Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:47 pm BST

PDB ID	:	5OA1 / pdb_00005oa1
EMDB ID	:	EMD-3727
Title	:	RNA polymerase I pre-initiation complex
Authors	:	Sadian, Y.; Tafur, L.; Kosinski, J.; Jakobi, A.J.; Muller, C.W.
Deposited on	:	2017-06-20
Resolution	:	4.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

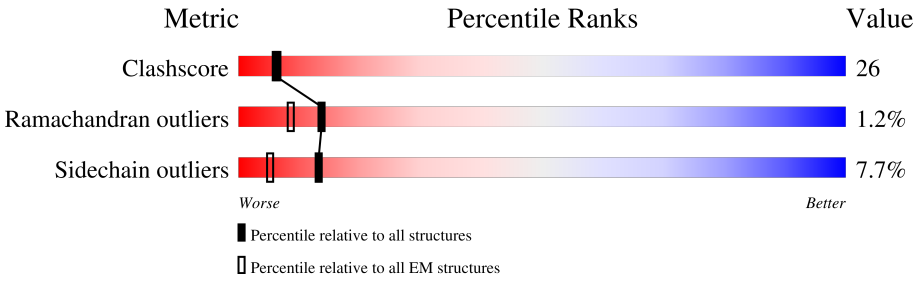
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1664	67% 20% 12%
2	B	1203	70% 25%
3	C	335	67% 23% 9%
4	D	137	5% 35% 8% 57%
5	E	215	92% 7%
6	F	155	56% 8% 35%
7	G	326	10% 47% 14% 38%
8	H	146	77% 15% 8%

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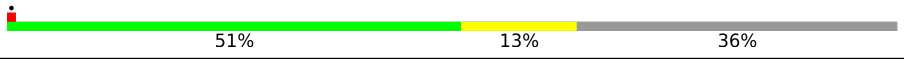
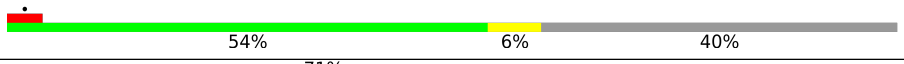
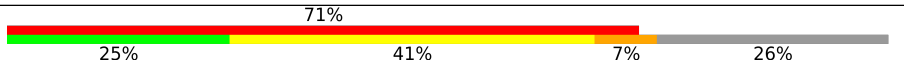
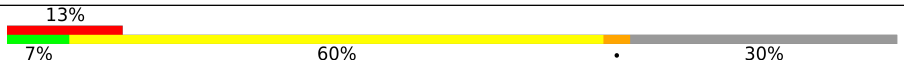
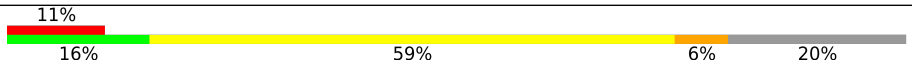
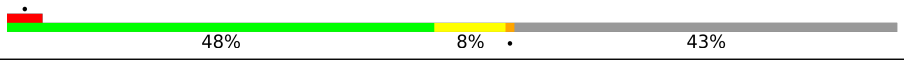
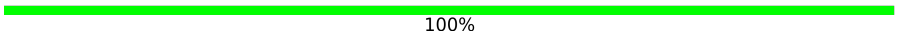
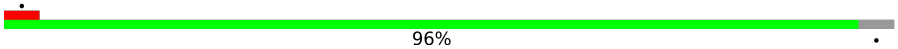
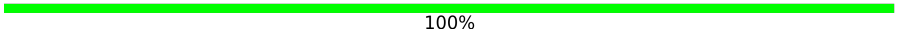
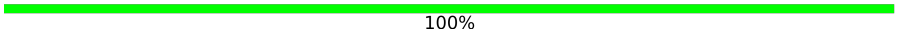
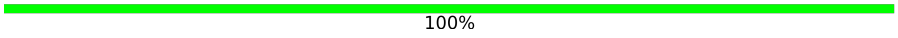
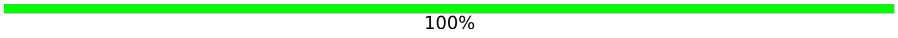
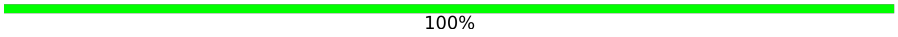
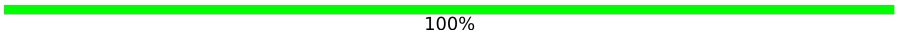
Mol	Chain	Length	Quality of chain
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	627	
16	S	70	
17	T	70	
18	U	514	
19	V	894	
20	W	507	
21	1	13	
22	2	19	
23	3	9	
23	9	9	
24	4	24	
25	5	16	
25	Q	16	
26	6	10	
26	8	10	
27	7	25	
28	P	22	
29	Z	15	
30	Y	12	

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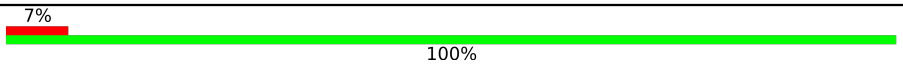
Mol	Chain	Length	Quality of chain
31	R	27	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 43459 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 DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1458	11513	7277	1997	2177	62	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1175	9327	5899	1635	1743	50	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	304	2418	1536	414	460	8	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	59	467	293	80	94	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	215	1759	1116	310	321	12	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	823	522	144	154	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	202	Total	C	N	O	S	0	0
			1600	1026	276	293	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	134	Total	C	N	O	S	0	0
			1072	676	181	211	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	124	Total	C	N	O	S	0	0
			942	584	160	189	9		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	103	Total	C	N	O	S	0	0
			810	506	132	167	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	105	Total	C	N	O	0	0
			831	528	137	166		

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	139	Total	C	N	O	S	0	0
			1103	706	179	214	4		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	463	Total	C	N	O	S	0	0
			3811	2473	623	694	21		

- Molecule 16 is a DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	49	Total	C	N	O	P	0	0
			1028	486	210	283	49		

- Molecule 17 is a DNA chain called DNA (56-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	56	Total	C	N	O	P	0	0
			1128	543	183	346	56		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	U	291	Total	C	N	O	0	0
			1164	582	291	291		

- Molecule 19 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	288	Total	C	N	O	0	0
			1152	576	288	288		

- Molecule 20 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	W	168	Total	C	N	O	0	0
			672	336	168	168		

- Molecule 21 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	1	13	Total	C	N	O	0	0
			52	26	13	13		

- Molecule 22 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	2	19	Total	C	N	O	0	0
			76	38	19	19		

- Molecule 23 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	3	9	Total	C	N	O	0	0
			36	18	9	9		
23	9	9	Total	C	N	O	0	0
			36	18	9	9		

- Molecule 24 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	4	23	Total	C	N	O	0	0
			92	46	23	23		

- Molecule 25 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	5	16	Total	C	N	O	0	0
			64	32	16	16		
25	Q	16	Total	C	N	O	0	0
			64	32	16	16		

- Molecule 26 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	6	10	Total	C	N	O	0	0
			40	20	10	10		
26	8	10	Total	C	N	O	0	0
			40	20	10	10		

- Molecule 27 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	7	25	Total	C	N	O	0	0
			100	50	25	25		

- Molecule 28 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	P	22	Total	C	N	O	0	0
			88	44	22	22		

- Molecule 29 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Z	15	Total	C	N	O	0	0
			60	30	15	15		

- Molecule 30 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	12	Total	C	N	O	0	0
			48	24	12	12		

- Molecule 31 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	R	27	Total	C	N	O	0	0
			108	54	27	27		

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	A	2	Total	Zn	0
			2	2	
32	B	1	Total	Zn	0
			1	1	
32	I	2	Total	Zn	0
			2	2	

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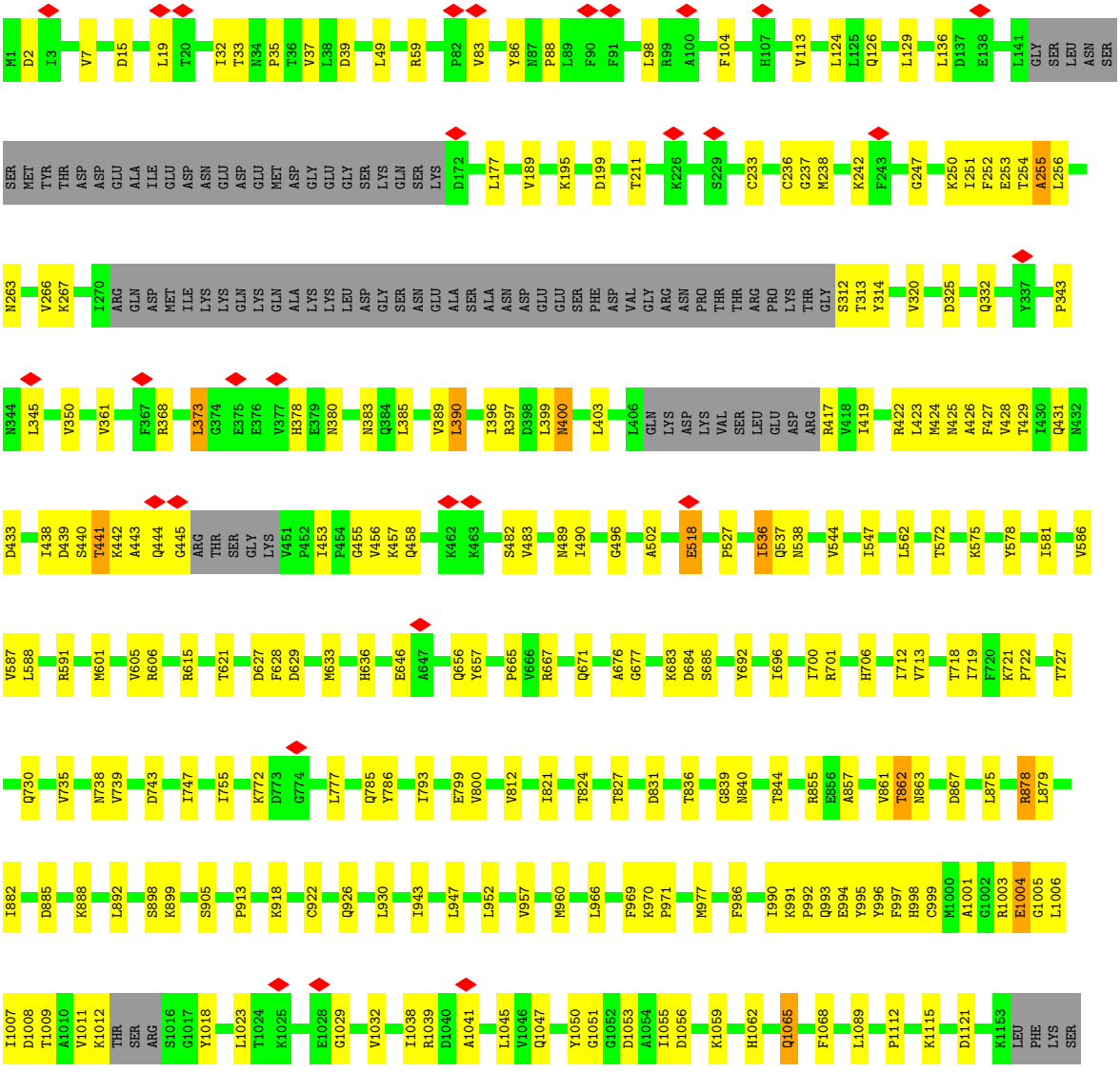
Mol	Chain	Residues	Atoms	AltConf
32	J	1	Total Zn 1 1	0
32	L	1	Total Zn 1 1	0

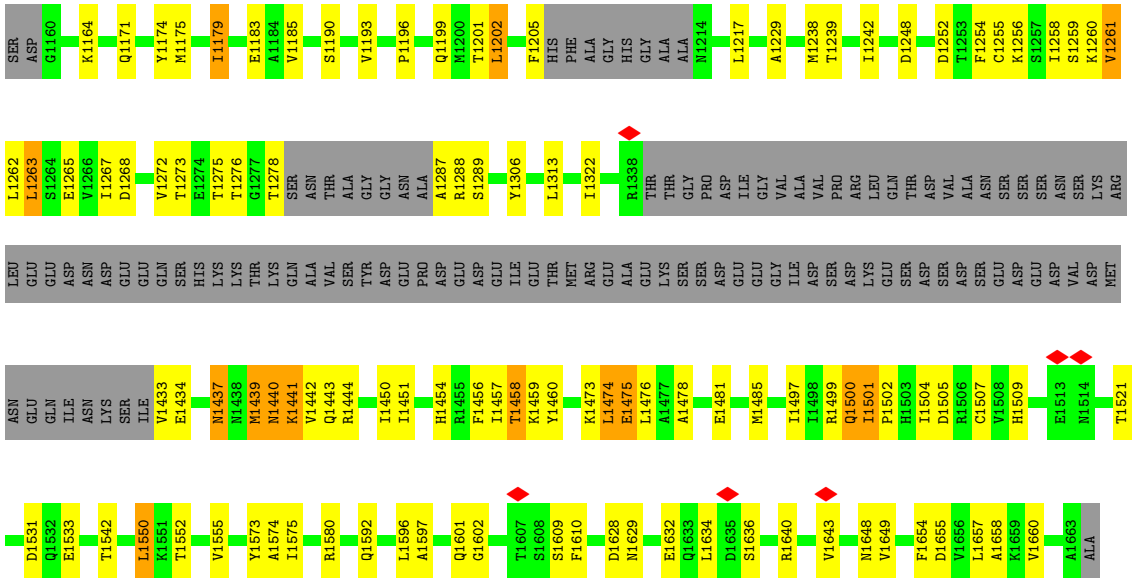
3 Residue-property plots (i)

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: DNA-directed RNA polymerase I subunit RPA190

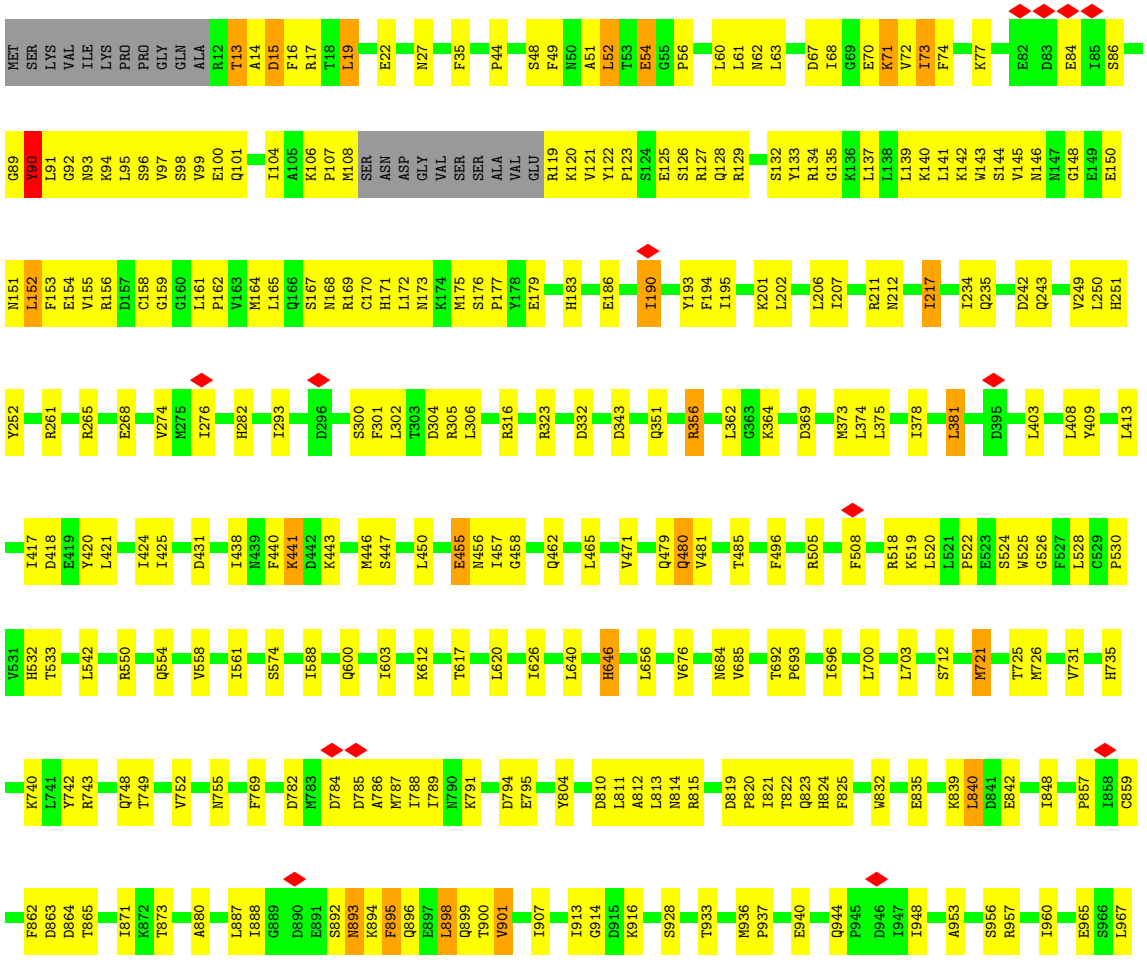
Chain A:

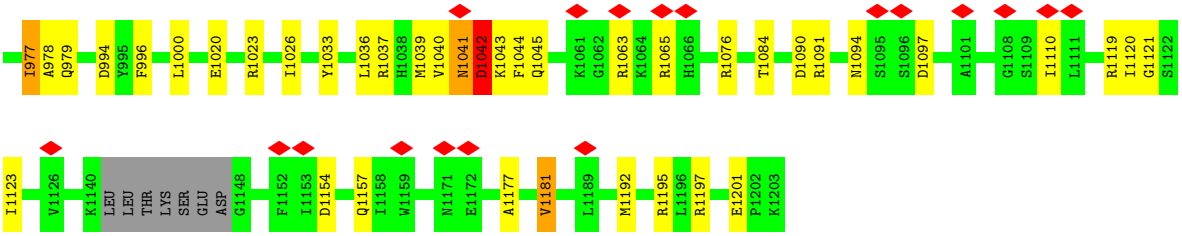




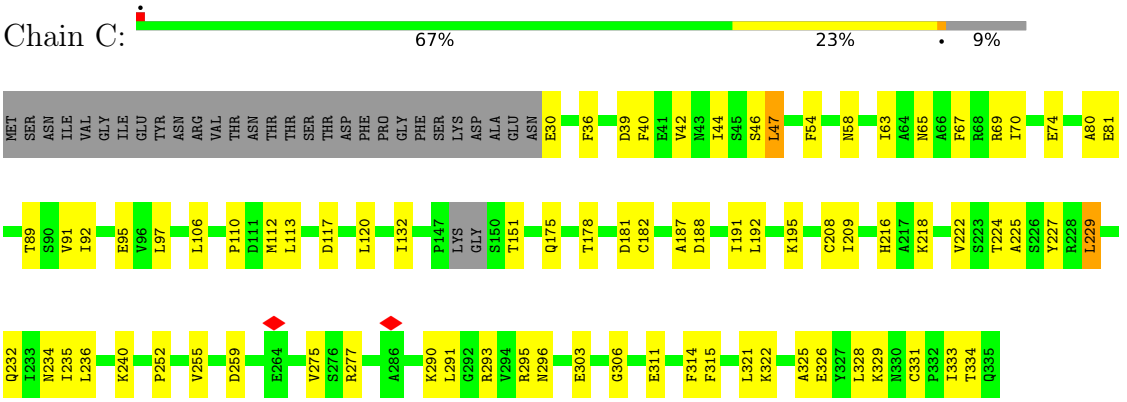
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

Chain B:

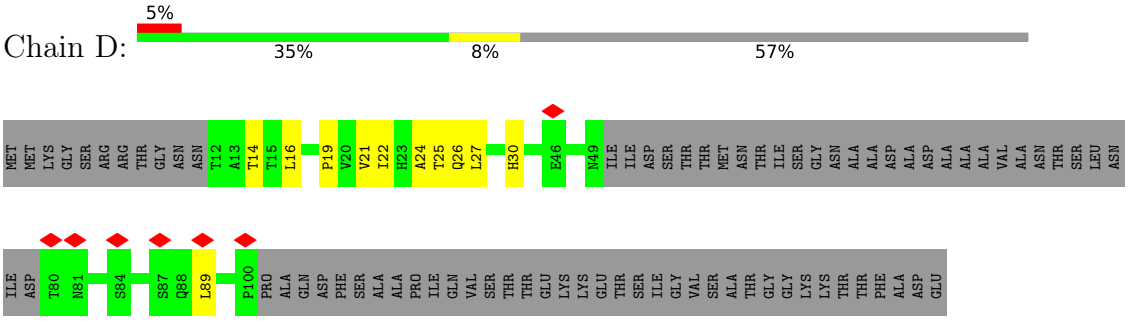




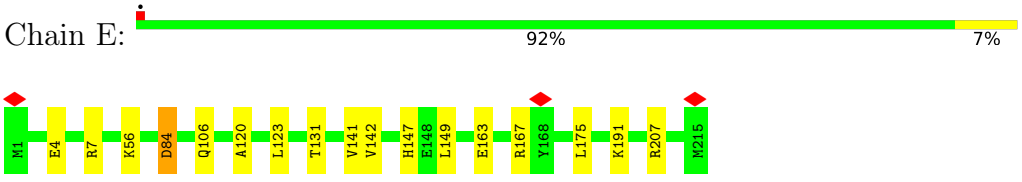
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



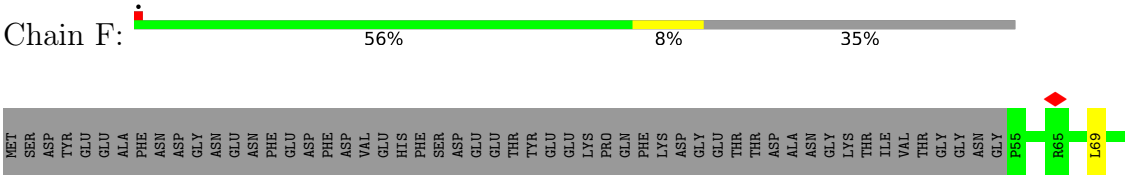
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

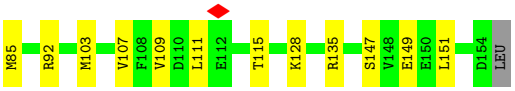


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

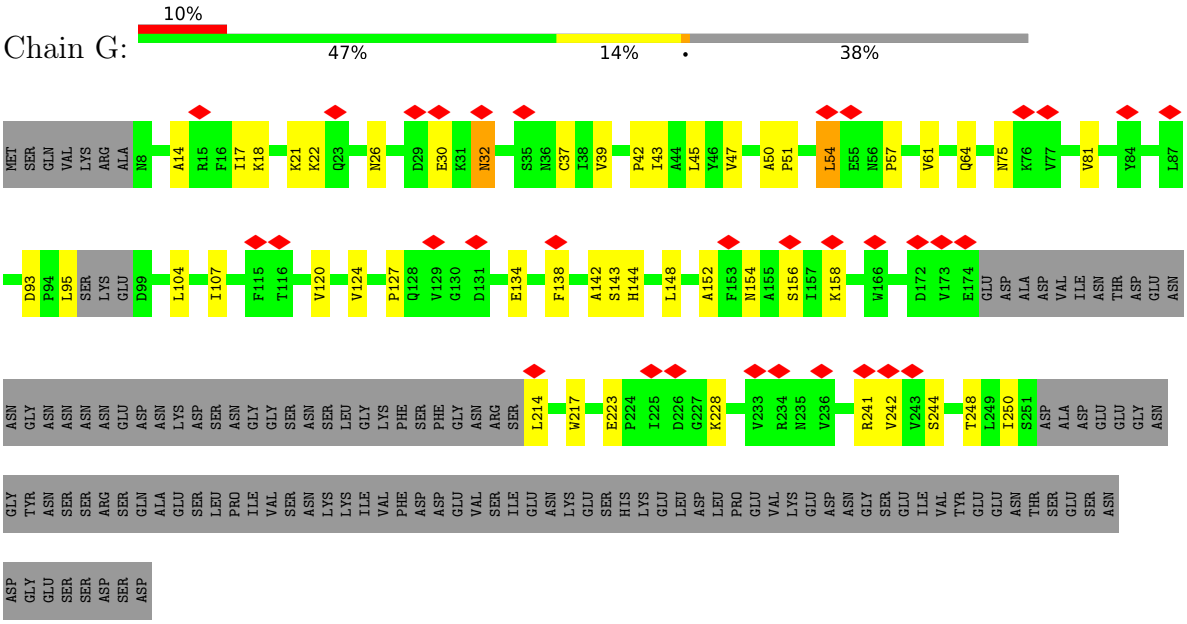


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

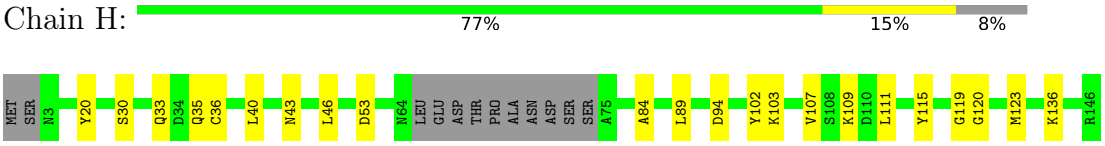




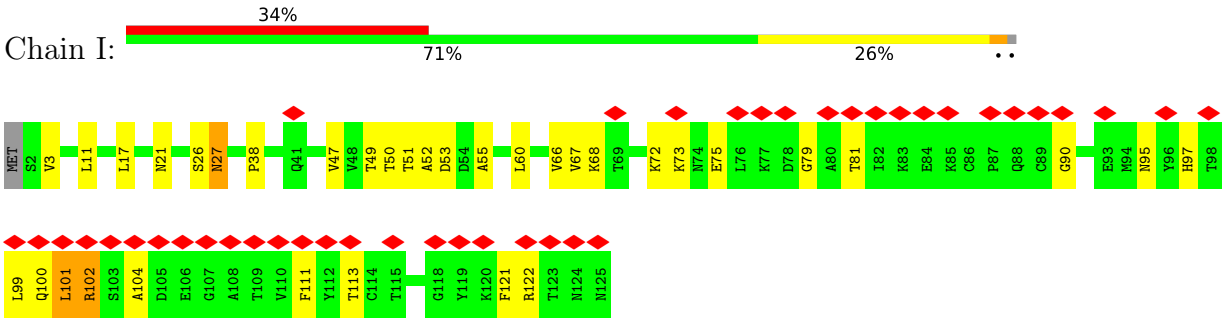
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43



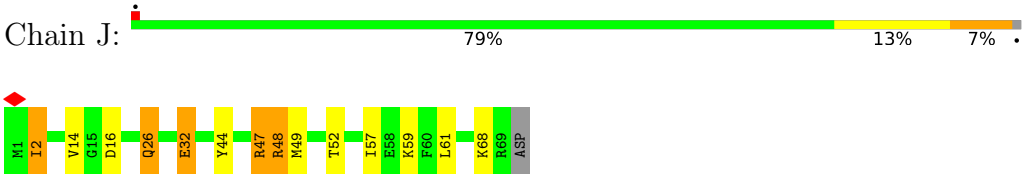
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

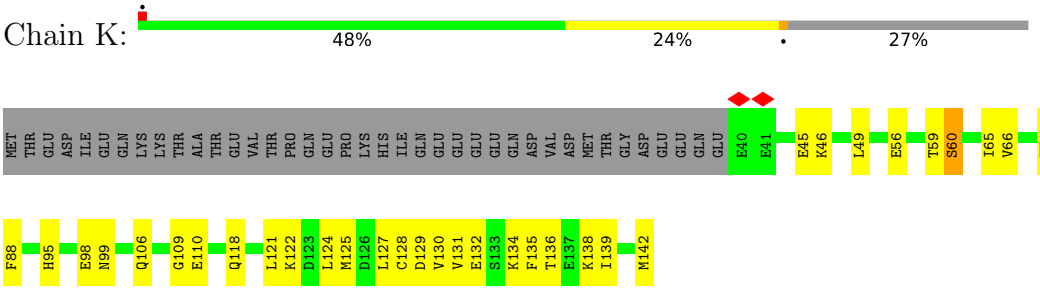


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



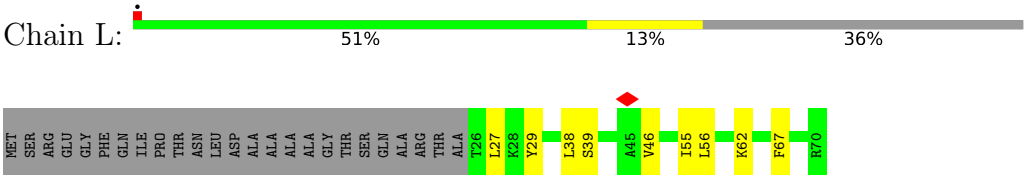
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



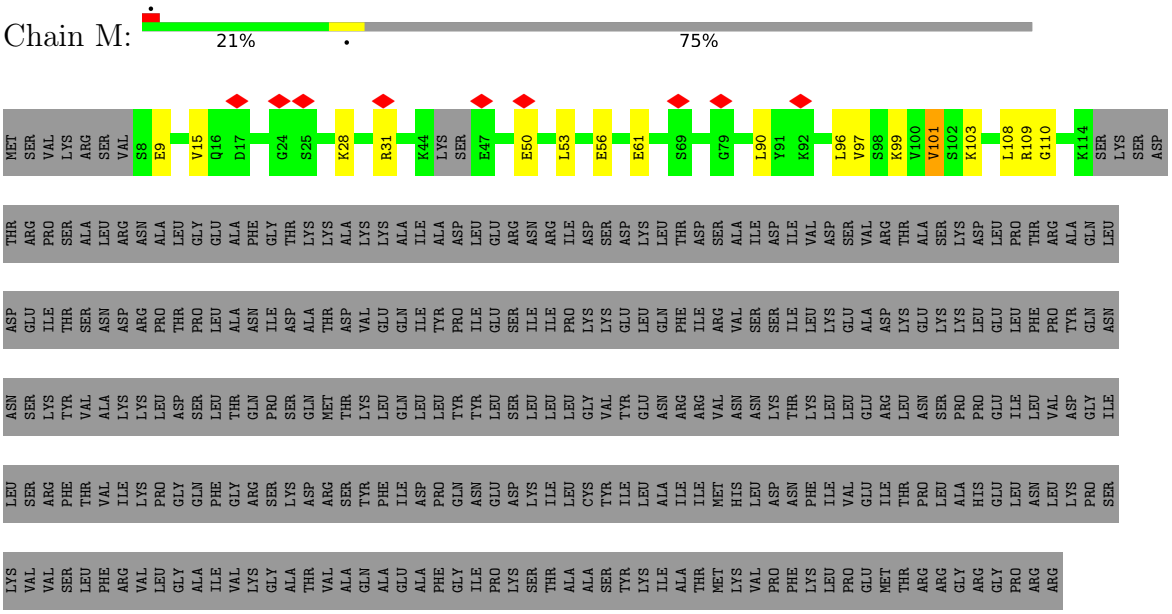
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



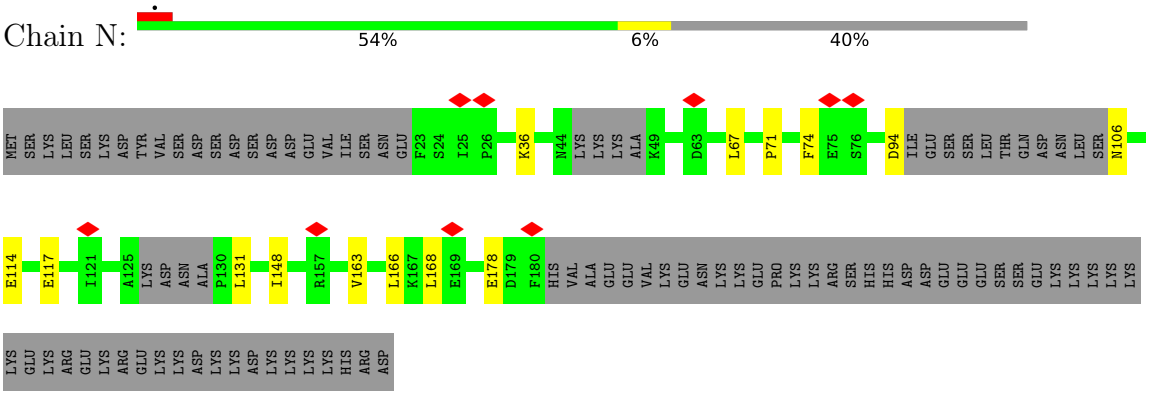
• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain M:



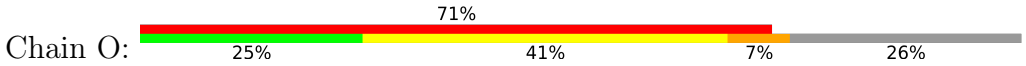
• Molecule 14: DNA-directed RNA polymerase I subunit RPA34

