Full wwPDB EM Validation Report

Nov 20, 2022 – 03:29 PM EST

PDB ID	:	7ML3
EMDB ID	:	EMD-23907
Title	:	General transcription factor TFIIH (weak binding)
Authors	:	Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on	:	2021-04-27
Resolution	:	7.60 Å(reported)
Based on initial model	:	5OQJ

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

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

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

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

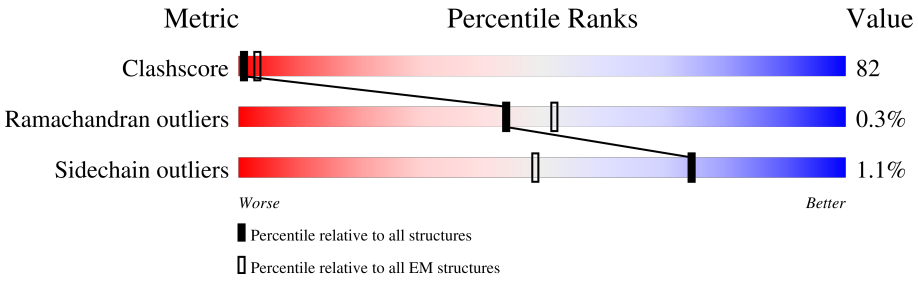
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 7.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	3	321	11% 23% 16% 57%
2	2	513	13% 42% 44% 10%
3	0	778	8% 23% 69% 5%
4	1	537	15% 41% 26% 32%
5	4	338	8% 32% 49% 16%
6	6	461	30% 42% 24%
7	5	72	22% 19% 64% 8% 8%
8	7	843	11% 23% 38% 35%

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Mol	Chain	Length	Quality of chain
9	N	30	
10	T	30	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	SF4	0	801	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 22648 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 BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	138	Total	C	N	O	S	0	0
			860	533	160	160	7		

- Molecule 2 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	460	Total	C	N	O	S	0	0
			3011	1856	562	584	9		

- Molecule 3 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	754	Total	C	N	O	S	0	0
			6108	3891	1032	1147	38		

- Molecule 4 is a protein called Tfb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	367	Total	C	N	O	S	0	0
			2411	1536	438	430	7		

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	113	UNK	ASP	conflict	UNP A0A7I9C5C2
4	114	UNK	MET	conflict	UNP A0A7I9C5C2

- Molecule 6 is a protein called General transcription and DNA repair factor IIH.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	351	Total	C	N	O	S	0	0
			2527	1590	454	456	27		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	412	UNK	ILE	conflict	UNP A0A7I9FQL5
6	413	UNK	LEU	conflict	UNP A0A7I9FQL5
6	414	UNK	LYS	conflict	UNP A0A7I9FQL5
6	415	UNK	ASN	conflict	UNP A0A7I9FQL5
6	416	UNK	HIS	conflict	UNP A0A7I9FQL5
6	417	UNK	LYS	conflict	UNP A0A7I9FQL5
6	418	UNK	ASN	conflict	UNP A0A7I9FQL5
6	419	UNK	ASP	conflict	UNP A0A7I9FQL5
6	420	UNK	LYS	conflict	UNP A0A7I9FQL5
6	421	UNK	LEU	conflict	UNP A0A7I9FQL5
6	422	UNK	LEU	conflict	UNP A0A7I9FQL5
6	423	UNK	THR	conflict	UNP A0A7I9FQL5
6	424	UNK	SER	conflict	UNP A0A7I9FQL5

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 8 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	548	Total	C	N	O	S	0	0
			3947	2438	729	757	23		

- Molecule 9 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	30	Total	C	N	O	P	0	0
			624	298	113	183	30		

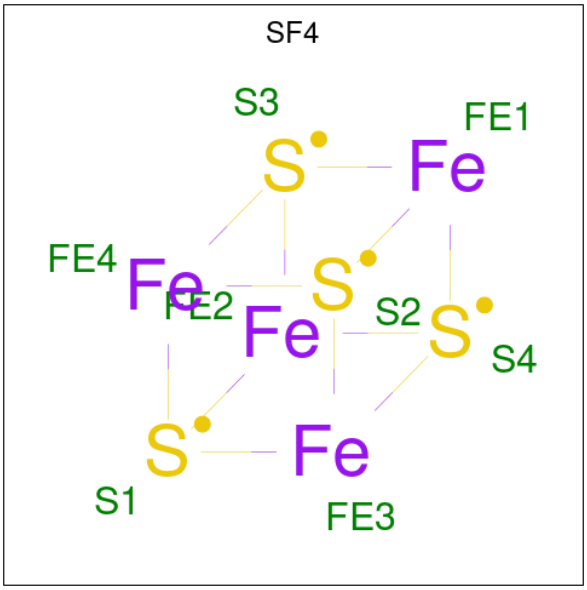
- Molecule 10 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	30	Total	C	N	O	P	0	0
			606	291	108	177	30		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	3	2	Total	Zn	0
			2	2	
11	4	1	Total	Zn	0
			1	1	
11	6	4	Total	Zn	0
			4	4	

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

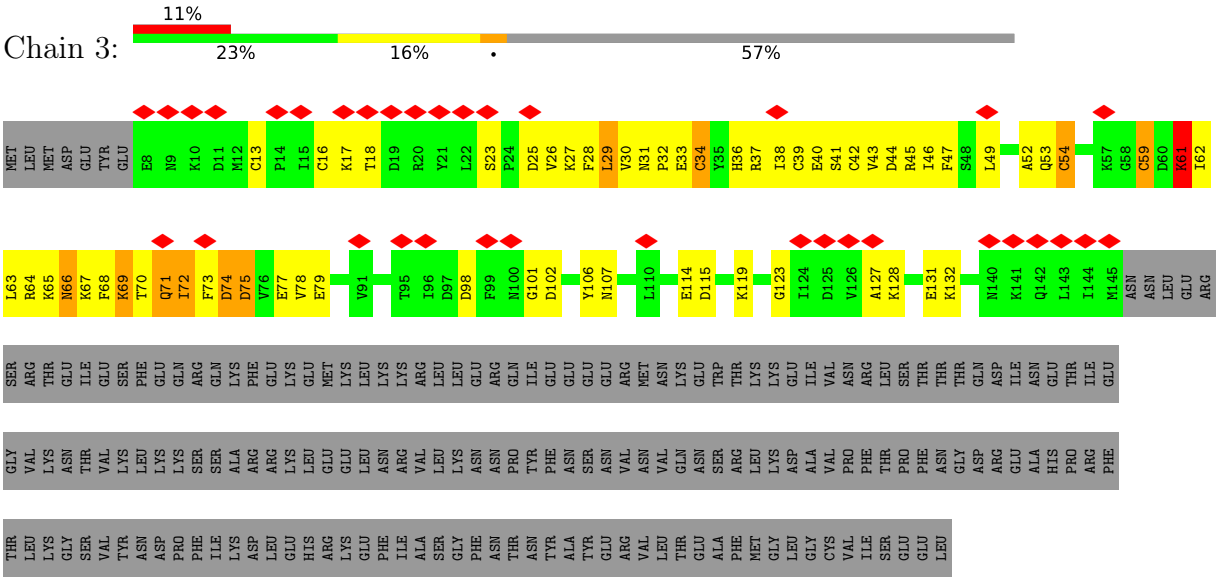


Mol	Chain	Residues	Atoms			AltConf
12	0	1	Total	Fe	S	0
			8	4	4	

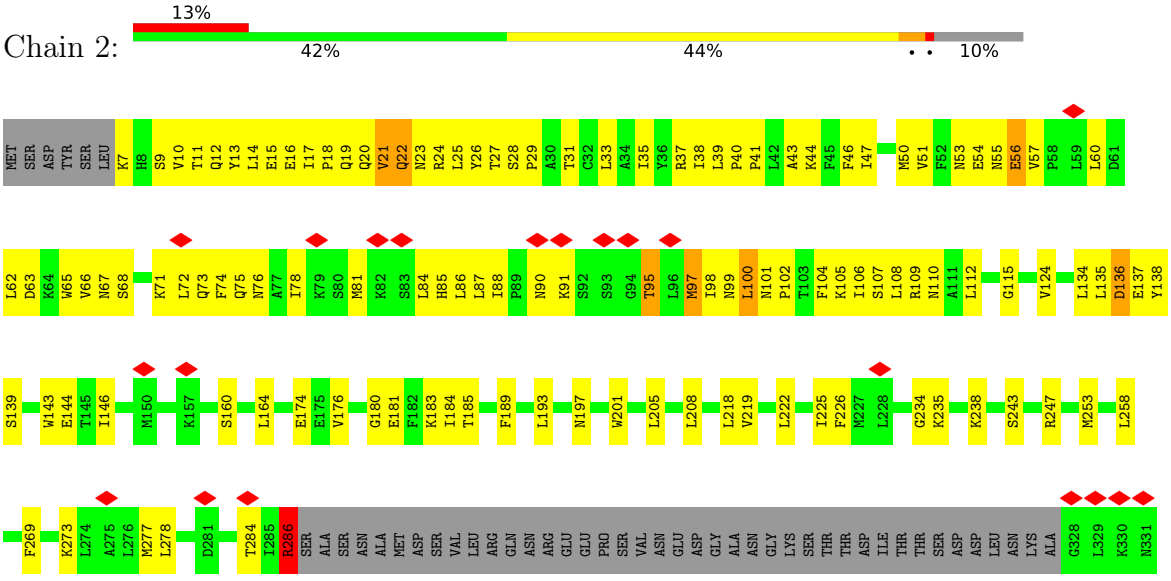
3 Residue-property plots (i)

