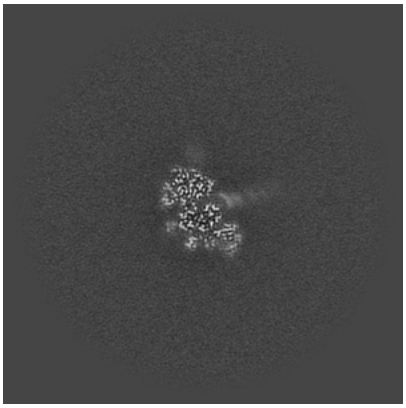
6.3.1 Primary map



X Index: 203



Y Index: 232

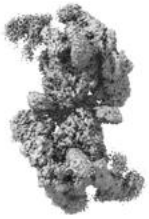


Z Index: 172

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

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

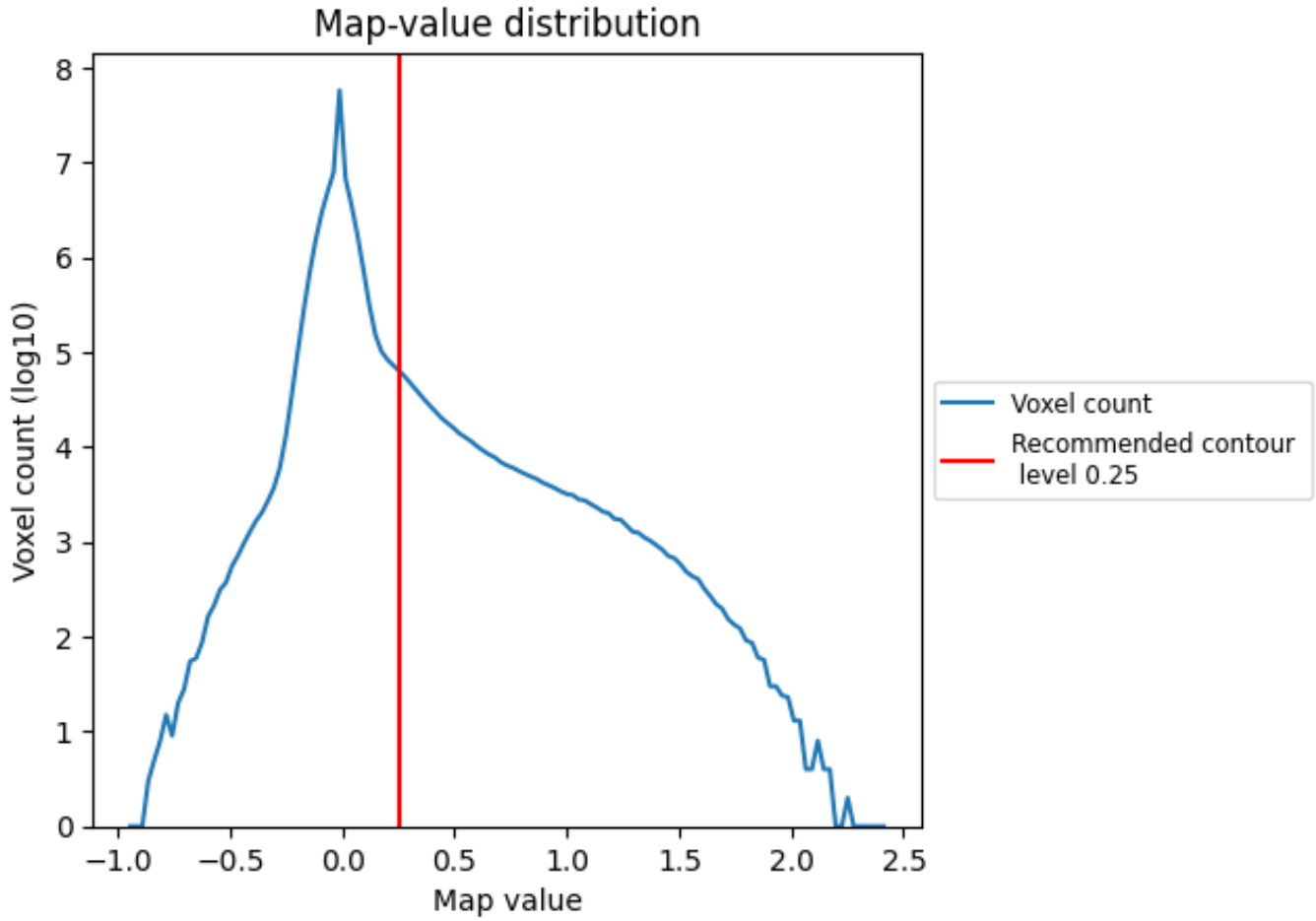
6.5 Mask visualisation (i)