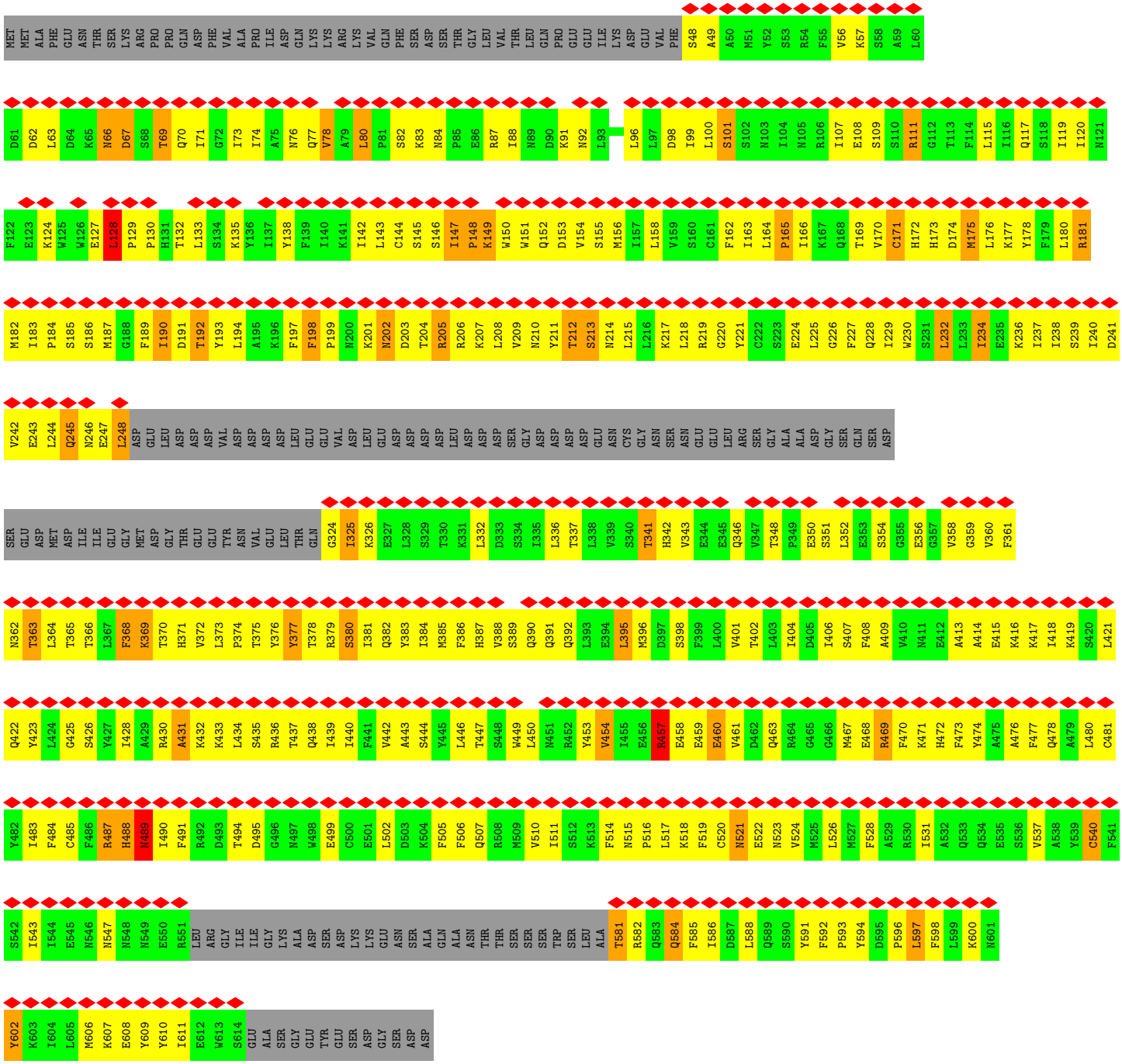
Chain N:



• Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3

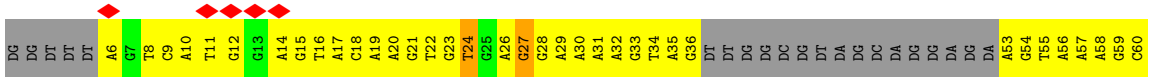
Chain O:





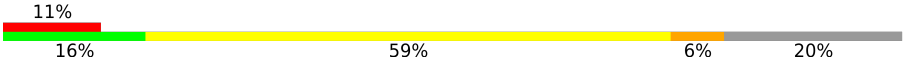
• Molecule 16: DNA (49-MER)

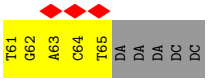
Chain S:



• Molecule 17: DNA (56-MER)

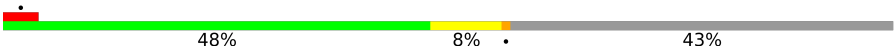
Chain T:

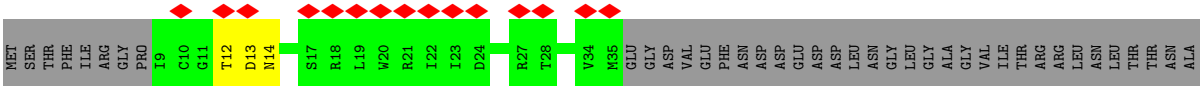


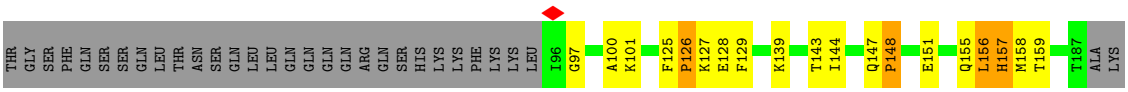


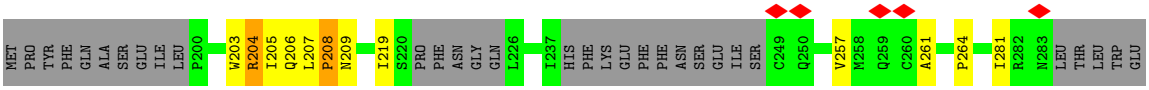
• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN7

Chain U:



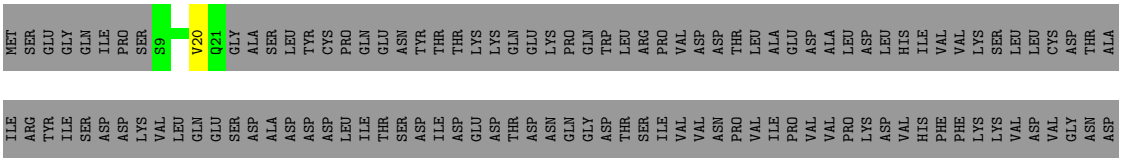


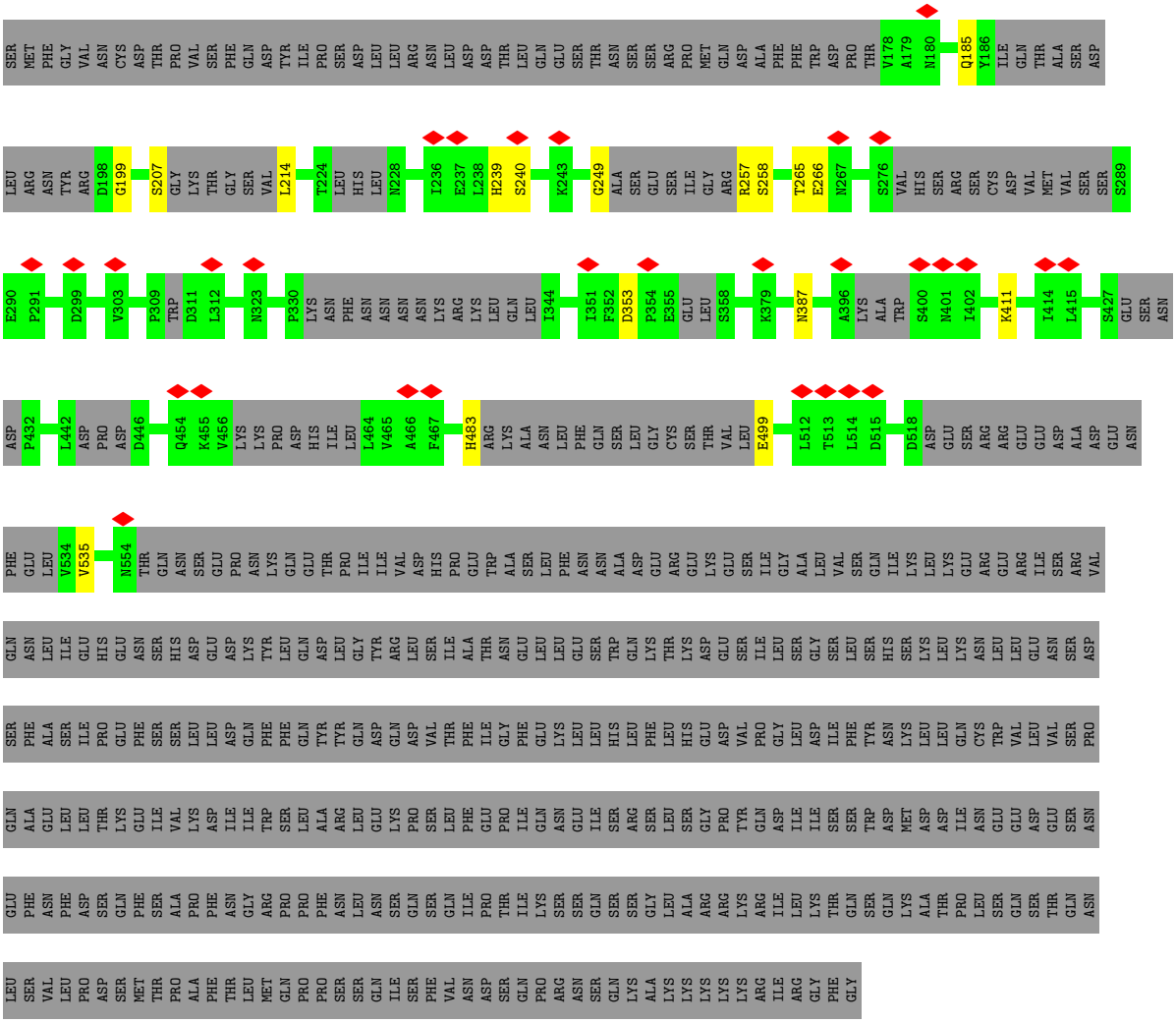




• Molecule 19: RNA polymerase I-specific transcription initiation factor RRN6

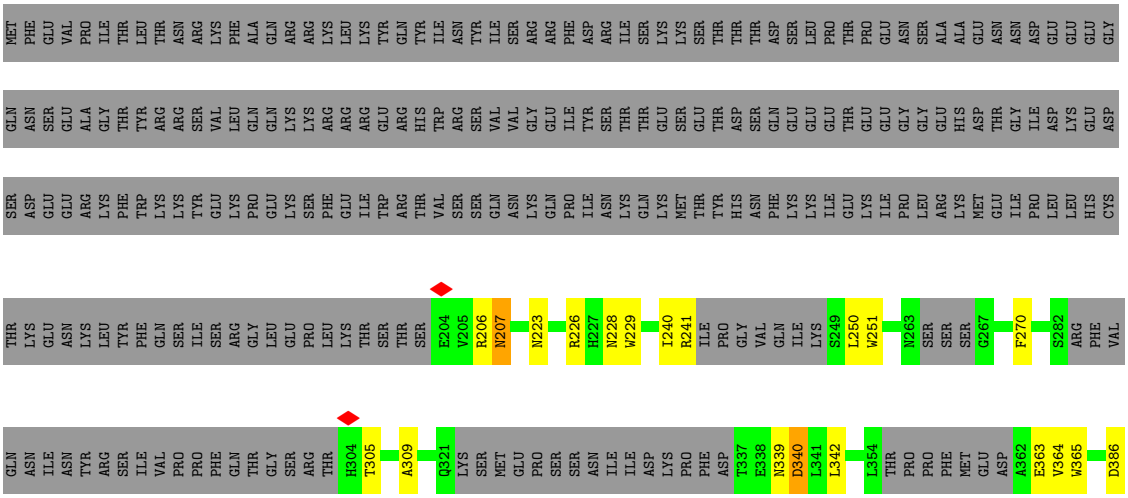
Chain V:

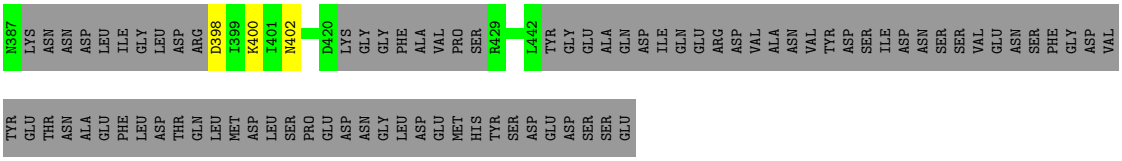




• Molecule 20: RNA polymerase I-specific transcription initiation factor RRN11

Chain W:





• Molecule 21: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 1: 100%

There are no outlier residues recorded for this chain.

• Molecule 22: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 2: 100%

There are no outlier residues recorded for this chain.

• Molecule 23: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 3: 100%

There are no outlier residues recorded for this chain.

• Molecule 23: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 9: 100%

There are no outlier residues recorded for this chain.

• Molecule 24: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 4: 96%

• Molecule 25: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 5: 100%

There are no outlier residues recorded for this chain.

• Molecule 25: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain Q: 100%

There are no outlier residues recorded for this chain.

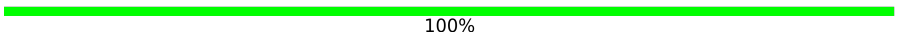
• Molecule 26: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 6:

There are no outlier residues recorded for this chain.

• Molecule 26: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

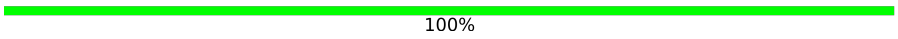
Chain 8:



There are no outlier residues recorded for this chain.

• Molecule 27: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 7:



There are no outlier residues recorded for this chain.

• Molecule 28: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

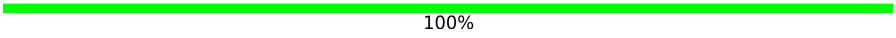
Chain P:

• Molecule 29: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain Z:

• Molecule 30: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

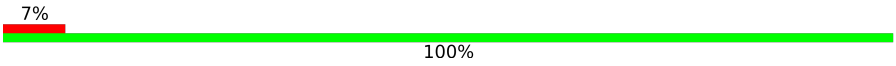
Chain Y:

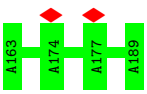


There are no outlier residues recorded for this chain.

• Molecule 31: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain R:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38589	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 ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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

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	0.39	0/11722	0.58	0/15832
2	B	0.38	0/9534	0.59	1/12889 (0.0%)
3	C	0.39	0/2469	0.61	0/3347
4	D	0.40	0/473	0.54	0/641
5	E	0.40	0/1795	0.55	0/2416
6	F	0.39	0/838	0.54	0/1129
7	G	0.39	0/1637	0.58	0/2226
8	H	0.39	0/1090	0.57	0/1476
9	I	0.40	0/955	0.56	0/1288
10	J	0.40	0/578	0.62	0/775
11	K	0.38	0/821	0.57	0/1108
12	L	0.38	0/361	0.61	0/478
13	M	0.38	0/846	0.53	0/1136
14	N	0.38	0/1124	0.52	0/1512
15	O	0.38	1/3897 (0.0%)	0.58	2/5268 (0.0%)
16	S	1.37	3/1160 (0.3%)	2.15	76/1790 (4.2%)
17	T	1.32	5/1256 (0.4%)	2.08	79/1930 (4.1%)
18	U	0.81	1/1155 (0.1%)	0.89	3/1428 (0.2%)
19	V	0.92	0/1136	0.91	0/1392
20	W	0.58	0/664	0.87	3/816 (0.4%)
21	1	0.53	0/51	0.92	0/62
22	2	0.54	0/75	0.97	0/92
23	3	0.15	0/35	0.27	0/42
23	9	0.55	0/35	0.95	0/42
24	4	0.39	0/91	0.69	0/112
25	5	0.54	0/63	0.97	0/77
25	Q	0.53	0/62	0.96	0/74
26	6	0.54	0/39	0.95	0/47
26	8	0.16	0/39	0.26	0/47
27	7	0.42	0/99	0.74	0/122
28	P	0.46	0/87	0.81	0/107
29	Z	0.49	0/59	0.95	0/72

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
30	Y	0.54	0/47	0.96	0/57
31	R	0.41	0/107	0.80	0/132
All	All	0.52	10/44400 (0.0%)	0.79	164/59962 (0.3%)

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
16	S	0	2
17	T	0	2
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	S	6	DA	O3'-P	10.54	1.73	1.61
17	T	43	DC	O3'-P	8.45	1.71	1.61
17	T	42	DT	O3'-P	8.06	1.70	1.61
15	O	198	PHE	C-N	-7.16	1.20	1.34
18	U	139	LYS	C-O	6.23	1.35	1.23
16	S	26	DA	N3-C4	5.77	1.38	1.34
17	T	47	DA	O3'-P	5.75	1.68	1.61
16	S	19	DA	N3-C4	5.48	1.38	1.34
17	T	35	DC	C1'-N1	5.23	1.56	1.49
17	T	47	DA	C4'-C3'	5.05	1.58	1.53

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	S	35	DA	N1-C6-N6	-11.19	111.89	118.60
17	T	63	DA	N1-C6-N6	-10.14	112.52	118.60
17	T	47	DA	O4'-C1'-N9	10.13	115.09	108.00
17	T	48	DC	N3-C2-O2	-9.96	114.93	121.90
17	T	63	DA	C5-C6-N1	9.24	122.32	117.70
16	S	29	DA	N1-C6-N6	-9.12	113.13	118.60
16	S	36	DG	N3-C2-N2	-8.98	113.61	119.90
16	S	32	DA	N1-C6-N6	-8.88	113.27	118.60
16	S	6	DA	OP1-P-O3'	8.85	124.66	105.20
16	S	21	DG	O4'-C1'-N9	8.53	113.97	108.00
16	S	23	DG	O4'-C1'-N9	8.49	113.94	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	42	DT	N1-C1'-C2'	8.44	128.63	112.60
17	T	56	DC	N3-C2-O2	-8.32	116.07	121.90
16	S	32	DA	C5-C6-N1	8.25	121.82	117.70
16	S	35	DA	C5-C6-N1	8.24	121.82	117.70
18	U	156	LEU	N-CA-C	-8.23	88.78	111.00
17	T	37	DA	C5-C6-N1	8.16	121.78	117.70
16	S	14	DA	N1-C6-N6	-8.10	113.74	118.60
16	S	31	DA	C5-C6-N1	7.86	121.63	117.70
16	S	9	DC	N3-C2-O2	-7.82	116.43	121.90
17	T	48	DC	N1-C2-O2	7.77	123.56	118.90
16	S	29	DA	C5-C6-N1	7.76	121.58	117.70
16	S	35	DA	C4-C5-C6	-7.75	113.13	117.00
17	T	39	DT	C6-C5-C7	-7.74	118.25	122.90
16	S	14	DA	C5-C6-N1	7.62	121.51	117.70
17	T	44	DC	N3-C2-O2	-7.47	116.67	121.90
15	O	460	GLU	N-CA-C	-7.42	90.95	111.00
17	T	36	DT	C2'-C3'-O3'	-7.41	88.15	112.60
17	T	47	DA	C5-C6-N1	7.32	121.36	117.70
18	U	148	PRO	N-CA-C	7.31	131.10	112.10
17	T	46	DC	N3-C2-O2	-7.30	116.79	121.90
16	S	30	DA	N1-C6-N6	-7.17	114.30	118.60
16	S	10	DA	C5-C6-N1	7.17	121.28	117.70
17	T	49	DA	N1-C6-N6	-7.16	114.30	118.60
16	S	30	DA	C5-C6-N1	7.14	121.27	117.70
17	T	56	DC	N1-C2-O2	7.11	123.17	118.90
17	T	55	DA	C5-C6-N1	7.04	121.22	117.70
16	S	14	DA	C4-C5-C6	-7.02	113.49	117.00
17	T	64	DC	N3-C2-O2	-7.01	116.99	121.90
16	S	19	DA	N1-C6-N6	-7.00	114.40	118.60
16	S	31	DA	N1-C6-N6	-7.00	114.40	118.60
17	T	51	DT	C6-C5-C7	-6.99	118.71	122.90
17	T	40	DT	C6-C5-C7	-6.92	118.75	122.90
17	T	49	DA	C5-C6-N1	6.83	121.11	117.70
17	T	60	DA	C5-C6-N1	6.80	121.10	117.70
16	S	17	DA	C5-C6-N1	6.79	121.10	117.70
16	S	20	DA	N1-C6-N6	-6.79	114.53	118.60
16	S	33	DG	N1-C6-O6	-6.79	115.83	119.90
17	T	58	DC	N3-C2-O2	-6.76	117.17	121.90
17	T	38	DC	N3-C2-O2	-6.75	117.17	121.90
17	T	50	DC	N3-C2-O2	-6.75	117.17	121.90
16	S	34	DT	C6-C5-C7	-6.72	118.87	122.90
17	T	59	DC	N3-C2-O2	-6.68	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	61	DT	N3-C2-O2	-6.67	118.30	122.30
16	S	16	DT	N3-C2-O2	-6.66	118.31	122.30
16	S	18	DC	N3-C2-O2	-6.66	117.24	121.90
17	T	49	DA	C4-C5-C6	-6.64	113.68	117.00
16	S	10	DA	N1-C6-N6	-6.64	114.61	118.60
16	S	9	DC	N1-C2-O2	6.63	122.88	118.90
16	S	24	DT	C6-C5-C7	-6.59	118.95	122.90
17	T	45	DT	C6-C5-C7	-6.58	118.95	122.90
17	T	60	DA	N1-C6-N6	-6.52	114.69	118.60
16	S	36	DG	N1-C6-O6	-6.45	116.03	119.90
16	S	26	DA	C5-C6-N1	6.44	120.92	117.70
17	T	60	DA	C4-C5-C6	-6.44	113.78	117.00
17	T	63	DA	C4-C5-C6	-6.43	113.79	117.00
16	S	10	DA	C4-C5-C6	-6.35	113.82	117.00
16	S	17	DA	N1-C6-N6	-6.35	114.79	118.60
17	T	53	DG	O4'-C1'-N9	6.35	112.45	108.00
16	S	31	DA	C4-C5-C6	-6.31	113.84	117.00
16	S	24	DT	N3-C2-O2	-6.31	118.51	122.30
17	T	57	DT	N3-C2-O2	-6.21	118.57	122.30
16	S	19	DA	C5-C6-N1	6.20	120.80	117.70
16	S	11	DT	N3-C2-O2	-6.19	118.58	122.30
16	S	8	DT	N3-C2-O2	-6.16	118.61	122.30
17	T	47	DA	O4'-C4'-C3'	6.16	109.69	106.00
17	T	42	DT	O4'-C1'-C2'	6.15	110.82	105.90
16	S	20	DA	C5-C6-N1	6.15	120.77	117.70
17	T	46	DC	N1-C2-O2	6.14	122.59	118.90
16	S	26	DA	N1-C6-N6	-6.12	114.93	118.60
16	S	17	DA	C4-C5-C6	-6.08	113.96	117.00
17	T	38	DC	N1-C2-O2	6.08	122.55	118.90
17	T	41	DT	C6-C5-C7	-6.08	119.25	122.90
16	S	27	DG	N1-C6-O6	-6.07	116.26	119.90
17	T	52	DT	C6-C5-C7	-6.01	119.29	122.90
20	W	309	ALA	N-CA-C	6.00	127.21	111.00
16	S	36	DG	O4'-C1'-N9	5.97	112.18	108.00
16	S	34	DT	O5'-P-OP2	-5.97	100.33	105.70
17	T	47	DA	C4'-C3'-O3'	5.94	124.54	109.70
17	T	57	DT	C6-C5-C7	-5.93	119.34	122.90
17	T	19	DA	O4'-C1'-N9	5.92	112.14	108.00
16	S	15	DG	N3-C2-N2	-5.91	115.76	119.90
17	T	47	DA	C4'-C3'-C2'	-5.90	97.79	103.10
16	S	20	DA	O4'-C1'-N9	5.89	112.13	108.00
17	T	43	DC	P-O3'-C3'	5.89	126.77	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	47	DA	C4-C5-C6	-5.88	114.06	117.00
17	T	37	DA	C4-C5-C6	-5.88	114.06	117.00
16	S	16	DT	C6-C5-C7	-5.86	119.38	122.90
20	W	400	LYS	N-CA-C	5.84	126.78	111.00
17	T	65	DT	C6-C5-C7	-5.82	119.41	122.90
16	S	30	DA	C4-C5-C6	-5.80	114.10	117.00
17	T	41	DT	N3-C2-O2	-5.79	118.83	122.30
16	S	28	DG	P-O3'-C3'	5.78	126.63	119.70
16	S	8	DT	C6-C5-C7	-5.73	119.46	122.90
16	S	23	DG	N1-C6-O6	-5.71	116.47	119.90
16	S	10	DA	O5'-P-OP2	-5.69	100.58	105.70
17	T	40	DT	N3-C2-O2	-5.66	118.90	122.30
17	T	48	DC	OP1-P-OP2	-5.64	111.14	119.60
16	S	32	DA	C4-C5-C6	-5.59	114.20	117.00
17	T	37	DA	O5'-P-OP2	-5.58	100.68	105.70
16	S	20	DA	C4-C5-C6	-5.58	114.21	117.00
17	T	51	DT	N3-C2-O2	-5.57	118.95	122.30
17	T	39	DT	O5'-P-OP2	-5.56	100.70	105.70
17	T	19	DA	O4'-C1'-C2'	5.54	110.33	105.90
16	S	22	DT	N3-C2-O2	-5.51	118.99	122.30
17	T	43	DC	C4'-C3'-O3'	-5.50	95.96	109.70
16	S	34	DT	N3-C2-O2	-5.49	119.00	122.30
17	T	50	DC	N1-C2-O2	5.49	122.19	118.90
17	T	50	DC	P-O3'-C3'	5.48	126.27	119.70
17	T	64	DC	N1-C2-O2	5.48	122.19	118.90
20	W	270	PHE	N-CA-C	5.47	125.78	111.00
16	S	22	DT	C6-C5-C7	-5.45	119.63	122.90
2	B	90	TYR	N-CA-C	5.43	125.66	111.00
16	S	15	DG	O4'-C1'-N9	5.42	111.79	108.00
17	T	59	DC	N1-C2-O2	5.42	122.15	118.90
17	T	51	DT	O4'-C1'-N1	5.42	111.79	108.00
17	T	37	DA	N1-C6-N6	-5.41	115.36	118.60
16	S	26	DA	C4-C5-C6	-5.38	114.31	117.00
17	T	55	DA	C4-C5-C6	-5.38	114.31	117.00
17	T	61	DT	C6-C5-C7	-5.37	119.68	122.90
16	S	28	DG	C4'-C3'-C2'	-5.36	98.28	103.10
16	S	21	DG	N1-C6-O6	-5.36	116.69	119.90
16	S	33	DG	O4'-C1'-N9	5.35	111.75	108.00
17	T	17	DG	O3'-P-O5'	5.35	114.16	104.00
16	S	19	DA	C4-C5-C6	-5.35	114.33	117.00
16	S	22	DT	O4'-C1'-N1	5.35	111.74	108.00
17	T	42	DT	P-O3'-C3'	5.34	126.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	S	28	DG	O4'-C1'-C2'	-5.32	101.64	105.90
17	T	62	DG	O4'-C1'-N9	5.31	111.72	108.00
16	S	28	DG	O4'-C1'-N9	5.28	111.70	108.00
17	T	40	DT	O4'-C1'-N1	5.26	111.69	108.00
17	T	35	DC	C2'-C3'-O3'	-5.26	95.25	112.60
17	T	58	DC	N1-C2-O2	5.25	122.05	118.90
17	T	52	DT	N3-C2-O2	-5.25	119.15	122.30
16	S	33	DG	N3-C2-N2	-5.22	116.24	119.90
16	S	34	DT	C5-C6-N1	-5.20	120.58	123.70
17	T	43	DC	O4'-C1'-N1	5.20	111.64	108.00
16	S	32	DA	O4'-C1'-N9	5.17	111.62	108.00
17	T	54	DT	N3-C2-O2	-5.15	119.21	122.30
17	T	39	DT	O4'-C1'-N1	5.15	111.60	108.00
18	U	151	GLU	N-CA-C	5.15	124.89	111.00
17	T	46	DC	O4'-C1'-N1	5.14	111.60	108.00
17	T	38	DC	N3-C4-C5	5.12	123.95	121.90
17	T	47	DA	N1-C6-N6	-5.12	115.53	118.60
16	S	23	DG	N3-C2-N2	-5.11	116.33	119.90
16	S	11	DT	C6-C5-C7	-5.10	119.84	122.90
16	S	12	DG	O4'-C1'-N9	5.10	111.57	108.00
16	S	20	DA	P-O3'-C3'	5.08	125.80	119.70
17	T	64	DC	O5'-P-OP2	-5.06	101.14	105.70
15	O	128	LEU	C-N-CD	5.05	139.01	128.40
17	T	44	DC	N1-C2-O2	5.03	121.92	118.90
16	S	18	DC	N1-C2-O2	5.02	121.91	118.90
16	S	28	DG	C5-C6-N1	5.01	114.01	111.50
17	T	57	DT	O4'-C1'-N1	5.00	111.50	108.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	S	24	DT	Sidechain
16	S	27	DG	Sidechain
17	T	38	DC	Sidechain
17	T	47	DA	Sidechain

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	11513	0	11582	500	0
2	B	9327	0	9191	643	0
3	C	2418	0	2401	60	0
4	D	467	0	468	4	0
5	E	1759	0	1788	7	0
6	F	823	0	841	7	0
7	G	1600	0	1594	115	0
8	H	1072	0	1042	26	0
9	I	942	0	935	50	0
10	J	569	0	585	14	0
11	K	810	0	801	49	0
12	L	359	0	381	36	0
13	M	831	0	820	11	0
14	N	1103	0	1106	5	0
15	O	3811	0	3792	805	0
16	S	1028	0	548	49	0
17	T	1128	0	637	57	0
18	U	1164	0	289	29	0
19	V	1152	0	292	5	0
20	W	672	0	166	9	0
21	1	52	0	12	0	0
22	2	76	0	18	0	0
23	3	36	0	8	0	0
23	9	36	0	8	0	0
24	4	92	0	22	0	0
25	5	64	0	15	0	0
25	Q	64	0	14	0	0
26	6	40	0	9	0	0
26	8	40	0	9	0	0
27	7	100	0	24	0	0
28	P	88	0	21	4	0
29	Z	60	0	14	4	0
30	Y	48	0	11	0	0
31	R	108	0	26	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
All	All	43459	0	39470	2074	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 26.