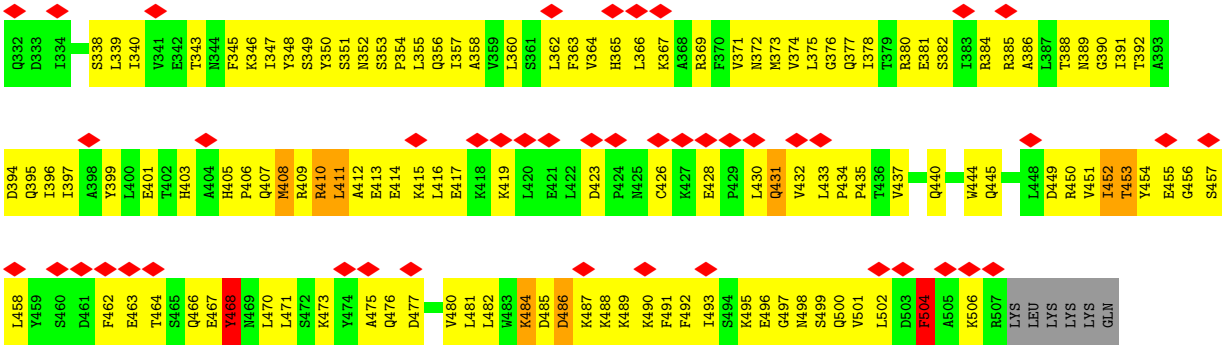
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: BJ4_G0050160.mRNA.1.CDS.1



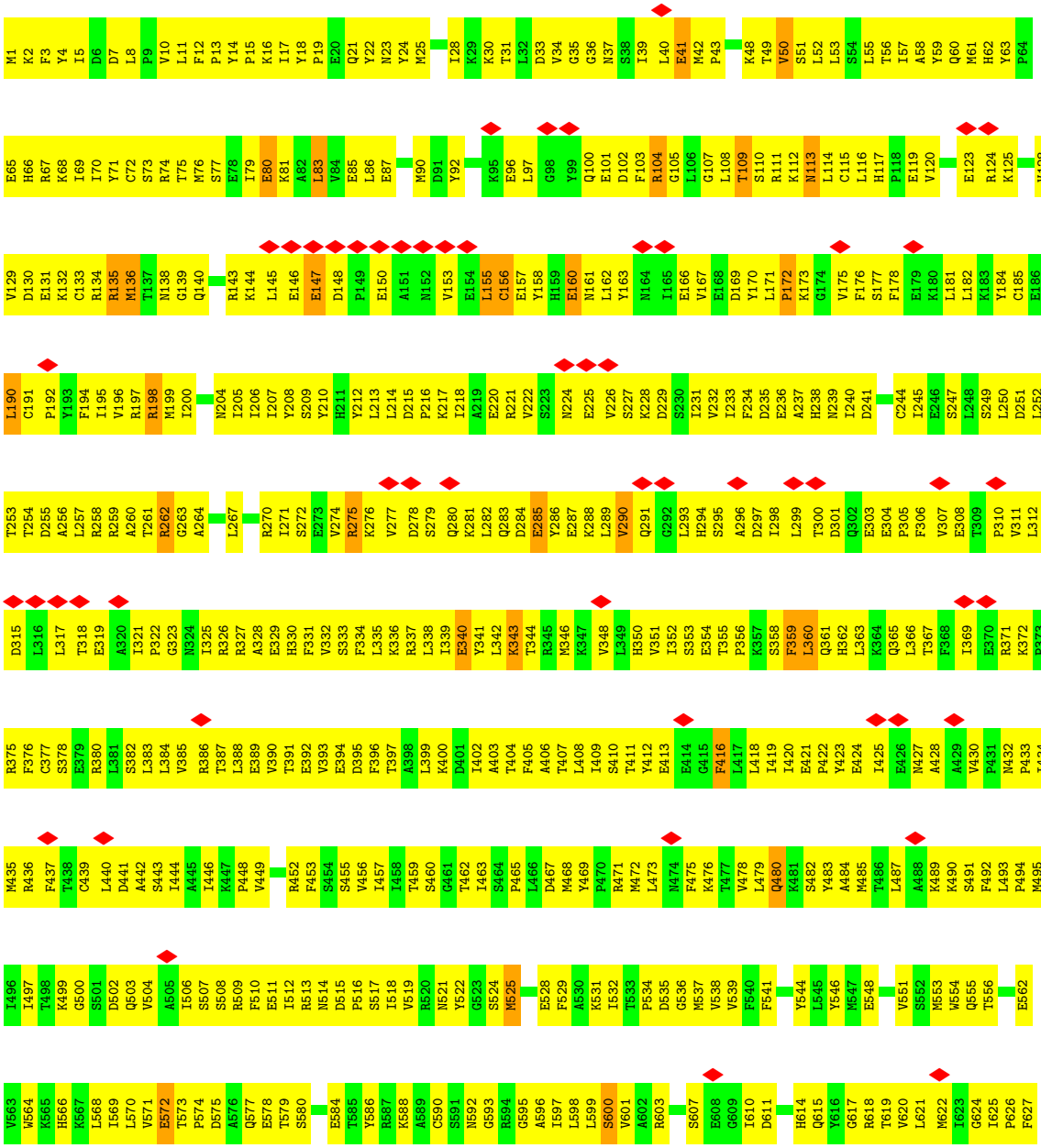
• Molecule 2: RNA polymerase II transcription factor B subunit 2





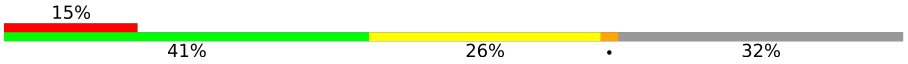
• Molecule 3: General transcription and DNA repair factor IIH helicase subunit XPD

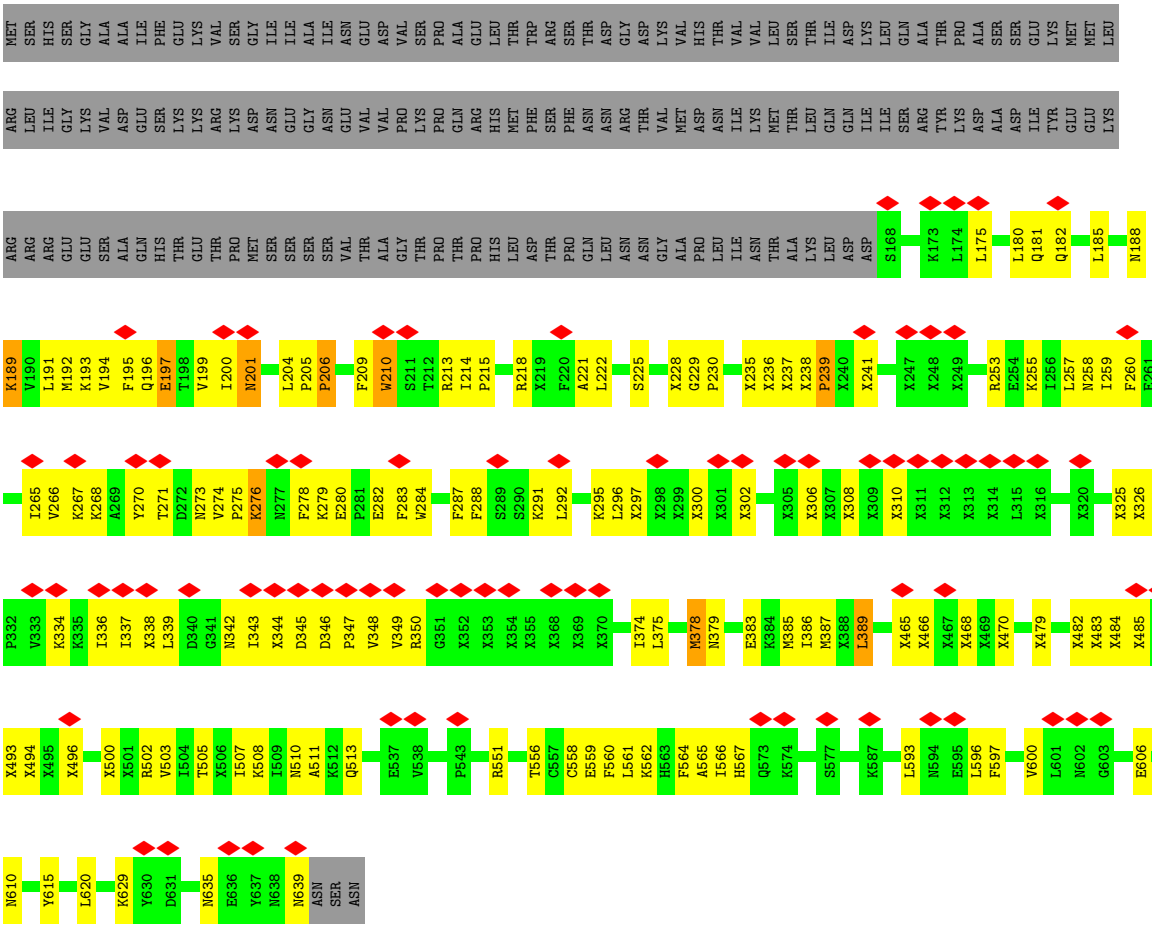
Chain 0:



• Molecule 4: Tfb1

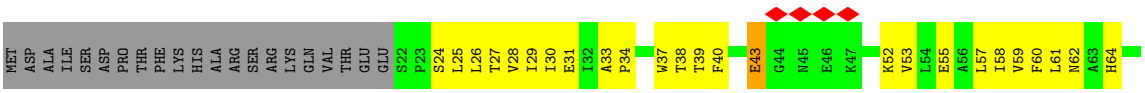
Chain 1:

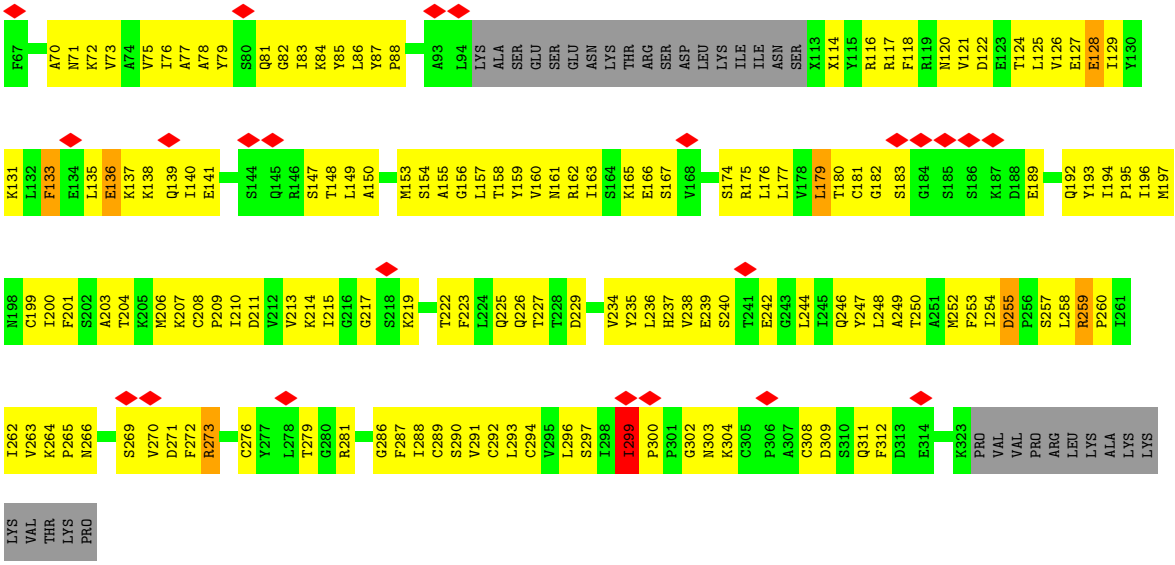




• Molecule 5: General transcription and DNA repair factor IIH subunit TFB4

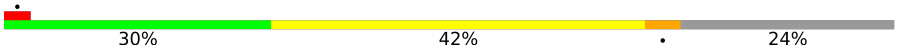
Chain 4:

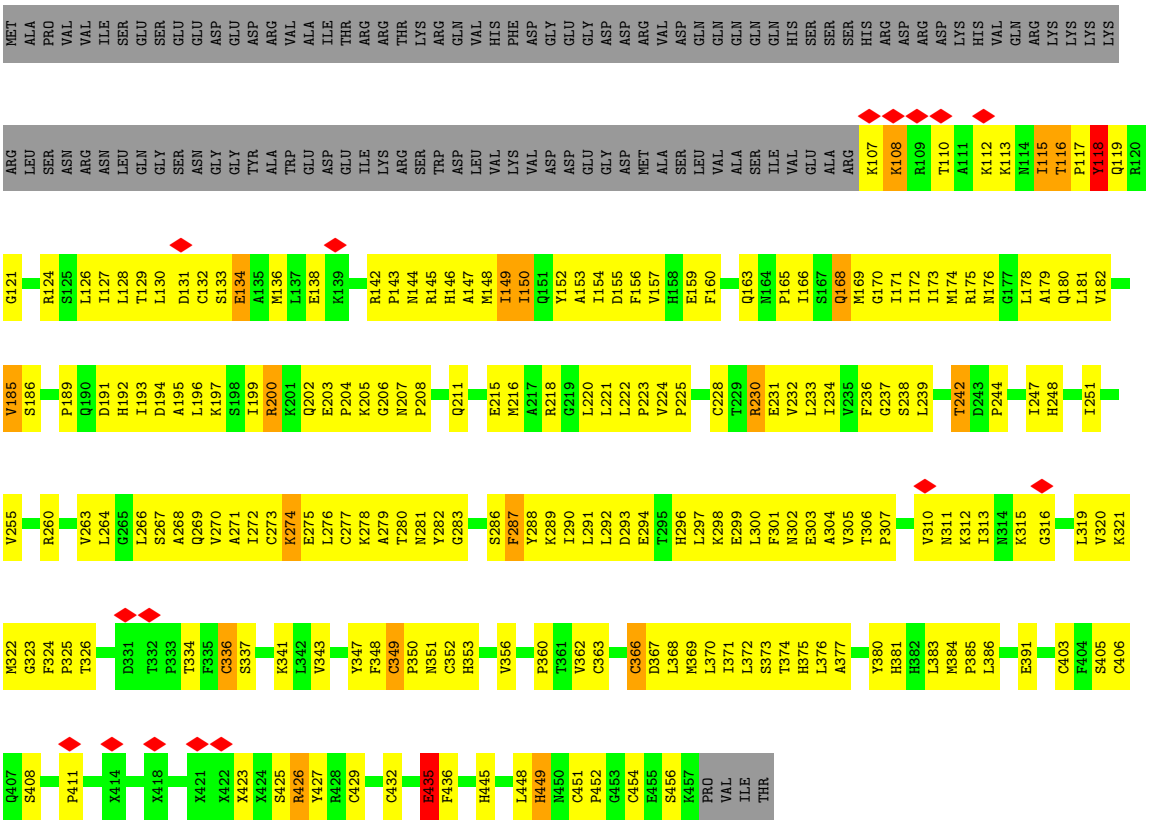




• Molecule 6: General transcription and DNA repair factor IIH

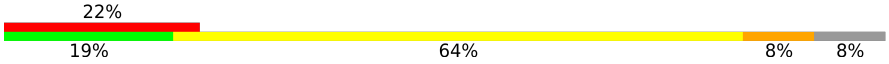
Chain 6:

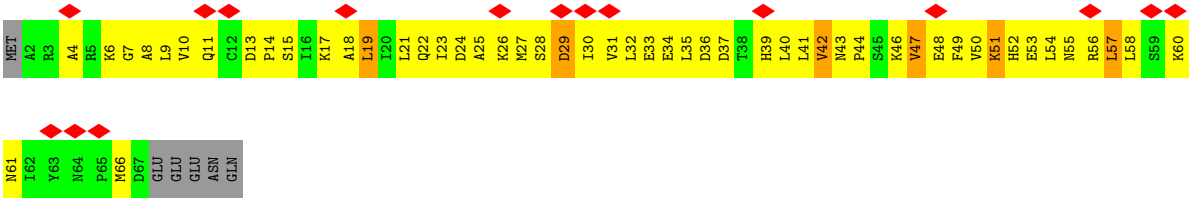




• Molecule 7: General transcription and DNA repair factor IIH subunit TFB5

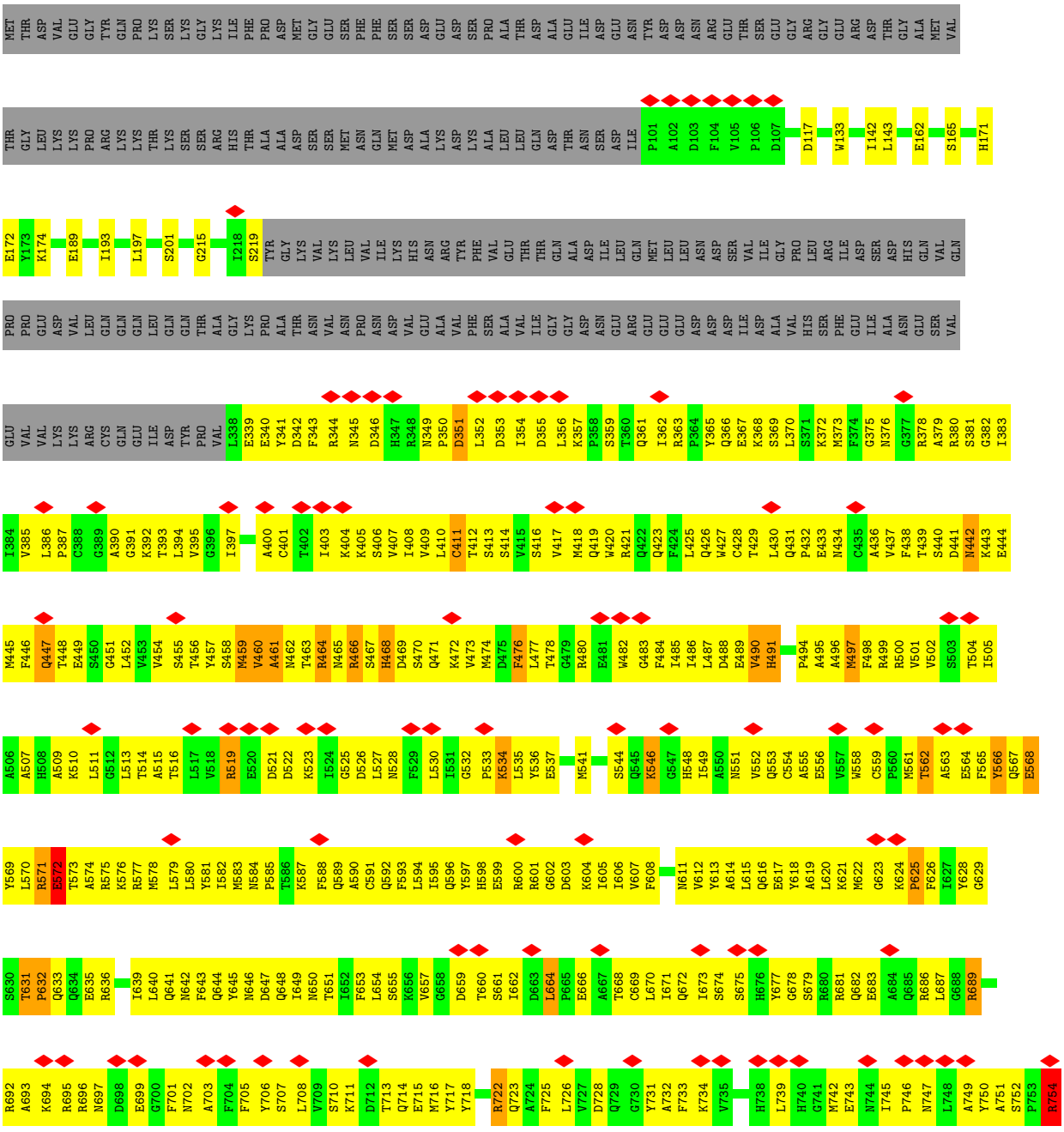
Chain 5:

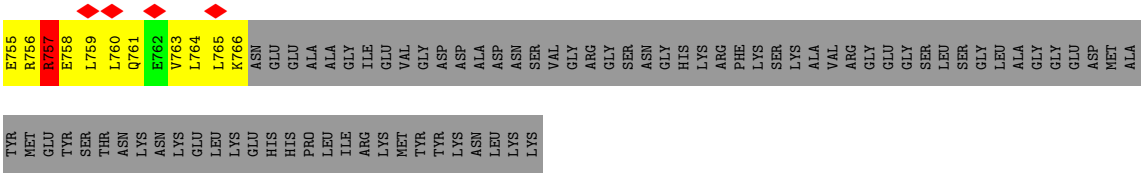




• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB

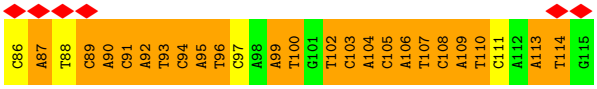
Chain 7:





• Molecule 9: non-template strand DNA

• Molecule 10: template strand DNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101497	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	273.47998, 273.47998, 272.41998	wwPDB
Map dimensions	258, 258, 257	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4

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	3	1.27	6/870 (0.7%)	0.84	7/1190 (0.6%)
2	2	1.03	19/3057 (0.6%)	1.20	16/4071 (0.4%)
3	0	0.81	27/6226 (0.4%)	0.79	23/8407 (0.3%)
4	1	0.62	7/1896 (0.4%)	0.60	2/2543 (0.1%)
5	4	0.84	8/2062 (0.4%)	0.77	8/2805 (0.3%)
6	6	1.04	14/2506 (0.6%)	0.84	6/3402 (0.2%)
7	5	0.73	3/502 (0.6%)	1.00	5/677 (0.7%)
8	7	1.06	29/4017 (0.7%)	1.13	32/5374 (0.6%)
9	N	2.51	44/700 (6.3%)	2.68	55/1081 (5.1%)
10	T	2.75	36/678 (5.3%)	2.77	48/1041 (4.6%)
All	All	1.12	193/22514 (0.9%)	1.15	202/30591 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	2
2	2	0	4
3	0	0	2
5	4	0	2
6	6	0	2
8	7	0	8
All	All	0	20