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

7 Map analysis

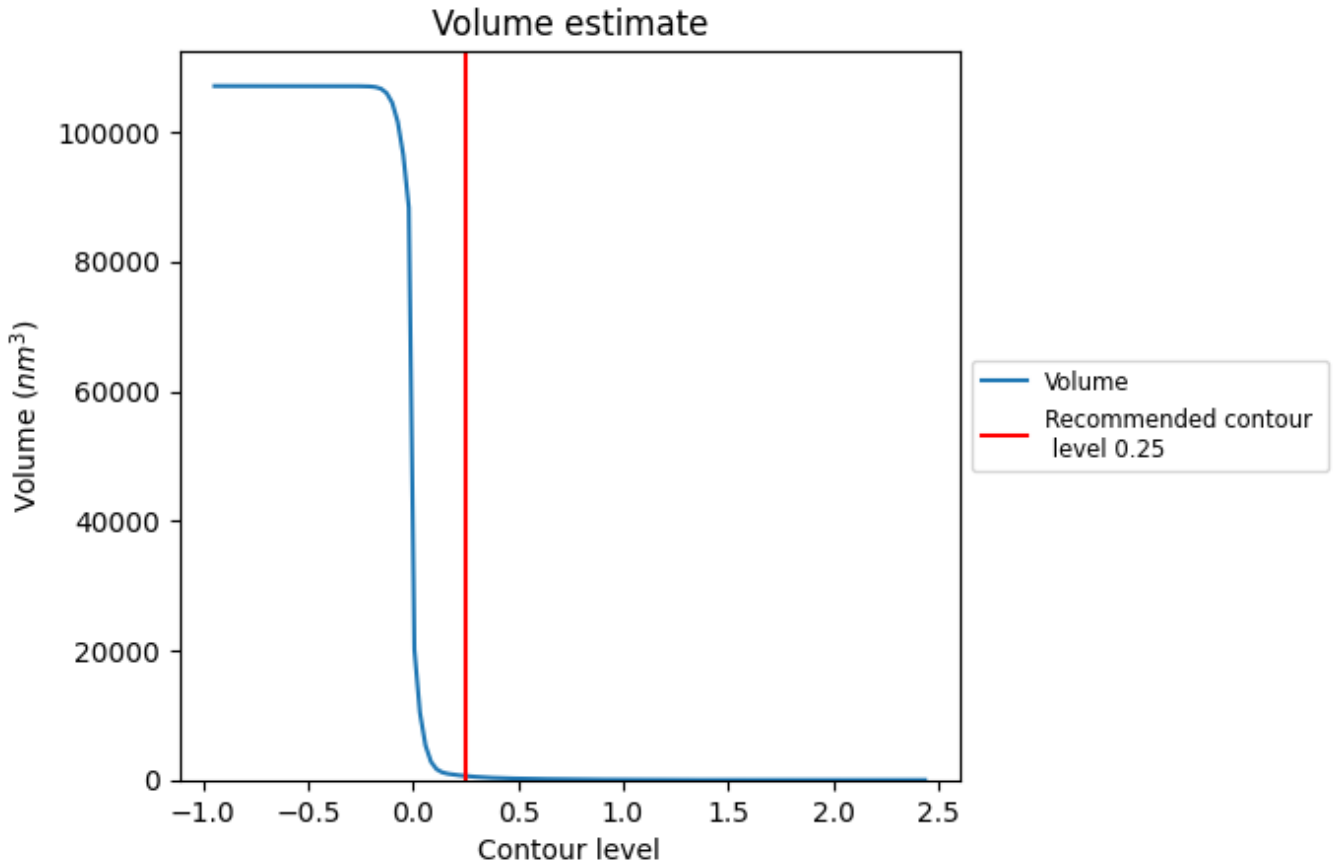
This section contains the results of statistical analysis of the map.

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.