All (2074) 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:1261:VAL:CG2	1:A:1306:TYR:HB3	1.20	1.66
15:O:162:PHE:CB	15:O:214:ASN:CB	1.76	1.62
2:B:74:PHE:CE2	2:B:94:LYS:CG	1.77	1.62
2:B:74:PHE:CE2	2:B:94:LYS:HG2	1.27	1.61
1:A:1261:VAL:HG21	1:A:1306:TYR:CB	1.21	1.59
1:A:1003:ARG:HH12	2:B:533:THR:CG2	1.05	1.57
2:B:73:ILE:CG2	2:B:425:ILE:HG23	1.20	1.57
15:O:372:VAL:HA	15:O:375:THR:CG2	1.12	1.56
7:G:138:PHE:CE1	15:O:181:ARG:HB3	1.40	1.55
2:B:1119:ARG:HB3	15:O:149:LYS:CE	1.13	1.55
2:B:1119:ARG:CB	15:O:149:LYS:HE3	1.33	1.54
2:B:811:LEU:CD2	2:B:899:GLN:HB3	1.10	1.54
7:G:138:PHE:CD2	15:O:182:MET:HB2	1.40	1.52
1:A:990:ILE:HD11	1:A:995:TYR:CD1	1.43	1.52
15:O:372:VAL:CA	15:O:375:THR:HG23	1.40	1.52
15:O:458:GLU:HA	15:O:461:VAL:CG2	1.26	1.50
2:B:811:LEU:HD22	2:B:899:GLN:CB	1.04	1.49
1:A:1202:LEU:CB	9:I:101:LEU:HD21	1.42	1.48
1:A:252:PHE:CE2	1:A:314:TYR:HB2	1.46	1.47
15:O:458:GLU:CA	15:O:461:VAL:HG23	1.28	1.47
2:B:74:PHE:CE1	2:B:94:LYS:CG	1.98	1.47
16:S:64:DT:N3	17:T:8:DA:C2	1.80	1.47
2:B:154:GLU:HG2	2:B:443:LYS:NZ	1.27	1.46
15:O:454:VAL:CB	15:O:514:PHE:HE2	1.30	1.45
2:B:1039:MET:CE	2:B:1042:ASP:HA	1.47	1.44
2:B:1119:ARG:CB	15:O:149:LYS:CE	1.83	1.44
7:G:143:SER:HB2	15:O:142:ILE:CG1	1.45	1.44
1:A:1202:LEU:HB3	9:I:101:LEU:CD2	1.44	1.43
2:B:898:LEU:CG	12:L:46:VAL:HG21	1.18	1.43
2:B:1120:ILE:N	15:O:149:LYS:HE2	1.27	1.42
2:B:898:LEU:HD22	12:L:46:VAL:CB	1.29	1.42
2:B:822:THR:CG2	2:B:864:ASP:N	1.77	1.42
2:B:74:PHE:CE1	2:B:94:LYS:CA	2.03	1.41
2:B:74:PHE:CZ	2:B:94:LYS:CB	2.04	1.41
1:A:1260:LYS:CD	1:A:1500:GLN:HA	1.29	1.40
2:B:154:GLU:CG	2:B:443:LYS:NZ	1.82	1.40
1:A:1457:ILE:CA	1:A:1473:LYS:O	1.66	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:PHE:CE2	15:O:182:MET:HB2	1.55	1.40
17:T:21:DG:H2'	17:T:22:DA:C5'	1.51	1.40
15:O:408:PHE:CZ	15:O:446:LEU:CD1	2.06	1.39
2:B:132:SER:HB2	2:B:134:ARG:NH1	1.07	1.38
15:O:408:PHE:CZ	15:O:446:LEU:HD11	1.58	1.38
15:O:138:TYR:CE2	15:O:142:ILE:HD11	1.56	1.37
2:B:887:LEU:HD21	12:L:56:LEU:CB	1.53	1.37
2:B:1120:ILE:HG12	15:O:150:TRP:CD2	1.57	1.37
2:B:819:ASP:OD1	2:B:820:PRO:HD2	1.20	1.37
2:B:822:THR:CG2	2:B:865:THR:H	1.35	1.37
2:B:106:LYS:NZ	2:B:171:HIS:ND1	1.67	1.37
15:O:471:LYS:HB2	15:O:585:PHE:CE1	1.58	1.37
15:O:372:VAL:CA	15:O:375:THR:CG2	1.99	1.35
2:B:1120:ILE:HG13	15:O:149:LYS:CD	1.56	1.35
15:O:454:VAL:HB	15:O:514:PHE:CE2	1.61	1.35
1:A:1450:ILE:HD13	1:A:1460:TYR:CD2	1.61	1.35
2:B:822:THR:HG23	2:B:864:ASP:CB	1.52	1.34
2:B:822:THR:HG22	2:B:864:ASP:N	1.06	1.34
16:S:62:DG:N2	17:T:10:DT:O2	1.58	1.34
2:B:822:THR:HG23	2:B:864:ASP:CA	1.56	1.33
1:A:250:LYS:HG2	1:A:252:PHE:CE1	1.63	1.32
2:B:822:THR:CG2	2:B:864:ASP:CA	2.05	1.32
16:S:64:DT:C2	17:T:8:DA:C2	2.17	1.32
2:B:1119:ARG:CB	15:O:149:LYS:NZ	1.82	1.32
7:G:143:SER:HB2	15:O:142:ILE:CD1	1.59	1.32
2:B:822:THR:CG2	2:B:865:THR:N	1.88	1.31
2:B:106:LYS:HD3	2:B:171:HIS:CE1	1.63	1.31
2:B:74:PHE:HE1	2:B:94:LYS:N	1.27	1.30
2:B:132:SER:CB	2:B:134:ARG:NH1	1.95	1.30
2:B:822:THR:HG21	2:B:865:THR:N	0.99	1.30
7:G:241:ARG:HD2	15:O:189:PHE:CD1	1.08	1.30
1:A:403:LEU:HD12	1:A:419:ILE:CG1	1.59	1.30
2:B:73:ILE:CG2	2:B:425:ILE:CG2	2.10	1.30
7:G:241:ARG:CD	15:O:189:PHE:CD1	1.97	1.29
7:G:241:ARG:CD	15:O:189:PHE:CE1	1.81	1.29
2:B:74:PHE:CE1	2:B:94:LYS:HG3	1.60	1.29
2:B:74:PHE:CZ	2:B:94:LYS:CD	2.15	1.29
15:O:198:PHE:CD2	15:O:232:LEU:HG	1.65	1.29
1:A:1457:ILE:C	1:A:1473:LYS:O	1.71	1.28
16:S:61:DA:H2	17:T:11:DG:N1	1.30	1.28
15:O:432:LYS:HG2	15:O:608:GLU:O	1.23	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:892:SER:O	2:B:895:PHE:CZ	1.88	1.27
17:T:21:DG:C2'	17:T:22:DA:H5"	1.64	1.27
2:B:106:LYS:HZ1	2:B:171:HIS:CG	1.53	1.26
2:B:887:LEU:HD23	12:L:56:LEU:O	1.31	1.26
15:O:454:VAL:CB	15:O:514:PHE:CE2	2.17	1.26
15:O:431:ALA:CB	15:O:434:LEU:HD11	1.63	1.26
2:B:900:THR:O	2:B:901:VAL:HG23	1.28	1.26
7:G:142:ALA:C	15:O:138:TYR:OH	1.73	1.25
2:B:143:TRP:NE1	2:B:440:PHE:HB3	1.47	1.25
2:B:887:LEU:CD2	12:L:56:LEU:O	1.82	1.25
1:A:439:ASP:HA	1:A:458:GLN:OE1	1.37	1.25
2:B:898:LEU:CD2	12:L:46:VAL:CB	1.80	1.25
2:B:1119:ARG:HB3	15:O:149:LYS:NZ	0.94	1.24
2:B:1120:ILE:N	15:O:149:LYS:CE	1.98	1.24
1:A:1322:ILE:HG21	1:A:1454:HIS:CD2	1.72	1.24
7:G:142:ALA:HB3	15:O:138:TYR:CE1	1.71	1.23
15:O:237:ILE:CB	15:O:381:ILE:HD12	1.68	1.23
1:A:33:THR:O	1:A:390:LEU:HD11	1.35	1.23
1:A:1009:THR:OG1	9:I:102:ARG:N	1.69	1.23
15:O:432:LYS:HB3	15:O:609:TYR:CA	1.69	1.23
7:G:143:SER:CB	15:O:142:ILE:CD1	2.17	1.22
1:A:1457:ILE:O	1:A:1473:LYS:O	1.58	1.22
7:G:138:PHE:CE1	15:O:181:ARG:CB	2.23	1.22
7:G:142:ALA:HB3	15:O:138:TYR:CZ	1.74	1.21
15:O:352:LEU:HD23	15:O:358:VAL:CG2	1.69	1.21
1:A:252:PHE:CE2	1:A:314:TYR:CB	2.22	1.21
2:B:74:PHE:CE1	2:B:94:LYS:HA	1.67	1.21
15:O:432:LYS:CG	15:O:608:GLU:O	1.87	1.21
1:A:1003:ARG:NH1	2:B:533:THR:HG21	0.88	1.21
2:B:154:GLU:CG	2:B:443:LYS:HZ3	1.49	1.20
15:O:373:LEU:HD11	15:O:416:LYS:CG	1.69	1.20
1:A:1260:LYS:CD	1:A:1500:GLN:CA	1.94	1.20
15:O:390:GLN:O	15:O:609:TYR:CE1	1.94	1.19
2:B:108:MET:HG3	2:B:171:HIS:CE1	1.78	1.19
15:O:162:PHE:O	15:O:210:ASN:O	1.61	1.19
15:O:237:ILE:CG2	15:O:381:ILE:HD12	1.73	1.19
15:O:352:LEU:CD2	15:O:358:VAL:HG22	1.71	1.19
15:O:432:LYS:CB	15:O:609:TYR:HA	1.71	1.19
7:G:143:SER:N	15:O:138:TYR:OH	1.76	1.19
7:G:241:ARG:HD2	15:O:189:PHE:CE1	1.55	1.18
2:B:887:LEU:CD2	12:L:56:LEU:HB2	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:CD2	1:A:453:ILE:HD13	1.74	1.18
1:A:1457:ILE:HA	1:A:1473:LYS:O	1.22	1.18
1:A:1457:ILE:HD12	1:A:1458:THR:N	1.57	1.18
15:O:370:THR:O	15:O:374:PRO:CD	1.92	1.18
15:O:426:SER:OG	15:O:594:TYR:HB2	1.42	1.17
2:B:73:ILE:HG21	2:B:425:ILE:CG2	1.68	1.17
15:O:247:GLU:OE1	15:O:325:ILE:HG12	1.42	1.17
1:A:385:LEU:HD11	1:A:453:ILE:CB	1.74	1.16
7:G:142:ALA:N	15:O:138:TYR:HE1	1.41	1.16
16:S:64:DT:N3	17:T:8:DA:N3	1.94	1.16
2:B:106:LYS:CD	2:B:171:HIS:CE1	2.28	1.16
7:G:242:VAL:HB	15:O:183:ILE:CG2	1.76	1.16
2:B:108:MET:CG	2:B:171:HIS:CE1	2.29	1.16
7:G:241:ARG:NE	15:O:190:ILE:HG22	1.60	1.16
15:O:237:ILE:HB	15:O:381:ILE:HD12	1.22	1.15
1:A:1261:VAL:HG21	1:A:1306:TYR:CG	1.82	1.15
1:A:1261:VAL:HG22	1:A:1306:TYR:CD1	1.81	1.15
7:G:154:ASN:OD1	15:O:184:PRO:CD	1.91	1.14
15:O:430:ARG:NH2	15:O:596:PRO:HD3	1.60	1.14
1:A:403:LEU:CD1	1:A:419:ILE:HG13	1.75	1.14
7:G:138:PHE:CD2	15:O:182:MET:CB	2.31	1.14
16:S:64:DT:C4	17:T:8:DA:N1	2.16	1.14
2:B:143:TRP:HE1	2:B:440:PHE:CB	1.59	1.13
16:S:61:DA:H2	17:T:11:DG:C2	1.65	1.13
1:A:1260:LYS:HD3	1:A:1500:GLN:CA	1.62	1.13
15:O:245:GLN:HG3	15:O:378:THR:HA	1.15	1.13
15:O:408:PHE:CE2	15:O:446:LEU:HD11	1.83	1.13
7:G:152:ALA:O	15:O:184:PRO:HG2	1.45	1.13
15:O:219:ARG:NH2	15:O:360:VAL:HG21	1.63	1.12
15:O:247:GLU:OE1	15:O:325:ILE:CG1	1.97	1.13
2:B:143:TRP:O	2:B:151:ASN:OD1	1.64	1.12
15:O:240:ILE:HG21	15:O:332:LEU:HB2	1.24	1.12
2:B:1120:ILE:HG12	15:O:150:TRP:CE3	1.68	1.12
1:A:385:LEU:HD21	1:A:453:ILE:CD1	1.78	1.12
2:B:108:MET:HE2	2:B:120:LYS:CA	1.78	1.12
2:B:1119:ARG:CA	15:O:149:LYS:HE3	1.78	1.12
15:O:454:VAL:HA	15:O:514:PHE:CZ	1.83	1.12
15:O:156:MET:HG3	15:O:197:PHE:CE2	1.83	1.11
15:O:454:VAL:CG2	15:O:514:PHE:HE2	1.62	1.11
1:A:1202:LEU:HD21	9:I:122:ARG:NH1	1.65	1.11
2:B:1120:ILE:CG1	15:O:150:TRP:CE3	2.31	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:241:ARG:CZ	15:O:190:ILE:HG22	1.80	1.11
2:B:108:MET:HE3	2:B:120:LYS:CB	1.80	1.11
7:G:143:SER:CB	15:O:142:ILE:HG12	1.81	1.11
1:A:385:LEU:CD1	1:A:453:ILE:HB	1.80	1.10
2:B:106:LYS:CE	2:B:171:HIS:ND1	2.15	1.10
2:B:49:PHE:HD1	2:B:167:SER:OG	1.35	1.10
2:B:145:VAL:HG23	2:B:440:PHE:HD2	1.13	1.10
2:B:894:LYS:O	2:B:895:PHE:CG	2.04	1.10
2:B:108:MET:HE2	2:B:120:LYS:HA	1.20	1.10
2:B:1120:ILE:HG13	15:O:149:LYS:HD3	1.29	1.10
16:S:61:DA:C2	17:T:11:DG:N1	2.14	1.10
2:B:49:PHE:CD1	2:B:167:SER:OG	2.03	1.10
2:B:74:PHE:HZ	2:B:94:LYS:CD	1.55	1.09
2:B:822:THR:HG23	2:B:864:ASP:HB2	1.14	1.09
15:O:408:PHE:CZ	15:O:446:LEU:HD13	1.81	1.09
15:O:447:THR:O	15:O:450:LEU:HB2	1.50	1.09
16:S:64:DT:C4	17:T:8:DA:C2	2.40	1.09
15:O:156:MET:SD	15:O:197:PHE:CZ	2.45	1.09
2:B:825:PHE:CD2	2:B:899:GLN:HA	1.70	1.09
3:C:92:ILE:HG12	10:J:2:ILE:HD11	1.32	1.09
15:O:138:TYR:CE2	15:O:142:ILE:CD1	2.36	1.09
15:O:152:GLN:HG2	15:O:193:TYR:OH	1.52	1.09
15:O:446:LEU:O	15:O:449:TRP:HB3	1.51	1.09
1:A:1199:GLN:O	9:I:122:ARG:NH2	1.86	1.09
2:B:108:MET:HA	2:B:121:VAL:HG12	1.11	1.08
2:B:134:ARG:HD3	2:B:462:GLN:OE1	1.53	1.08
15:O:129:PRO:CD	15:O:132:THR:HB	1.83	1.08
1:A:998:HIS:CD2	2:B:712:SER:HB2	1.88	1.08
2:B:108:MET:CA	2:B:121:VAL:HG12	1.82	1.07
15:O:138:TYR:CZ	15:O:142:ILE:HD11	1.89	1.07
2:B:139:LEU:CD2	2:B:420:TYR:CE2	2.36	1.07
15:O:201:LYS:HD2	15:O:239:SER:OG	1.54	1.07
1:A:250:LYS:CG	1:A:252:PHE:CE1	2.38	1.07
1:A:252:PHE:HE2	1:A:314:TYR:CB	1.65	1.07
2:B:106:LYS:NZ	2:B:171:HIS:CE1	2.23	1.07
18:U:436:LEU:O	18:U:438:PHE:N	1.87	1.07
2:B:1119:ARG:HB2	15:O:149:LYS:HE3	1.33	1.07
15:O:162:PHE:CA	15:O:214:ASN:CB	2.33	1.07
15:O:435:SER:HB3	15:O:438:GLN:HG3	1.37	1.07
2:B:123:PRO:HG3	2:B:172:LEU:HD11	1.36	1.07
1:A:990:ILE:CD1	1:A:995:TYR:CD1	2.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:THR:CG2	2:B:864:ASP:C	2.23	1.06
15:O:198:PHE:CD1	15:O:236:LYS:HE3	1.90	1.06
1:A:252:PHE:CD2	1:A:314:TYR:HA	1.91	1.06
1:A:1256:LYS:O	1:A:1259:SER:HB2	1.55	1.06
2:B:1039:MET:CE	2:B:1042:ASP:CA	2.33	1.06
2:B:1041:ASN:O	2:B:1043:LYS:N	1.88	1.06
2:B:154:GLU:HG3	2:B:443:LYS:NZ	1.68	1.06
1:A:444:GLN:HG3	1:A:445:GLY:H	0.89	1.06
1:A:1261:VAL:CG2	1:A:1306:TYR:CD1	2.39	1.06
15:O:240:ILE:HG22	15:O:332:LEU:HD22	1.08	1.06
2:B:813:LEU:HD12	2:B:814:ASN:OD1	1.54	1.05
2:B:106:LYS:HG2	2:B:107:PRO:HD2	1.35	1.05
7:G:154:ASN:OD1	15:O:184:PRO:HD3	1.54	1.05
15:O:156:MET:SD	15:O:197:PHE:HZ	1.77	1.05
15:O:428:ILE:HG23	15:O:439:ILE:HG21	1.38	1.05
15:O:425:GLY:HA2	15:O:483:ILE:HD11	1.34	1.05
1:A:1601:GLN:HE21	16:S:57:DA:H5"	1.22	1.05
2:B:159:GLY:HA3	2:B:456:ASN:HA	1.36	1.05
15:O:152:GLN:CG	15:O:193:TYR:OH	2.04	1.05
15:O:240:ILE:CG2	15:O:332:LEU:HD22	1.87	1.05
1:A:252:PHE:CE2	1:A:314:TYR:CD1	2.45	1.05
2:B:145:VAL:CG2	2:B:440:PHE:HD2	1.69	1.05
2:B:900:THR:O	2:B:901:VAL:CG2	2.04	1.05
2:B:1120:ILE:H	15:O:149:LYS:CE	1.63	1.05
7:G:138:PHE:CZ	15:O:181:ARG:HB3	1.92	1.05
15:O:129:PRO:HD2	15:O:132:THR:HB	1.32	1.05
15:O:198:PHE:CZ	15:O:236:LYS:HG3	1.92	1.05
1:A:250:LYS:HG2	1:A:252:PHE:HE1	0.90	1.04
2:B:73:ILE:HG22	2:B:425:ILE:HG23	1.35	1.04
16:S:64:DT:O4	17:T:8:DA:C6	2.10	1.04
1:A:252:PHE:CZ	1:A:314:TYR:HD1	1.76	1.04
2:B:825:PHE:HD2	2:B:899:GLN:HA	0.92	1.04
2:B:898:LEU:HD22	12:L:46:VAL:HB	1.34	1.04
2:B:1039:MET:HE3	2:B:1042:ASP:HA	1.38	1.04
2:B:1039:MET:HE2	2:B:1042:ASP:HA	1.39	1.04
7:G:242:VAL:HB	15:O:183:ILE:HG22	1.35	1.04
2:B:74:PHE:CE1	2:B:94:LYS:N	2.18	1.04
15:O:241:ASP:OD1	15:O:378:THR:HG22	1.58	1.04
1:A:385:LEU:HD21	1:A:453:ILE:HD13	1.07	1.04
2:B:142:LYS:HG3	2:B:153:PHE:CE1	1.92	1.04
2:B:887:LEU:HD21	12:L:56:LEU:HB2	1.04	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:VAL:CG2	1:A:1306:TYR:CG	2.39	1.04
1:A:1451:ILE:HG12	1:A:1458:THR:O	1.58	1.04
2:B:144:SER:CA	2:B:151:ASN:OD1	2.06	1.04
2:B:822:THR:O	2:B:863:ASP:HA	1.55	1.03
15:O:390:GLN:NE2	15:O:432:LYS:H	1.54	1.03
16:S:61:DA:C2	17:T:11:DG:N2	2.25	1.03
1:A:444:GLN:HG3	1:A:445:GLY:N	1.72	1.03
2:B:106:LYS:CD	2:B:171:HIS:HE1	1.68	1.03
2:B:1120:ILE:HG13	15:O:149:LYS:HD2	1.40	1.03
7:G:242:VAL:CG1	15:O:185:SER:H	1.71	1.03
15:O:431:ALA:HB1	15:O:434:LEU:HD11	1.34	1.03
1:A:438:ILE:O	1:A:455:GLY:HA3	1.58	1.03
2:B:74:PHE:CE1	2:B:94:LYS:CB	2.34	1.03
2:B:108:MET:HE3	2:B:120:LYS:HB2	1.06	1.03
15:O:431:ALA:HB3	15:O:434:LEU:HD11	1.37	1.03
1:A:1261:VAL:HG13	1:A:1306:TYR:CD1	1.94	1.03
2:B:154:GLU:CG	2:B:443:LYS:HZ1	1.56	1.02
15:O:488:HIS:CG	15:O:489:ASN:H	1.74	1.02
15:O:174:ASP:HA	15:O:177:LYS:HE2	1.40	1.02
1:A:439:ASP:OD1	1:A:458:GLN:NE2	1.92	1.01
1:A:800:VAL:HG23	1:A:1068:PHE:CZ	1.94	1.01
2:B:811:LEU:CG	2:B:899:GLN:HB3	1.90	1.01
15:O:237:ILE:HB	15:O:381:ILE:CD1	1.88	1.01
15:O:369:LYS:O	15:O:373:LEU:N	1.91	1.01
2:B:106:LYS:CE	2:B:171:HIS:CE1	2.44	1.01
2:B:108:MET:CE	2:B:120:LYS:HB2	1.90	1.01
2:B:825:PHE:CD2	2:B:899:GLN:CA	2.39	1.01
15:O:372:VAL:HA	15:O:375:THR:HG21	1.04	1.01
20:W:223:ASN:O	20:W:226:ARG:O	1.79	1.01
2:B:74:PHE:HE1	2:B:94:LYS:CA	1.55	1.01
2:B:143:TRP:C	2:B:151:ASN:OD1	1.98	1.00
7:G:143:SER:HB2	15:O:142:ILE:HG12	1.01	1.00
15:O:201:LYS:CD	15:O:239:SER:OG	2.09	1.00
2:B:1121:GLY:H	15:O:149:LYS:HD3	1.24	1.00
7:G:143:SER:CB	15:O:142:ILE:HD13	1.88	1.00
2:B:1119:ARG:C	15:O:149:LYS:HE3	1.81	1.00
15:O:352:LEU:HA	15:O:358:VAL:HG23	1.44	1.00
1:A:444:GLN:CG	1:A:445:GLY:H	1.73	1.00
1:A:683:LYS:HB2	8:H:20:TYR:CE1	1.97	1.00
2:B:1039:MET:HE2	2:B:1042:ASP:CA	1.91	1.00
2:B:1120:ILE:CG1	15:O:150:TRP:CD2	2.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:64:DT:C4	17:T:8:DA:C6	2.48	1.00
2:B:90:TYR:CZ	2:B:92:GLY:HA2	1.97	1.00
2:B:139:LEU:HD23	2:B:420:TYR:CE2	1.96	1.00
2:B:822:THR:HG21	2:B:864:ASP:C	1.82	1.00
7:G:138:PHE:CE2	15:O:182:MET:CB	2.43	1.00
2:B:142:LYS:HG3	2:B:153:PHE:HE1	1.27	1.00
2:B:1120:ILE:HD12	15:O:149:LYS:O	1.56	1.00
15:O:370:THR:O	15:O:374:PRO:CG	2.09	1.00
15:O:428:ILE:HD12	15:O:439:ILE:HG23	1.44	1.00
2:B:914:GLY:HA3	2:B:1040:VAL:HG21	1.43	0.99
15:O:240:ILE:HG21	15:O:332:LEU:CB	1.92	0.99
7:G:241:ARG:CZ	15:O:190:ILE:CG2	2.40	0.99
15:O:440:ILE:HG23	15:O:491:PHE:HE1	1.27	0.99
7:G:142:ALA:CB	15:O:138:TYR:CE1	2.43	0.99
15:O:373:LEU:HD11	15:O:416:LYS:HG3	1.43	0.99
15:O:471:LYS:CB	15:O:585:PHE:CE1	2.45	0.99
2:B:811:LEU:HB3	2:B:899:GLN:OE1	1.62	0.99
28:P:134:ALA:O	29:Z:148:ALA:O	1.80	0.99
2:B:813:LEU:CD1	2:B:814:ASN:OD1	2.10	0.99
7:G:242:VAL:HG11	15:O:185:SER:H	1.27	0.99
15:O:240:ILE:CG2	15:O:332:LEU:HD13	1.93	0.99
2:B:893:ASN:OD1	2:B:895:PHE:CZ	1.97	0.98
1:A:998:HIS:HD2	2:B:712:SER:HB2	1.26	0.98
2:B:139:LEU:HD21	2:B:420:TYR:CE2	1.98	0.98
15:O:348:THR:HG22	15:O:351:SER:HB3	1.41	0.98
1:A:373:LEU:HD21	1:A:378:HIS:CD2	1.99	0.98
7:G:242:VAL:CG1	15:O:185:SER:N	2.25	0.98
16:S:61:DA:C2	17:T:11:DG:C2	2.52	0.98
2:B:74:PHE:CE2	2:B:94:LYS:CD	2.39	0.98
2:B:1119:ARG:HB3	15:O:149:LYS:HZ1	1.27	0.98
16:S:65:DG:N2	17:T:7:DA:C2	2.32	0.98
15:O:352:LEU:HD23	15:O:358:VAL:HG22	1.00	0.97
15:O:454:VAL:CG2	15:O:514:PHE:CE2	2.44	0.97
16:S:57:DA:N6	17:T:14:DT:O4	1.97	0.97
7:G:241:ARG:NH2	15:O:190:ILE:CG2	2.27	0.97
2:B:811:LEU:HD22	2:B:899:GLN:CG	1.94	0.97
2:B:106:LYS:HD3	2:B:171:HIS:HE1	0.80	0.97
2:B:1120:ILE:HB	15:O:153:ASP:OD1	1.64	0.97
2:B:156:ARG:HD3	2:B:450:LEU:HD12	1.47	0.97
7:G:242:VAL:CB	15:O:183:ILE:HG22	1.95	0.97
15:O:158:LEU:HD23	15:O:172:HIS:HD2	1.25	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:59:DG:N2	17:T:13:DT:O2	1.98	0.97
1:A:1261:VAL:HG13	1:A:1306:TYR:CE1	1.99	0.96
15:O:423:TYR:HD1	15:O:594:TYR:CE2	1.82	0.96
1:A:252:PHE:CZ	1:A:314:TYR:CD1	2.54	0.96
1:A:683:LYS:HD2	8:H:20:TYR:CE2	2.00	0.96
15:O:458:GLU:CA	15:O:461:VAL:CG2	2.08	0.96
2:B:158:CYS:O	2:B:455:GLU:O	1.84	0.96
2:B:819:ASP:OD1	2:B:820:PRO:CD	2.14	0.96
1:A:1202:LEU:HD13	9:I:101:LEU:HD11	1.44	0.96
16:S:61:DA:N3	17:T:11:DG:N2	2.14	0.96
1:A:991:LYS:HD2	1:A:994:GLU:OE1	1.65	0.95
2:B:1119:ARG:CB	15:O:149:LYS:HZ2	1.60	0.95
15:O:156:MET:CG	15:O:197:PHE:CE2	2.48	0.95
1:A:252:PHE:CD2	1:A:314:TYR:CA	2.49	0.95
1:A:719:ILE:HD13	8:H:43:ASN:HD22	1.31	0.95
1:A:1199:GLN:O	9:I:122:ARG:CZ	2.13	0.95
2:B:894:LYS:O	2:B:895:PHE:CD2	2.18	0.95
1:A:380:ASN:CB	1:A:383:ASN:OD1	2.13	0.95
19:V:185:GLN:O	19:V:199:GLY:HA3	1.65	0.95
2:B:74:PHE:HE1	2:B:93:ASN:C	1.68	0.95
2:B:887:LEU:HD23	2:B:887:LEU:H	1.30	0.95
1:A:990:ILE:CD1	1:A:995:TYR:HD1	1.74	0.95
1:A:1261:VAL:CG1	1:A:1306:TYR:CD1	2.49	0.95
2:B:822:THR:HG22	2:B:863:ASP:C	1.84	0.95
2:B:821:ILE:HG21	2:B:899:GLN:HE22	1.28	0.95
7:G:142:ALA:N	15:O:138:TYR:CE1	2.33	0.95
1:A:252:PHE:CE2	1:A:314:TYR:HD1	1.84	0.95
1:A:1261:VAL:HG22	1:A:1306:TYR:HD1	1.18	0.95
2:B:144:SER:HA	2:B:151:ASN:OD1	1.64	0.95
2:B:811:LEU:CB	2:B:899:GLN:OE1	2.15	0.94
3:C:42:VAL:HB	11:K:138:LYS:HG3	1.47	0.94
7:G:143:SER:OG	15:O:142:ILE:HD13	1.66	0.94
15:O:63:LEU:HD12	15:O:71:ILE:HG13	1.47	0.94
2:B:96:SER:N	2:B:144:SER:O	2.00	0.94
17:T:21:DG:C2'	17:T:22:DA:C5'	2.35	0.94
15:O:358:VAL:O	15:O:362:ASN:ND2	2.00	0.94
1:A:1322:ILE:CG2	1:A:1454:HIS:HD2	1.81	0.94
15:O:417:LYS:HD2	15:O:472:HIS:CE1	2.02	0.94
16:S:65:DG:N1	17:T:7:DA:N1	2.15	0.94
15:O:454:VAL:HG23	15:O:514:PHE:CE2	2.01	0.94
2:B:1119:ARG:C	15:O:149:LYS:CE	2.35	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:342:HIS:O	15:O:346:GLN:HG2	1.68	0.94
2:B:892:SER:O	2:B:895:PHE:HZ	1.29	0.94
15:O:342:HIS:CD2	15:O:346:GLN:HE21	1.85	0.94
7:G:241:ARG:HG2	15:O:186:SER:HA	1.48	0.94
1:A:252:PHE:CD2	1:A:314:TYR:HB2	2.02	0.93
1:A:439:ASP:OD1	1:A:457:LYS:HB3	1.67	0.93
2:B:141:LEU:HD21	2:B:424:ILE:HD13	1.49	0.93
15:O:240:ILE:HG22	15:O:332:LEU:CD2	1.98	0.93
15:O:241:ASP:CG	15:O:378:THR:HG22	1.89	0.93
2:B:161:LEU:CA	2:B:458:GLY:HA2	1.97	0.93
2:B:898:LEU:HD23	2:B:898:LEU:H	1.32	0.93
2:B:145:VAL:HG23	2:B:440:PHE:CD2	2.03	0.93
2:B:93:ASN:HB2	2:B:146:ASN:OD1	1.69	0.93
2:B:108:MET:CE	2:B:120:LYS:CB	2.46	0.93
15:O:372:VAL:N	15:O:375:THR:HG23	1.82	0.93
2:B:94:LYS:O	2:B:145:VAL:HA	1.69	0.92
1:A:1261:VAL:HG23	1:A:1306:TYR:HB3	1.47	0.92
15:O:147:ILE:O	15:O:149:LYS:N	2.03	0.92
2:B:168:ASN:HA	2:B:173:ASN:HD22	1.33	0.92
15:O:408:PHE:HZ	15:O:446:LEU:HD11	1.25	0.92
2:B:108:MET:HA	2:B:121:VAL:CG1	1.97	0.92
18:U:446:TYR:CA	18:U:450:THR:O	2.17	0.92
2:B:821:ILE:HG22	2:B:823:GLN:H	1.34	0.92
2:B:73:ILE:HG22	2:B:425:ILE:CG2	1.88	0.92
15:O:224:GLU:OE1	15:O:224:GLU:N	2.01	0.92
15:O:386:PHE:HD2	15:O:606:MET:HE1	1.32	0.92
15:O:426:SER:OG	15:O:594:TYR:CB	2.18	0.92
15:O:234:ILE:CG2	15:O:371:HIS:HD2	1.81	0.92
1:A:1202:LEU:HD22	9:I:101:LEU:CD2	2.00	0.92
2:B:154:GLU:HG3	2:B:443:LYS:CE	2.00	0.92
15:O:240:ILE:HG21	15:O:332:LEU:HD13	1.51	0.92
15:O:408:PHE:HZ	15:O:446:LEU:CD1	1.74	0.92
15:O:435:SER:CB	15:O:438:GLN:HG3	1.98	0.91
16:S:65:DG:C2	17:T:7:DA:C2	2.59	0.91
1:A:438:ILE:C	1:A:455:GLY:HA3	1.89	0.91
1:A:250:LYS:CG	1:A:252:PHE:HE1	1.78	0.91
2:B:143:TRP:HZ2	2:B:440:PHE:CD1	1.89	0.91
3:C:67:PHE:CE2	11:K:131:VAL:HG11	2.06	0.91
15:O:219:ARG:NH2	15:O:360:VAL:CG2	2.32	0.91
15:O:342:HIS:CE1	15:O:346:GLN:HG3	2.05	0.91
1:A:483:VAL:HG21	2:B:1040:VAL:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:372:VAL:HA	15:O:375:THR:HG23	0.96	0.91
15:O:390:GLN:NE2	15:O:609:TYR:HB3	1.86	0.91
2:B:108:MET:CE	2:B:120:LYS:CA	2.48	0.91
2:B:1119:ARG:HB3	15:O:149:LYS:HZ2	1.14	0.91
15:O:426:SER:CB	15:O:594:TYR:HB2	2.01	0.91
2:B:162:PRO:CG	2:B:465:LEU:HD12	2.01	0.90
1:A:1456:PHE:O	1:A:1475:GLU:N	2.03	0.90
1:A:1322:ILE:HG21	1:A:1454:HIS:HD2	1.16	0.90
1:A:373:LEU:HD21	1:A:378:HIS:NE2	1.86	0.90
2:B:108:MET:CG	2:B:171:HIS:NE2	2.33	0.90
7:G:142:ALA:H	15:O:138:TYR:HE1	0.96	0.90
15:O:129:PRO:CG	15:O:132:THR:HB	2.01	0.90
15:O:386:PHE:HD2	15:O:606:MET:CE	1.83	0.90
7:G:143:SER:OG	15:O:142:ILE:CD1	2.18	0.90
2:B:132:SER:HB2	2:B:134:ARG:HH12	1.32	0.90
15:O:240:ILE:CG2	15:O:332:LEU:HB2	2.01	0.90
1:A:1202:LEU:CG	9:I:101:LEU:HD21	2.02	0.90
2:B:811:LEU:HD11	2:B:825:PHE:CZ	2.05	0.90
1:A:722:PRO:CD	8:H:46:LEU:HB3	2.01	0.90
2:B:811:LEU:HD22	2:B:899:GLN:CA	2.01	0.90
15:O:158:LEU:HD23	15:O:172:HIS:CD2	2.07	0.89
1:A:1260:LYS:HD2	1:A:1500:GLN:CA	1.52	0.89
2:B:74:PHE:CE1	2:B:93:ASN:C	2.43	0.89
2:B:108:MET:CE	2:B:120:LYS:HA	2.02	0.89
2:B:132:SER:OG	2:B:462:GLN:NE2	2.05	0.89
1:A:380:ASN:HB3	1:A:383:ASN:OD1	1.68	0.89
1:A:722:PRO:HG2	8:H:46:LEU:HD22	1.51	0.89
15:O:198:PHE:CG	15:O:236:LYS:HE3	2.06	0.89
1:A:1003:ARG:HH11	2:B:533:THR:HG21	1.36	0.89
15:O:457:ARG:HA	15:O:460:GLU:HB2	1.55	0.89
2:B:894:LYS:C	2:B:895:PHE:CD1	2.46	0.89
2:B:1041:ASN:CG	2:B:1044:PHE:HB2	1.91	0.89
15:O:432:LYS:HB2	15:O:609:TYR:C	1.92	0.89
15:O:478:GLN:HE21	15:O:592:PHE:HZ	1.19	0.89
15:O:194:LEU:O	15:O:232:LEU:HD21	1.72	0.89
15:O:421:LEU:HD13	15:O:476:ALA:HB2	1.54	0.89
1:A:1202:LEU:CD2	9:I:122:ARG:NH1	2.36	0.89
15:O:370:THR:O	15:O:374:PRO:HD3	1.72	0.89
15:O:454:VAL:HA	15:O:514:PHE:HZ	1.34	0.89
16:S:54:DG:O6	17:T:17:DG:N1	1.73	0.89
1:A:380:ASN:ND2	1:A:383:ASN:OD1	2.04	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:VAL:HG12	1:A:1265:GLU:HB2	1.55	0.88
2:B:1119:ARG:CG	15:O:149:LYS:HZ2	1.86	0.88
15:O:488:HIS:O	15:O:490:ILE:N	2.06	0.88
1:A:800:VAL:HG23	1:A:1068:PHE:HZ	1.36	0.88
1:A:1202:LEU:HD11	9:I:111:PHE:CZ	2.08	0.88
7:G:142:ALA:CB	15:O:138:TYR:CZ	2.56	0.88
1:A:1450:ILE:HD13	1:A:1460:TYR:HD2	1.05	0.88
15:O:459:GLU:O	15:O:463:GLN:HG3	1.73	0.88
1:A:440:SER:O	1:A:443:ALA:N	2.06	0.88
2:B:108:MET:HG3	2:B:171:HIS:NE2	1.89	0.88
15:O:488:HIS:ND1	15:O:489:ASN:N	2.21	0.88
15:O:198:PHE:HD2	15:O:232:LEU:CG	1.86	0.88
1:A:995:TYR:CE2	1:A:999:CYS:SG	2.67	0.88
2:B:887:LEU:HD21	12:L:56:LEU:CA	2.04	0.88
15:O:417:LYS:CD	15:O:472:HIS:CE1	2.57	0.88
16:S:64:DT:C2	17:T:8:DA:H2	1.92	0.88
15:O:432:LYS:CB	15:O:609:TYR:CA	2.41	0.88
1:A:1450:ILE:HG21	1:A:1460:TYR:CB	2.03	0.88
1:A:947:LEU:HD23	1:A:998:HIS:HD1	1.39	0.87
1:A:252:PHE:HE2	1:A:314:TYR:HB2	0.81	0.87
2:B:898:LEU:CB	12:L:46:VAL:HG21	2.02	0.87
1:A:1202:LEU:CD2	9:I:101:LEU:CD2	2.52	0.87
2:B:819:ASP:CG	2:B:820:PRO:HD2	1.94	0.87
15:O:219:ARG:HH21	15:O:360:VAL:CG2	1.86	0.87
2:B:106:LYS:NZ	2:B:171:HIS:CG	2.29	0.87
1:A:385:LEU:HD11	1:A:453:ILE:HB	0.89	0.87
15:O:366:THR:O	15:O:370:THR:HG23	1.75	0.87
15:O:521:ASN:HD22	15:O:524:VAL:H	1.22	0.87
1:A:712:ILE:H	11:K:106:GLN:HE22	1.22	0.86
2:B:74:PHE:CZ	2:B:94:LYS:CG	0.83	0.86
2:B:49:PHE:HD1	2:B:167:SER:HG	0.89	0.86
1:A:1202:LEU:CD2	9:I:101:LEU:HD21	2.04	0.86
2:B:1119:ARG:CA	15:O:149:LYS:CE	2.44	0.86
15:O:390:GLN:O	15:O:609:TYR:HE1	1.52	0.86
3:C:47:LEU:HD13	11:K:142:MET:HE2	1.56	0.86
15:O:163:ILE:HG22	15:O:211:TYR:HB2	1.57	0.86
2:B:91:LEU:H	2:B:91:LEU:HD12	1.38	0.86
16:S:64:DT:C2	17:T:8:DA:N3	2.36	0.86
1:A:1322:ILE:CG2	1:A:1454:HIS:CD2	2.55	0.86
2:B:90:TYR:CE1	2:B:92:GLY:HA2	2.10	0.86
2:B:119:ARG:NE	2:B:119:ARG:O	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1120:ILE:CD1	15:O:149:LYS:O	2.19	0.86
15:O:243:GLU:HA	15:O:246:ASN:ND2	1.90	0.86
1:A:719:ILE:HG21	8:H:46:LEU:HD12	1.58	0.85
2:B:822:THR:O	2:B:864:ASP:N	2.09	0.85
1:A:990:ILE:HD12	1:A:995:TYR:HA	1.58	0.85
1:A:1278:THR:HG1	1:A:1287:ALA:N	1.74	0.85
15:O:181:ARG:CB	15:O:181:ARG:HH11	1.90	0.85
2:B:99:VAL:HG23	2:B:421:LEU:HD21	1.58	0.85
2:B:165:LEU:HD21	2:B:195:ILE:CD1	2.06	0.85
2:B:1041:ASN:OD1	2:B:1044:PHE:HB2	1.76	0.85
2:B:1119:ARG:HD2	15:O:149:LYS:NZ	1.92	0.85
1:A:399:LEU:HD21	1:A:422:ARG:HG3	1.58	0.85
15:O:198:PHE:HD2	15:O:232:LEU:HG	1.05	0.85
1:A:1260:LYS:HD3	1:A:1500:GLN:HA	0.85	0.85
15:O:373:LEU:HB3	15:O:374:PRO:HD3	1.58	0.85
1:A:996:TYR:CD1	2:B:525:TRP:CE3	2.64	0.85
2:B:887:LEU:CG	12:L:56:LEU:HB2	2.07	0.85
2:B:1119:ARG:CD	15:O:149:LYS:NZ	2.39	0.85
15:O:457:ARG:O	15:O:460:GLU:HB2	1.76	0.85
15:O:417:LYS:HB3	15:O:472:HIS:NE2	1.91	0.85
2:B:139:LEU:HD21	2:B:420:TYR:CD2	2.11	0.85
15:O:361:PHE:O	15:O:365:THR:HG23	1.78	0.84
15:O:371:HIS:O	15:O:375:THR:CG2	2.24	0.84
15:O:408:PHE:CE2	15:O:446:LEU:CD1	2.50	0.84
1:A:957:VAL:HG21	1:A:997:PHE:CD1	2.12	0.84
1:A:1275:THR:CG2	1:A:1289:SER:HB2	2.07	0.84
2:B:887:LEU:CD2	12:L:56:LEU:C	2.45	0.84
15:O:396:MET:HE1	15:O:434:LEU:HD12	1.56	0.84
2:B:108:MET:HG3	2:B:171:HIS:HE1	1.42	0.84
15:O:447:THR:HG22	15:O:480:LEU:HD22	1.58	0.84
15:O:521:ASN:ND2	15:O:523:ASN:H	1.74	0.84
1:A:1202:LEU:CD1	9:I:111:PHE:CZ	2.59	0.84
1:A:1601:GLN:HE21	16:S:57:DA:C5'	1.90	0.84
15:O:467:MET:HG3	15:O:519:PHE:CZ	2.13	0.84
1:A:252:PHE:CD2	1:A:314:TYR:CB	2.59	0.84
2:B:914:GLY:HA3	2:B:1040:VAL:CG2	1.92	0.84
2:B:898:LEU:CG	12:L:46:VAL:CG2	1.86	0.84
15:O:352:LEU:O	15:O:358:VAL:HG21	1.77	0.84
15:O:390:GLN:NE2	15:O:432:LYS:N	2.25	0.84
18:U:203:TRP:O	18:U:206:GLN:N	2.09	0.84
2:B:158:CYS:C	2:B:455:GLU:O	2.16	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:THR:CG2	2:B:864:ASP:CB	2.45	0.84
15:O:240:ILE:CB	15:O:332:LEU:HD13	2.07	0.84
15:O:242:VAL:HA	15:O:378:THR:HG21	1.60	0.84
15:O:372:VAL:CA	15:O:375:THR:HG21	1.89	0.84
1:A:252:PHE:CE2	1:A:314:TYR:CG	2.66	0.83
2:B:107:PRO:O	2:B:121:VAL:CG1	2.26	0.83
1:A:403:LEU:CD1	1:A:419:ILE:CG1	2.46	0.83
15:O:162:PHE:HA	15:O:214:ASN:CB	2.09	0.83
15:O:181:ARG:HH11	15:O:181:ARG:HB2	1.41	0.83
15:O:237:ILE:HG22	15:O:381:ILE:HD12	1.60	0.83
15:O:454:VAL:HB	15:O:514:PHE:HE2	0.99	0.83
15:O:471:LYS:HB2	15:O:585:PHE:HE1	1.00	0.83
1:A:403:LEU:HD12	1:A:419:ILE:HG13	0.87	0.83
2:B:74:PHE:CE2	2:B:94:LYS:HD2	2.11	0.83
15:O:359:GLY:HA2	15:O:362:ASN:HD22	1.43	0.83
15:O:386:PHE:CD2	15:O:606:MET:CE	2.62	0.83
1:A:799:GLU:HG2	1:A:1062:HIS:CG	2.14	0.83
15:O:440:ILE:HG23	15:O:491:PHE:CE1	2.13	0.83
15:O:458:GLU:HA	15:O:461:VAL:HG21	1.58	0.83
2:B:106:LYS:HZ2	2:B:171:HIS:CE1	1.97	0.83
2:B:161:LEU:HD12	2:B:161:LEU:O	1.78	0.83
15:O:240:ILE:HG21	15:O:332:LEU:CD1	2.08	0.83
1:A:1202:LEU:CD2	9:I:122:ARG:HH12	1.91	0.83
15:O:422:GLN:NE2	15:O:592:PHE:CE2	2.45	0.83
2:B:1119:ARG:CG	15:O:149:LYS:NZ	2.42	0.83
15:O:242:VAL:N	15:O:378:THR:HG21	1.94	0.83
2:B:74:PHE:HZ	2:B:94:LYS:CB	1.63	0.82
15:O:156:MET:CG	15:O:197:PHE:CZ	2.61	0.82
2:B:91:LEU:HD23	2:B:343:ASP:HA	1.61	0.82
2:B:894:LYS:C	2:B:895:PHE:CG	2.49	0.82
2:B:132:SER:CB	2:B:134:ARG:HH12	1.87	0.82
2:B:822:THR:HG22	2:B:864:ASP:H	1.00	0.82
15:O:386:PHE:CD2	15:O:606:MET:HE1	2.14	0.82
15:O:454:VAL:CA	15:O:514:PHE:CE2	2.62	0.82
15:O:245:GLN:HG3	15:O:378:THR:CA	2.05	0.82
15:O:398:SER:O	15:O:401:VAL:HG12	1.78	0.82
18:U:415:LYS:O	18:U:418:PRO:O	1.98	0.82
2:B:74:PHE:CZ	2:B:94:LYS:HG3	0.62	0.82
7:G:138:PHE:HE1	15:O:181:ARG:HD2	1.44	0.82
7:G:143:SER:CB	15:O:142:ILE:CG1	2.35	0.82
2:B:73:ILE:HG23	2:B:425:ILE:HD12	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:823:GLN:O	2:B:824:HIS:CG	2.33	0.82
1:A:1003:ARG:NH1	2:B:533:THR:CG2	1.84	0.82
1:A:1450:ILE:HG21	1:A:1460:TYR:CG	2.15	0.82
2:B:1119:ARG:CD	15:O:149:LYS:HZ1	1.92	0.82
15:O:457:ARG:CA	15:O:460:GLU:HB2	2.09	0.82
15:O:383:TYR:CD2	15:O:597:LEU:HD22	2.15	0.82
15:O:369:LYS:HE2	15:O:370:THR:CG2	2.10	0.81
1:A:1202:LEU:CD1	9:I:111:PHE:HZ	1.92	0.81
2:B:1120:ILE:CG1	15:O:149:LYS:HD3	2.10	0.81
15:O:246:ASN:OD1	15:O:247:GLU:N	2.11	0.81
15:O:371:HIS:C	15:O:375:THR:HG23	2.01	0.81
15:O:428:ILE:CG2	15:O:439:ILE:HG21	2.09	0.81
20:W:386:ASP:O	20:W:398:ASP:N	2.13	0.81
2:B:108:MET:HG2	2:B:171:HIS:NE2	1.95	0.81
1:A:683:LYS:HB2	8:H:20:TYR:CZ	2.13	0.81
1:A:1601:GLN:NE2	16:S:57:DA:H5"	1.93	0.81
2:B:132:SER:HB2	2:B:134:ARG:HH11	0.99	0.81
2:B:811:LEU:HD11	2:B:825:PHE:CE2	2.16	0.81
15:O:488:HIS:CG	15:O:489:ASN:N	2.40	0.81
20:W:206:ARG:O	20:W:207:ASN:O	1.99	0.81
1:A:1450:ILE:CD1	1:A:1460:TYR:HD2	1.92	0.81
15:O:457:ARG:C	15:O:460:GLU:HB2	2.01	0.81
2:B:161:LEU:HB3	2:B:458:GLY:HA2	1.62	0.81
7:G:142:ALA:CA	15:O:138:TYR:CE1	2.64	0.81
15:O:371:HIS:O	15:O:375:THR:HG23	1.79	0.81
7:G:244:SER:OG	15:O:148:PRO:HG2	1.79	0.81
15:O:237:ILE:CG2	15:O:381:ILE:CD1	2.57	0.81
2:B:1121:GLY:N	15:O:149:LYS:HD3	1.95	0.81
2:B:822:THR:CG2	2:B:864:ASP:HB2	2.06	0.80
1:A:252:PHE:HD2	1:A:314:TYR:CA	1.92	0.80
1:A:1261:VAL:CG2	1:A:1306:TYR:CB	2.01	0.80
2:B:1121:GLY:O	15:O:152:GLN:OE1	1.99	0.80
2:B:99:VAL:CG2	2:B:421:LEU:HD21	2.12	0.80
2:B:145:VAL:CG2	2:B:440:PHE:CD2	2.60	0.80
2:B:169:ARG:HA	2:B:169:ARG:HE	1.43	0.80
2:B:132:SER:CB	2:B:134:ARG:HH11	1.74	0.80
7:G:138:PHE:HE1	15:O:181:ARG:CB	1.87	0.80
18:U:97:GLY:H	18:U:101:LYS:N	1.79	0.80
1:A:683:LYS:HD2	8:H:20:TYR:CZ	2.17	0.80
2:B:822:THR:CG2	2:B:864:ASP:H	1.67	0.80
1:A:250:LYS:HD2	1:A:252:PHE:HZ	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:HD12	1:A:426:ALA:HB1	1.64	0.80
7:G:241:ARG:NH2	15:O:190:ILE:HG21	1.97	0.80
15:O:129:PRO:HG2	15:O:132:THR:HB	1.63	0.80
15:O:387:HIS:HB2	15:O:606:MET:SD	2.21	0.80
15:O:243:GLU:O	15:O:246:ASN:OD1	1.99	0.79
15:O:454:VAL:HA	15:O:514:PHE:CE2	2.16	0.79
15:O:584:GLN:OE1	15:O:584:GLN:N	2.11	0.79
18:U:436:LEU:O	18:U:439:ILE:N	2.14	0.79
1:A:722:PRO:HD2	8:H:46:LEU:HB3	1.64	0.79
1:A:1202:LEU:HD22	9:I:101:LEU:CD1	2.12	0.79
2:B:144:SER:N	2:B:151:ASN:OD1	2.14	0.79
2:B:154:GLU:HG2	2:B:443:LYS:HZ3	0.99	0.79
15:O:240:ILE:HG21	15:O:332:LEU:CG	2.11	0.79
15:O:436:ARG:O	15:O:440:ILE:HG13	1.82	0.79
2:B:74:PHE:CE2	2:B:94:LYS:HG3	1.80	0.79
15:O:166:ILE:CD1	15:O:213:SER:OG	2.30	0.79
2:B:1039:MET:HE1	2:B:1042:ASP:HA	1.63	0.79
19:V:185:GLN:O	19:V:199:GLY:CA	2.31	0.79
1:A:1439:MET:HE1	1:A:1444:ARG:HG2	1.64	0.78
2:B:142:LYS:CG	2:B:153:PHE:HE1	1.95	0.78
2:B:154:GLU:HG3	2:B:443:LYS:HE2	1.64	0.78
15:O:219:ARG:HH22	15:O:360:VAL:HG21	1.47	0.78
18:U:155:GLN:C	18:U:157:HIS:N	2.34	0.78
18:U:156:LEU:O	18:U:159:THR:N	2.14	0.78
2:B:98:SER:HB3	2:B:142:LYS:HB3	1.63	0.78
15:O:478:GLN:NE2	15:O:592:PHE:HZ	1.81	0.78
1:A:1601:GLN:NE2	16:S:57:DA:C5'	2.45	0.78
2:B:74:PHE:HE2	2:B:94:LYS:HD2	1.45	0.78
2:B:156:ARG:HD3	2:B:450:LEU:CD1	2.13	0.78
15:O:372:VAL:C	15:O:375:THR:HG23	2.04	0.78
17:T:21:DG:H5'	17:T:21:DG:H8	1.47	0.78
2:B:887:LEU:HD21	12:L:56:LEU:C	2.03	0.78
15:O:219:ARG:HH21	15:O:360:VAL:HG21	1.45	0.78
15:O:234:ILE:CG2	15:O:371:HIS:CD2	2.66	0.78
7:G:138:PHE:HD2	15:O:182:MET:HB2	1.43	0.78
15:O:425:GLY:HA2	15:O:483:ILE:CD1	2.13	0.78
15:O:360:VAL:O	15:O:364:LEU:HG	1.83	0.78
1:A:722:PRO:CG	8:H:46:LEU:HB3	2.14	0.78
2:B:1120:ILE:HB	15:O:153:ASP:CG	2.04	0.78
15:O:369:LYS:HB3	15:O:369:LYS:HZ3	1.48	0.78
1:A:373:LEU:CD2	1:A:378:HIS:CD2	2.67	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:243:GLU:HA	15:O:246:ASN:HD21	1.46	0.78
1:A:957:VAL:HG11	1:A:997:PHE:HE1	1.48	0.77
15:O:423:TYR:CD1	15:O:594:TYR:CE2	2.72	0.77
1:A:947:LEU:HD23	1:A:998:HIS:ND1	2.00	0.77
15:O:240:ILE:HB	15:O:332:LEU:HD13	1.66	0.77
15:O:158:LEU:CD2	15:O:172:HIS:CD2	2.67	0.77
15:O:234:ILE:HG21	15:O:371:HIS:CD2	2.18	0.77
15:O:373:LEU:CD1	15:O:416:LYS:HG3	2.13	0.77
2:B:898:LEU:HD23	12:L:46:VAL:CG2	1.26	0.77
2:B:161:LEU:CB	2:B:458:GLY:HA2	2.13	0.77
15:O:359:GLY:O	15:O:363:THR:HG22	1.85	0.77
15:O:241:ASP:OD1	15:O:378:THR:CG2	2.33	0.77
2:B:90:TYR:CE2	2:B:92:GLY:HA2	2.19	0.77
15:O:129:PRO:HG2	15:O:132:THR:CB	2.14	0.77
1:A:977:MET:HE1	1:A:993:GLN:HB2	1.67	0.77
2:B:73:ILE:HG21	2:B:425:ILE:HG23	0.77	0.77
2:B:887:LEU:CD2	12:L:56:LEU:CB	2.44	0.77
2:B:1120:ILE:CG1	15:O:149:LYS:CD	2.52	0.77
7:G:143:SER:CB	15:O:142:ILE:HD11	2.15	0.77
15:O:174:ASP:O	15:O:177:LYS:HG2	1.85	0.76
15:O:174:ASP:CA	15:O:177:LYS:HE2	2.12	0.76
2:B:1120:ILE:HG12	15:O:150:TRP:CE2	2.20	0.76
2:B:1121:GLY:H	15:O:149:LYS:CD	1.98	0.76
15:O:242:VAL:CA	15:O:378:THR:HG21	2.14	0.76
1:A:1456:PHE:O	1:A:1474:LEU:HA	1.85	0.76
2:B:96:SER:HB3	2:B:144:SER:HB2	1.67	0.76
15:O:430:ARG:NH2	15:O:596:PRO:CD	2.44	0.76
15:O:484:PHE:CE1	15:O:502:LEU:CD1	2.69	0.76
15:O:62:ASP:HB3	15:O:67:ASP:OD2	1.86	0.76
15:O:230:TRP:CE2	15:O:364:LEU:HD21	2.21	0.76
1:A:957:VAL:HG11	1:A:997:PHE:CE1	2.21	0.76
15:O:414:ALA:O	15:O:418:ILE:HD12	1.85	0.76
1:A:1005:GLY:HA3	9:I:100:GLN:HB3	1.68	0.76
1:A:1009:THR:OG1	9:I:101:LEU:C	2.24	0.75
2:B:71:LYS:O	2:B:97:VAL:HG12	1.87	0.75
15:O:484:PHE:CE1	15:O:502:LEU:HD12	2.21	0.75
1:A:1202:LEU:HD13	9:I:111:PHE:HZ	1.51	0.75
1:A:1457:ILE:HA	1:A:1473:LYS:C	2.06	0.75
2:B:132:SER:HB2	2:B:134:ARG:CZ	2.12	0.75
3:C:69:ARG:NH1	11:K:71:THR:OG1	2.19	0.75
15:O:369:LYS:HE2	15:O:370:THR:HG23	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:143:SER:HB2	15:O:142:ILE:HD11	1.65	0.75
15:O:447:THR:O	15:O:450:LEU:CB	2.33	0.75
1:A:1278:THR:O	1:A:1287:ALA:N	2.19	0.75
15:O:432:LYS:CB	15:O:609:TYR:C	2.54	0.75
7:G:143:SER:N	15:O:138:TYR:CZ	2.54	0.75
15:O:432:LYS:HG2	15:O:608:GLU:C	2.06	0.75
2:B:143:TRP:HE1	2:B:440:PHE:HB3	0.69	0.75
2:B:822:THR:O	2:B:863:ASP:CA	2.35	0.75
15:O:484:PHE:HE1	15:O:502:LEU:HD12	1.52	0.75
2:B:164:MET:HE2	2:B:194:PHE:CE1	2.21	0.75
2:B:898:LEU:HD21	12:L:46:VAL:CB	1.82	0.75