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	34	CYS	CB-SG	-30.99	1.29	1.82
6	6	366	CYS	CB-SG	-24.74	1.40	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	504	PHE	CE1-CZ	-22.91	0.93	1.37
6	6	426	ARG	CZ-NH2	21.06	1.60	1.33
8	7	572	GLU	CG-CD	19.68	1.81	1.51
10	T	104	DA	C2'-C1'	19.55	1.72	1.52
10	T	102	DT	C4-O4	-19.41	1.05	1.23
10	T	90	DA	C2'-C1'	18.96	1.71	1.52
2	2	468	TYR	CD2-CE2	18.86	1.67	1.39
6	6	426	ARG	NE-CZ	-18.74	1.08	1.33
3	0	156	CYS	CB-SG	-18.62	1.50	1.82
10	T	104	DA	O4'-C1'	-17.97	1.20	1.42
10	T	90	DA	O4'-C1'	-17.32	1.21	1.42
2	2	504	PHE	CG-CD2	-17.28	1.12	1.38
10	T	92	DA	O4'-C1'	-16.66	1.22	1.42
10	T	106	DA	O4'-C1'	-16.55	1.22	1.42
5	4	136	GLU	CG-CD	-15.95	1.28	1.51
3	0	742	GLU	CD-OE1	-15.30	1.08	1.25
8	7	757	ARG	NE-CZ	15.27	1.52	1.33
5	4	136	GLU	CD-OE2	14.68	1.41	1.25
8	7	757	ARG	CZ-NH1	14.31	1.51	1.33
8	7	568	GLU	CG-CD	-14.01	1.30	1.51
2	2	56	GLU	CG-CD	13.09	1.71	1.51
9	N	80	DG	O4'-C1'	12.74	1.57	1.42
8	7	757	ARG	CD-NE	12.71	1.68	1.46
8	7	757	ARG	CG-CD	-12.51	1.20	1.51
2	2	286	ARG	CZ-NH2	12.27	1.49	1.33
8	7	490	VAL	CB-CG2	-12.20	1.27	1.52
10	T	92	DA	C2'-C1'	12.10	1.64	1.52
10	T	106	DA	C2'-C1'	12.08	1.64	1.52
3	0	340	GLU	CD-OE1	-11.80	1.12	1.25
2	2	468	TYR	CD1-CE1	11.62	1.56	1.39
2	2	486	ASP	CB-CG	-11.61	1.27	1.51
9	N	64	DA	C2-N3	-11.51	1.23	1.33
10	T	87	DA	O4'-C1'	-11.06	1.28	1.42
2	2	286	ARG	CZ-NH1	11.00	1.47	1.33
10	T	102	DT	N1-C2	-10.99	1.29	1.38
8	7	464	ARG	CG-CD	-10.86	1.24	1.51
8	7	689	ARG	CB-CG	-10.51	1.24	1.52
6	6	426	ARG	CZ-NH1	10.40	1.46	1.33
8	7	566	TYR	CD2-CE2	-10.29	1.24	1.39
8	7	722	ARG	CZ-NH2	-10.19	1.19	1.33
4	1	210	TRP	CE3-CZ3	-10.14	1.21	1.38
5	4	136	GLU	CD-OE1	9.98	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	447	GLN	CD-NE2	-9.92	1.08	1.32
3	0	680	VAL	CB-CG2	-9.85	1.32	1.52
5	4	43	GLU	CD-OE1	-9.83	1.14	1.25
8	7	754	ARG	N-CA	-9.80	1.26	1.46
6	6	406	CYS	CB-SG	-9.66	1.65	1.82
10	T	87	DA	C2'-C1'	9.56	1.61	1.52
2	2	56	GLU	CB-CG	-9.36	1.34	1.52
8	7	572	GLU	CD-OE1	9.28	1.35	1.25
8	7	572	GLU	CB-CG	9.16	1.69	1.52
10	T	102	DT	O4'-C1'	-9.12	1.31	1.42
9	N	52	DA	N7-C5	-8.99	1.33	1.39
9	N	66	DA	N7-C5	-8.92	1.33	1.39
8	7	566	TYR	CE2-CZ	8.88	1.50	1.38
9	N	67	DT	O4'-C1'	8.76	1.52	1.42
2	2	56	GLU	CD-OE2	8.73	1.35	1.25
9	N	53	DT	O4'-C1'	8.73	1.52	1.42
8	7	754	ARG	CB-CG	-8.64	1.29	1.52
1	3	54	CYS	CB-SG	-8.62	1.67	1.82
10	T	99	DA	O4'-C1'	-8.45	1.32	1.42
10	T	113	DA	O4'-C1'	-8.45	1.32	1.42
4	1	378	MET	CG-SD	-8.38	1.59	1.81
1	3	61	LYS	CD-CE	-8.35	1.30	1.51
10	T	109	DA	O4'-C1'	-8.34	1.32	1.42
10	T	95	DA	O4'-C1'	-8.29	1.32	1.42
3	0	343	LYS	CE-NZ	-8.27	1.28	1.49
10	T	113	DA	C2'-C1'	8.26	1.60	1.52
2	2	286	ARG	CD-NE	-8.23	1.32	1.46
10	T	99	DA	C2'-C1'	8.16	1.60	1.52
3	0	285	GLU	CD-OE1	-8.08	1.16	1.25
7	5	51	LYS	CE-NZ	-8.05	1.28	1.49
9	N	65	DC	C2'-C1'	7.97	1.60	1.52
2	2	431	GLN	CD-OE1	-7.96	1.06	1.24
5	4	128	GLU	CG-CD	-7.91	1.40	1.51
9	N	64	DA	C6-N1	-7.78	1.30	1.35
3	0	600	SER	CB-OG	-7.72	1.32	1.42
6	6	336	CYS	CB-SG	-7.71	1.69	1.82
9	N	52	DA	C6-N1	-7.69	1.30	1.35
9	N	53	DT	N3-C4	7.61	1.44	1.38
10	T	91	DC	N3-C4	7.61	1.39	1.33
9	N	65	DC	O4'-C1'	-7.58	1.33	1.42
2	2	286	ARG	NE-CZ	-7.54	1.23	1.33
10	T	105	DC	N3-C4	7.54	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	67	DT	C4'-O4'	7.52	1.52	1.45
10	T	114	DT	N1-C2	-7.50	1.32	1.38
9	N	53	DT	C4'-O4'	7.46	1.52	1.45
9	N	65	DC	N1-C2	7.40	1.47	1.40
4	1	210	TRP	CD2-CE3	-7.30	1.29	1.40
10	T	95	DA	C2'-C1'	7.28	1.59	1.52
7	5	47	VAL	CB-CG2	-7.27	1.37	1.52
10	T	109	DA	C2'-C1'	7.22	1.59	1.52
3	0	480	GLN	CD-NE2	-7.22	1.14	1.32
8	7	571	ARG	NE-CZ	-7.18	1.23	1.33
3	0	80	GLU	CD-OE1	-7.16	1.17	1.25
3	0	113	ASN	CB-CG	-7.12	1.34	1.51
10	T	103	DC	O4'-C1'	-7.08	1.33	1.42
10	T	102	DT	C4'-O4'	7.08	1.52	1.45
3	0	359	PHE	CG-CD2	-7.00	1.28	1.38
9	N	75	DG	C2'-C1'	-6.93	1.45	1.52
9	N	63	DG	C2'-C1'	-6.92	1.45	1.52
9	N	61	DG	C2'-C1'	-6.86	1.45	1.52
6	6	200	ARG	CZ-NH2	-6.85	1.24	1.33
3	0	359	PHE	CE1-CZ	-6.76	1.24	1.37
8	7	447	GLN	CD-OE1	-6.69	1.09	1.24
9	N	64	DA	N7-C5	-6.54	1.35	1.39
10	T	113	DA	C6-N1	-6.52	1.30	1.35
3	0	696	TRP	CE3-CZ3	-6.45	1.27	1.38
3	0	155	LEU	CG-CD1	-6.43	1.28	1.51
10	T	103	DC	C2'-C1'	6.42	1.58	1.52
3	0	160	GLU	CB-CG	-6.41	1.40	1.52
8	7	466	ARG	NE-CZ	6.38	1.41	1.33
8	7	566	TYR	CZ-OH	6.38	1.48	1.37
8	7	566	TYR	CD1-CE1	-6.37	1.29	1.39
3	0	190	LEU	CG-CD2	-6.34	1.28	1.51
10	T	96	DT	O4'-C1'	-6.33	1.34	1.42
10	T	110	DT	O4'-C1'	-6.31	1.34	1.42
3	0	642	MET	SD-CE	-6.30	1.42	1.77
9	N	65	DC	N3-C4	6.24	1.38	1.33
8	7	568	GLU	CB-CG	-6.24	1.40	1.52
10	T	114	DT	N3-C4	6.23	1.43	1.38
5	4	273	ARG	CZ-NH2	-6.22	1.25	1.33
1	3	69	LYS	CE-NZ	-6.21	1.33	1.49
2	2	136	ASP	CA-C	6.19	1.69	1.52
9	N	54	DT	O4'-C1'	6.15	1.49	1.42
8	7	464	ARG	NE-CZ	6.14	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	21	VAL	CB-CG2	-6.14	1.40	1.52
1	3	59	CYS	CB-SG	6.12	1.92	1.82
9	N	68	DT	O4'-C1'	6.12	1.49	1.42
8	7	447	GLN	CB-CG	-6.10	1.36	1.52
3	0	275	ARG	CZ-NH1	-6.04	1.25	1.33
6	6	168	GLN	CD-OE1	-6.03	1.10	1.24
4	1	210	TRP	CZ3-CH2	-6.03	1.30	1.40
10	T	89	DC	O4'-C1'	-6.03	1.35	1.42
10	T	100	DT	N1-C2	-6.00	1.33	1.38
10	T	102	DT	C4-C5	-5.96	1.39	1.45
7	5	42	VAL	CB-CG1	-5.94	1.40	1.52
4	1	201	ASN	CG-OD1	-5.94	1.10	1.24
9	N	64	DA	N3-C4	-5.93	1.31	1.34
2	2	504	PHE	CE2-CZ	-5.87	1.26	1.37
3	0	359	PHE	CD2-CE2	-5.82	1.27	1.39
5	4	299	ILE	N-CA	5.75	1.57	1.46
6	6	200	ARG	CB-CG	-5.73	1.37	1.52
3	0	343	LYS	CG-CD	-5.70	1.33	1.52
8	7	491	HIS	CB-CG	-5.70	1.39	1.50
6	6	349	CYS	CB-SG	5.69	1.92	1.82
2	2	22	GLN	CG-CD	-5.67	1.38	1.51
8	7	571	ARG	CZ-NH2	5.66	1.40	1.33
4	1	197	GLU	CG-CD	-5.65	1.43	1.51
2	2	100	LEU	CG-CD1	-5.63	1.31	1.51
3	0	636	LYS	CE-NZ	-5.62	1.35	1.49
9	N	54	DT	C5-C7	5.60	1.53	1.50
9	N	66	DA	N9-C4	-5.59	1.34	1.37
1	3	74	ASP	CB-CG	-5.55	1.40	1.51
9	N	66	DA	N3-C4	-5.54	1.31	1.34
9	N	63	DG	O4'-C1'	5.54	1.48	1.42
9	N	52	DA	N1-C2	5.53	1.39	1.34
6	6	185	VAL	CB-CG2	-5.52	1.41	1.52
3	0	104	ARG	CZ-NH2	-5.50	1.25	1.33
3	0	416	PHE	CE1-CZ	-5.47	1.26	1.37
9	N	52	DA	N9-C4	-5.44	1.34	1.37
9	N	68	DT	C5-C7	5.43	1.53	1.50
8	7	754	ARG	CA-C	5.42	1.67	1.52
9	N	52	DA	N3-C4	-5.42	1.31	1.34
8	7	476	PHE	CA-CB	-5.39	1.42	1.53
9	N	75	DG	O4'-C1'	5.38	1.48	1.42
9	N	51	DC	N3-C4	5.34	1.37	1.33
6	6	287	PHE	CE2-CZ	-5.30	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	61	DG	O4'-C1'	5.29	1.48	1.42
10	T	102	DT	C2-N3	-5.28	1.33	1.37
9	N	67	DT	C4'-C3'	-5.28	1.47	1.52
3	0	290	VAL	CB-CG1	-5.27	1.41	1.52
6	6	134	GLU	CG-CD	-5.24	1.44	1.51
3	0	572	GLU	CB-CG	-5.22	1.42	1.52
9	N	65	DC	C2-O2	5.22	1.29	1.24
9	N	53	DT	C4'-C3'	-5.21	1.47	1.52
4	1	206	PRO	CB-CG	-5.21	1.23	1.50
10	T	89	DC	C2'-C1'	5.21	1.57	1.52
5	4	133	PHE	C-O	-5.20	1.13	1.23
6	6	149	ILE	CG1-CD1	-5.16	1.14	1.50
9	N	59	DA	C4'-C3'	-5.13	1.47	1.52
9	N	66	DA	C6-N1	-5.12	1.31	1.35
9	N	73	DA	C4'-C3'	-5.12	1.47	1.52
9	N	77	DG	C2'-C1'	-5.11	1.47	1.52
9	N	72	DG	N7-C5	-5.09	1.36	1.39
3	0	147	GLU	CG-CD	-5.07	1.44	1.51
2	2	408	MET	SD-CE	-5.05	1.49	1.77
3	0	50	VAL	CB-CG2	-5.03	1.42	1.52
9	N	64	DA	C5-C4	5.02	1.42	1.38
9	N	72	DG	N3-C4	-5.01	1.31	1.35
9	N	68	DT	C5'-C4'	5.00	1.56	1.51