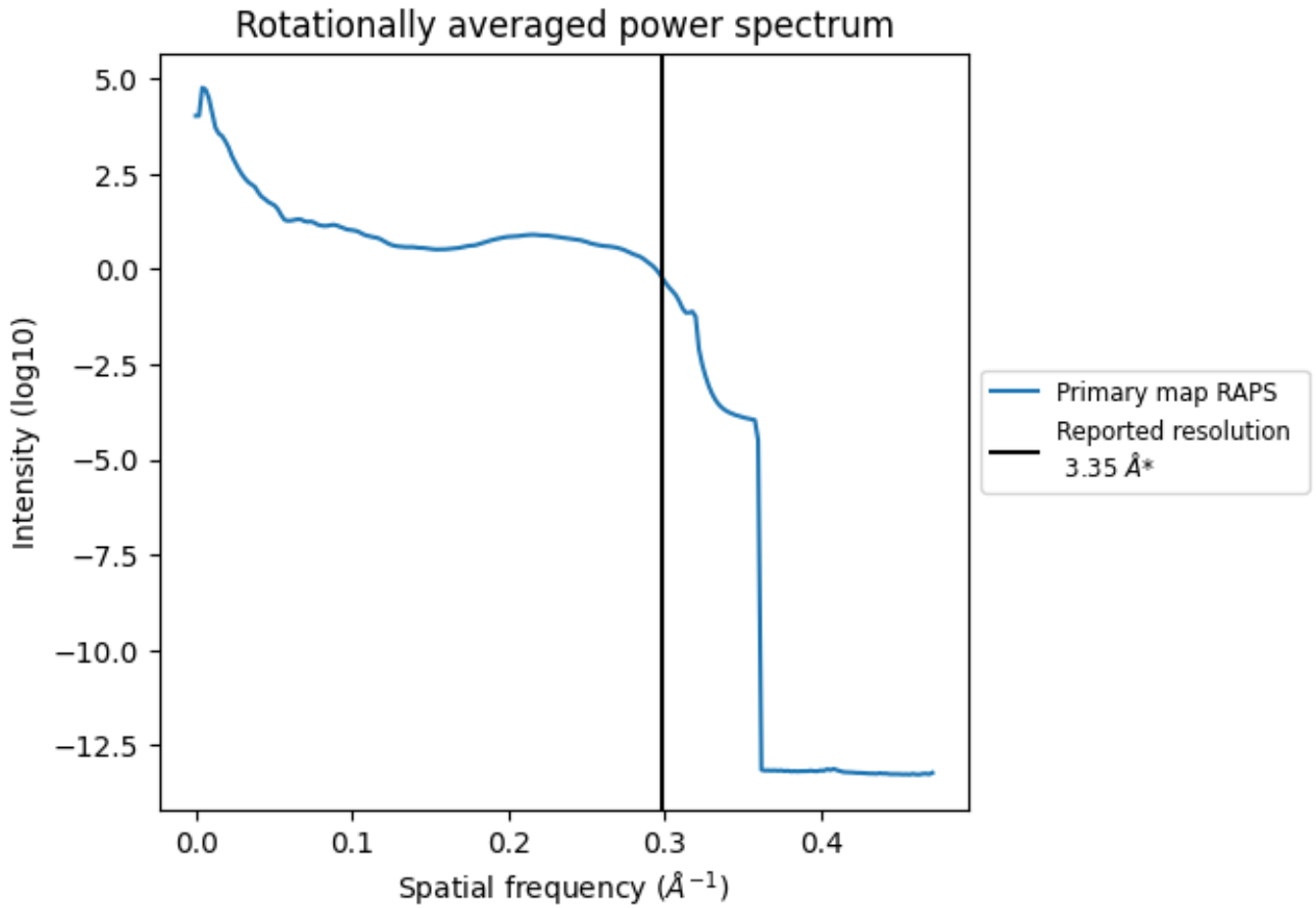
7.2 Volume estimate



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 $Å^{-1}$

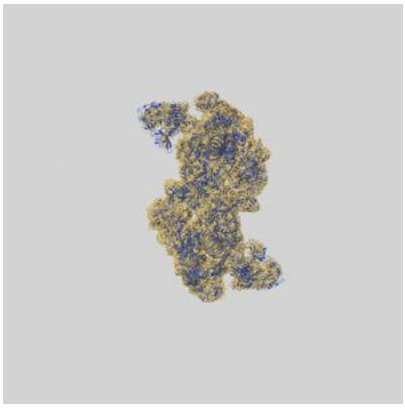
8 Fourier-Shell correlation

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

9 Map-model fit

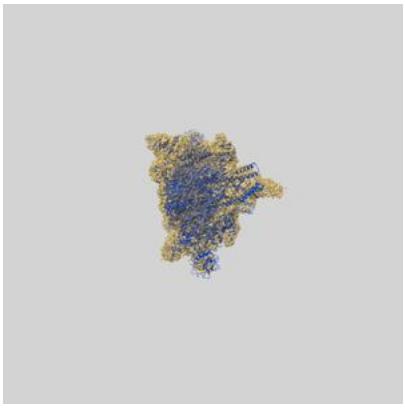