7:G:244:SER:CB	15:O:148:PRO:HG2	2.17	0.75
17:T:21:DG:H5'	17:T:21:DG:C8	2.22	0.75
2:B:16:PHE:HD2	2:B:978:ALA:HB2	1.51	0.75
2:B:898:LEU:HD23	2:B:898:LEU:N	2.01	0.75
15:O:428:ILE:HD12	15:O:439:ILE:CG2	2.16	0.75
7:G:242:VAL:HG11	15:O:185:SER:N	1.94	0.74
15:O:166:ILE:HD13	15:O:213:SER:OG	1.86	0.74
18:U:436:LEU:O	18:U:437:THR:C	2.26	0.74
15:O:372:VAL:N	15:O:375:THR:CG2	2.44	0.74
7:G:138:PHE:CE1	15:O:181:ARG:HD2	2.21	0.74
15:O:143:LEU:HD11	15:O:150:TRP:CD1	2.22	0.74
15:O:201:LYS:HD3	15:O:239:SER:OG	1.88	0.74
16:S:56:DA:N6	17:T:15:DT:O4	2.15	0.74
2:B:104:ILE:HB	2:B:169:ARG:HD2	1.69	0.74
2:B:106:LYS:HE3	2:B:171:HIS:ND1	2.01	0.74
15:O:245:GLN:HA	15:O:245:GLN:HE21	1.51	0.74
2:B:96:SER:HB3	2:B:144:SER:O	1.87	0.74
15:O:198:PHE:CE2	15:O:232:LEU:HG	2.22	0.74
15:O:359:GLY:HA2	15:O:362:ASN:ND2	2.02	0.74
15:O:234:ILE:HG22	15:O:371:HIS:HD2	1.53	0.74
15:O:342:HIS:NE2	15:O:346:GLN:NE2	2.34	0.74
2:B:152:LEU:HD22	2:B:152:LEU:N	2.01	0.74
15:O:432:LYS:HB3	15:O:609:TYR:HA	0.81	0.74
2:B:90:TYR:O	2:B:91:LEU:C	2.20	0.73
2:B:108:MET:C	2:B:119:ARG:HH21	1.92	0.73
2:B:168:ASN:HA	2:B:173:ASN:ND2	2.03	0.73
15:O:120:ILE:CD1	15:O:150:TRP:CE3	2.71	0.73
1:A:385:LEU:CD1	1:A:453:ILE:CG2	2.66	0.73
18:U:203:TRP:O	18:U:205:ILE:N	2.21	0.73
15:O:186:SER:O	15:O:190:ILE:HG22	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:VAL:CG1	2:B:441:LYS:HD2	2.18	0.73
2:B:106:LYS:CG	2:B:107:PRO:HD2	2.17	0.73
2:B:822:THR:HG23	2:B:864:ASP:C	2.01	0.73
3:C:329:LYS:HD2	11:K:122:LYS:HG3	1.69	0.73
7:G:241:ARG:HD3	15:O:189:PHE:CE1	1.37	0.73
15:O:101:SER:HB3	15:O:142:ILE:HD12	1.69	0.73
15:O:158:LEU:CD2	15:O:172:HIS:HD2	2.01	0.73
15:O:421:LEU:CD1	15:O:476:ALA:HB2	2.18	0.73
15:O:488:HIS:CD2	15:O:489:ASN:OD1	2.42	0.73
1:A:439:ASP:OD2	1:A:457:LYS:HD3	1.88	0.73
2:B:54:GLU:HB2	2:B:168:ASN:ND2	2.04	0.73
15:O:440:ILE:CG2	15:O:491:PHE:HE1	2.00	0.73
2:B:894:LYS:O	2:B:895:PHE:CD1	2.41	0.73
7:G:142:ALA:CA	15:O:138:TYR:HE1	1.99	0.73
15:O:162:PHE:O	15:O:210:ASN:C	2.27	0.73
15:O:241:ASP:C	15:O:378:THR:HG21	2.08	0.73
1:A:1007:ILE:O	1:A:1011:VAL:HG22	1.88	0.73
1:A:1450:ILE:HG21	1:A:1460:TYR:HB3	1.71	0.73
15:O:454:VAL:CA	15:O:514:PHE:CZ	2.67	0.73
15:O:348:THR:CG2	15:O:351:SER:HB3	2.19	0.72
15:O:373:LEU:HD11	15:O:416:LYS:HG2	1.65	0.72
15:O:407:SER:HB2	15:O:408:PHE:CD1	2.22	0.72
2:B:51:ALA:O	2:B:60:LEU:CD2	2.37	0.72
15:O:156:MET:SD	15:O:197:PHE:CE2	2.82	0.72
15:O:238:ILE:HD11	15:O:371:HIS:HB3	1.70	0.72
1:A:824:THR:HG23	2:B:1023:ARG:HB2	1.71	0.72
2:B:106:LYS:HG2	2:B:107:PRO:CD	2.14	0.72
15:O:194:LEU:CD2	15:O:225:LEU:HD11	2.19	0.72
15:O:352:LEU:CA	15:O:358:VAL:HG23	2.19	0.72
15:O:361:PHE:CE1	15:O:365:THR:HG21	2.24	0.72
15:O:240:ILE:CG2	15:O:332:LEU:CD1	2.67	0.72
15:O:356:GLU:O	15:O:360:VAL:HG23	1.88	0.72
15:O:371:HIS:C	15:O:375:THR:CG2	2.58	0.72
1:A:1454:HIS:HB2	1:A:1457:ILE:CG1	2.20	0.72
1:A:1499:ARG:O	1:A:1500:GLN:HB2	1.88	0.72
15:O:158:LEU:HD22	15:O:172:HIS:HA	1.71	0.72
15:O:225:LEU:O	15:O:225:LEU:HD13	1.89	0.72
15:O:370:THR:O	15:O:374:PRO:HG3	1.87	0.72
1:A:439:ASP:OD1	1:A:458:GLN:CD	2.27	0.72
7:G:241:ARG:HE	15:O:190:ILE:HG22	1.52	0.72
15:O:163:ILE:HA	15:O:211:TYR:N	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:390:GLN:HE22	15:O:432:LYS:N	1.86	0.72
1:A:799:GLU:OE1	1:A:1062:HIS:HB2	1.89	0.71
1:A:1256:LYS:C	1:A:1259:SER:HB2	2.10	0.71
3:C:54:PHE:CD2	11:K:135:PHE:HE1	2.08	0.71
2:B:823:GLN:HG2	2:B:863:ASP:HB3	1.71	0.71
1:A:438:ILE:O	1:A:455:GLY:CA	2.36	0.71
3:C:222:VAL:HG21	3:C:225:ALA:HB2	1.73	0.71
3:C:325:ALA:HB3	11:K:125:MET:HG3	1.71	0.71
15:O:352:LEU:O	15:O:358:VAL:CG2	2.39	0.71
16:S:53:DA:N6	17:T:18:DC:H42	1.88	0.71
2:B:898:LEU:HD23	12:L:46:VAL:HG21	1.02	0.71
2:B:1041:ASN:O	2:B:1044:PHE:N	2.23	0.71
3:C:47:LEU:HD13	11:K:142:MET:CE	2.20	0.71
7:G:158:LYS:CG	15:O:146:SER:OG	2.34	0.71
15:O:237:ILE:HG22	15:O:381:ILE:HB	1.71	0.71
1:A:1439:MET:CE	1:A:1444:ARG:HG2	2.20	0.71
2:B:164:MET:HB2	2:B:194:PHE:CE2	2.25	0.71
15:O:459:GLU:O	15:O:463:GLN:CG	2.37	0.71
2:B:139:LEU:CD2	2:B:420:TYR:CD2	2.71	0.71
7:G:241:ARG:CG	15:O:186:SER:HA	2.18	0.71
1:A:489:ASN:HB2	11:K:95:HIS:CD2	2.25	0.71
1:A:1202:LEU:HD22	9:I:101:LEU:HD22	1.73	0.71
15:O:128:LEU:HB3	15:O:129:PRO:CD	2.20	0.71
15:O:447:THR:CG2	15:O:480:LEU:HD22	2.21	0.71
7:G:152:ALA:O	15:O:184:PRO:CG	2.33	0.71
1:A:1440:ASN:O	1:A:1443:GLN:HB2	1.91	0.71
1:A:247:GLY:O	1:A:442:LYS:NZ	2.24	0.70
1:A:878:ARG:HD2	9:I:67:VAL:HG12	1.72	0.70
15:O:66:ASN:HD22	15:O:66:ASN:N	1.89	0.70
2:B:91:LEU:H	2:B:91:LEU:CD1	2.03	0.70
2:B:811:LEU:CD1	2:B:825:PHE:CE2	2.74	0.70
15:O:225:LEU:O	15:O:227:PHE:N	2.24	0.70
18:U:12:THR:O	18:U:14:ASN:O	2.08	0.70
1:A:1278:THR:OG1	1:A:1287:ALA:CB	2.39	0.70
7:G:158:LYS:HG2	15:O:146:SER:OG	1.92	0.70
15:O:152:GLN:HG3	15:O:193:TYR:OH	1.89	0.70
15:O:198:PHE:CE1	15:O:236:LYS:HG3	2.25	0.70
1:A:990:ILE:HD11	1:A:995:TYR:CG	2.21	0.70
2:B:154:GLU:HG2	2:B:443:LYS:HZ1	1.14	0.70
1:A:799:GLU:HG2	1:A:1062:HIS:CD2	2.27	0.70
15:O:471:LYS:HB2	15:O:585:PHE:CZ	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:O	1:A:390:LEU:CD1	2.28	0.70
2:B:1041:ASN:O	2:B:1042:ASP:C	2.29	0.70
2:B:74:PHE:HZ	2:B:94:LYS:CG	0.55	0.69
2:B:74:PHE:CD1	2:B:94:LYS:HA	2.25	0.69
2:B:162:PRO:HG3	2:B:465:LEU:HD12	1.74	0.69
2:B:887:LEU:CD2	2:B:887:LEU:H	2.04	0.69
1:A:1256:LYS:HA	1:A:1259:SER:HB2	1.74	0.69
15:O:373:LEU:HD12	15:O:373:LEU:O	1.91	0.69
2:B:811:LEU:HB2	2:B:899:GLN:OE1	1.92	0.69
2:B:108:MET:SD	2:B:171:HIS:CE1	2.86	0.69
1:A:1457:ILE:O	1:A:1459:LYS:N	2.22	0.69
2:B:898:LEU:CD2	12:L:46:VAL:HG23	1.17	0.69
7:G:242:VAL:CB	15:O:183:ILE:CG2	2.58	0.69
15:O:343:VAL:CG1	15:O:388:VAL:CG2	2.71	0.69
15:O:369:LYS:HB3	15:O:369:LYS:NZ	2.04	0.69
1:A:396:ILE:CD1	1:A:426:ALA:HB1	2.23	0.69
1:A:990:ILE:HD12	1:A:995:TYR:CA	2.22	0.69
2:B:161:LEU:HA	2:B:458:GLY:HA2	1.75	0.69
15:O:369:LYS:O	15:O:373:LEU:CB	2.41	0.69
16:S:65:DG:N1	17:T:7:DA:C2	2.58	0.69
15:O:220:GLY:O	15:O:221:TYR:CD1	2.46	0.69
1:A:1012:LYS:HB2	1:A:1012:LYS:NZ	2.08	0.69
2:B:123:PRO:CG	2:B:172:LEU:HD11	2.19	0.69
15:O:373:LEU:CB	15:O:374:PRO:HD3	2.22	0.69
16:S:64:DT:N3	17:T:8:DA:C4	2.48	0.69
1:A:1457:ILE:HD12	1:A:1458:THR:CA	2.24	0.68
2:B:813:LEU:HD13	2:B:813:LEU:O	1.93	0.68
2:B:68:ILE:HG21	2:B:418:ASP:OD2	1.92	0.68
15:O:597:LEU:HD12	15:O:598:PHE:H	1.58	0.68
18:U:155:GLN:C	18:U:157:HIS:H	1.93	0.68
1:A:253:GLU:HB3	1:A:313:THR:H	1.58	0.68
1:A:721:LYS:HD3	8:H:94:ASP:O	1.94	0.68
1:A:439:ASP:CA	1:A:458:GLN:OE1	2.29	0.68
1:A:977:MET:CE	1:A:993:GLN:HB2	2.22	0.68
1:A:990:ILE:HG13	1:A:995:TYR:HB2	1.75	0.68
1:A:996:TYR:CD1	2:B:525:TRP:CZ3	2.81	0.68
15:O:390:GLN:HE21	15:O:432:LYS:H	1.38	0.68
1:A:396:ILE:HD12	1:A:426:ALA:CB	2.23	0.68
2:B:811:LEU:CD2	2:B:899:GLN:CB	2.00	0.68
1:A:719:ILE:HG21	8:H:46:LEU:CD1	2.23	0.68
1:A:1023:LEU:HB3	1:A:1190:SER:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:240:ILE:CG2	15:O:332:LEU:CD2	2.63	0.68
15:O:458:GLU:HG3	15:O:514:PHE:CZ	2.29	0.68
1:A:1256:LYS:HA	1:A:1259:SER:CB	2.24	0.68
2:B:1120:ILE:CG1	15:O:149:LYS:HD2	2.22	0.68
15:O:108:GLU:HB2	15:O:147:ILE:HD11	1.75	0.68
15:O:241:ASP:CG	15:O:380:SER:HB2	2.14	0.68
15:O:474:TYR:HB3	15:O:520:CYS:SG	2.33	0.68
1:A:1261:VAL:HG22	1:A:1306:TYR:CB	2.21	0.68
3:C:40:PHE:HE2	11:K:134:LYS:HB2	1.59	0.68
1:A:33:THR:C	1:A:390:LEU:HD11	2.11	0.68
1:A:250:LYS:HD2	1:A:252:PHE:CZ	2.26	0.68
1:A:1003:ARG:CZ	2:B:533:THR:HG21	2.06	0.68
15:O:372:VAL:HA	15:O:375:THR:CB	2.17	0.68
15:O:390:GLN:CB	15:O:609:TYR:CD1	2.76	0.68
15:O:390:GLN:CD	15:O:609:TYR:HB3	2.15	0.68
15:O:417:LYS:HD3	15:O:472:HIS:HE1	1.57	0.68
3:C:229:LEU:HB3	3:C:293:ARG:HG2	1.76	0.67
2:B:165:LEU:HD12	2:B:165:LEU:N	2.08	0.67
7:G:241:ARG:CZ	15:O:190:ILE:HG21	2.24	0.67
16:S:53:DA:H62	17:T:18:DC:H42	1.42	0.67
2:B:123:PRO:HG3	2:B:172:LEU:CD1	2.19	0.67
18:U:155:GLN:O	18:U:157:HIS:N	2.23	0.67
3:C:40:PHE:HD2	11:K:134:LYS:HG3	1.59	0.67
2:B:128:GLN:HB2	12:L:55:ILE:HD13	1.76	0.67
2:B:1041:ASN:O	2:B:1041:ASN:ND2	2.27	0.67
1:A:403:LEU:HD12	1:A:419:ILE:HG12	1.72	0.67
2:B:74:PHE:CD1	2:B:93:ASN:O	2.48	0.67
15:O:241:ASP:C	15:O:378:THR:CG2	2.63	0.67
1:A:1256:LYS:O	1:A:1259:SER:CB	2.39	0.67
15:O:146:SER:O	15:O:148:PRO:HD3	1.95	0.67
1:A:947:LEU:CD2	1:A:998:HIS:ND1	2.58	0.67
2:B:97:VAL:HG11	2:B:425:ILE:HD11	1.76	0.67
15:O:428:ILE:O	15:O:487:ARG:NE	2.24	0.67
15:O:368:PHE:O	15:O:372:VAL:HG23	1.94	0.67
1:A:800:VAL:CG2	1:A:1068:PHE:CZ	2.76	0.66
2:B:74:PHE:CZ	2:B:94:LYS:HG2	1.01	0.66
2:B:107:PRO:O	2:B:121:VAL:HG11	1.94	0.66
17:T:21:DG:H2'	17:T:22:DA:H5"	0.73	0.66
2:B:60:LEU:HD22	2:B:60:LEU:N	2.09	0.66
2:B:96:SER:CA	2:B:144:SER:O	2.44	0.66
1:A:396:ILE:CD1	1:A:426:ALA:CB	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:GLU:HG2	2:B:140:LYS:HZ2	1.60	0.66
2:B:161:LEU:CA	2:B:458:GLY:CA	2.71	0.66
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.77	0.66
2:B:811:LEU:HD12	2:B:811:LEU:N	2.10	0.66
15:O:390:GLN:HB3	15:O:609:TYR:CD1	2.30	0.66
15:O:458:GLU:CG	15:O:514:PHE:CZ	2.79	0.66
1:A:250:LYS:CD	1:A:252:PHE:CZ	2.79	0.66
1:A:1202:LEU:CD2	9:I:101:LEU:HD22	2.26	0.66
1:A:1261:VAL:HA	1:A:1265:GLU:OE1	1.96	0.66
1:A:1202:LEU:HD22	9:I:122:ARG:HH12	1.59	0.66
1:A:1456:PHE:C	1:A:1474:LEU:HA	2.16	0.66
2:B:108:MET:HG2	2:B:171:HIS:CE1	2.25	0.66
15:O:174:ASP:HA	15:O:177:LYS:CE	2.22	0.66
2:B:72:VAL:HG11	2:B:94:LYS:HE3	1.78	0.66
2:B:141:LEU:HD21	2:B:424:ILE:CD1	2.22	0.66
2:B:108:MET:CG	2:B:171:HIS:HE2	2.08	0.66
2:B:129:ARG:O	2:B:129:ARG:HG3	1.94	0.66
15:O:108:GLU:HG3	15:O:108:GLU:O	1.96	0.66
1:A:399:LEU:HD21	1:A:422:ARG:CG	2.25	0.66
1:A:1260:LYS:CG	1:A:1500:GLN:HA	2.24	0.66
1:A:439:ASP:OD1	1:A:458:GLN:OE1	2.14	0.65
15:O:371:HIS:O	15:O:375:THR:HG22	1.95	0.65
1:A:1254:PHE:CE2	1:A:1258:ILE:HD11	2.31	0.65
2:B:77:LYS:O	2:B:90:TYR:CD2	2.49	0.65
2:B:156:ARG:CD	2:B:450:LEU:CD1	2.74	0.65
2:B:165:LEU:HD21	2:B:195:ILE:HD11	1.77	0.65
2:B:175:MET:CE	2:B:183:HIS:ND1	2.59	0.65
15:O:241:ASP:HA	15:O:380:SER:HB2	1.78	0.65
1:A:440:SER:O	1:A:442:LYS:N	2.30	0.65
15:O:219:ARG:HH21	15:O:360:VAL:HG22	1.60	0.65
2:B:156:ARG:NH2	2:B:447:SER:HA	2.12	0.65
1:A:250:LYS:CG	1:A:252:PHE:CZ	2.79	0.65
1:A:1454:HIS:CB	1:A:1457:ILE:CG1	2.74	0.65
1:A:1574:ALA:HB2	9:I:121:PHE:HA	1.79	0.65
2:B:1041:ASN:C	2:B:1043:LYS:N	2.50	0.65
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.77	0.65
2:B:1120:ILE:H	15:O:149:LYS:HE2	0.68	0.65
3:C:63:ILE:HG21	11:K:127:LEU:HD21	1.79	0.65
15:O:392:GLN:HB2	15:O:395:LEU:HD22	1.79	0.65
15:O:454:VAL:HG23	15:O:458:GLU:HG3	1.78	0.65
1:A:772:LYS:HE3	8:H:102:TYR:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:PHE:CE1	2:B:94:LYS:HG2	1.96	0.65
15:O:431:ALA:HB1	15:O:434:LEU:CD1	2.21	0.65
15:O:434:LEU:HD12	15:O:434:LEU:N	2.11	0.65
18:U:203:TRP:O	18:U:204:ARG:C	2.35	0.65
2:B:887:LEU:HD21	12:L:56:LEU:HB3	1.71	0.65
15:O:343:VAL:CG1	15:O:388:VAL:HG23	2.27	0.65
2:B:90:TYR:CZ	2:B:92:GLY:CA	2.78	0.65
2:B:169:ARG:HA	2:B:169:ARG:NE	2.12	0.65
2:B:811:LEU:CD2	2:B:899:GLN:CG	2.62	0.65
15:O:129:PRO:CG	15:O:132:THR:CB	2.74	0.65
15:O:430:ARG:HH21	15:O:596:PRO:HD3	1.55	0.65
15:O:488:HIS:NE2	15:O:489:ASN:OD1	2.29	0.65
2:B:51:ALA:O	2:B:60:LEU:HD23	1.96	0.64
3:C:315:PHE:CE1	11:K:136:THR:OG1	2.50	0.64
15:O:241:ASP:CB	15:O:380:SER:HB2	2.26	0.64
16:S:64:DT:O4	17:T:8:DA:C5	2.49	0.64
2:B:815:ARG:NH1	2:B:821:ILE:CD1	2.36	0.64
15:O:370:THR:O	15:O:374:PRO:HD2	1.93	0.64
1:A:1456:PHE:HB3	1:A:1475:GLU:N	2.12	0.64
2:B:139:LEU:HD23	2:B:420:TYR:CZ	2.33	0.64
2:B:913:ILE:O	2:B:1040:VAL:HG21	1.97	0.64
15:O:170:VAL:HG13	15:O:171:CYS:N	2.12	0.64
15:O:343:VAL:HG11	15:O:388:VAL:CG2	2.27	0.64
15:O:428:ILE:HD12	15:O:439:ILE:HD12	1.79	0.64
2:B:141:LEU:CD2	2:B:424:ILE:HD13	2.26	0.64
2:B:152:LEU:HD22	2:B:152:LEU:H	1.61	0.64
17:T:21:DG:C2'	17:T:22:DA:O5'	2.44	0.64
2:B:815:ARG:NH1	2:B:821:ILE:HD11	1.68	0.64
15:O:510:VAL:HG13	15:O:517:LEU:HD11	1.79	0.64
1:A:439:ASP:CG	1:A:457:LYS:HB3	2.17	0.64
1:A:1450:ILE:HD13	1:A:1460:TYR:CE2	2.25	0.64
1:A:1454:HIS:CB	1:A:1457:ILE:HG12	2.28	0.64
2:B:154:GLU:CG	2:B:443:LYS:CE	2.68	0.64
2:B:107:PRO:HA	2:B:135:GLY:HA2	1.79	0.64
2:B:558:VAL:HA	2:B:561:ILE:HD12	1.80	0.64
15:O:422:GLN:NE2	15:O:592:PHE:CD2	2.65	0.64
15:O:447:THR:HA	15:O:450:LEU:HD12	1.80	0.64
1:A:253:GLU:CB	1:A:313:THR:H	2.11	0.64
1:A:1262:LEU:HD22	1:A:1497:ILE:HG22	1.80	0.64
2:B:97:VAL:CG1	2:B:425:ILE:HD11	2.28	0.64
2:B:813:LEU:HD13	2:B:813:LEU:C	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:PHE:CD2	11:K:134:LYS:HG3	2.33	0.64
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.63	0.63
1:A:1457:ILE:CD1	1:A:1458:THR:N	2.50	0.63
2:B:164:MET:HB2	2:B:194:PHE:CZ	2.32	0.63
2:B:190:ILE:H	2:B:190:ILE:HD13	1.64	0.63
15:O:181:ARG:HB2	15:O:181:ARG:NH1	2.13	0.63
15:O:435:SER:HB3	15:O:438:GLN:CG	2.23	0.63
15:O:454:VAL:HG23	15:O:458:GLU:CG	2.28	0.63
1:A:990:ILE:CD1	1:A:995:TYR:HB2	2.29	0.63
1:A:1256:LYS:CA	1:A:1259:SER:HB2	2.29	0.63
20:W:339:ASN:O	20:W:342:LEU:N	2.31	0.63
1:A:878:ARG:HD2	9:I:67:VAL:CG1	2.28	0.63
7:G:148:LEU:HD21	15:O:181:ARG:O	1.98	0.63
15:O:373:LEU:N	15:O:374:PRO:CD	2.61	0.63
2:B:73:ILE:C	2:B:73:ILE:HD12	2.18	0.63
2:B:164:MET:CE	2:B:194:PHE:CZ	2.82	0.63
2:B:108:MET:CG	2:B:171:HIS:HE1	1.99	0.63
15:O:240:ILE:CG2	15:O:332:LEU:CG	2.76	0.63
15:O:368:PHE:CE2	15:O:382:GLN:HA	2.33	0.63
2:B:73:ILE:HG22	2:B:425:ILE:HG21	1.79	0.63
15:O:383:TYR:CE2	15:O:597:LEU:HD22	2.33	0.63
15:O:430:ARG:HH22	15:O:596:PRO:HD3	1.58	0.63
1:A:713:VAL:H	1:A:738:ASN:HD21	1.47	0.63
1:A:990:ILE:CD1	1:A:995:TYR:CB	2.77	0.63
2:B:1119:ARG:HB2	15:O:149:LYS:CE	2.04	0.63
15:O:144:CYS:O	15:O:148:PRO:HG3	1.99	0.63
15:O:181:ARG:HH11	15:O:181:ARG:CG	2.12	0.63
1:A:996:TYR:CD1	2:B:525:TRP:HE3	2.14	0.62
2:B:168:ASN:OD1	2:B:173:ASN:ND2	2.32	0.62
15:O:98:ASP:OD2	15:O:135:LYS:HD3	1.99	0.62
15:O:198:PHE:CD1	15:O:236:LYS:CE	2.78	0.62
15:O:457:ARG:O	15:O:460:GLU:CB	2.47	0.62
17:T:7:DA:H2"	17:T:8:DA:H5"	1.79	0.62
1:A:719:ILE:HD13	8:H:43:ASN:ND2	2.08	0.62
1:A:1457:ILE:C	1:A:1457:ILE:HD12	2.18	0.62
15:O:426:SER:OG	15:O:594:TYR:CA	2.46	0.62
15:O:471:LYS:HG3	15:O:472:HIS:N	2.14	0.62
15:O:454:VAL:HG23	15:O:458:GLU:OE2	1.98	0.62
15:O:460:GLU:O	15:O:469:ARG:NH1	2.32	0.62
1:A:701:ARG:H	1:A:706:HIS:HD2	1.46	0.62
2:B:164:MET:HE2	2:B:194:PHE:CZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:245:GLN:HA	15:O:245:GLN:NE2	2.14	0.62
15:O:247:GLU:OE1	15:O:325:ILE:HG13	1.95	0.62
2:B:137:LEU:HD23	2:B:158:CYS:CB	2.30	0.62
2:B:161:LEU:HD12	2:B:161:LEU:C	2.20	0.62
2:B:143:TRP:CZ2	2:B:440:PHE:CD1	2.80	0.62
2:B:96:SER:CB	2:B:144:SER:O	2.47	0.62
2:B:159:GLY:CA	2:B:456:ASN:HA	2.22	0.62
7:G:143:SER:OG	15:O:142:ILE:HD11	1.98	0.62
15:O:225:LEU:HD13	15:O:225:LEU:C	2.19	0.62
15:O:379:ARG:CB	15:O:382:GLN:HE22	2.12	0.62
15:O:581:THR:HA	15:O:584:GLN:NE2	2.15	0.62
1:A:1202:LEU:HB3	9:I:101:LEU:HD21	0.67	0.62
15:O:151:TRP:CZ2	15:O:176:LEU:HD23	2.35	0.62
15:O:158:LEU:HB3	15:O:172:HIS:HB3	1.82	0.62
15:O:368:PHE:CE2	15:O:385:MET:HB2	2.34	0.62
1:A:1038:ILE:HB	1:A:1047:GLN:HB2	1.82	0.62
15:O:56:VAL:HG21	15:O:99:ILE:HD12	1.82	0.62
15:O:343:VAL:HG12	15:O:388:VAL:HG23	1.82	0.62
15:O:450:LEU:O	15:O:454:VAL:HG12	2.00	0.62
15:O:454:VAL:HG23	15:O:458:GLU:CD	2.19	0.62
1:A:1261:VAL:HG12	1:A:1265:GLU:CB	2.29	0.61
15:O:417:LYS:HD3	15:O:472:HIS:CE1	2.33	0.61
2:B:1120:ILE:HG13	15:O:149:LYS:CE	2.29	0.61
15:O:155:SER:HA	15:O:158:LEU:HD12	1.81	0.61
15:O:447:THR:HG22	15:O:480:LEU:CD2	2.28	0.61
18:U:436:LEU:C	18:U:438:PHE:N	2.52	0.61
1:A:990:ILE:HD12	1:A:995:TYR:CB	2.30	0.61
1:A:1202:LEU:HD11	9:I:111:PHE:CE1	2.35	0.61
1:A:1454:HIS:HB2	1:A:1457:ILE:HG12	1.81	0.61
2:B:887:LEU:HD11	12:L:56:LEU:CD1	2.30	0.61
9:I:72:LYS:HB2	9:I:75:GLU:HB2	1.80	0.61
15:O:152:GLN:HG2	15:O:193:TYR:HH	1.63	0.61
15:O:241:ASP:OD1	15:O:379:ARG:C	2.39	0.61
15:O:447:THR:CG2	15:O:480:LEU:CD2	2.79	0.61
1:A:657:TYR:HA	1:A:667:ARG:HG3	1.82	0.61
1:A:991:LYS:CD	1:A:994:GLU:OE1	2.44	0.61
1:A:1457:ILE:O	1:A:1473:LYS:C	2.38	0.61
2:B:108:MET:C	2:B:121:VAL:HG12	2.20	0.61
15:O:348:THR:HG22	15:O:351:SER:CB	2.26	0.61
15:O:428:ILE:HG23	15:O:439:ILE:CG2	2.23	0.61
1:A:1450:ILE:CD1	1:A:1460:TYR:CD2	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:369:LYS:HG3	15:O:406:ILE:HD11	1.83	0.61
1:A:1261:VAL:HG21	1:A:1306:TYR:HB3	0.63	0.61
2:B:175:MET:HE3	2:B:183:HIS:ND1	2.16	0.61
3:C:44:ILE:HD12	11:K:138:LYS:O	2.00	0.61
2:B:165:LEU:HD21	2:B:195:ILE:HD12	1.81	0.61
15:O:67:ASP:OD1	15:O:69:THR:HB	2.00	0.61
1:A:1003:ARG:HE	2:B:520:LEU:HB2	1.66	0.61
2:B:900:THR:C	2:B:901:VAL:HG23	2.18	0.61
15:O:396:MET:SD	15:O:434:LEU:HA	2.41	0.61
2:B:74:PHE:HD1	2:B:93:ASN:O	1.83	0.60
2:B:176:SER:OG	2:B:177:PRO:HD2	2.01	0.60
2:B:811:LEU:HD21	2:B:825:PHE:CE2	2.35	0.60
1:A:722:PRO:HD2	8:H:46:LEU:HD13	1.83	0.60
1:A:1275:THR:HG23	1:A:1289:SER:HB2	1.82	0.60
2:B:68:ILE:O	2:B:68:ILE:HG22	2.00	0.60
2:B:90:TYR:CE2	2:B:92:GLY:CA	2.84	0.60
2:B:91:LEU:HD23	2:B:343:ASP:CA	2.29	0.60
15:O:100:LEU:HD22	15:O:107:ILE:HD11	1.82	0.60
15:O:423:TYR:HD1	15:O:594:TYR:CZ	2.19	0.60
15:O:457:ARG:HA	15:O:460:GLU:CB	2.30	0.60
2:B:811:LEU:HD21	2:B:825:PHE:CD2	2.35	0.60
3:C:322:LYS:HD2	11:K:129:ASP:OD1	2.01	0.60
1:A:1262:LEU:CD2	1:A:1497:ILE:HG22	2.31	0.60
7:G:138:PHE:CE1	15:O:181:ARG:CG	2.84	0.60
2:B:156:ARG:HH21	2:B:447:SER:HA	1.67	0.60
15:O:431:ALA:HB3	15:O:434:LEU:CD1	2.23	0.60
16:S:58:DA:C2	17:T:14:DT:O2	2.54	0.60
1:A:878:ARG:NH1	9:I:66:VAL:HB	2.17	0.60
7:G:152:ALA:C	15:O:184:PRO:HG2	2.22	0.60
15:O:467:MET:HG3	15:O:519:PHE:CE2	2.36	0.60
1:A:947:LEU:CD2	1:A:998:HIS:HD1	2.14	0.60
1:A:1003:ARG:NH2	2:B:530:PRO:O	2.34	0.60
2:B:100:GLU:HG2	2:B:140:LYS:NZ	2.16	0.60
10:J:48:ARG:O	10:J:52:THR:HB	2.02	0.60
2:B:1039:MET:HE3	2:B:1042:ASP:CA	2.18	0.60
2:B:89:GLY:O	2:B:91:LEU:N	2.34	0.60
2:B:162:PRO:HG2	2:B:465:LEU:HD12	1.82	0.60
1:A:385:LEU:HD11	1:A:453:ILE:CG2	2.28	0.60
2:B:96:SER:HB3	2:B:144:SER:CB	2.31	0.60
2:B:98:SER:HB3	2:B:142:LYS:HD2	1.83	0.60
1:A:996:TYR:HD1	2:B:525:TRP:CZ3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:154:ASN:CB	15:O:183:ILE:HG12	2.31	0.59
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.83	0.59
2:B:1120:ILE:CD1	15:O:150:TRP:CE3	2.86	0.59
28:P:135:ALA:CA	29:Z:149:ALA:O	2.50	0.59
1:A:1457:ILE:HD12	1:A:1458:THR:H	1.62	0.59
2:B:749:THR:O	10:J:52:THR:HG23	2.01	0.59
2:B:823:GLN:O	2:B:824:HIS:CD2	2.55	0.59
2:B:1119:ARG:CD	15:O:149:LYS:HZ2	2.12	0.59
15:O:582:ARG:O	15:O:586:ILE:HG13	2.01	0.59
2:B:1120:ILE:CD1	15:O:150:TRP:CD2	2.85	0.59
7:G:142:ALA:CA	15:O:138:TYR:OH	2.50	0.59
15:O:348:THR:HG23	15:O:351:SER:H	1.68	0.59
18:U:156:LEU:O	18:U:158:MET:N	2.35	0.59
2:B:84:GLU:HG3	2:B:86:SER:H	1.67	0.59
7:G:142:ALA:CB	15:O:138:TYR:OH	2.50	0.59
7:G:154:ASN:ND2	15:O:183:ILE:CG1	2.65	0.59
3:C:275:VAL:HG21	3:C:293:ARG:HH21	1.66	0.59
5:E:147:HIS:HD2	5:E:149:LEU:H	1.50	0.59
2:B:70:GLU:HG2	2:B:98:SER:HB2	1.84	0.59
9:I:11:LEU:HD22	13:M:31:ARG:HG3	1.84	0.59
15:O:487:ARG:HH11	15:O:487:ARG:CG	2.14	0.59
18:U:127:LYS:C	18:U:129:PHE:N	2.56	0.59
1:A:380:ASN:CG	1:A:383:ASN:OD1	2.41	0.59
1:A:1012:LYS:O	1:A:1012:LYS:HG2	2.02	0.59
1:A:1202:LEU:HB3	9:I:101:LEU:CG	2.28	0.59
1:A:1202:LEU:CD1	9:I:101:LEU:HD11	2.25	0.59
2:B:154:GLU:CD	2:B:443:LYS:HZ3	2.06	0.59
13:M:61:GLU:HB3	13:M:101:VAL:HG23	1.84	0.59
1:A:1456:PHE:O	1:A:1474:LEU:CA	2.51	0.59
2:B:887:LEU:CD2	12:L:56:LEU:CA	2.77	0.59
15:O:241:ASP:O	15:O:378:THR:CG2	2.51	0.59
15:O:373:LEU:N	15:O:374:PRO:HD2	2.17	0.59
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.85	0.59
15:O:377:TYR:O	15:O:378:THR:OG1	2.21	0.59
1:A:629:ASP:HA	2:B:785:ASP:HB3	1.84	0.58
7:G:241:ARG:NH2	15:O:190:ILE:HG22	2.06	0.58
1:A:1278:THR:OG1	1:A:1287:ALA:HB2	2.03	0.58
2:B:91:LEU:CD2	2:B:343:ASP:HA	2.33	0.58
2:B:123:PRO:HA	2:B:133:TYR:CE1	2.38	0.58
2:B:211:ARG:HH22	2:B:243:GLN:HE22	1.49	0.58
15:O:164:LEU:O	15:O:165:PRO:O	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:242:VAL:CG2	15:O:183:ILE:HG22	2.33	0.58
2:B:822:THR:HA	2:B:864:ASP:OD2	2.03	0.58
1:A:439:ASP:CG	1:A:458:GLN:HE22	2.07	0.58
1:A:998:HIS:CD2	2:B:712:SER:CB	2.76	0.58
2:B:96:SER:CB	2:B:144:SER:HB2	2.33	0.58
2:B:175:MET:HE1	2:B:183:HIS:HB2	1.86	0.58
3:C:95:GLU:HG3	12:L:67:PHE:CE1	2.38	0.58
7:G:154:ASN:CG	15:O:184:PRO:HD3	2.23	0.58
1:A:727:THR:HG22	1:A:730:GLN:HG3	1.85	0.58
1:A:1261:VAL:CG1	1:A:1306:TYR:CG	2.87	0.58
2:B:91:LEU:HD12	2:B:91:LEU:N	2.11	0.58
7:G:143:SER:CA	15:O:138:TYR:OH	2.50	0.58
15:O:454:VAL:CG2	15:O:458:GLU:OE2	2.51	0.58
2:B:90:TYR:C	2:B:92:GLY:N	2.56	0.58
2:B:748:GLN:HB3	10:J:52:THR:HG22	1.85	0.58
3:C:67:PHE:CZ	11:K:131:VAL:HG11	2.38	0.58
15:O:369:LYS:CE	15:O:370:THR:HG22	2.33	0.58
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.85	0.58
2:B:162:PRO:HG2	2:B:409:TYR:OH	2.03	0.58
2:B:822:THR:HG22	2:B:822:THR:O	2.02	0.58
3:C:321:LEU:HD23	11:K:128:CYS:SG	2.43	0.58
15:O:101:SER:HB3	15:O:142:ILE:CD1	2.33	0.58
1:A:482:SER:HA	2:B:1041:ASN:OD1	2.04	0.58
2:B:89:GLY:O	2:B:91:LEU:HD12	2.04	0.58
2:B:108:MET:HG3	2:B:171:HIS:HE2	1.67	0.58
7:G:138:PHE:HE1	15:O:181:ARG:CD	2.14	0.58
15:O:230:TRP:CZ2	15:O:364:LEU:HD11	2.39	0.58
2:B:145:VAL:HG21	2:B:440:PHE:CD2	2.37	0.58
1:A:399:LEU:HD21	1:A:422:ARG:CD	2.33	0.57
1:A:1456:PHE:C	1:A:1475:GLU:H	2.08	0.57
15:O:174:ASP:O	15:O:177:LYS:CG	2.52	0.57
15:O:458:GLU:CB	15:O:461:VAL:CG2	2.80	0.57
15:O:173:HIS:CD2	15:O:217:LYS:HG2	2.39	0.57
15:O:484:PHE:CD1	15:O:502:LEU:HD13	2.39	0.57
15:O:487:ARG:O	15:O:490:ILE:HB	2.04	0.57
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.85	0.57
1:A:1450:ILE:CG2	1:A:1460:TYR:CB	2.80	0.57
2:B:108:MET:HB3	2:B:120:LYS:HA	1.86	0.57
1:A:389:VAL:HG22	1:A:433:ASP:CG	2.25	0.57
2:B:839:LYS:HG3	2:B:857:PRO:HD2	1.86	0.57
2:B:1039:MET:HE2	2:B:1042:ASP:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:359:GLY:CA	15:O:362:ASN:HD22	2.16	0.57
1:A:1001:ALA:O	1:A:1004:GLU:HG3	2.05	0.57
15:O:440:ILE:CG2	15:O:491:PHE:CE1	2.82	0.57
1:A:396:ILE:HG13	1:A:426:ALA:CB	2.35	0.57
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.86	0.57
15:O:63:LEU:HD23	15:O:111:ARG:HD2	1.87	0.57
15:O:154:VAL:O	15:O:158:LEU:HG	2.05	0.57
15:O:417:LYS:HB3	15:O:472:HIS:CE1	2.39	0.57
16:S:65:DG:C2	17:T:7:DA:H2	2.18	0.57
1:A:396:ILE:CG1	1:A:426:ALA:HB1	2.34	0.57
1:A:1202:LEU:HD22	9:I:101:LEU:HD13	1.86	0.57
2:B:137:LEU:HD23	2:B:158:CYS:HB2	1.86	0.57
2:B:1041:ASN:OD1	2:B:1044:PHE:CB	2.51	0.57
7:G:142:ALA:C	15:O:138:TYR:CZ	2.77	0.57
15:O:428:ILE:CD1	15:O:439:ILE:HD12	2.33	0.57
15:O:607:LYS:HG3	15:O:608:GLU:N	2.17	0.57
16:S:63:DT:H2"	16:S:64:DT:H3'	1.86	0.57
2:B:914:GLY:CA	2:B:1040:VAL:HG21	2.28	0.57
15:O:98:ASP:OD2	15:O:135:LYS:NZ	2.35	0.57
15:O:158:LEU:HD22	15:O:172:HIS:CB	2.35	0.57
15:O:205:ARG:O	15:O:209:VAL:HG12	2.05	0.57
15:O:390:GLN:HB2	15:O:609:TYR:CD1	2.37	0.57
15:O:484:PHE:CE1	15:O:502:LEU:HD13	2.39	0.57
2:B:143:TRP:O	2:B:151:ASN:HA	2.05	0.57
15:O:66:ASN:N	15:O:66:ASN:ND2	2.53	0.57
15:O:190:ILE:HA	15:O:193:TYR:CD2	2.39	0.57
15:O:369:LYS:HD3	15:O:373:LEU:HD22	1.85	0.57
1:A:1456:PHE:HB3	1:A:1475:GLU:H	1.69	0.56
7:G:154:ASN:OD1	15:O:184:PRO:HD2	1.98	0.56
15:O:109:SER:OG	15:O:111:ARG:HG3	2.05	0.56
15:O:128:LEU:HD22	15:O:129:PRO:HD3	1.86	0.56
15:O:422:GLN:NE2	15:O:592:PHE:CZ	2.69	0.56
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.87	0.56
2:B:1041:ASN:C	2:B:1043:LYS:H	2.07	0.56
15:O:98:ASP:CG	15:O:135:LYS:HD3	2.26	0.56
15:O:247:GLU:HB3	15:O:325:ILE:HD11	1.86	0.56
18:U:126:PRO:O	18:U:129:PHE:N	2.30	0.56
1:A:332:GLN:HE22	1:A:350:VAL:H	1.51	0.56
1:A:1262:LEU:N	1:A:1265:GLU:OE1	2.38	0.56
2:B:107:PRO:O	2:B:121:VAL:HG13	2.06	0.56
3:C:42:VAL:CB	11:K:138:LYS:HG3	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:369:LYS:O	15:O:373:LEU:HB3	2.04	0.56
15:O:447:THR:HA	15:O:450:LEU:CG	2.35	0.56
15:O:458:GLU:HG2	15:O:514:PHE:CZ	2.41	0.56
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.85	0.56
1:A:990:ILE:CG1	1:A:995:TYR:HB2	2.36	0.56
1:A:1008:ASP:HA	1:A:1011:VAL:CG2	2.36	0.56
7:G:138:PHE:CD2	15:O:182:MET:CG	2.87	0.56
2:B:106:LYS:HD3	2:B:108:MET:HG3	1.87	0.56
11:K:46:LYS:HA	11:K:66:VAL:HG22	1.88	0.56
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.86	0.56
15:O:421:LEU:HD13	15:O:476:ALA:CB	2.31	0.56
15:O:391:GLN:OE1	15:O:609:TYR:OH	2.23	0.56
15:O:408:PHE:CE1	15:O:446:LEU:HD13	2.35	0.56
1:A:400:ASN:OD1	1:A:423:LEU:HD11	2.06	0.56
1:A:1454:HIS:CB	1:A:1457:ILE:HG13	2.36	0.56
1:A:701:ARG:H	1:A:706:HIS:CD2	2.24	0.56
15:O:432:LYS:HB2	15:O:610:TYR:N	2.20	0.56
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.87	0.56
1:A:712:ILE:N	11:K:106:GLN:HE22	2.01	0.56
2:B:96:SER:O	2:B:144:SER:N	2.35	0.56
3:C:326:GLU:HA	11:K:125:MET:SD	2.46	0.56
15:O:447:THR:C	15:O:450:LEU:H	2.09	0.56
1:A:1256:LYS:HA	1:A:1259:SER:OG	2.06	0.55
2:B:108:MET:SD	2:B:171:HIS:HE1	2.29	0.55
2:B:815:ARG:HD2	2:B:821:ILE:HA	1.88	0.55
15:O:396:MET:HE1	15:O:434:LEU:CD1	2.30	0.55
15:O:447:THR:HA	15:O:450:LEU:CD1	2.35	0.55
1:A:719:ILE:CD1	8:H:43:ASN:HD22	2.12	0.55
2:B:300:SER:HB3	9:I:49:THR:HG22	1.87	0.55
2:B:721:MET:HG3	2:B:1036:LEU:HD21	1.88	0.55
2:B:840:LEU:HD21	2:B:857:PRO:HB2	1.87	0.55
15:O:517:LEU:HD12	15:O:543:ILE:HG21	1.88	0.55
2:B:142:LYS:HA	2:B:153:PHE:CD1	2.41	0.55
1:A:385:LEU:CD1	1:A:453:ILE:CB	2.56	0.55
2:B:791:LYS:O	2:B:795:GLU:HG2	2.06	0.55
15:O:360:VAL:O	15:O:363:THR:HG23	2.06	0.55
1:A:399:LEU:HD11	1:A:422:ARG:HD2	1.87	0.55
1:A:943:ILE:HG12	2:B:960:ILE:HD11	1.87	0.55
1:A:990:ILE:HD11	1:A:995:TYR:HD1	0.82	0.55
1:A:1261:VAL:HG11	1:A:1306:TYR:CG	2.41	0.55
2:B:811:LEU:CD2	2:B:825:PHE:CE2	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:371:HIS:C	15:O:374:PRO:HD2	2.27	0.55
15:O:432:LYS:HG3	15:O:608:GLU:O	1.96	0.55
2:B:90:TYR:CD1	2:B:92:GLY:HA2	2.41	0.55
2:B:161:LEU:HA	2:B:458:GLY:CA	2.35	0.55
15:O:169:THR:HA	15:O:172:HIS:ND1	2.22	0.55
15:O:158:LEU:HD22	15:O:172:HIS:CA	2.36	0.55
15:O:343:VAL:CG1	15:O:388:VAL:HG21	2.36	0.55
15:O:369:LYS:HD2	15:O:369:LYS:C	2.27	0.55
15:O:487:ARG:NH2	15:O:611:ILE:HD12	2.22	0.55
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.07	0.55
1:A:1276:THR:HG23	1:A:1276:THR:O	2.07	0.55
15:O:129:PRO:HG2	15:O:132:THR:OG1	2.06	0.55
15:O:238:ILE:CD1	15:O:371:HIS:HB3	2.37	0.55
15:O:488:HIS:C	15:O:490:ILE:N	2.59	0.55
1:A:1275:THR:HG22	1:A:1289:SER:HB2	1.85	0.54
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.89	0.54
13:M:9:GLU:HG2	14:N:71:PRO:HB3	1.89	0.54
15:O:69:THR:O	15:O:73:ILE:HG13	2.07	0.54
15:O:432:LYS:CB	15:O:608:GLU:O	2.55	0.54
15:O:147:ILE:O	15:O:147:ILE:HG22	2.07	0.54
15:O:423:TYR:CD1	15:O:594:TYR:CZ	2.95	0.54
1:A:373:LEU:HD11	1:A:378:HIS:NE2	2.22	0.54
1:A:990:ILE:CD1	1:A:995:TYR:CG	2.84	0.54
2:B:122:TYR:HB3	2:B:123:PRO:HD2	1.89	0.54
15:O:484:PHE:CD1	15:O:502:LEU:CD1	2.89	0.54
1:A:396:ILE:HD12	1:A:426:ALA:C	2.28	0.54
7:G:134:GLU:HB3	7:G:228:LYS:HE2	1.89	0.54
15:O:241:ASP:CA	15:O:380:SER:HB2	2.38	0.54
1:A:253:GLU:HB3	1:A:312:SER:HA	1.89	0.54
2:B:90:TYR:O	2:B:92:GLY:N	2.41	0.54
2:B:108:MET:HE2	2:B:120:LYS:N	2.22	0.54
2:B:813:LEU:HD13	2:B:814:ASN:OD1	2.01	0.54
2:B:857:PRO:HB3	2:B:871:ILE:HD13	1.89	0.54
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.88	0.54
15:O:191:ASP:O	15:O:194:LEU:HB2	2.06	0.54
15:O:488:HIS:C	15:O:490:ILE:H	2.10	0.54
1:A:905:SER:HB2	9:I:81:THR:O	2.08	0.54
3:C:325:ALA:CB	11:K:125:MET:HG3	2.38	0.54
15:O:166:ILE:HD11	15:O:213:SER:OG	2.06	0.54
15:O:386:PHE:CD2	15:O:606:MET:HE2	2.40	0.54
1:A:1457:ILE:C	1:A:1459:LYS:H	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:SER:OG	2:B:177:PRO:CD	2.56	0.54
15:O:156:MET:HG3	15:O:197:PHE:HE2	1.61	0.54
1:A:380:ASN:HB3	1:A:383:ASN:HB2	1.90	0.54
1:A:863:ASN:OD1	9:I:68:LYS:HE3	2.08	0.54
1:A:1062:HIS:HA	1:A:1065:GLN:HB2	1.90	0.54
15:O:100:LEU:HD22	15:O:107:ILE:CD1	2.38	0.54
2:B:108:MET:CA	2:B:121:VAL:CG1	2.68	0.54
2:B:175:MET:HE3	2:B:183:HIS:CG	2.43	0.54
2:B:895:PHE:CD2	2:B:896:GLN:HG3	2.43	0.54
7:G:138:PHE:HD2	15:O:182:MET:CG	2.21	0.54
15:O:391:GLN:NE2	15:O:609:TYR:CE2	2.76	0.54
1:A:676:ALA:HB2	1:A:821:ILE:HD13	1.90	0.54
2:B:323:ARG:HH22	2:B:351:GLN:HE22	1.56	0.54
2:B:1041:ASN:ND2	2:B:1044:PHE:N	2.56	0.54
3:C:315:PHE:HE1	11:K:136:THR:OG1	1.90	0.54
7:G:154:ASN:HB3	15:O:183:ILE:HG12	1.89	0.54
15:O:164:LEU:HB3	15:O:165:PRO:HD2	1.89	0.54
15:O:343:VAL:HG11	15:O:388:VAL:HG21	1.89	0.54
15:O:426:SER:HB3	15:O:594:TYR:HD2	1.72	0.54
1:A:1450:ILE:HG21	1:A:1460:TYR:CD2	2.42	0.53
15:O:189:PHE:CD1	15:O:190:ILE:N	2.76	0.53
1:A:627:ASP:HB2	2:B:785:ASP:OD2	2.07	0.53
1:A:1657:LEU:HD11	6:F:135:ARG:HB2	1.89	0.53
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.90	0.53
15:O:63:LEU:CD2	15:O:111:ARG:HD2	2.38	0.53
15:O:447:THR:O	15:O:450:LEU:N	2.39	0.53
1:A:1450:ILE:CG2	1:A:1460:TYR:HB3	2.36	0.53
15:O:390:GLN:HB2	15:O:609:TYR:CG	2.43	0.53
28:P:134:ALA:O	29:Z:148:ALA:C	2.47	0.53
1:A:970:LYS:HE2	2:B:685:VAL:HG21	1.90	0.53
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	1.90	0.53
3:C:333:ILE:HD11	11:K:118:GLN:HE21	1.74	0.53
15:O:447:THR:HA	15:O:450:LEU:HG	1.88	0.53
1:A:799:GLU:OE1	1:A:1062:HIS:ND1	2.41	0.53
3:C:92:ILE:CG1	10:J:2:ILE:HD11	2.21	0.53
3:C:232:GLN:HE21	3:C:234:ASN:HD21	1.55	0.53
5:E:131:THR:HG21	5:E:191:LYS:HE2	1.91	0.53
15:O:368:PHE:CZ	15:O:385:MET:HB2	2.43	0.53
1:A:444:GLN:CG	1:A:445:GLY:N	2.44	0.53
1:A:1457:ILE:O	1:A:1458:THR:OG1	2.23	0.53
2:B:73:ILE:HD12	2:B:73:ILE:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ILE:HG23	10:J:57:ILE:HG21	1.90	0.53
15:O:352:LEU:HD22	15:O:358:VAL:HG22	1.81	0.53
1:A:385:LEU:HG	1:A:453:ILE:HG21	1.90	0.53
1:A:1261:VAL:CG1	1:A:1306:TYR:CE1	2.80	0.53
2:B:72:VAL:HG11	2:B:94:LYS:CE	2.39	0.53
2:B:888:ILE:N	2:B:888:ILE:HD12	2.24	0.53
7:G:81:VAL:HA	7:G:124:VAL:HG12	1.90	0.53
15:O:206:ARG:HA	15:O:209:VAL:HG12	1.91	0.53
15:O:218:LEU:HD23	15:O:229:ILE:HD11	1.90	0.53
1:A:1056:ASP:HB3	1:A:1059:LYS:HD3	1.91	0.53
15:O:342:HIS:O	15:O:346:GLN:CG	2.51	0.53
1:A:83:VAL:HG11	1:A:427:PHE:CE1	2.44	0.53
1:A:1454:HIS:HB3	1:A:1457:ILE:HG13	1.90	0.53
1:A:1499:ARG:O	1:A:1500:GLN:CB	2.57	0.53
15:O:155:SER:HB2	15:O:176:LEU:HD21	1.91	0.53
2:B:172:LEU:HD22	2:B:175:MET:SD	2.49	0.53
15:O:337:THR:O	15:O:341:THR:OG1	2.27	0.53
1:A:368:ARG:O	1:A:380:ASN:ND2	2.42	0.52
20:W:363:GLU:C	20:W:365:TRP:H	2.12	0.52
1:A:385:LEU:HD12	1:A:453:ILE:CG2	2.40	0.52
1:A:1261:VAL:CB	1:A:1306:TYR:CD1	2.92	0.52
2:B:282:HIS:HD2	13:M:99:LYS:HD2	1.73	0.52
15:O:147:ILE:HG22	15:O:149:LYS:HB3	1.91	0.52
15:O:520:CYS:O	15:O:521:ASN:O	2.27	0.52
1:A:1573:TYR:O	9:I:122:ARG:HB3	2.08	0.52
2:B:293:ILE:HG12	2:B:302:LEU:HD23	1.92	0.52
2:B:979:GLN:HG2	2:B:996:PHE:HE1	1.73	0.52
1:A:489:ASN:HB2	11:K:95:HIS:HD2	1.71	0.52
1:A:898:SER:O	9:I:79:GLY:HA3	2.09	0.52
3:C:36:PHE:CD2	11:K:130:VAL:HG11	2.44	0.52
9:I:95:ASN:HB2	9:I:113:THR:HB	1.90	0.52
15:O:459:GLU:C	15:O:461:VAL:N	2.61	0.52
15:O:499:GLU:O	15:O:502:LEU:HG	2.09	0.52
1:A:799:GLU:CG	1:A:1062:HIS:CG	2.90	0.52
7:G:138:PHE:CE1	15:O:181:ARG:CD	2.91	0.52
15:O:402:THR:O	15:O:406:ILE:HG13	2.10	0.52
15:O:458:GLU:CG	15:O:514:PHE:CE2	2.92	0.52
1:A:1239:THR:HB	1:A:1542:THR:HB	1.92	0.52
2:B:815:ARG:NH2	2:B:821:ILE:HD11	1.78	0.52
7:G:242:VAL:HB	15:O:183:ILE:HG23	1.78	0.52
1:A:588:LEU:HB2	1:A:636:HIS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:VAL:CG1	1:A:1265:GLU:HB2	2.36	0.52
7:G:156:SER:OG	15:O:145:SER:O	2.16	0.52
13:M:28:LYS:HD2	14:N:106:ASN:HB2	1.90	0.52
15:O:415:GLU:O	15:O:419:LYS:HG3	2.10	0.52
15:O:98:ASP:OD2	15:O:135:LYS:CE	2.58	0.52
15:O:237:ILE:CB	15:O:381:ILE:CD1	2.57	0.52
15:O:446:LEU:O	15:O:449:TRP:CB	2.42	0.52
2:B:811:LEU:CD1	2:B:811:LEU:N	2.73	0.52
15:O:156:MET:HE2	15:O:193:TYR:CE1	2.43	0.52
15:O:248:LEU:HD23	15:O:248:LEU:O	2.10	0.52
15:O:457:ARG:O	15:O:461:VAL:HG23	2.10	0.52