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	286	ARG	NE-CZ-NH2	-49.68	95.46	120.30
8	7	757	ARG	NE-CZ-NH1	27.93	134.26	120.30
10	T	102	DT	O4'-C1'-N1	26.90	126.83	108.00
10	T	92	DA	O4'-C1'-N9	26.29	126.41	108.00
10	T	106	DA	O4'-C1'-N9	26.22	126.35	108.00
8	7	466	ARG	NE-CZ-NH1	25.86	133.23	120.30
8	7	571	ARG	NE-CZ-NH1	-23.63	108.49	120.30
6	6	426	ARG	NE-CZ-NH2	-21.18	109.71	120.30
10	T	104	DA	O4'-C1'-N9	20.86	122.60	108.00
10	T	90	DA	O4'-C1'-N9	20.39	122.27	108.00
9	N	53	DT	O4'-C1'-N1	-19.13	94.61	108.00
9	N	67	DT	O4'-C1'-N1	-19.08	94.64	108.00
2	2	486	ASP	CB-CG-OD1	-17.11	102.90	118.30
10	T	102	DT	C5-C4-O4	-16.91	113.06	124.90
6	6	435	GLU	CB-CA-C	-16.54	77.33	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	286	ARG	NH1-CZ-NH2	16.39	137.43	119.40
10	T	102	DT	O4'-C4'-C3'	16.34	115.81	106.00
2	2	97	MET	CG-SD-CE	16.07	125.91	100.20
3	0	642	MET	CG-SD-CE	-15.95	74.69	100.20
9	N	73	DA	O4'-C1'-N9	-15.81	96.93	108.00
9	N	59	DA	O4'-C1'-N9	-15.68	97.03	108.00
9	N	66	DA	O4'-C1'-N9	-15.11	97.42	108.00
9	N	52	DA	O4'-C1'-N9	-15.00	97.50	108.00
8	7	757	ARG	NH1-CZ-NH2	-14.50	103.45	119.40
10	T	102	DT	O4'-C1'-C2'	14.17	117.23	105.90
7	5	19	LEU	CB-CG-CD1	-14.08	87.06	111.00
8	7	757	ARG	CD-NE-CZ	13.99	143.18	123.60
10	T	102	DT	N3-C4-O4	13.97	128.28	119.90
2	2	504	PHE	CG-CD2-CE2	-13.86	105.56	120.80
5	4	273	ARG	NE-CZ-NH2	-13.42	113.59	120.30
9	N	69	DG	O4'-C1'-N9	13.33	117.33	108.00
9	N	55	DG	O4'-C1'-N9	13.29	117.31	108.00
9	N	72	DG	O4'-C1'-N9	-13.12	98.82	108.00
9	N	58	DG	O4'-C1'-N9	-13.10	98.83	108.00
2	2	504	PHE	CZ-CE2-CD2	13.03	135.74	120.10
9	N	54	DT	O4'-C1'-N1	-12.69	99.12	108.00
9	N	80	DG	O4'-C1'-N9	-12.69	99.12	108.00
9	N	68	DT	O4'-C1'-N1	-12.66	99.14	108.00
9	N	70	DA	O4'-C1'-N9	-12.49	99.25	108.00
9	N	56	DA	O4'-C1'-N9	-12.41	99.31	108.00
9	N	67	DT	O4'-C1'-C2'	-12.40	95.98	105.90
8	7	722	ARG	NE-CZ-NH2	-12.39	114.10	120.30
9	N	53	DT	O4'-C1'-C2'	-12.39	95.99	105.90
3	0	275	ARG	NE-CZ-NH1	12.23	126.42	120.30
10	T	102	DT	C1'-O4'-C4'	-11.91	98.19	110.10
9	N	64	DA	C6-N1-C2	11.79	125.67	118.60
9	N	64	DA	C5-C6-N1	-11.48	111.96	117.70
10	T	104	DA	O4'-C4'-C3'	11.33	112.80	106.00
8	7	466	ARG	NH1-CZ-NH2	-11.25	107.03	119.40
10	T	90	DA	O4'-C4'-C3'	11.24	112.74	106.00
9	N	67	DT	O4'-C4'-C3'	-11.22	99.27	106.00
9	N	53	DT	O4'-C4'-C3'	-11.17	99.30	106.00
10	T	103	DC	O4'-C1'-N1	10.85	115.59	108.00
8	7	722	ARG	NE-CZ-NH1	10.78	125.69	120.30
3	0	155	LEU	CB-CG-CD1	-10.73	92.76	111.00
8	7	466	ARG	CD-NE-CZ	10.69	138.57	123.60
8	7	572	GLU	OE1-CD-OE2	-10.68	110.49	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	7	519	ARG	NE-CZ-NH2	-10.58	115.01	120.30
8	7	754	ARG	O-C-N	-10.55	105.82	122.70
10	T	92	DA	O4'-C1'-C2'	10.41	114.23	105.90
10	T	106	DA	O4'-C1'-C2'	10.36	114.19	105.90
3	0	275	ARG	NH1-CZ-NH2	-10.35	108.02	119.40
8	7	519	ARG	NE-CZ-NH1	10.34	125.47	120.30
3	0	109	THR	CA-CB-CG2	-10.24	98.07	112.40
3	0	275	ARG	NE-CZ-NH2	10.23	125.42	120.30
3	0	136	MET	CG-SD-CE	-10.15	83.96	100.20
8	7	754	ARG	CA-CB-CG	9.98	135.35	113.40
10	T	106	DA	O4'-C4'-C3'	9.85	111.91	106.00
10	T	89	DC	O4'-C1'-N1	9.81	114.87	108.00
8	7	568	GLU	CG-CD-OE2	-9.69	98.93	118.30
8	7	757	ARG	CG-CD-NE	9.55	131.85	111.80
10	T	92	DA	O4'-C4'-C3'	9.46	111.68	106.00
2	2	408	MET	CG-SD-CE	-9.45	85.07	100.20
10	T	102	DT	C2-N3-C4	-9.23	121.66	127.20
1	3	34	CYS	CA-CB-SG	9.14	130.45	114.00
9	N	78	DA	O4'-C1'-N9	-8.76	101.87	108.00
10	T	87	DA	O4'-C1'-N9	8.65	114.06	108.00
10	T	96	DT	O4'-C1'-N1	8.60	114.02	108.00
10	T	110	DT	O4'-C1'-N1	8.54	113.98	108.00
8	7	689	ARG	NE-CZ-NH1	8.50	124.55	120.30
9	N	64	DA	N1-C6-N6	8.38	123.63	118.60
10	T	91	DC	N1-C2-O2	-8.37	113.88	118.90
5	4	133	PHE	O-C-N	-8.36	109.33	122.70
8	7	464	ARG	NE-CZ-NH1	-8.28	116.16	120.30
8	7	459	MET	CG-SD-CE	-8.26	86.98	100.20
10	T	105	DC	N1-C2-O2	-8.24	113.95	118.90
2	2	56	GLU	CG-CD-OE2	8.22	134.74	118.30
8	7	497	MET	CG-SD-CE	-8.14	87.18	100.20
2	2	411	LEU	CB-CG-CD1	8.12	124.81	111.00
8	7	568	GLU	CG-CD-OE1	8.11	134.53	118.30
7	5	19	LEU	CA-CB-CG	-8.07	96.75	115.30
2	2	504	PHE	CB-CG-CD1	7.89	126.32	120.80
5	4	136	GLU	OE1-CD-OE2	7.87	132.74	123.30
8	7	664	LEU	CB-CG-CD1	7.83	124.32	111.00
2	2	486	ASP	OD1-CG-OD2	7.66	137.85	123.30
5	4	128	GLU	CG-CD-OE1	-7.65	102.99	118.30
8	7	754	ARG	CB-CA-C	7.64	125.68	110.40
3	0	636	LYS	CD-CE-NZ	7.57	129.10	111.70
1	3	69	LYS	CD-CE-NZ	-7.54	94.36	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	6	426	ARG	NH1-CZ-NH2	7.52	127.67	119.40
9	N	64	DA	O4'-C4'-C3'	-7.51	101.49	106.00
4	1	210	TRP	CE3-CZ3-CH2	7.39	129.32	121.20
9	N	80	DG	O4'-C1'-C2'	-7.38	99.99	105.90
8	7	689	ARG	NE-CZ-NH2	-7.27	116.67	120.30