This section contains information regarding the fit between EMDB map EMD-31138 and PDB model 7EGQ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay



X

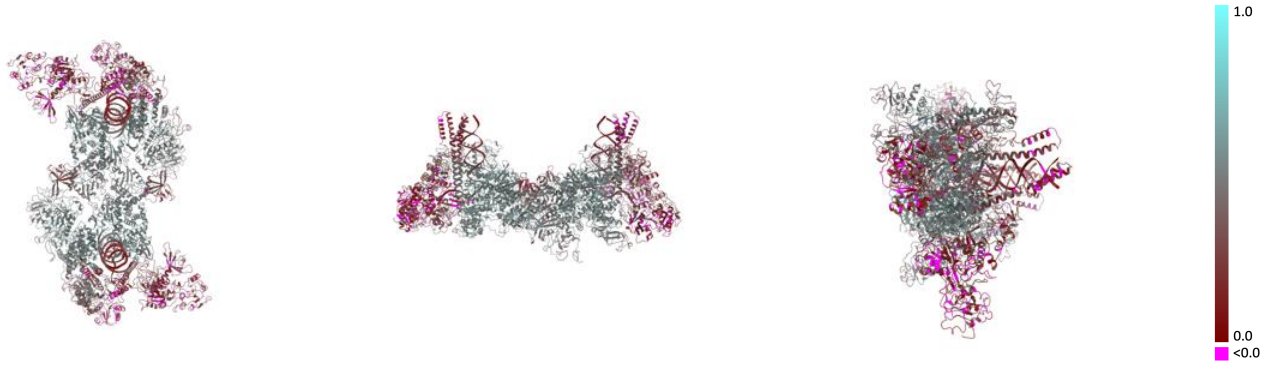
Y



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.

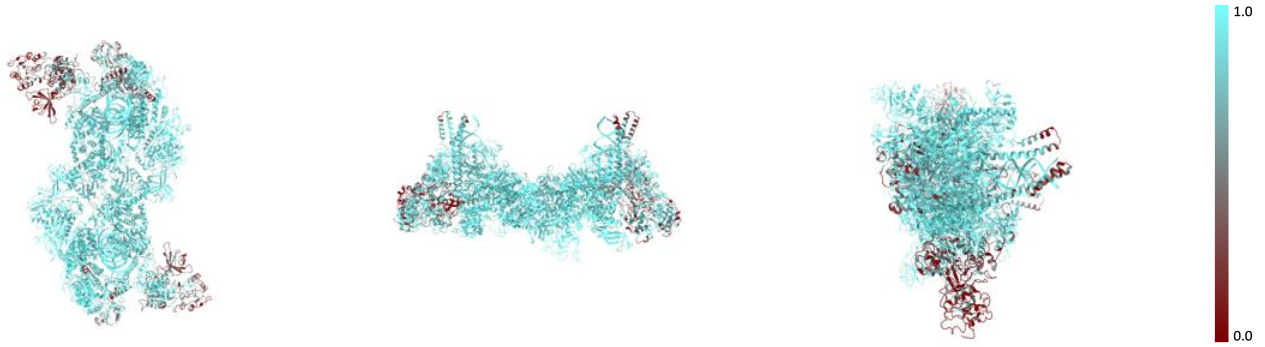
9.2 Q-score mapped to coordinate model



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.