2:B:60:LEU:HD12	2:B:242:ASP:HA	1.91	0.52
2:B:161:LEU:HA	2:B:458:GLY:O	2.10	0.51
15:O:379:ARG:CB	15:O:382:GLN:NE2	2.74	0.51
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.93	0.51
15:O:352:LEU:HA	15:O:358:VAL:CG2	2.31	0.51
2:B:60:LEU:CD2	2:B:60:LEU:N	2.74	0.51
2:B:137:LEU:HD23	2:B:158:CYS:HB3	1.92	0.51
7:G:50:ALA:H	7:G:64:GLN:HE22	1.56	0.51
15:O:383:TYR:CZ	15:O:597:LEU:HB2	2.46	0.51
16:S:64:DT:O2	17:T:8:DA:N3	2.42	0.51
2:B:145:VAL:HG13	2:B:441:LYS:HD2	1.91	0.51
2:B:646:HIS:H	2:B:646:HIS:CD2	2.28	0.51
15:O:359:GLY:CA	15:O:362:ASN:ND2	2.73	0.51
15:O:518:LYS:HD3	15:O:519:PHE:CZ	2.45	0.51
2:B:164:MET:HE3	2:B:194:PHE:CZ	2.46	0.51
2:B:165:LEU:N	2:B:165:LEU:CD1	2.73	0.51
2:B:900:THR:HG22	2:B:901:VAL:N	2.25	0.51
2:B:1121:GLY:HA2	15:O:152:GLN:HB3	1.92	0.51
1:A:1440:ASN:HA	1:A:1444:ARG:NE	2.25	0.51
1:A:1478:ALA:HB1	9:I:21:ASN:HB3	1.92	0.51
2:B:158:CYS:HB3	2:B:457:ILE:HD12	1.91	0.51
15:O:459:GLU:HG3	15:O:460:GLU:N	2.25	0.51
17:T:21:DG:H8	17:T:21:DG:C5'	2.22	0.51
1:A:977:MET:HE1	1:A:993:GLN:OE1	2.10	0.51
1:A:1260:LYS:HE3	1:A:1504:ILE:O	2.11	0.51
2:B:815:ARG:HD2	2:B:821:ILE:HG23	1.92	0.51
1:A:777:LEU:O	8:H:120:GLY:HA2	2.10	0.51
15:O:241:ASP:O	15:O:378:THR:HG23	2.10	0.51
1:A:380:ASN:HB3	1:A:383:ASN:CG	2.32	0.51
1:A:440:SER:O	1:A:441:THR:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:GLU:HG3	6:F:115:THR:HG21	1.93	0.51
2:B:145:VAL:HG11	2:B:441:LYS:HD2	1.91	0.51
13:M:53:LEU:HB2	13:M:96:LEU:HD22	1.93	0.51
15:O:488:HIS:CE1	15:O:489:ASN:H	2.27	0.51
16:S:57:DA:C2	17:T:15:DT:C2	2.99	0.51
1:A:1229:ALA:CB	1:A:1597:ALA:HB2	2.41	0.51
2:B:56:PRO:HG2	2:B:554:GLN:HE22	1.76	0.51
2:B:72:VAL:CG1	2:B:94:LYS:HE3	2.41	0.51
2:B:822:THR:OG1	2:B:865:THR:HG23	2.11	0.51
2:B:1120:ILE:C	15:O:153:ASP:OD1	2.49	0.51
15:O:247:GLU:OE1	15:O:325:ILE:CD1	2.57	0.51
15:O:444:SER:O	15:O:447:THR:OG1	2.23	0.51
15:O:478:GLN:OE1	15:O:521:ASN:HB2	2.10	0.51
17:T:21:DG:C2	17:T:22:DA:C1'	2.93	0.51
1:A:403:LEU:CG	1:A:419:ILE:HG12	2.41	0.50
1:A:1501:ILE:HG23	1:A:1504:ILE:HB	1.91	0.50
2:B:1119:ARG:HD2	15:O:149:LYS:HZ2	1.73	0.50
7:G:242:VAL:HG11	15:O:183:ILE:C	2.31	0.50
1:A:250:LYS:CD	1:A:252:PHE:CE1	2.93	0.50
1:A:1439:MET:CE	1:A:1444:ARG:CG	2.87	0.50
2:B:98:SER:O	2:B:142:LYS:N	2.38	0.50
15:O:151:TRP:HZ2	15:O:176:LEU:HA	1.76	0.50
2:B:101:GLN:HB3	2:B:140:LYS:HE3	1.94	0.50
15:O:198:PHE:CD2	15:O:232:LEU:CG	2.60	0.50
15:O:324:GLY:O	15:O:326:LYS:N	2.44	0.50
1:A:861:VAL:HG21	1:A:892:LEU:HA	1.94	0.50
1:A:957:VAL:HG21	1:A:997:PHE:HD1	1.70	0.50
1:A:1012:LYS:NZ	1:A:1012:LYS:CB	2.74	0.50
2:B:91:LEU:HD23	2:B:343:ASP:CB	2.41	0.50
18:U:12:THR:O	18:U:13:ASP:C	2.47	0.50
1:A:918:LYS:HE2	1:A:922:CYS:HB3	1.93	0.50
2:B:1039:MET:CE	2:B:1042:ASP:N	2.75	0.50
7:G:154:ASN:CG	15:O:183:ILE:HG12	2.32	0.50
15:O:208:LEU:O	15:O:212:THR:HG23	2.12	0.50
15:O:591:TYR:HE2	15:O:593:PRO:HG3	1.77	0.50
16:S:64:DT:C5	17:T:8:DA:N1	2.77	0.50
1:A:1202:LEU:HD22	9:I:101:LEU:HD11	1.93	0.50
2:B:574:SER:HB2	13:M:97:VAL:HG11	1.94	0.50
15:O:591:TYR:CE2	15:O:593:PRO:HG3	2.46	0.50
18:U:257:VAL:O	18:U:261:ALA:N	2.37	0.50
1:A:88:PRO:HG2	1:A:438:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:PRO:HD2	8:H:46:LEU:CB	2.37	0.50
1:A:1278:THR:OG1	1:A:1287:ALA:HB3	2.10	0.50
2:B:165:LEU:HD12	2:B:165:LEU:H	1.77	0.50
15:O:468:GLU:C	15:O:470:PHE:N	2.65	0.50
15:O:471:LYS:CG	15:O:472:HIS:N	2.75	0.50
2:B:74:PHE:CD1	2:B:93:ASN:C	2.84	0.50
15:O:443:ALA:O	15:O:447:THR:HG23	2.12	0.50
1:A:426:ALA:HA	1:A:429:THR:HG22	1.93	0.50
1:A:1261:VAL:CG1	1:A:1265:GLU:CB	2.89	0.50
2:B:98:SER:N	2:B:142:LYS:O	2.43	0.50
2:B:137:LEU:CG	2:B:158:CYS:HB2	2.41	0.50
16:S:64:DT:C4	17:T:8:DA:C5	2.98	0.50
1:A:1039:ARG:HD2	1:A:1045:LEU:HA	1.94	0.49
2:B:1039:MET:HE2	2:B:1042:ASP:CB	2.41	0.49
15:O:177:LYS:HG3	15:O:178:TYR:N	2.27	0.49
15:O:507:GLN:O	15:O:511:ILE:HG23	2.12	0.49
16:S:57:DA:H2"	16:S:58:DA:C8	2.47	0.49
18:U:208:PRO:O	18:U:209:ASN:C	2.49	0.49
1:A:1440:ASN:H	1:A:1440:ASN:HD22	1.59	0.49
1:A:1441:LYS:HG2	1:A:1442:VAL:N	2.26	0.49
1:A:986:PHE:HB2	2:B:960:ILE:HD12	1.95	0.49
1:A:995:TYR:CD2	1:A:999:CYS:SG	3.05	0.49
15:O:173:HIS:CD2	15:O:217:LYS:CG	2.95	0.49
15:O:234:ILE:O	15:O:238:ILE:HG13	2.12	0.49
15:O:453:TYR:CE1	15:O:473:PHE:HB2	2.47	0.49
16:S:60:DC:H2"	16:S:61:DA:C8	2.47	0.49
16:S:62:DG:N2	17:T:10:DT:C2	2.64	0.49
18:U:203:TRP:C	18:U:205:ILE:N	2.63	0.49
1:A:263:ASN:HA	1:A:266:VAL:HG22	1.94	0.49
2:B:106:LYS:HD3	2:B:108:MET:SD	2.52	0.49
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.94	0.49
3:C:216:HIS:HD2	3:C:218:LYS:H	1.59	0.49
7:G:51:PRO:HA	7:G:54:LEU:HD13	1.95	0.49
16:S:65:DG:H2"	16:S:66:DA:C8	2.46	0.49
17:T:21:DG:N2	17:T:22:DA:H1'	2.28	0.49
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.94	0.49
1:A:996:TYR:HD1	2:B:525:TRP:CE3	2.26	0.49
1:A:1007:ILE:CD1	2:B:518:ARG:HD3	2.42	0.49
2:B:121:VAL:HG23	2:B:125:GLU:OE1	2.12	0.49
2:B:887:LEU:HD11	12:L:56:LEU:HD12	1.93	0.49
15:O:242:VAL:HA	15:O:378:THR:CG2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:434:LEU:CD1	15:O:434:LEU:N	2.75	0.49
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.95	0.49
1:A:1038:ILE:HD12	1:A:1185:VAL:HG21	1.94	0.49
7:G:138:PHE:CZ	15:O:181:ARG:CB	2.77	0.49
15:O:138:TYR:CD2	15:O:142:ILE:CD1	2.92	0.49
15:O:368:PHE:CD2	15:O:385:MET:HG2	2.47	0.49
1:A:799:GLU:OE1	1:A:1062:HIS:CG	2.66	0.49
2:B:143:TRP:HZ2	2:B:440:PHE:HD1	1.49	0.49
2:B:154:GLU:OE1	2:B:154:GLU:N	2.45	0.49
2:B:175:MET:HE2	2:B:179:GLU:HB3	1.95	0.49
15:O:368:PHE:C	15:O:368:PHE:CD1	2.86	0.49
1:A:252:PHE:HD2	1:A:314:TYR:N	2.10	0.49
2:B:740:LYS:HA	2:B:804:TYR:O	2.12	0.49
1:A:242:LYS:HB2	1:A:254:THR:OG1	2.13	0.49
2:B:139:LEU:HD11	2:B:417:ILE:HD11	1.95	0.49
2:B:893:ASN:OD1	2:B:895:PHE:HZ	1.80	0.49
15:O:173:HIS:CE1	15:O:217:LYS:HB3	2.48	0.49
15:O:199:PRO:HB2	15:O:208:LEU:HD23	1.95	0.49
15:O:426:SER:HB3	15:O:594:TYR:HB2	1.88	0.49
15:O:440:ILE:HD13	15:O:491:PHE:CD1	2.48	0.49
15:O:446:LEU:C	15:O:449:TRP:HB3	2.30	0.49
2:B:67:ASP:O	2:B:356:ARG:NH2	2.46	0.49
15:O:361:PHE:CD1	15:O:361:PHE:C	2.86	0.49
15:O:369:LYS:HE2	15:O:370:THR:N	2.28	0.49
15:O:430:ARG:O	15:O:431:ALA:O	2.31	0.49
1:A:1509:HIS:O	9:I:73:LYS:HE3	2.13	0.48
15:O:176:LEU:HD13	15:O:218:LEU:HD13	1.95	0.48
15:O:369:LYS:O	15:O:373:LEU:CA	2.60	0.48
18:U:127:LYS:O	18:U:129:PHE:N	2.46	0.48
1:A:440:SER:C	1:A:442:LYS:N	2.66	0.48
2:B:143:TRP:CE2	2:B:440:PHE:HB3	2.38	0.48
2:B:916:LYS:HB3	2:B:1036:LEU:HD12	1.95	0.48
3:C:113:LEU:HD11	3:C:132:ILE:HD12	1.94	0.48
15:O:158:LEU:HD22	15:O:172:HIS:CD2	2.46	0.48
15:O:163:ILE:HG22	15:O:207:LYS:O	2.13	0.48
28:P:135:ALA:O	29:Z:149:ALA:CA	2.61	0.48
1:A:977:MET:CE	1:A:994:GLU:HG3	2.42	0.48
15:O:175:MET:HE2	15:O:175:MET:HA	1.95	0.48
1:A:799:GLU:CD	1:A:1062:HIS:HB2	2.33	0.48
2:B:480:GLN:HE21	2:B:508:PHE:H	1.61	0.48
2:B:731:VAL:HG21	10:J:59:LYS:HG2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:242:VAL:HG21	15:O:183:ILE:O	2.13	0.48
15:O:383:TYR:CG	15:O:597:LEU:HD22	2.47	0.48
17:T:21:DG:N3	17:T:22:DA:O4'	2.46	0.48
2:B:134:ARG:CD	2:B:462:GLN:OE1	2.44	0.48
2:B:700:LEU:HA	2:B:703:LEU:HD12	1.95	0.48
1:A:35:PRO:CD	1:A:390:LEU:HD12	2.44	0.48
1:A:836:THR:HG23	1:A:839:GLY:H	1.78	0.48
1:A:1278:THR:HG1	1:A:1287:ALA:CB	2.26	0.48
1:A:1640:ARG:HH11	1:A:1648:ASN:HB3	1.78	0.48
11:K:95:HIS:HB3	11:K:98:GLU:HG2	1.96	0.48
15:O:241:ASP:OD1	15:O:380:SER:HB2	2.12	0.48
15:O:468:GLU:C	15:O:470:PHE:H	2.15	0.48
15:O:484:PHE:O	15:O:488:HIS:HB3	2.14	0.48
17:T:22:DA:H2'	17:T:23:DA:H8	1.79	0.48
1:A:977:MET:HE2	1:A:994:GLU:HG3	1.96	0.48
13:M:109:ARG:HG3	13:M:110:GLY:H	1.77	0.48
15:O:151:TRP:CZ2	15:O:176:LEU:HA	2.49	0.48
15:O:237:ILE:HG22	15:O:381:ILE:CD1	2.34	0.48
2:B:72:VAL:CB	2:B:94:LYS:HE3	2.44	0.48
2:B:165:LEU:CD1	2:B:165:LEU:H	2.27	0.48
1:A:995:TYR:CD2	1:A:995:TYR:C	2.86	0.48
1:A:1012:LYS:HB2	1:A:1012:LYS:HZ3	1.77	0.48
2:B:77:LYS:HG2	2:B:90:TYR:HE2	1.78	0.48
2:B:90:TYR:CD2	2:B:92:GLY:HA2	2.49	0.48
1:A:403:LEU:CD1	1:A:419:ILE:HG12	2.35	0.48
1:A:1038:ILE:HD11	1:A:1050:TYR:HB2	1.96	0.48
2:B:93:ASN:CB	2:B:146:ASN:OD1	2.51	0.48
2:B:165:LEU:HD22	2:B:193:TYR:CE2	2.49	0.48
16:S:58:DA:H2	17:T:14:DT:O2	1.95	0.48
1:A:1634:LEU:HD13	1:A:1643:VAL:HG11	1.96	0.47
15:O:107:ILE:O	15:O:109:SER:N	2.46	0.47
15:O:408:PHE:CD2	15:O:449:TRP:CE2	3.02	0.47
1:A:126:GLN:HB3	1:A:343:PRO:HD3	1.96	0.47
1:A:1322:ILE:HD13	1:A:1454:HIS:NE2	2.29	0.47
2:B:96:SER:HB3	2:B:144:SER:C	2.34	0.47
3:C:315:PHE:HZ	11:K:136:THR:HA	1.79	0.47
7:G:18:LYS:HA	7:G:21:LYS:HD2	1.95	0.47
15:O:129:PRO:O	15:O:133:LEU:CB	2.62	0.47
15:O:206:ARG:HA	15:O:209:VAL:CG1	2.44	0.47
15:O:477:PHE:CE2	15:O:481:CYS:SG	3.07	0.47
18:U:127:LYS:C	18:U:129:PHE:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:416:ILE:O	18:U:417:PHE:C	2.52	0.47
1:A:419:ILE:HD12	1:A:422:ARG:HE	1.79	0.47
1:A:1275:THR:HG23	1:A:1275:THR:O	2.14	0.47
2:B:137:LEU:CD2	2:B:158:CYS:HB2	2.44	0.47
15:O:488:HIS:O	15:O:491:PHE:N	2.38	0.47
1:A:1012:LYS:CB	1:A:1012:LYS:HZ3	2.28	0.47
7:G:47:VAL:HG21	7:G:61:VAL:HG13	1.96	0.47
7:G:142:ALA:CA	15:O:138:TYR:CZ	2.93	0.47
16:S:53:DA:N6	17:T:18:DC:N4	2.58	0.47
1:A:671:GLN:HE22	2:B:784:ASP:HB2	1.80	0.47
1:A:799:GLU:OE1	1:A:1062:HIS:CB	2.61	0.47
2:B:107:PRO:CB	2:B:133:TYR:CE2	2.97	0.47
2:B:375:LEU:HA	2:B:378:ILE:HD12	1.96	0.47
2:B:1121:GLY:HA3	15:O:149:LYS:O	2.14	0.47
15:O:194:LEU:HD21	15:O:225:LEU:HD11	1.96	0.47
15:O:225:LEU:HD12	15:O:229:ILE:HG13	1.96	0.47
16:S:65:DG:N2	17:T:7:DA:H2	2.04	0.47
1:A:502:ALA:HA	1:A:581:ILE:CG2	2.43	0.47
1:A:1260:LYS:CB	1:A:1500:GLN:HA	2.44	0.47
2:B:656:LEU:HB3	14:N:148:ILE:HG12	1.97	0.47
2:B:823:GLN:HG2	2:B:863:ASP:CB	2.43	0.47
3:C:42:VAL:O	11:K:138:LYS:CE	2.62	0.47
8:H:103:LYS:HB3	8:H:115:TYR:HB2	1.96	0.47
15:O:146:SER:C	15:O:148:PRO:HD3	2.34	0.47
15:O:352:LEU:CA	15:O:358:VAL:CG2	2.90	0.47
1:A:238:MET:HG2	1:A:267:LYS:HB2	1.79	0.47
1:A:385:LEU:HD12	1:A:453:ILE:HG22	1.97	0.47
1:A:396:ILE:CG1	1:A:426:ALA:CB	2.92	0.47
1:A:629:ASP:HB3	2:B:785:ASP:CG	2.35	0.47
1:A:1196:PRO:HB2	1:A:1575:ILE:HG21	1.96	0.47
2:B:91:LEU:CD1	2:B:91:LEU:N	2.73	0.47
2:B:1041:ASN:CG	2:B:1044:PHE:CB	2.75	0.47
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.95	0.47
5:E:56:LYS:HE2	5:E:84:ASP:H	1.80	0.47
15:O:91:LYS:HG3	15:O:92:ASN:N	2.28	0.47
15:O:128:LEU:HB3	15:O:129:PRO:HD2	1.97	0.47
15:O:232:LEU:HD12	15:O:232:LEU:HA	1.74	0.47
15:O:369:LYS:HD2	15:O:370:THR:HA	1.95	0.47
15:O:460:GLU:O	15:O:469:ARG:NH2	2.47	0.47
20:W:363:GLU:O	20:W:365:TRP:N	2.40	0.47
1:A:727:THR:H	1:A:730:GLN:HE21	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LEU:HG	2:B:158:CYS:HB2	1.96	0.47
2:B:887:LEU:HD23	2:B:887:LEU:N	2.11	0.47
15:O:237:ILE:CG2	15:O:381:ILE:CG1	2.93	0.47
15:O:506:PHE:HD2	15:O:537:VAL:CG1	2.28	0.47
1:A:32:ILE:HG21	1:A:49:LEU:HD13	1.96	0.47
1:A:1610:PHE:CD2	1:A:1632:GLU:HG2	2.49	0.47
2:B:49:PHE:CE1	2:B:167:SER:OG	2.53	0.47
2:B:810:ASP:OD1	2:B:812:ALA:HB3	2.15	0.47
1:A:538:ASN:HA	1:A:575:LYS:HG2	1.96	0.47
1:A:1008:ASP:HA	1:A:1011:VAL:HG22	1.95	0.47
1:A:1258:ILE:HD12	1:A:1507:CYS:SG	2.55	0.47
2:B:1120:ILE:CB	15:O:153:ASP:OD1	2.51	0.47
1:A:253:GLU:HB3	1:A:313:THR:N	2.28	0.46
2:B:821:ILE:HG21	2:B:899:GLN:NE2	2.13	0.46
2:B:887:LEU:CD1	12:L:56:LEU:HB2	2.45	0.46
15:O:407:SER:CB	15:O:408:PHE:CD1	2.95	0.46
15:O:426:SER:HB3	15:O:594:TYR:CD2	2.50	0.46
15:O:428:ILE:CG2	15:O:439:ILE:CG2	2.86	0.46
1:A:800:VAL:HG23	1:A:1068:PHE:CE2	2.48	0.46
1:A:986:PHE:CB	2:B:960:ILE:HD12	2.46	0.46
2:B:95:LEU:HD12	2:B:95:LEU:N	2.30	0.46
2:B:123:PRO:HA	2:B:133:TYR:CD1	2.51	0.46
15:O:391:GLN:HE22	15:O:609:TYR:HE2	1.61	0.46
1:A:991:LYS:HB2	1:A:994:GLU:CD	2.35	0.46
2:B:63:LEU:N	2:B:63:LEU:CD1	2.77	0.46
2:B:99:VAL:HG21	2:B:421:LEU:HD21	1.95	0.46
2:B:823:GLN:C	2:B:824:HIS:CG	2.84	0.46
6:F:128:LYS:HD2	6:F:149:GLU:HA	1.97	0.46
20:W:339:ASN:O	20:W:340:ASP:C	2.52	0.46
1:A:718:THR:HG21	8:H:119:GLY:HA3	1.97	0.46
2:B:104:ILE:O	2:B:169:ARG:NH1	2.48	0.46
2:B:107:PRO:HB2	2:B:133:TYR:CE2	2.51	0.46
2:B:894:LYS:O	2:B:895:PHE:CE2	2.65	0.46
8:H:107:VAL:O	8:H:111:LEU:HB2	2.15	0.46
15:O:372:VAL:CG1	15:O:423:TYR:OH	2.64	0.46
15:O:388:VAL:HG13	15:O:389:SER:N	2.31	0.46
19:V:249:GLY:HA3	19:V:257:ARG:N	2.30	0.46
1:A:373:LEU:CD2	1:A:378:HIS:NE2	2.70	0.46
1:A:700:ILE:HD11	1:A:735:VAL:HA	1.97	0.46
1:A:862:THR:OG1	1:A:878:ARG:HB3	2.15	0.46
15:O:120:ILE:HD13	15:O:150:TRP:CE3	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:602:TYR:O	15:O:606:MET:HG2	2.15	0.46
1:A:536:ILE:HD11	1:A:575:LYS:HD3	1.96	0.46
1:A:879:LEU:HA	1:A:882:ILE:HD12	1.97	0.46
3:C:229:LEU:HD23	3:C:293:ARG:HB3	1.97	0.46
1:A:19:LEU:HG	2:B:1195:ARG:HB2	1.98	0.46
1:A:601:MET:SD	1:A:656:GLN:HG3	2.56	0.46
1:A:1018:TYR:CE1	17:T:19:DA:OP1	2.69	0.46
1:A:1263:LEU:HD22	1:A:1267:ILE:HD11	1.98	0.46
2:B:54:GLU:HB2	2:B:168:ASN:HD22	1.77	0.46
15:O:74:ILE:O	15:O:78:VAL:HG13	2.16	0.46
15:O:148:PRO:HB3	15:O:183:ILE:HD13	1.98	0.46
15:O:234:ILE:HG22	15:O:371:HIS:CD2	2.42	0.46
1:A:537:GLN:HB2	1:A:578:TYR:HE1	1.81	0.46
1:A:1006:LEU:HD22	9:I:104:ALA:HB2	1.98	0.46
1:A:1112:PRO:HD2	1:A:1115:LYS:HB2	1.97	0.46
1:A:1658:ALA:HB2	7:G:107:ILE:HD11	1.98	0.46
2:B:54:GLU:HB2	2:B:168:ASN:HD21	1.78	0.46
3:C:54:PHE:CD2	11:K:135:PHE:CE1	2.97	0.46
15:O:237:ILE:HG22	15:O:381:ILE:CB	2.45	0.46
15:O:433:LYS:HG3	15:O:433:LYS:O	2.16	0.46
1:A:1012:LYS:HB2	1:A:1012:LYS:HZ2	1.81	0.46
2:B:362:LEU:HD22	2:B:369:ASP:HB3	1.97	0.46
3:C:44:ILE:HG21	11:K:142:MET:SD	2.56	0.46
5:E:4:GLU:HG2	5:E:7:ARG:HH12	1.80	0.46
7:G:143:SER:HG	15:O:142:ILE:HD13	1.78	0.46
7:G:14:ALA:HA	7:G:17:ILE:HD12	1.97	0.46
19:V:483:HIS:C	19:V:499:GLU:N	2.70	0.46
1:A:35:PRO:HG3	1:A:390:LEU:HD12	1.98	0.45
1:A:380:ASN:HB3	1:A:383:ASN:CB	2.45	0.45
1:A:396:ILE:HG13	1:A:426:ALA:HB1	1.98	0.45
2:B:721:MET:O	2:B:725:THR:HG23	2.16	0.45
2:B:898:LEU:CD2	12:L:46:VAL:CG2	0.47	0.45
15:O:174:ASP:C	15:O:177:LYS:HG2	2.36	0.45
15:O:369:LYS:HE2	15:O:370:THR:HG22	1.87	0.45
15:O:459:GLU:O	15:O:463:GLN:CB	2.63	0.45
15:O:468:GLU:O	15:O:470:PHE:N	2.49	0.45
1:A:1601:GLN:NE2	16:S:57:DA:H5'	2.27	0.45
2:B:815:ARG:NH2	2:B:821:ILE:CD1	2.49	0.45
7:G:241:ARG:HG2	15:O:186:SER:CA	2.34	0.45
1:A:83:VAL:HG11	1:A:427:PHE:HE1	1.81	0.45
1:A:255:ALA:O	1:A:256:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:LEU:HD13	2:B:193:TYR:O	2.16	0.45
2:B:892:SER:O	2:B:895:PHE:CE2	2.61	0.45
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.98	0.45
15:O:234:ILE:HD13	15:O:234:ILE:HA	1.74	0.45
15:O:396:MET:HE1	15:O:433:LYS:C	2.36	0.45
20:W:240:ILE:O	20:W:241:ARG:C	2.55	0.45
1:A:429:THR:O	1:A:433:ASP:HB2	2.15	0.45
2:B:815:ARG:NH1	2:B:815:ARG:HB2	2.31	0.45
2:B:880:ALA:HB2	2:B:907:ILE:HG13	1.98	0.45
2:B:977:ILE:HD13	14:N:163:VAL:HG21	1.99	0.45
15:O:148:PRO:HB3	15:O:183:ILE:CD1	2.46	0.45
15:O:169:THR:O	15:O:170:VAL:C	2.54	0.45
15:O:426:SER:OG	15:O:594:TYR:C	2.55	0.45
15:O:447:THR:HB	15:O:505:PHE:CE2	2.51	0.45
15:O:459:GLU:O	15:O:463:GLN:N	2.50	0.45
17:T:22:DA:H2'	17:T:23:DA:C8	2.52	0.45
1:A:628:PHE:C	2:B:785:ASP:HB2	2.37	0.45
1:A:1322:ILE:CD1	1:A:1454:HIS:NE2	2.79	0.45
3:C:36:PHE:CE2	11:K:130:VAL:HG11	2.52	0.45
3:C:63:ILE:HG21	11:K:127:LEU:CD2	2.45	0.45
15:O:138:TYR:CE2	15:O:142:ILE:HD12	2.43	0.45
1:A:1005:GLY:O	9:I:100:GLN:O	2.34	0.45
1:A:1288:ARG:HB2	1:A:1476:LEU:HB2	1.98	0.45
3:C:229:LEU:HD21	3:C:295:ARG:HA	1.99	0.45
15:O:376:TYR:O	15:O:377:TYR:C	2.55	0.45
15:O:390:GLN:C	15:O:609:TYR:CE1	2.81	0.45
17:T:21:DG:C3'	17:T:22:DA:C5'	2.93	0.45
1:A:862:THR:HG21	1:A:875:LEU:HD12	1.99	0.45
1:A:1032:VAL:HG21	1:A:1179:ILE:HG12	1.99	0.45
2:B:108:MET:HA	2:B:121:VAL:H	1.81	0.45
15:O:98:ASP:OD2	15:O:135:LYS:CD	2.64	0.45
1:A:456:VAL:HG21	2:B:1192:MET:HG3	1.99	0.45
2:B:72:VAL:O	2:B:72:VAL:HG23	2.15	0.45
2:B:898:LEU:HD23	12:L:46:VAL:HG23	1.20	0.45
2:B:1120:ILE:HD13	15:O:150:TRP:CE3	2.52	0.45
15:O:170:VAL:CG1	15:O:171:CYS:N	2.78	0.45
15:O:352:LEU:HD23	15:O:358:VAL:HG23	1.85	0.45
15:O:384:ILE:HA	15:O:602:TYR:OH	2.17	0.45
15:O:458:GLU:HG3	15:O:514:PHE:CE2	2.51	0.45
15:O:521:ASN:ND2	15:O:523:ASN:N	2.54	0.45
18:U:445:ARG:O	18:U:450:THR:CA	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1454:HIS:HB3	1:A:1457:ILE:CG1	2.44	0.45
2:B:90:TYR:O	2:B:90:TYR:CD2	2.70	0.45
15:O:190:ILE:HD13	15:O:190:ILE:C	2.36	0.45
15:O:391:GLN:CD	15:O:609:TYR:OH	2.55	0.45
15:O:454:VAL:HB	15:O:514:PHE:CD2	2.37	0.45
15:O:487:ARG:CG	15:O:487:ARG:NH1	2.73	0.45
1:A:1029:GLY:HA3	1:A:1041:ALA:HB2	1.99	0.45
11:K:56:GLU:OE1	11:K:56:GLU:HA	2.17	0.45
1:A:992:PRO:HB2	2:B:676:VAL:HG11	1.98	0.44
15:O:239:SER:O	15:O:243:GLU:HG2	2.16	0.44
15:O:458:GLU:CB	15:O:461:VAL:HG21	2.47	0.44
15:O:485:CYS:SG	15:O:531:ILE:HD12	2.56	0.44
15:O:506:PHE:CG	15:O:528:PHE:HZ	2.34	0.44
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.52	0.44
2:B:811:LEU:CB	2:B:899:GLN:HB3	2.45	0.44
2:B:898:LEU:H	12:L:46:VAL:HG21	1.82	0.44
7:G:30:GLU:HG2	7:G:32:ASN:HB2	1.99	0.44
7:G:148:LEU:HD11	15:O:181:ARG:O	2.18	0.44
15:O:69:THR:HG22	15:O:70:GLN:N	2.31	0.44
15:O:156:MET:CE	15:O:193:TYR:CE1	3.00	0.44
15:O:158:LEU:HD22	15:O:172:HIS:CG	2.52	0.44
15:O:241:ASP:HA	15:O:380:SER:CB	2.46	0.44
15:O:368:PHE:HE2	15:O:382:GLN:HA	1.81	0.44
15:O:383:TYR:O	15:O:386:PHE:N	2.51	0.44
15:O:467:MET:HE1	15:O:470:PHE:HE2	1.82	0.44
17:T:21:DG:C2	17:T:22:DA:O4'	2.70	0.44
1:A:657:TYR:O	1:A:665:PRO:HA	2.17	0.44
15:O:372:VAL:O	15:O:375:THR:OG1	2.24	0.44
15:O:458:GLU:HA	15:O:461:VAL:HG23	0.48	0.44
2:B:823:GLN:HA	2:B:862:PHE:O	2.17	0.44
3:C:40:PHE:HE2	11:K:134:LYS:CB	2.29	0.44
3:C:110:PRO:C	3:C:112:MET:H	2.20	0.44
7:G:242:VAL:CG1	15:O:183:ILE:CG2	2.96	0.44
15:O:458:GLU:CA	15:O:461:VAL:HG21	2.29	0.44
15:O:488:HIS:O	15:O:489:ASN:C	2.54	0.44
1:A:238:MET:HB3	1:A:267:LYS:HD3	1.99	0.44
1:A:719:ILE:CD1	8:H:43:ASN:ND2	2.76	0.44
2:B:127:ARG:HG3	2:B:195:ILE:HD13	1.99	0.44
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.99	0.44
15:O:488:HIS:CE1	15:O:489:ASN:OD1	2.71	0.44
2:B:1097:ASP:OD2	2:B:1181:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:VAL:HG12	5:E:142:VAL:HG23	2.00	0.44
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.99	0.44
15:O:413:ALA:HB1	15:O:415:GLU:OE1	2.18	0.44
1:A:1260:LYS:HD3	1:A:1501:ILE:N	2.32	0.44
3:C:63:ILE:HD12	11:K:127:LEU:HD22	2.00	0.44
15:O:76:ASN:O	15:O:80:LEU:HD13	2.18	0.44
15:O:143:LEU:HD11	15:O:150:TRP:HD1	1.77	0.44
15:O:237:ILE:HD13	15:O:384:ILE:HD11	2.00	0.44
2:B:13:THR:HG21	2:B:977:ILE:HB	1.99	0.44
15:O:189:PHE:HA	15:O:192:THR:HG23	1.99	0.44
15:O:373:LEU:CB	15:O:374:PRO:CD	2.94	0.44
15:O:408:PHE:HZ	15:O:446:LEU:CD2	2.30	0.44
15:O:478:GLN:NE2	15:O:592:PHE:CZ	2.69	0.44
15:O:581:THR:HA	15:O:584:GLN:CD	2.38	0.44
2:B:15:ASP:HA	2:B:978:ALA:HB3	2.00	0.44
2:B:19:LEU:HD11	10:J:26:GLN:HG2	2.00	0.44
2:B:895:PHE:HD2	2:B:896:GLN:HG3	1.82	0.44
3:C:314:PHE:CE2	11:K:135:PHE:CD1	3.06	0.44
5:E:120:ALA:HA	5:E:123:LEU:HD12	2.00	0.44
13:M:9:GLU:HA	14:N:71:PRO:HA	2.00	0.44
1:A:692:TYR:O	1:A:696:ILE:HG12	2.17	0.43
1:A:1012:LYS:HD3	1:A:1201:THR:HA	1.19	0.43
2:B:145:VAL:HG21	2:B:440:PHE:HB2	1.99	0.43
2:B:813:LEU:CD1	2:B:813:LEU:C	2.86	0.43
15:O:377:TYR:O	15:O:377:TYR:CD2	2.71	0.43
1:A:799:GLU:HB2	1:A:1062:HIS:CE1	2.53	0.43
2:B:108:MET:C	2:B:119:ARG:NH2	2.66	0.43
7:G:242:VAL:CG1	15:O:183:ILE:HG22	2.45	0.43
15:O:460:GLU:O	15:O:469:ARG:CZ	2.67	0.43
19:V:207:SER:CA	19:V:214:LEU:N	2.81	0.43
1:A:252:PHE:HD2	1:A:314:TYR:HA	1.51	0.43
2:B:62:ASN:HD22	2:B:62:ASN:N	2.14	0.43
2:B:301:PHE:O	2:B:305:ARG:HG2	2.18	0.43
2:B:811:LEU:HD13	2:B:899:GLN:C	2.38	0.43
2:B:1120:ILE:N	15:O:149:LYS:CD	2.76	0.43
15:O:78:VAL:HA	15:O:88:ILE:HG22	2.00	0.43
15:O:245:GLN:CG	15:O:378:THR:HG23	2.48	0.43
15:O:457:ARG:HA	15:O:460:GLU:CG	2.49	0.43
15:O:468:GLU:HG2	15:O:469:ARG:N	2.33	0.43
18:U:436:LEU:C	18:U:438:PHE:H	2.18	0.43
1:A:1440:ASN:HD22	1:A:1440:ASN:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	2.00	0.43
2:B:156:ARG:NH2	2:B:446:MET:O	2.52	0.43
2:B:251:HIS:HE1	2:B:261:ARG:HD2	1.84	0.43
3:C:91:VAL:HG21	10:J:61:LEU:HD23	2.00	0.43
9:I:97:HIS:HB3	9:I:111:PHE:HB2	2.01	0.43
15:O:129:PRO:HD2	15:O:132:THR:CB	2.25	0.43
18:U:97:GLY:H	18:U:100:ALA:C	2.19	0.43
1:A:233:CYS:HB3	1:A:236:CYS:O	2.18	0.43
1:A:385:LEU:HD21	1:A:453:ILE:HD12	1.88	0.43
1:A:1255:CYS:O	1:A:1259:SER:OG	2.21	0.43
2:B:898:LEU:HD21	12:L:46:VAL:CG2	0.66	0.43
7:G:241:ARG:CD	15:O:186:SER:CA	2.95	0.43
2:B:815:ARG:CD	2:B:821:ILE:HG23	2.49	0.43
6:F:107:VAL:HG12	6:F:109:VAL:H	1.84	0.43
15:O:56:VAL:CG2	15:O:99:ILE:HD12	2.47	0.43
15:O:66:ASN:CG	15:O:111:ARG:NH1	2.72	0.43
15:O:356:GLU:OE1	15:O:356:GLU:HA	2.19	0.43
15:O:369:LYS:NZ	15:O:369:LYS:CB	2.73	0.43
2:B:211:ARG:HH22	2:B:243:GLN:NE2	2.16	0.43
2:B:887:LEU:CD2	2:B:887:LEU:N	2.76	0.43
10:J:32:GLU:H	10:J:32:GLU:HG2	1.53	0.43
15:O:202:ASN:OD1	15:O:202:ASN:N	2.52	0.43
15:O:413:ALA:C	15:O:415:GLU:N	2.72	0.43
15:O:515:ASN:N	15:O:516:PRO:HD3	2.33	0.43
1:A:629:ASP:CA	2:B:785:ASP:HB3	2.49	0.43
2:B:100:GLU:CG	2:B:140:LYS:NZ	2.82	0.43
2:B:936:MET:HG3	2:B:937:PRO:HD2	2.01	0.43
2:B:1120:ILE:O	15:O:153:ASP:OD1	2.35	0.43
15:O:108:GLU:HB2	15:O:147:ILE:CD1	2.47	0.43
15:O:124:LYS:O	15:O:127:GLU:HB2	2.18	0.43
1:A:1439:MET:HE1	1:A:1444:ARG:CG	2.43	0.43
2:B:403:LEU:HD21	2:B:408:LEU:HD13	2.00	0.43
6:F:85:MET:HB2	6:F:151:LEU:HB3	2.01	0.43
15:O:521:ASN:HD22	15:O:523:ASN:H	1.59	0.43
1:A:996:TYR:CE1	2:B:525:TRP:CE3	3.06	0.43
1:A:996:TYR:CE1	2:B:525:TRP:HE3	2.36	0.43
9:I:27:ASN:HA	9:I:38:PRO:HD3	1.99	0.43
15:O:230:TRP:CE2	15:O:364:LEU:CD2	2.99	0.43
15:O:245:GLN:O	15:O:248:LEU:N	2.40	0.43
2:B:161:LEU:C	2:B:161:LEU:CD1	2.86	0.42
2:B:175:MET:CE	2:B:183:HIS:CG	3.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:811:LEU:HB2	2:B:899:GLN:CB	2.49	0.42
15:O:169:THR:O	15:O:172:HIS:N	2.52	0.42
15:O:431:ALA:HB3	15:O:434:LEU:HD21	2.00	0.42
1:A:389:VAL:HA	1:A:433:ASP:OD2	2.19	0.42
2:B:139:LEU:CD2	2:B:417:ILE:CD1	2.97	0.42
2:B:164:MET:N	2:B:194:PHE:CE2	2.87	0.42
2:B:748:GLN:HB3	10:J:52:THR:CG2	2.47	0.42
4:D:30:HIS:HA	7:G:39:VAL:HG23	2.00	0.42
15:O:467:MET:CG	15:O:519:PHE:CZ	2.96	0.42
18:U:143:THR:O	18:U:144:ILE:C	2.57	0.42
20:W:228:ASN:O	20:W:229:TRP:C	2.56	0.42
7:G:241:ARG:HD3	15:O:186:SER:HB2	2.01	0.42
15:O:173:HIS:HE1	15:O:214:ASN:O	2.02	0.42
15:O:181:ARG:NH1	15:O:181:ARG:CG	2.77	0.42
15:O:434:LEU:HD23	15:O:439:ILE:HG13	2.00	0.42
15:O:447:THR:HB	15:O:505:PHE:CZ	2.55	0.42
1:A:400:ASN:O	1:A:400:ASN:ND2	2.49	0.42
1:A:721:LYS:HB3	8:H:94:ASP:O	2.18	0.42
1:A:885:ASP:HB3	1:A:888:LYS:HB2	2.01	0.42
1:A:1437:ASN:HD22	1:A:1437:ASN:HA	1.65	0.42
2:B:71:LYS:HB3	2:B:425:ILE:HG13	2.01	0.42
15:O:48:SER:O	15:O:49:ALA:C	2.57	0.42
15:O:124:LYS:HD3	15:O:127:GLU:OE2	2.20	0.42
15:O:336:LEU:HD11	15:O:380:SER:O	2.19	0.42
1:A:536:ILE:HG23	1:A:544:VAL:HB	2.02	0.42
1:A:827:THR:HG21	2:B:1026:ILE:HA	2.02	0.42
1:A:1457:ILE:C	1:A:1457:ILE:CD1	2.85	0.42
2:B:887:LEU:HD11	12:L:56:LEU:HB2	2.02	0.42
15:O:352:LEU:CD2	15:O:358:VAL:CG2	2.56	0.42
1:A:739:VAL:HG11	1:A:812:VAL:HG21	2.00	0.42
9:I:11:LEU:HB3	13:M:31:ARG:HB2	2.01	0.42
11:K:60:SER:HB3	11:K:106:GLN:HG2	2.02	0.42
15:O:163:ILE:CG2	15:O:211:TYR:HB2	2.38	0.42
15:O:244:LEU:HD23	15:O:244:LEU:O	2.20	0.42
15:O:369:LYS:HE3	15:O:370:THR:HG22	1.99	0.42
15:O:430:ARG:O	15:O:610:TYR:HA	2.20	0.42
1:A:86:TYR:H	1:A:431:GLN:HE22	1.67	0.42
1:A:489:ASN:CB	11:K:95:HIS:CD2	2.99	0.42
1:A:966:LEU:HD23	2:B:522:PRO:HB3	2.02	0.42
3:C:329:LYS:NZ	11:K:122:LYS:HE3	2.34	0.42
15:O:404:ILE:CD1	15:O:442:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:447:THR:HG21	15:O:480:LEU:HD21	2.02	0.42
15:O:515:ASN:HD21	15:O:547:ASN:HD21	1.67	0.42
1:A:1053:ASP:HB2	1:A:1174:TYR:OH	2.20	0.42
2:B:190:ILE:HD11	2:B:496:PHE:HE2	1.85	0.42
2:B:561:ILE:HG12	2:B:620:LEU:HD12	2.01	0.42
2:B:953:ALA:O	2:B:957:ARG:HG2	2.19	0.42
4:D:24:ALA:HA	7:G:43:ILE:HG22	2.02	0.42
15:O:369:LYS:C	15:O:369:LYS:CD	2.86	0.42
15:O:390:GLN:NE2	15:O:431:ALA:HA	2.34	0.42
15:O:447:THR:O	15:O:450:LEU:CA	2.68	0.42
1:A:35:PRO:CG	1:A:390:LEU:HD12	2.50	0.42
1:A:991:LYS:O	1:A:992:PRO:C	2.58	0.42
2:B:62:ASN:N	2:B:62:ASN:ND2	2.67	0.42
2:B:90:TYR:O	2:B:90:TYR:CG	2.71	0.42
4:D:19:PRO:HG2	4:D:22:ILE:HD11	2.01	0.42
15:O:170:VAL:HG13	15:O:171:CYS:H	1.79	0.42
2:B:132:SER:OG	2:B:134:ARG:NH1	2.47	0.42
2:B:162:PRO:CB	2:B:465:LEU:HD12	2.48	0.42
11:K:46:LYS:O	11:K:65:ILE:HA	2.19	0.42
15:O:66:ASN:ND2	15:O:111:ARG:CZ	2.83	0.42
15:O:199:PRO:HD3	15:O:211:TYR:CG	2.54	0.42
15:O:409:ALA:O	15:O:417:LYS:HE2	2.20	0.42
16:S:54:DG:H2'	16:S:55:DT:H71	2.02	0.42
1:A:502:ALA:HA	1:A:581:ILE:HG22	2.01	0.41
1:A:646:GLU:HB3	2:B:1084:THR:OG1	2.20	0.41
1:A:1550:LEU:HD12	1:A:1555:VAL:HA	2.02	0.41
2:B:95:LEU:HA	2:B:145:VAL:HG23	2.02	0.41
3:C:252:PRO:HD2	3:C:255:VAL:HG21	2.02	0.41
15:O:96:LEU:O	15:O:100:LEU:HG	2.20	0.41
1:A:389:VAL:HG22	1:A:433:ASP:OD1	2.20	0.41
1:A:1007:ILE:HD13	2:B:518:ARG:HD3	2.02	0.41
2:B:788:ILE:HB	2:B:948:ILE:HB	2.01	0.41
3:C:65:ASN:HA	3:C:227:TYR:HE2	1.85	0.41
10:J:48:ARG:HE	10:J:49:MET:HE2	1.85	0.41
15:O:487:ARG:NH1	15:O:487:ARG:HG3	2.34	0.41
1:A:124:LEU:HD21	1:A:189:VAL:HA	2.01	0.41
1:A:250:LYS:CD	1:A:252:PHE:HZ	2.15	0.41
1:A:591:ARG:HB2	1:A:633:MET:HG2	2.02	0.41
1:A:1018:TYR:CD1	17:T:19:DA:OP1	2.72	0.41
2:B:97:VAL:HA	2:B:142:LYS:O	2.20	0.41
2:B:150:GLU:HA	2:B:150:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:VAL:HB	2:B:261:ARG:HB3	2.01	0.41
2:B:898:LEU:HD22	12:L:46:VAL:CG2	0.94	0.41
2:B:1119:ARG:HB2	15:O:149:LYS:HG3	2.02	0.41
3:C:44:ILE:HD12	11:K:138:LYS:C	2.40	0.41
15:O:128:LEU:HD13	15:O:132:THR:HG22	2.02	0.41
15:O:173:HIS:CG	15:O:217:LYS:HG3	2.55	0.41
1:A:1654:PHE:CE2	6:F:92:ARG:HD3	2.56	0.41
2:B:162:PRO:O	2:B:409:TYR:OH	2.24	0.41
2:B:1121:GLY:N	15:O:149:LYS:O	2.54	0.41
3:C:187:ALA:HB1	3:C:306:GLY:HA3	2.02	0.41
3:C:328:LEU:HD13	11:K:121:LEU:HD21	2.01	0.41
7:G:143:SER:N	15:O:138:TYR:CE1	2.87	0.41
15:O:342:HIS:CD2	15:O:346:GLN:NE2	2.68	0.41
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	2.02	0.41
1:A:1238:MET:HB2	1:A:1521:THR:HB	2.01	0.41
1:A:1459:LYS:HB2	1:A:1473:LYS:HB2	2.02	0.41
2:B:526:GLY:HA2	2:B:696:ILE:HA	2.02	0.41
3:C:311:GLU:HB3	11:K:139:ILE:HD11	2.03	0.41
15:O:56:VAL:HG23	15:O:57:LYS:N	2.35	0.41
15:O:77:GLN:HG2	15:O:88:ILE:HB	2.01	0.41
15:O:471:LYS:CB	15:O:585:PHE:HE1	1.94	0.41
1:A:98:LEU:HD13	1:A:320:VAL:HG13	2.03	0.41
1:A:396:ILE:CD1	1:A:426:ALA:HB3	2.51	0.41
1:A:424:MET:O	1:A:428:VAL:HG23	2.21	0.41
1:A:755:ILE:HG12	1:A:930:LEU:HB3	2.03	0.41
1:A:1229:ALA:HB2	1:A:1597:ALA:HB2	2.02	0.41
2:B:145:VAL:HB	2:B:440:PHE:HB2	2.02	0.41
2:B:162:PRO:HG3	2:B:462:GLN:HA	2.03	0.41
2:B:207:ILE:HB	2:B:505:ARG:HA	2.02	0.41
2:B:217:ILE:HD11	2:B:235:GLN:HB2	2.02	0.41
2:B:612:LYS:HD3	2:B:626:ILE:HD11	2.01	0.41
3:C:80:ALA:HA	3:C:208:CYS:HA	2.03	0.41
3:C:191:ILE:HA	10:J:16:ASP:HB3	2.02	0.41
7:G:26:ASN:ND2	7:G:37:CYS:HA	2.35	0.41
7:G:45:LEU:HD11	7:G:120:VAL:HG12	2.02	0.41
7:G:244:SER:HB2	15:O:148:PRO:HG2	2.01	0.41
9:I:52:ALA:HB3	9:I:55:ALA:HB2	2.02	0.41
15:O:107:ILE:O	15:O:107:ILE:CG2	2.69	0.41
15:O:225:LEU:C	15:O:225:LEU:CD1	2.86	0.41
15:O:588:LEU:HD23	15:O:588:LEU:HA	1.88	0.41
16:S:67:DA:H2"	16:S:68:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ALA:HB1	2:B:755:ASN:HD21	1.84	0.41
2:B:811:LEU:CD2	2:B:825:PHE:CD2	3.04	0.41
8:H:35:GLN:HB3	8:H:111:LEU:HD21	2.01	0.41
15:O:115:LEU:O	15:O:119:ILE:HG13	2.21	0.41
15:O:150:TRP:O	15:O:154:VAL:HG23	2.21	0.41
15:O:240:ILE:CG2	15:O:332:LEU:CB	2.75	0.41
1:A:385:LEU:CG	1:A:453:ILE:HB	2.48	0.41
1:A:970:LYS:HG2	1:A:971:PRO:HD2	2.02	0.41
2:B:68:ILE:CG2	2:B:418:ASP:OD2	2.66	0.41
2:B:100:GLU:OE1	2:B:100:GLU:N	2.54	0.41
2:B:140:LYS:HB3	2:B:155:VAL:HG22	2.01	0.41
2:B:144:SER:HB3	2:B:148:GLY:HA2	2.03	0.41
12:L:29:TYR:HD2	12:L:39:SER:HA	1.85	0.41
17:T:6:DC:H2"	17:T:7:DA:C8	2.56	0.41
1:A:966:LEU:HB2	1:A:969:PHE:HD2	1.85	0.41
1:A:996:TYR:HD2	1:A:996:TYR:O	2.04	0.41
1:A:1006:LEU:HD22	9:I:104:ALA:CB	2.51	0.41
1:A:1272:VAL:HG11	1:A:1485:MET:HB3	2.03	0.41
2:B:73:ILE:C	2:B:73:ILE:CD1	2.85	0.41
2:B:128:GLN:NE2	2:B:735:HIS:HA	2.36	0.41
2:B:128:GLN:CB	12:L:55:ILE:HD13	2.48	0.41
2:B:132:SER:H	2:B:134:ARG:HH12	1.68	0.41
2:B:170:CYS:SG	2:B:171:HIS:N	2.93	0.41
2:B:1041:ASN:CB	2:B:1044:PHE:HB2	2.47	0.41
3:C:175:GLN:HB3	3:C:178:THR:HG22	2.03	0.41
4:D:26:GLN:HB2	7:G:42:PRO:HG2	2.03	0.41
13:M:15:VAL:HG12	13:M:90:LEU:HB2	2.03	0.41
15:O:198:PHE:HD2	15:O:232:LEU:CD2	2.32	0.41
15:O:342:HIS:NE2	15:O:346:GLN:HG3	2.34	0.41
15:O:422:GLN:HB3	15:O:593:PRO:HD3	2.02	0.41
15:O:423:TYR:CE1	15:O:593:PRO:HB2	2.55	0.41
15:O:430:ARG:NH2	15:O:596:PRO:CG	2.84	0.41
15:O:458:GLU:HG2	15:O:461:VAL:HG21	2.02	0.41
1:A:35:PRO:N	1:A:390:LEU:HD12	2.36	0.41
1:A:855:ARG:HH21	1:A:867:ASP:HB3	1.86	0.41
1:A:857:ALA:HB2	1:A:899:LYS:HD2	2.03	0.41
2:B:94:LYS:HB3	2:B:94:LYS:HE2	1.84	0.41
2:B:106:LYS:HD3	2:B:108:MET:CG	2.50	0.41
2:B:600:GLN:HA	2:B:603:ILE:HD12	2.02	0.41
11:K:109:GLY:O	11:K:110:GLU:HG2	2.21	0.41
15:O:173:HIS:NE2	15:O:217:LYS:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:386:PHE:CE2	15:O:606:MET:CE	3.03	0.41
1:A:490:ILE:HG22	1:A:606:ARG:HD3	2.04	0.40
1:A:1260:LYS:HD3	1:A:1500:GLN:C	2.33	0.40
2:B:108:MET:HE2	2:B:108:MET:HB3	1.98	0.40
2:B:201:LYS:HD3	2:B:465:LEU:O	2.20	0.40
2:B:811:LEU:HB2	2:B:899:GLN:HB2	2.03	0.40
2:B:887:LEU:HD22	12:L:56:LEU:O	2.00	0.40
1:A:636:HIS:HD2	2:B:1091:ARG:HH21	1.68	0.40
1:A:1041:ALA:HB1	1:A:1636:SER:HA	2.02	0.40
2:B:44:PRO:O	2:B:48:SER:HB2	2.20	0.40
2:B:97:VAL:HG12	2:B:425:ILE:HD11	2.03	0.40
2:B:1084:THR:HG23	2:B:1084:THR:O	2.21	0.40
3:C:328:LEU:HB2	11:K:121:LEU:HD22	2.02	0.40
7:G:241:ARG:CD	15:O:186:SER:HA	2.50	0.40
15:O:128:LEU:HD23	15:O:128:LEU:HA	1.90	0.40
1:A:251:ILE:HD12	1:A:320:VAL:HG21	2.03	0.40
1:A:1439:MET:O	1:A:1439:MET:SD	2.79	0.40
2:B:49:PHE:O	2:B:52:LEU:HB2	2.22	0.40
8:H:30:SER:HB3	8:H:36:CYS:HB3	2.03	0.40
15:O:237:ILE:HD13	15:O:384:ILE:CD1	2.52	0.40
1:A:1121:ASP:HA	5:E:207:ARG:HH22	1.86	0.40
2:B:693:PRO:O	2:B:696:ILE:HG12	2.22	0.40
15:O:147:ILE:HG22	15:O:149:LYS:CB	2.51	0.40
15:O:163:ILE:HG22	15:O:211:TYR:CB	2.42	0.40
1:A:104:PHE:CZ	1:A:267:LYS:HE2	2.56	0.40
1:A:253:GLU:O	1:A:312:SER:CB	2.70	0.40
15:O:83:LYS:HG3	15:O:84:ASN:N	2.37	0.40
15:O:163:ILE:HD12	15:O:207:LYS:HG2	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	1438/1664 (86%)	1365 (95%)	67 (5%)	6 (0%)	30	67
2	B	1169/1203 (97%)	1093 (94%)	71 (6%)	5 (0%)	30	67
3	C	300/335 (90%)	285 (95%)	15 (5%)	0	100	100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
7	G	196/326 (60%)	184 (94%)	11 (6%)	1 (0%)	25	63
8	H	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	16	53
9	I	122/125 (98%)	109 (89%)	11 (9%)	2 (2%)	8	37
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	101/142 (71%)	96 (95%)	5 (5%)	0	100	100
12	L	43/70 (61%)	39 (91%)	4 (9%)	0	100	100
13	M	101/415 (24%)	93 (92%)	8 (8%)	0	100	100
14	N	131/233 (56%)	123 (94%)	8 (6%)	0	100	100
15	O	457/627 (73%)	400 (88%)	38 (8%)	19 (4%)	2	18
18	U	273/514 (53%)	245 (90%)	14 (5%)	14 (5%)	1	16
19	V	256/894 (29%)	235 (92%)	11 (4%)	10 (4%)	2	19
20	W	152/507 (30%)	141 (93%)	4 (3%)	7 (5%)	2	17
21	1	11/13 (85%)	11 (100%)	0	0	100	100
22	2	17/19 (90%)	17 (100%)	0	0	100	100
23	3	7/9 (78%)	7 (100%)	0	0	100	100
23	9	7/9 (78%)	7 (100%)	0	0	100	100
24	4	21/24 (88%)	21 (100%)	0	0	100	100
25	5	14/16 (88%)	14 (100%)	0	0	100	100
25	Q	12/16 (75%)	12 (100%)	0	0	100	100
26	6	8/10 (80%)	8 (100%)	0	0	100	100
26	8	8/10 (80%)	8 (100%)	0	0	100	100
27	7	23/25 (92%)	23 (100%)	0	0	100	100
28	P	20/22 (91%)	20 (100%)	0	0	100	100
29	Z	13/15 (87%)	13 (100%)	0	0	100	100
30	Y	10/12 (83%)	10 (100%)	0	0	100	100
31	R	25/27 (93%)	25 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5498/8005 (69%)	5135 (93%)	298 (5%)	65 (1%)	14 43