6	6	230	ARG	NE-CZ-NH2	7.25	123.93	120.30
3	0	198	ARG	NE-CZ-NH2	7.24	123.92	120.30
3	0	600	SER	N-CA-CB	-7.22	99.67	110.50
1	3	61	LYS	CD-CE-NZ	-7.10	95.37	111.70
10	T	94	DC	N1-C2-O2	-7.00	114.70	118.90
10	T	108	DC	N1-C2-O2	-6.99	114.70	118.90
3	0	41	GLU	OE1-CD-OE2	-6.98	114.92	123.30
3	0	675	ASP	CB-CG-OD1	6.94	124.55	118.30
1	3	74	ASP	CB-CG-OD1	-6.91	112.08	118.30
9	N	66	DA	O4'-C4'-C3'	-6.90	101.74	104.50
8	7	571	ARG	NH1-CZ-NH2	6.88	126.96	119.40
9	N	63	DG	O4'-C1'-N9	-6.83	103.22	108.00
10	T	102	DT	N3-C2-O2	-6.81	118.22	122.30
10	T	91	DC	C2-N3-C4	-6.76	116.52	119.90
9	N	52	DA	O4'-C4'-C3'	-6.75	101.80	104.50
10	T	105	DC	C2-N3-C4	-6.71	116.55	119.90
1	3	59	CYS	CA-CB-SG	6.71	126.07	114.00
10	T	99	DA	O4'-C4'-C3'	6.67	110.00	106.00
10	T	113	DA	O4'-C4'-C3'	6.61	109.97	106.00
2	2	504	PHE	CB-CG-CD2	-6.56	116.21	120.80
6	6	150	ILE	CA-CB-CG2	-6.53	97.84	110.90
9	N	64	DA	O4'-C1'-N9	-6.51	103.44	108.00
9	N	66	DA	N9-C1'-C2'	6.50	124.94	112.60
10	T	102	DT	P-O3'-C3'	6.49	127.48	119.70
7	5	19	LEU	CD1-CG-CD2	6.40	129.71	110.50
9	N	75	DG	O4'-C1'-N9	-6.39	103.53	108.00
9	N	52	DA	N9-C1'-C2'	6.39	124.73	112.60
9	N	61	DG	O4'-C1'-N9	-6.38	103.53	108.00
10	T	114	DT	C2-N3-C4	-6.29	123.43	127.20
9	N	52	DA	C6-N1-C2	6.26	122.36	118.60
10	T	114	DT	N1-C2-N3	6.25	118.35	114.60
8	7	562	THR	CA-CB-CG2	-6.25	103.65	112.40
3	0	525	MET	CG-SD-CE	-6.24	90.22	100.20
5	4	128	GLU	OE1-CD-OE2	6.17	130.70	123.30
9	N	57	DT	O4'-C1'-N1	-6.17	103.68	108.00
9	N	71	DT	O4'-C1'-N1	-6.15	103.69	108.00
3	0	633	ARG	N-CA-CB	-6.08	99.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	4	273	ARG	NH1-CZ-NH2	6.05	126.05	119.40
3	0	572	GLU	OE1-CD-OE2	-6.03	116.06	123.30
3	0	262	ARG	NE-CZ-NH2	-6.03	117.29	120.30
5	4	179	LEU	CA-CB-CG	6.00	129.10	115.30
9	N	54	DT	C5-C4-O4	-5.99	120.71	124.90
9	N	54	DT	O4'-C4'-C3'	-5.95	102.12	104.50
3	0	156	CYS	CA-CB-SG	5.94	124.70	114.00
8	7	754	ARG	CA-C-O	5.94	132.57	120.10
3	0	600	SER	CA-CB-OG	5.90	127.13	111.20
9	N	68	DT	O4'-C4'-C3'	-5.89	102.14	104.50
10	T	109	DA	O4'-C1'-N9	5.89	112.12	108.00
9	N	68	DT	C5-C4-O4	-5.88	120.78	124.90
2	2	56	GLU	OE1-CD-OE2	-5.86	116.27	123.30
10	T	95	DA	O4'-C1'-N9	5.83	112.08	108.00
10	T	87	DA	O4'-C4'-C3'	5.82	109.49	106.00
2	2	135	LEU	C-N-CA	-5.81	107.17	121.70
9	N	59	DA	O4'-C1'-C2'	-5.77	101.28	105.90
9	N	73	DA	O4'-C1'-C2'	-5.76	101.29	105.90
9	N	77	DG	O4'-C1'-N9	-5.76	103.97	108.00
10	T	102	DT	N3-C4-C5	5.76	118.66	115.20
9	N	52	DA	C5-C6-N1	-5.68	114.86	117.70
10	T	102	DT	N1-C2-N3	5.68	118.01	114.60
9	N	64	DA	O4'-C1'-C2'	-5.65	101.38	105.90
10	T	104	DA	C4'-C3'-C2'	-5.63	98.03	103.10
9	N	79	DT	O4'-C1'-N1	-5.61	104.07	108.00
10	T	90	DA	C4'-C3'-C2'	-5.58	98.08	103.10
7	5	29	ASP	CB-CG-OD2	5.58	123.32	118.30
8	7	447	GLN	CG-CD-OE1	5.56	132.73	121.60
10	T	114	DT	N3-C2-O2	-5.49	119.01	122.30
10	T	102	DT	C4'-C3'-C2'	-5.47	98.17	103.10
3	0	104	ARG	NE-CZ-NH1	5.47	123.03	120.30
3	0	109	THR	OG1-CB-CG2	5.45	122.54	110.00
10	T	107	DT	O4'-C1'-N1	5.44	111.81	108.00
10	T	93	DT	O4'-C1'-N1	5.44	111.81	108.00
9	N	51	DC	O4'-C4'-C3'	5.42	109.25	106.00
8	7	572	GLU	CB-CA-C	-5.41	99.59	110.40
10	T	113	DA	C6-N1-C2	5.38	121.83	118.60
8	7	351	ASP	CB-CG-OD2	5.35	123.12	118.30
9	N	54	DT	N3-C4-O4	5.33	123.10	119.90
9	N	68	DT	N3-C4-O4	5.33	123.10	119.90
8	7	566	TYR	CB-CG-CD2	-5.31	117.81	121.00
4	1	206	PRO	N-CA-CB	-5.30	96.77	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	66	DA	O4'-C1'-C2'	-5.29	101.67	105.90
1	3	29	LEU	CB-CG-CD2	5.27	119.97	111.00
10	T	113	DA	N1-C2-N3	-5.27	126.67	129.30
3	0	83	LEU	CB-CG-CD2	-5.26	102.05	111.00
9	N	80	DG	O4'-C4'-C3'	-5.25	102.40	104.50
6	6	242	THR	C-N-CA	-5.21	108.66	121.70
2	2	56	GLU	CG-CD-OE1	-5.18	107.94	118.30
8	7	351	ASP	CB-CG-OD1	-5.17	113.65	118.30
3	0	360	LEU	CA-CB-CG	5.17	127.19	115.30
2	2	95	THR	CA-CB-CG2	-5.14	105.20	112.40
9	N	54	DT	O4'-C1'-C2'	-5.13	101.80	105.90
5	4	259	ARG	NE-CZ-NH1	5.12	122.86	120.30
9	N	52	DA	O4'-C1'-C2'	-5.11	101.82	105.90
3	0	135	ARG	NE-CZ-NH2	-5.09	117.75	120.30
9	N	68	DT	O4'-C1'-C2'	-5.04	101.87	105.90
1	3	29	LEU	CD1-CG-CD2	-5.02	95.43	110.50
7	5	57	LEU	CB-CG-CD2	-5.02	102.46	111.00
9	N	66	DA	C5-C6-N1	-5.01	115.19	117.70
10	T	105	DC	C6-N1-C2	5.01	122.30	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	0	629	TYR	Peptide
3	0	631	GLU	Peptide
2	2	286	ARG	Sidechain
2	2	468	TYR	Sidechain
2	2	504	PHE	Sidechain
2	2	68	SER	Peptide
1	3	71	GLN	Peptide
1	3	75	ASP	Peptide
5	4	255	ASP	Peptide
5	4	299	ILE	Peptide
6	6	435	GLU	Mainchain
6	6	449	HIS	Peptide
8	7	442	ASN	Peptide
8	7	460	VAL	Peptide
8	7	461	ALA	Peptide
8	7	468	HIS	Peptide
8	7	572	GLU	Sidechain
8	7	631	THR	Peptide