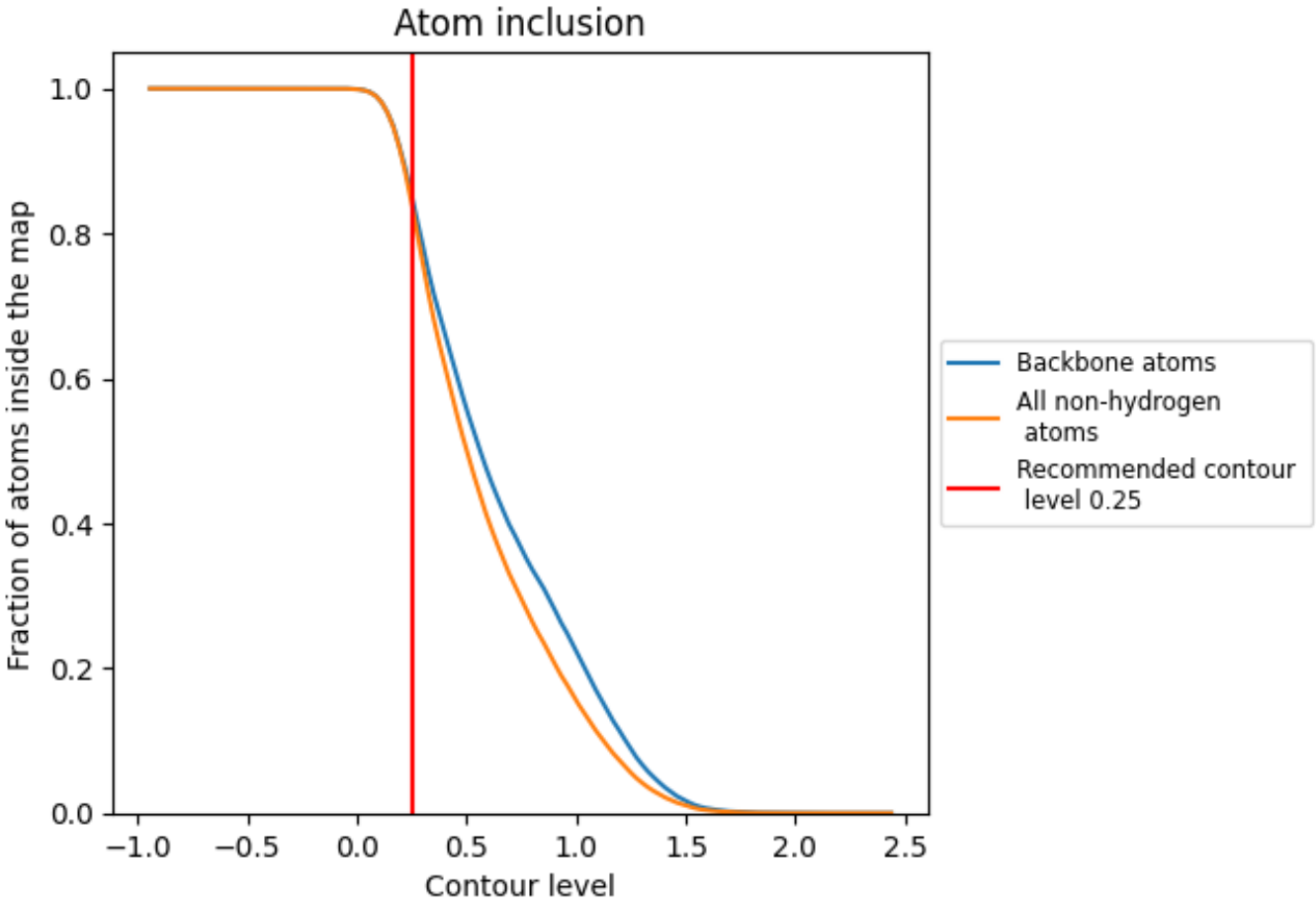
9.3 Atom inclusion mapped to coordinate model



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	0.8397	0.3840
A	0.9721	0.5200
B	0.8542	0.3890
C	0.9545	0.5070
D	0.8711	0.3790
E	0.6985	0.2140
F	0.3209	0.1710
G	0.9482	0.3630
H	0.9926	0.4660
I	0.9064	0.2680
J	0.9711	0.2770
K	0.9853	0.5130
L	0.8936	0.2740
M	0.9653	0.2800
N	0.9780	0.5320
O	0.9268	0.4190
P	0.9582	0.5070
Q	0.9205	0.4000
R	0.8713	0.3000
S	0.5356	0.1800
T	0.9318	0.3380
U	0.9915	0.4590
X	0.9673	0.4760