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1441	LYS
1	A	1500	GLN
2	B	90	TYR
2	B	1042	ASP
15	O	165	PRO
15	O	226	GLY
15	O	325	ILE
15	O	380	SER
15	O	431	ALA
15	O	489	ASN
15	O	521	ASN
15	O	540	CYS
15	O	600	LYS
18	U	125	PHE
18	U	128	GLU
18	U	147	GLN
18	U	148	PRO
18	U	207	LEU
18	U	208	PRO
18	U	264	PRO
18	U	437	THR
19	V	239	HIS
19	V	258	SER
19	V	387	ASN
19	V	411	LYS
20	W	207	ASN
20	W	251	TRP
20	W	402	ASN
1	A	441	THR
15	O	488	HIS
18	U	157	HIS
18	U	204	ARG
18	U	219	ILE
19	V	20	VAL
19	V	266	GLU
1	A	237	GLY
1	A	255	ALA

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Mol	Chain	Res	Type
2	B	532	HIS
2	B	1154	ASP
15	O	82	SER
15	O	130	PRO
15	O	148	PRO
15	O	377	TYR
15	O	457	ARG
15	O	469	ARG
19	V	240	SER
19	V	265	THR
19	V	353	ASP
20	W	305	THR
1	A	1458	THR
15	O	187	MET
18	U	405	ASP
20	W	250	LEU
20	W	340	ASP
9	I	26	SER
20	W	364	VAL
2	B	901	VAL
8	H	84	ALA
15	O	147	ILE
15	O	128	LEU
18	U	126	PRO
18	U	281	ILE
19	V	535	VAL
7	G	127	PRO
9	I	90	GLY

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	1287/1465 (88%)	1210 (94%)	77 (6%)	16 38
2	B	1024/1053 (97%)	932 (91%)	92 (9%)	8 25
3	C	269/296 (91%)	244 (91%)	25 (9%)	7 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	56/116 (48%)	50 (89%)	6 (11%)	5 20
5	E	197/197 (100%)	192 (98%)	5 (2%)	42 62
6	F	90/137 (66%)	86 (96%)	4 (4%)	24 46
7	G	180/291 (62%)	167 (93%)	13 (7%)	12 32
8	H	116/128 (91%)	111 (96%)	5 (4%)	25 47
9	I	109/110 (99%)	98 (90%)	11 (10%)	6 21
10	J	64/65 (98%)	57 (89%)	7 (11%)	5 19
11	K	93/130 (72%)	84 (90%)	9 (10%)	6 22
12	L	40/57 (70%)	37 (92%)	3 (8%)	11 31
13	M	94/371 (25%)	89 (95%)	5 (5%)	19 41
14	N	128/220 (58%)	118 (92%)	10 (8%)	10 29
15	O	427/576 (74%)	378 (88%)	49 (12%)	4 18
All	All	4174/5212 (80%)	3853 (92%)	321 (8%)	13 30

All (321) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	39	ASP
1	A	59	ARG
1	A	113	VAL
1	A	129	LEU
1	A	136	LEU
1	A	177	LEU
1	A	195	LYS
1	A	199	ASP
1	A	211	THR
1	A	325	ASP
1	A	345	LEU
1	A	361	VAL
1	A	373	LEU
1	A	390	LEU
1	A	397	ARG
1	A	400	ASN
1	A	417	ARG
1	A	425	ASN
1	A	518	GLU
1	A	536	ILE

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Mol	Chain	Res	Type
1	A	562	LEU
1	A	572	THR
1	A	586	VAL
1	A	587	VAL
1	A	621	THR
1	A	684	ASP
1	A	685	SER
1	A	743	ASP
1	A	747	ILE
1	A	831	ASP
1	A	840	ASN
1	A	844	THR
1	A	862	THR
1	A	878	ARG
1	A	952	LEU
1	A	960	MET
1	A	1004	GLU
1	A	1065	GLN
1	A	1089	LEU
1	A	1164	LYS
1	A	1171	GLN
1	A	1175	MET
1	A	1179	ILE
1	A	1183	GLU
1	A	1193	VAL
1	A	1202	LEU
1	A	1205	PHE
1	A	1217	LEU
1	A	1242	ILE
1	A	1248	ASP
1	A	1252	ASP
1	A	1261	VAL
1	A	1263	LEU
1	A	1268	ASP
1	A	1273	THR
1	A	1313	LEU
1	A	1433	VAL
1	A	1434	GLU
1	A	1437	ASN
1	A	1439	MET
1	A	1440	ASN
1	A	1474	LEU

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Mol	Chain	Res	Type
1	A	1475	GLU
1	A	1481	GLU
1	A	1501	ILE
1	A	1502	PRO
1	A	1505	ASP
1	A	1531	ASP
1	A	1533	GLU
1	A	1550	LEU
1	A	1552	THR
1	A	1592	GLN
1	A	1609	SER
1	A	1628	ASP
1	A	1629	ASN
1	A	1649	VAL
2	B	13	THR
2	B	15	ASP
2	B	17	ARG
2	B	19	LEU
2	B	22	GLU
2	B	27	ASN
2	B	35	PHE
2	B	52	LEU
2	B	54	GLU
2	B	61	LEU
2	B	71	LYS
2	B	73	ILE
2	B	126	SER
2	B	152	LEU
2	B	186	GLU
2	B	190	ILE
2	B	202	LEU
2	B	206	LEU
2	B	212	ASN
2	B	217	ILE
2	B	234	ILE
2	B	250	LEU
2	B	265	ARG
2	B	268	GLU
2	B	274	VAL
2	B	276	ILE
2	B	304	ASP
2	B	306	LEU

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Mol	Chain	Res	Type
2	B	316	ARG
2	B	332	ASP
2	B	356	ARG
2	B	364	LYS
2	B	373	MET
2	B	374	LEU
2	B	381	LEU
2	B	413	LEU
2	B	431	ASP
2	B	438	ILE
2	B	441	LYS
2	B	455	GLU
2	B	471	VAL
2	B	479	GLN
2	B	480	GLN
2	B	481	VAL
2	B	485	THR
2	B	519	LYS
2	B	542	LEU
2	B	550	ARG
2	B	588	ILE
2	B	617	THR
2	B	640	LEU
2	B	646	HIS
2	B	684	ASN
2	B	692	THR
2	B	721	MET
2	B	743	ARG
2	B	752	VAL
2	B	782	ASP
2	B	787	MET
2	B	789	ILE
2	B	794	ASP
2	B	832	TRP
2	B	835	GLU
2	B	840	LEU
2	B	842	GLU
2	B	848	ILE
2	B	859	CYS
2	B	873	THR
2	B	893	ASN
2	B	895	PHE

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Mol	Chain	Res	Type
2	B	898	LEU
2	B	933	THR
2	B	940	GLU
2	B	944	GLN
2	B	956	SER
2	B	965	GLU
2	B	967	LEU
2	B	977	ILE
2	B	994	ASP
2	B	1000	LEU
2	B	1020	GLU
2	B	1033	TYR
2	B	1037	ARG
2	B	1041	ASN
2	B	1042	ASP
2	B	1065	ARG
2	B	1076	ARG
2	B	1110	ILE
2	B	1123	ILE
2	B	1157	GLN
2	B	1181	VAL
2	B	1201	GLU
3	C	30	GLU
3	C	39	ASP
3	C	46	SER
3	C	47	LEU
3	C	81	GLU
3	C	89	THR
3	C	97	LEU
3	C	106	LEU
3	C	117	ASP
3	C	120	LEU
3	C	151	THR
3	C	181	ASP
3	C	182	CYS
3	C	188	ASP
3	C	209	ILE
3	C	224	THR
3	C	229	LEU
3	C	235	ILE
3	C	240	LYS
3	C	259	ASP

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Mol	Chain	Res	Type
3	C	277	ARG
3	C	291	LEU
3	C	303	GLU
3	C	331	CYS
3	C	334	THR
4	D	14	THR
4	D	16	LEU
4	D	21	VAL
4	D	25	THR
4	D	27	LEU
4	D	89	LEU
5	E	84	ASP
5	E	106	GLN
5	E	163	GLU
5	E	167	ARG
5	E	175	LEU
6	F	69	LEU
6	F	103	MET
6	F	111	LEU
6	F	147	SER
7	G	22	LYS
7	G	32	ASN
7	G	54	LEU
7	G	75	ASN
7	G	93	ASP
7	G	95	LEU
7	G	104	LEU
7	G	144	HIS
7	G	214	LEU
7	G	217	TRP
7	G	223	GLU
7	G	248	THR
7	G	250	ILE
8	H	33	GLN
8	H	53	ASP
8	H	89	LEU
8	H	109	LYS
8	H	136	LYS
9	I	3	VAL
9	I	17	LEU
9	I	27	ASN
9	I	47	VAL

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Mol	Chain	Res	Type
9	I	50	THR
9	I	51	THR
9	I	53	ASP
9	I	60	LEU
9	I	99	LEU
9	I	101	LEU
9	I	102	ARG
10	J	2	ILE
10	J	14	VAL
10	J	26	GLN
10	J	32	GLU
10	J	47	ARG
10	J	48	ARG
10	J	68	LYS
11	K	45	GLU
11	K	49	LEU
11	K	59	THR
11	K	60	SER
11	K	72	LEU
11	K	77	ARG
11	K	99	ASN
11	K	124	LEU
11	K	132	GLU
12	L	27	LEU
12	L	38	LEU
12	L	62	LYS
13	M	50	GLU
13	M	56	GLU
13	M	101	VAL
13	M	103	LYS
13	M	108	LEU
14	N	36	LYS
14	N	67	LEU
14	N	74	PHE
14	N	94	ASP
14	N	114	GLU
14	N	117	GLU
14	N	131	LEU
14	N	166	LEU
14	N	168	LEU
14	N	178	GLU
15	O	66	ASN

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Mol	Chain	Res	Type
15	O	67	ASP
15	O	69	THR
15	O	78	VAL
15	O	80	LEU
15	O	87	ARG
15	O	101	SER
15	O	111	ARG
15	O	117	GLN
15	O	149	LYS
15	O	171	CYS
15	O	175	MET
15	O	180	LEU
15	O	181	ARG
15	O	190	ILE
15	O	192	THR
15	O	202	ASN
15	O	203	ASP
15	O	204	THR
15	O	205	ARG
15	O	212	THR
15	O	213	SER
15	O	215	LEU
15	O	228	GLN
15	O	232	LEU
15	O	234	ILE
15	O	245	GLN
15	O	248	LEU
15	O	341	THR
15	O	350	GLU
15	O	354	SER
15	O	363	THR
15	O	368	PHE
15	O	369	LYS
15	O	395	LEU
15	O	437	THR
15	O	454	VAL
15	O	457	ARG
15	O	487	ARG
15	O	489	ASN
15	O	494	THR
15	O	495	ASP
15	O	522	GLU

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Mol	Chain	Res	Type
15	O	526	LEU
15	O	540	CYS
15	O	581	THR
15	O	584	GLN
15	O	597	LEU
15	O	602	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	GLN
1	A	431	GLN
1	A	580	HIS
1	A	590	ASN
1	A	592	GLN
1	A	636	HIS
1	A	671	GLN
1	A	693	GLN
1	A	706	HIS
1	A	730	GLN
1	A	738	ASN
1	A	926	GLN
1	A	1026	GLN
1	A	1036	ASN
1	A	1072	ASN
1	A	1113	HIS
1	A	1128	ASN
1	A	1437	ASN
1	A	1440	ASN
1	A	1443	GLN
1	A	1599	ASN
1	A	1601	GLN
2	B	62	ASN
2	B	168	ASN
2	B	173	ASN
2	B	212	ASN
2	B	243	GLN
2	B	251	HIS
2	B	282	HIS
2	B	351	GLN
2	B	361	HIS
2	B	400	GLN

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Mol	Chain	Res	Type
2	B	462	GLN
2	B	480	GLN
2	B	646	HIS
2	B	686	HIS
2	B	695	ASN
2	B	724	GLN
2	B	755	ASN
2	B	823	GLN
2	B	896	GLN
2	B	975	HIS
2	B	987	ASN
2	B	999	GLN
2	B	1053	ASN
2	B	1114	GLN
3	C	130	ASN
3	C	216	HIS
3	C	232	GLN
3	C	335	GLN
4	D	30	HIS
5	E	147	HIS
5	E	179	GLN
7	G	20	HIS
7	G	32	ASN
7	G	64	GLN
7	G	65	HIS
7	G	140	GLN
7	G	150	HIS
8	H	35	GLN
8	H	43	ASN
9	I	21	ASN
9	I	97	HIS
9	I	124	ASN
9	I	125	ASN
11	K	106	GLN
11	K	118	GLN
13	M	16	GLN
14	N	132	GLN
15	O	66	ASN
15	O	70	GLN
15	O	172	HIS
15	O	173	HIS
15	O	245	GLN

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Mol	Chain	Res	Type
15	O	346	GLN
15	O	362	ASN
15	O	371	HIS
15	O	390	GLN
15	O	472	HIS
15	O	497	ASN
15	O	507	GLN
15	O	521	ASN
15	O	547	ASN
15	O	549	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	103:ALA	C	105:ALA	N	5.80

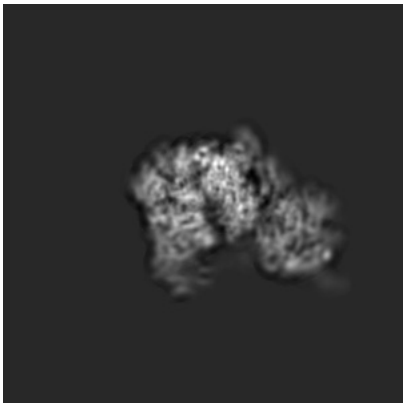
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3727. These allow visual inspection of the internal detail of the map and identification of artifacts.

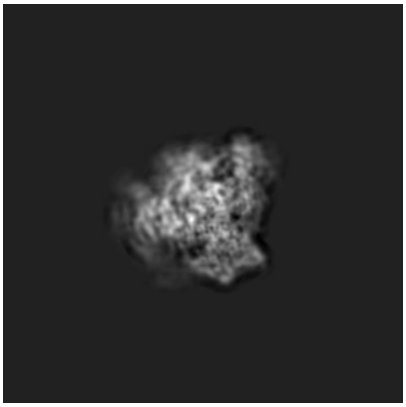
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

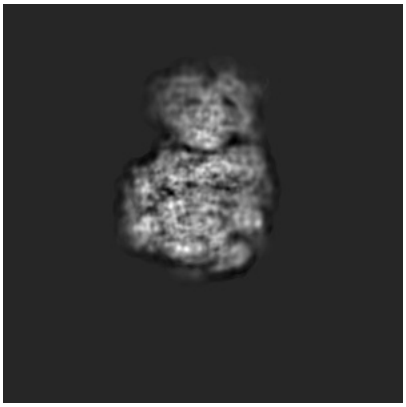
6.1.1 Primary map



X



Y



Z

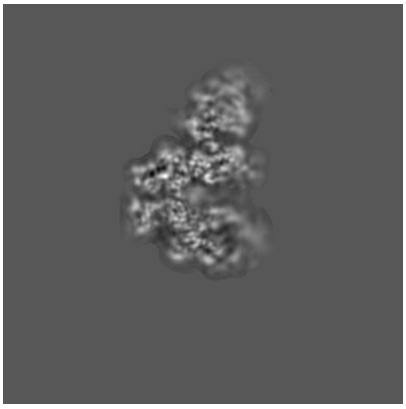
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 144

Y Index: 144

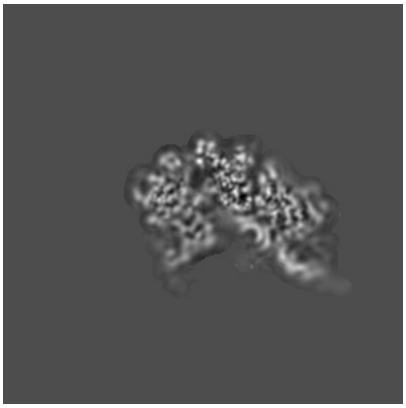


Z Index: 144

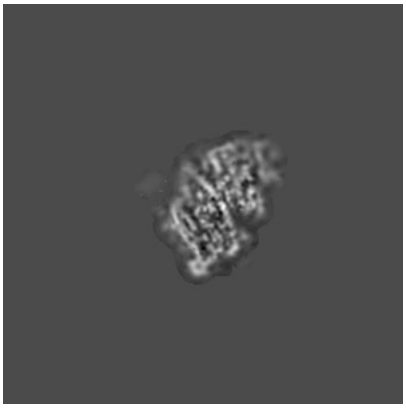
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

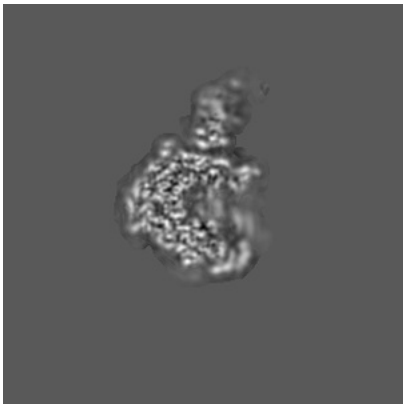
6.3.1 Primary map



X Index: 150



Y Index: 168

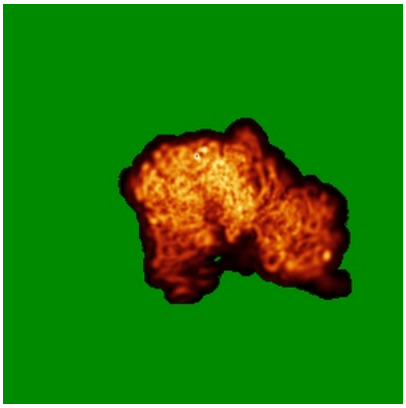


Z Index: 152

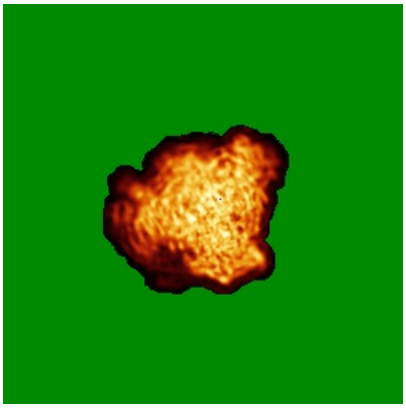
The images above show the largest variance slices of the map in three orthogonal directions.

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

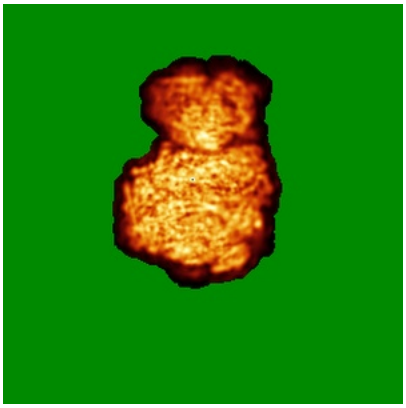
6.4.1 Primary map



X



Y

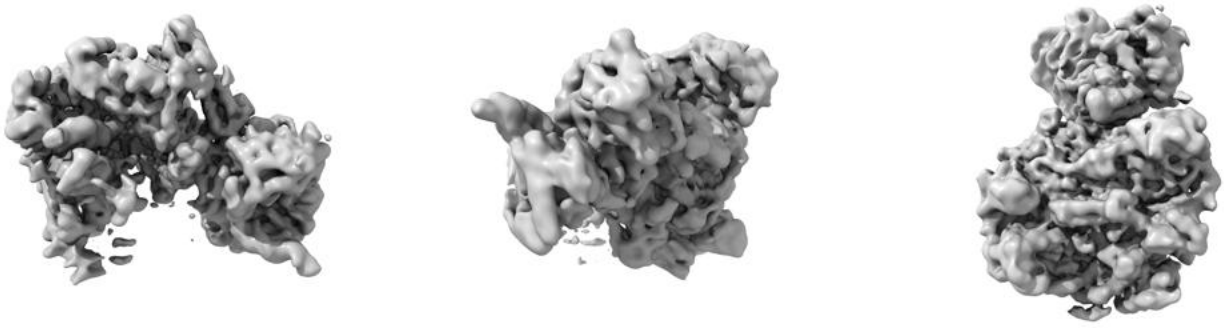


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

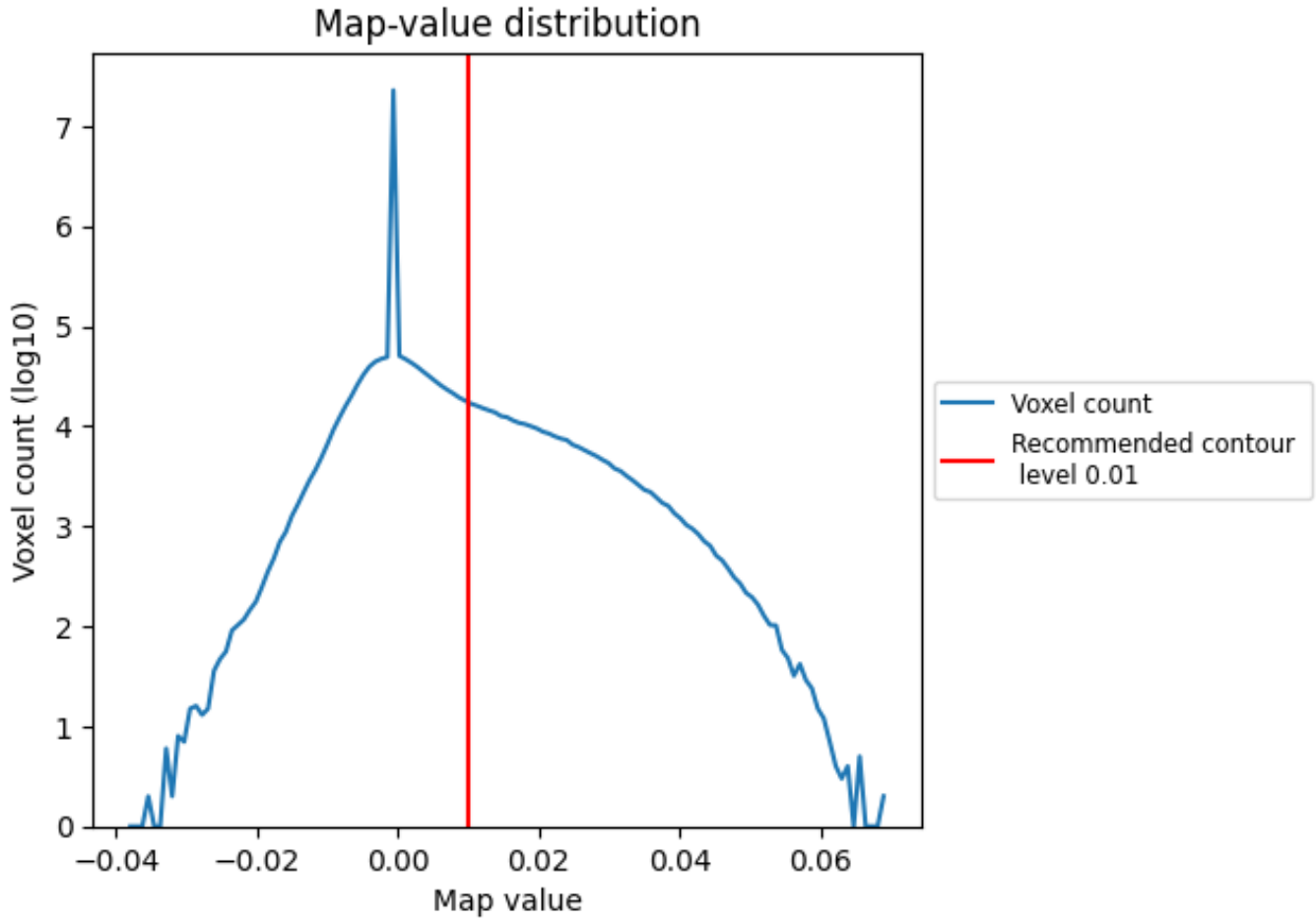
6.6 Mask visualisation (i)

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

7 Map analysis

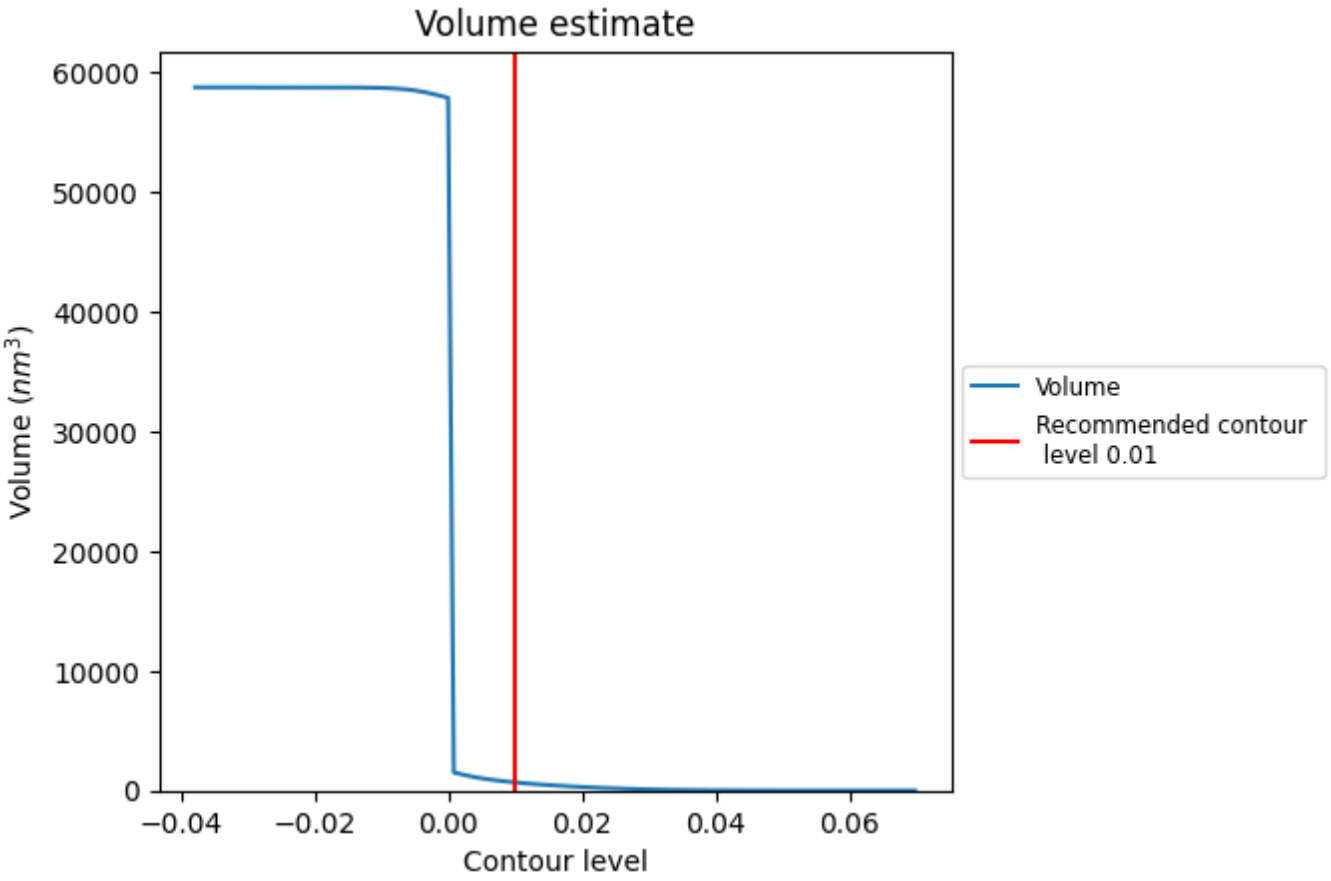
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

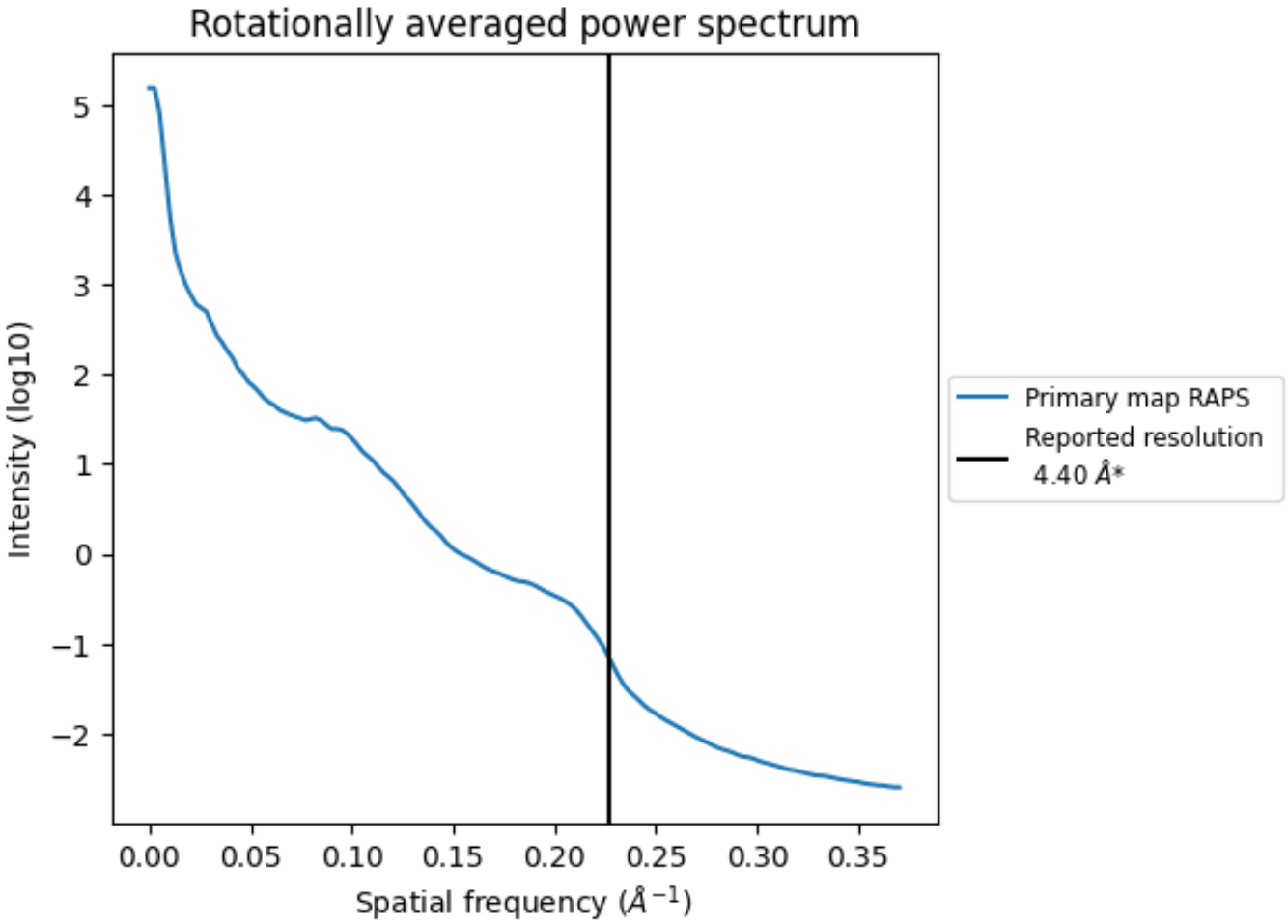
7.2 Volume estimate



The volume at the recommended contour level is 676 nm^3; this corresponds to an approximate mass of 611 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 0.227 Å^{-1}

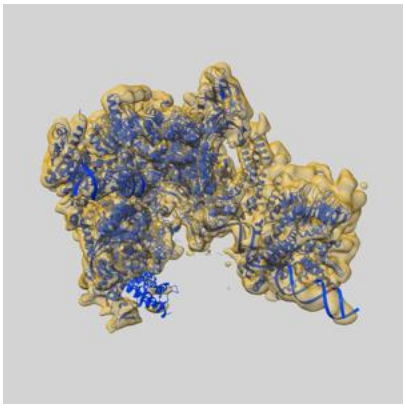
8 Fourier-Shell correlation (i)

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

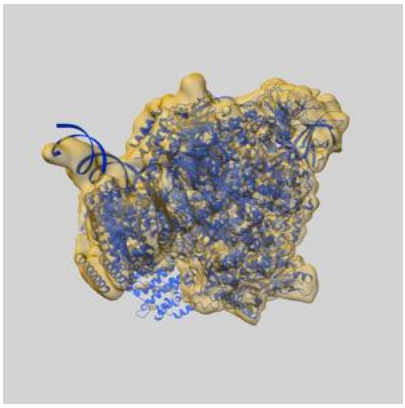
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3727 and PDB model 5OA1. Per-residue inclusion information can be found in section 3 on page 11.

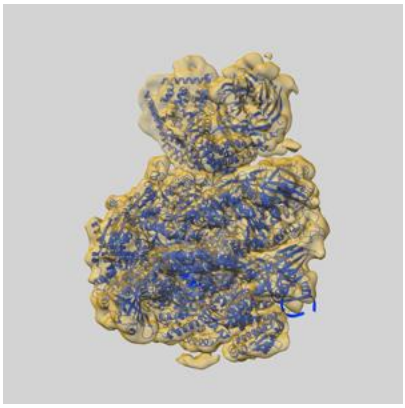
9.1 Map-model overlay



X



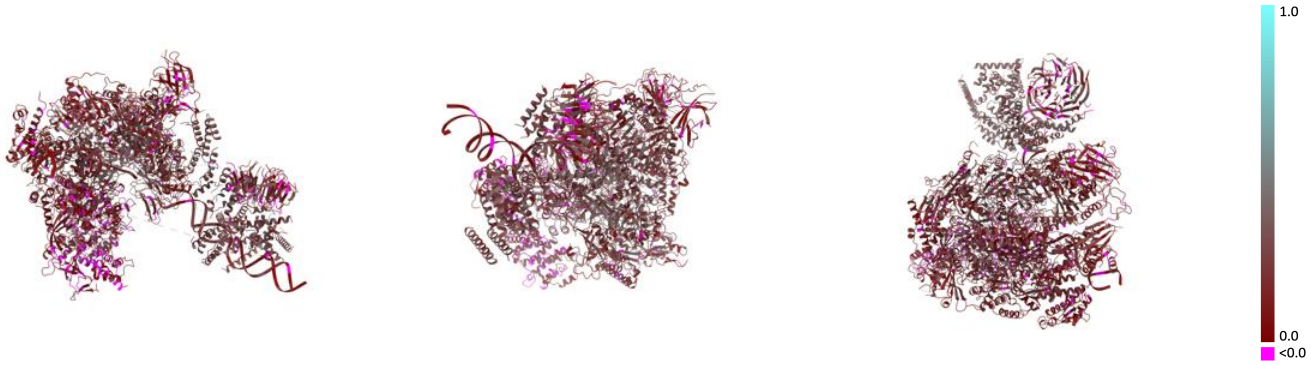
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

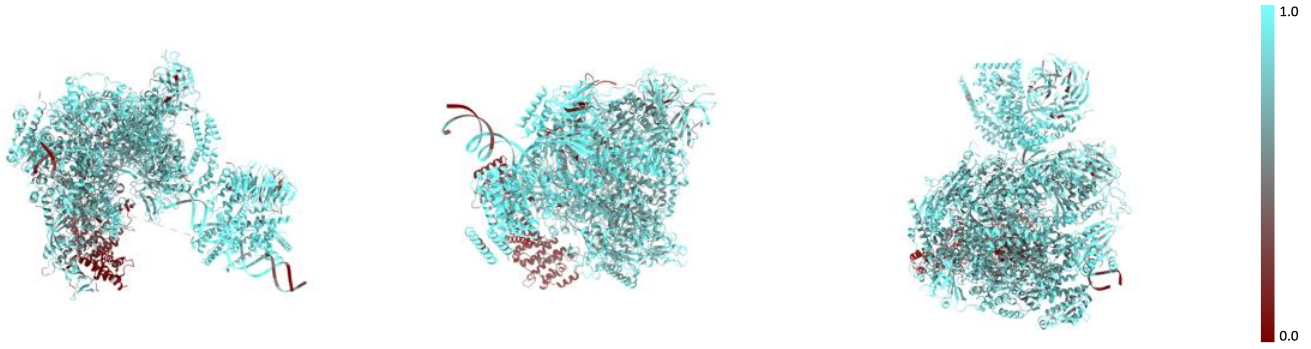
9.2 Q-score mapped to coordinate model



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.

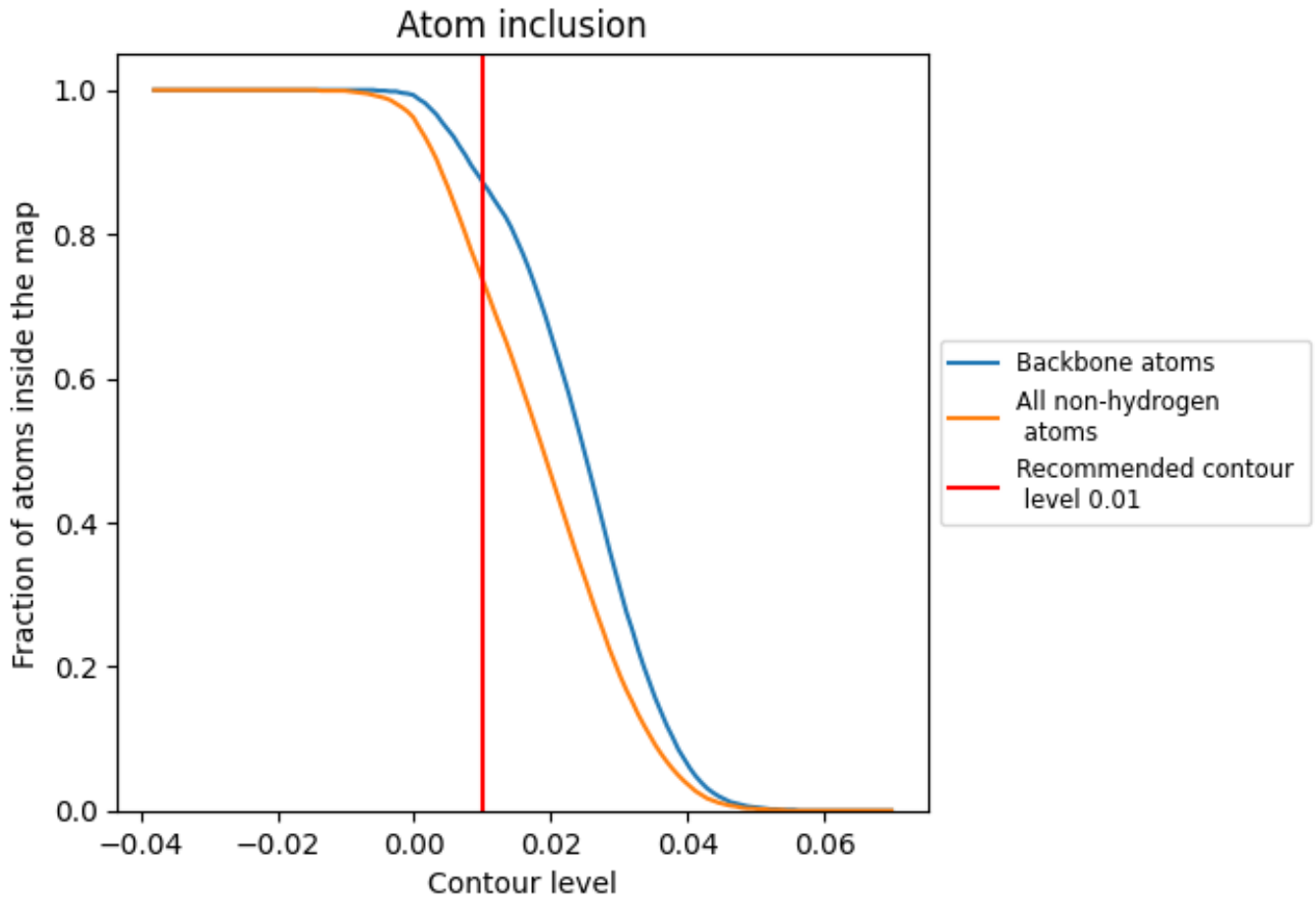
9.3 Atom inclusion mapped to coordinate model



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7370	0.1890
1	1.0000	0.3030
2	1.0000	0.2910
3	1.0000	0.2960
4	0.9570	0.3080
5	1.0000	0.3090
6	1.0000	0.3370
7	1.0000	0.3200
8	1.0000	0.2560
9	1.0000	0.3100
A	0.8020	0.1940
B	0.7980	0.2350
C	0.8540	0.2140
D	0.7150	0.1440
E	0.8180	0.1730
F	0.8000	0.1840
G	0.6950	0.0930
H	0.8970	0.2140
I	0.5560	0.1360
J	0.8330	0.2440
K	0.8340	0.1920
L	0.7810	0.2000
M	0.7460	0.1400
N	0.7520	0.1660
O	0.0440	0.0600
P	0.9430	0.2990
Q	0.9690	0.2640
R	0.8980	0.2740
S	0.7530	0.1600
T	0.7510	0.1720
U	0.9130	0.2880
V	0.8500	0.1500
W	0.9780	0.3230
Y	1.0000	0.3080
Z	1.0000	0.3170