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Mol	Chain	Res	Type	Group
8	7	632	PRO	Peptide
8	7	757	ARG	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	3	860	0	621	127	0
2	2	3011	0	2600	427	0
3	0	6108	0	6165	1150	0
4	1	2411	0	1882	220	0
5	4	2041	0	1954	302	0
6	6	2527	0	2321	404	0
7	5	498	0	506	129	0
8	7	3947	0	3575	814	0
9	N	624	0	342	87	0
10	T	606	0	339	44	0
11	3	2	0	0	0	0
11	4	1	0	0	0	0
11	6	4	0	0	0	0
12	0	8	0	0	4	0
All	All	22648	0	20305	3535	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 82.

All (3535) 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)
2:2:501:VAL:HA	2:2:504:PHE:CE2	1.33	1.63
3:0:614:HIS:CE1	3:0:675:ASP:HA	1.28	1.61
2:2:380:ARG:HH11	2:2:444:TRP:CB	1.16	1.57
8:7:757:ARG:CD	8:7:757:ARG:NE	1.68	1.51
8:7:572:GLU:CD	8:7:572:GLU:CG	1.81	1.47
2:2:501:VAL:HA	2:2:504:PHE:CD2	1.55	1.39
2:2:501:VAL:HG13	2:2:504:PHE:CZ	1.60	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:239:ASN:OD1	3:0:664:GLN:NE2	1.60	1.33
8:7:489:GLU:HG3	8:7:491:HIS:CE1	1.65	1.30
2:2:19:GLN:NE2	2:2:85:HIS:HB3	1.46	1.29
2:2:136:ASP:O	2:2:286:ARG:NH2	1.60	1.29
3:0:356:PRO:HA	3:0:359:PHE:CE2	1.67	1.29
8:7:401:CYS:O	8:7:404:LYS:NZ	1.62	1.29
2:2:136:ASP:CA	2:2:286:ARG:NH2	1.96	1.29
2:2:501:VAL:CA	2:2:504:PHE:CE2	2.15	1.29
8:7:754:ARG:O	8:7:757:ARG:HD3	1.32	1.27
2:2:504:PHE:CZ	2:2:504:PHE:CD1	1.97	1.27
3:0:135:ARG:HA	3:0:138:ASN:ND2	1.45	1.27
1:3:36:HIS:HE1	1:3:59:CYS:SG	1.58	1.26
2:2:17:ILE:O	2:2:22:GLN:NE2	1.66	1.26
3:0:167:VAL:HA	3:0:198:ARG:NH2	1.50	1.26
8:7:446:PHE:HD2	8:7:447:GLN:NE2	1.30	1.25
8:7:465:ASN:HB3	8:7:471:GLN:NE2	1.47	1.25
2:2:136:ASP:CA	2:2:286:ARG:HH22	1.48	1.25
8:7:568:GLU:CD	8:7:571:ARG:HE	1.37	1.25
2:2:136:ASP:C	2:2:286:ARG:NH2	1.90	1.25
8:7:447:GLN:HG3	8:7:476:PHE:CD1	1.72	1.25
8:7:458:SER:HA	8:7:462:ASN:OD1	1.28	1.25
2:2:504:PHE:CE2	2:2:504:PHE:CE1	1.85	1.25
6:6:197:LYS:HD3	6:6:200:ARG:NH2	1.52	1.25
2:2:136:ASP:C	2:2:286:ARG:CZ	2.05	1.25
8:7:571:ARG:NH2	8:7:572:GLU:OE2	1.69	1.24
2:2:431:GLN:OE1	2:2:434:PRO:HA	1.34	1.24
2:2:136:ASP:CA	2:2:286:ARG:CZ	2.15	1.24
3:0:614:HIS:CE1	3:0:675:ASP:CA	2.21	1.24
3:0:111:ARG:NH1	3:0:130:ASP:OD1	1.70	1.23
8:7:571:ARG:NH1	8:7:572:GLU:OE1	1.69	1.23
2:2:380:ARG:NH1	2:2:444:TRP:CB	2.01	1.21
3:0:356:PRO:HA	3:0:359:PHE:CZ	1.74	1.21
6:6:224:VAL:O	6:6:230:ARG:NH2	1.74	1.21
3:0:572:GLU:OE2	3:0:600:SER:HB2	1.38	1.20
1:3:44:ASP:HA	1:3:47:PHE:CE2	1.78	1.19
3:0:312:LEU:HD11	3:0:448:PRO:HG3	1.25	1.18
3:0:577:GLN:NE2	3:0:578:GLU:HG2	1.54	1.18
3:0:104:ARG:NH2	3:0:172:PRO:O	1.74	1.18
3:0:639:LEU:HA	3:0:642:MET:CE	1.70	1.18
8:7:568:GLU:OE2	8:7:571:ARG:NH2	1.77	1.18
8:7:754:ARG:HB2	8:7:757:ARG:NH1	1.57	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:381:HIS:CE1	6:6:449:HIS:CD2	2.32	1.17
3:0:251:ASP:HB2	3:0:436:ARG:HD3	1.24	1.16
3:0:327:ARG:HB3	3:0:330:HIS:HD2	1.05	1.16
2:2:497:GLY:HA2	2:2:500:GLN:NE2	1.59	1.16
3:0:374:LEU:HD22	3:0:410:SER:HB2	1.19	1.16
2:2:136:ASP:O	2:2:286:ARG:CZ	1.94	1.15
3:0:250:LEU:HA	4:1:350:ARG:HG2	1.29	1.15
5:4:255:ASP:O	5:4:259:ARG:NH1	1.77	1.15
8:7:494:PRO:HG2	8:7:497:MET:CE	1.76	1.15
2:2:354:PRO:HA	2:2:357:ILE:HG12	1.23	1.14
3:0:79:ILE:HG23	3:0:207:ILE:HD12	1.24	1.14
8:7:491:HIS:HA	8:7:519:ARG:NH2	1.60	1.14
3:0:220:GLU:OE2	3:0:221:ARG:HG3	1.46	1.14
6:6:116:THR:H	6:6:117:PRO:CD	1.61	1.14
3:0:493:LEU:HD22	3:0:495:MET:HE1	1.17	1.14
8:7:469:ASP:HA	8:7:472:LYS:HE2	1.17	1.13
8:7:552:VAL:HG11	8:7:731:TYR:CD1	1.83	1.12
3:0:69:ILE:HG23	3:0:231:ILE:HG13	1.31	1.12
8:7:401:CYS:C	8:7:404:LYS:HZ2	1.53	1.12
8:7:457:TYR:OH	8:7:487:LEU:HD22	1.47	1.12
8:7:580:LEU:HA	8:7:583:MET:HE3	1.16	1.12
8:7:356:LEU:HD12	8:7:404:LYS:HZ3	1.13	1.11
2:2:19:GLN:HE22	2:2:85:HIS:CB	1.61	1.11
1:3:34:CYS:HB3	1:3:61:LYS:NZ	1.64	1.11
2:2:17:ILE:HG12	2:2:21:VAL:HG21	1.24	1.10
2:2:367:LYS:HB2	2:2:375:LEU:HD23	1.16	1.10
8:7:568:GLU:OE2	8:7:571:ARG:NE	1.83	1.10
3:0:166:GLU:HG3	3:0:198:ARG:HH11	1.06	1.10
4:1:206:PRO:CB	4:1:210:TRP:HZ3	1.63	1.10
8:7:494:PRO:HG2	8:7:497:MET:HE1	1.22	1.10
8:7:604:LYS:HZ1	8:7:694:LYS:HE3	1.12	1.10
8:7:754:ARG:HA	8:7:757:ARG:HD2	1.31	1.10
2:2:56:GLU:HG2	2:2:97:MET:HG3	1.27	1.09
3:0:39:ILE:HG23	3:0:480:GLN:HG3	1.34	1.09
8:7:446:PHE:CE2	8:7:472:LYS:HD2	1.85	1.09
8:7:664:LEU:HG	8:7:689:ARG:CG	1.80	1.09
3:0:144:LYS:HA	3:0:147:GLU:OE2	1.52	1.09
8:7:655:SER:HB2	8:7:657:VAL:HG12	1.35	1.09
7:5:51:LYS:HZ2	7:5:54:LEU:HD22	1.06	1.09
8:7:446:PHE:CD2	8:7:447:GLN:NE2	2.21	1.09
1:3:34:CYS:HB3	1:3:61:LYS:HZ1	1.12	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:631:THR:O	8:7:633:GLN:NE2	1.86	1.08
6:6:278:LYS:HG3	6:6:283:GLY:O	1.54	1.08
1:3:31:ASN:OD1	1:3:32:PRO:HD2	1.53	1.08
8:7:613:TYR:CB	8:7:766:LYS:HG2	1.83	1.08
4:1:222:LEU:HD21	6:6:216:MET:HG2	1.30	1.08
3:0:259:ARG:HG2	3:0:262:ARG:HH22	1.18	1.08
1:3:32:PRO:HD3	1:3:69:LYS:HZ3	0.98	1.07
6:6:150:ILE:HG21	6:6:200:ARG:CG	1.84	1.07
3:0:259:ARG:HG2	3:0:262:ARG:NH2	1.67	1.07
3:0:339:ILE:O	3:0:343:LYS:NZ	1.88	1.07
3:0:708:LEU:HB3	3:0:712:MET:SD	1.92	1.07
4:1:593:LEU:HD21	4:1:620:LEU:HD21	1.35	1.07
5:4:176:LEU:HD11	5:4:210:ILE:HG23	1.35	1.07
6:6:116:THR:HG21	6:6:385:PRO:HG2	1.35	1.07
2:2:475:ALA:HB1	2:2:481:LEU:HG	1.31	1.07
8:7:754:ARG:CB	8:7:757:ARG:CZ	2.32	1.07
1:3:36:HIS:CE1	1:3:59:CYS:SG	2.47	1.07
2:2:468:TYR:OH	2:2:484:LYS:HD3	1.53	1.07
3:0:254:THR:HA	3:0:257:LEU:HD13	1.37	1.07
8:7:568:GLU:OE2	8:7:571:ARG:CZ	2.01	1.07
8:7:577:ARG:NH1	8:7:714:GLN:OE1	1.86	1.07
8:7:664:LEU:HG	8:7:689:ARG:HG3	1.09	1.06
6:6:150:ILE:HG21	6:6:200:ARG:HG2	1.34	1.06
7:5:49:PHE:HA	7:5:52:HIS:ND1	1.69	1.06
3:0:167:VAL:HA	3:0:198:ARG:CZ	1.85	1.05
8:7:447:GLN:HA	8:7:476:PHE:CZ	1.90	1.05
3:0:531:LYS:HG2	3:0:566:HIS:HE1	1.20	1.05
3:0:312:LEU:HG	3:0:313:PRO:HD2	1.36	1.05
3:0:493:LEU:HD22	3:0:495:MET:CE	1.88	1.04
3:0:621:LEU:HG	3:0:680:VAL:CG2	1.87	1.04
3:0:472:MET:HG3	3:0:473:LEU:HG	1.36	1.04
7:5:51:LYS:NZ	7:5:54:LEU:HD22	1.72	1.04
8:7:571:ARG:NH1	8:7:572:GLU:CD	2.08	1.04
8:7:580:LEU:HA	8:7:583:MET:CE	1.85	1.04
1:3:27:LYS:NZ	1:3:29:LEU:HA	1.70	1.04
2:2:15:GLU:HB3	2:2:84:LEU:HD12	1.37	1.04
2:2:56:GLU:CG	2:2:97:MET:HG3	1.87	1.04
8:7:563:ALA:O	8:7:567:GLN:NE2	1.90	1.04
5:4:273:ARG:HH22	6:6:372:LEU:C	1.61	1.04
3:0:327:ARG:HB3	3:0:330:HIS:CD2	1.92	1.03
4:1:325:UNK:O	4:1:329:LEU:HD23	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:408:MET:CE	2:2:411:LEU:HD13	1.89	1.03
4:1:375:LEU:HA	4:1:378:MET:SD	1.98	1.03
8:7:754:ARG:O	8:7:757:ARG:CD	2.05	1.03
3:0:570:LEU:HD22	3:0:586:TYR:HB2	1.41	1.03
6:6:116:THR:H	6:6:117:PRO:HD2	1.16	1.03
8:7:356:LEU:CD1	8:7:404:LYS:HZ3	1.71	1.03
1:3:114:GLU:C	3:0:330:HIS:HE1	1.60	1.03
3:0:77:SER:HA	3:0:80:GLU:OE1	1.57	1.03
1:3:32:PRO:HD3	1:3:69:LYS:NZ	1.73	1.02
8:7:489:GLU:CG	8:7:491:HIS:CE1	2.42	1.02
3:0:353:SER:HB3	3:0:419:ILE:HD13	1.42	1.02
8:7:489:GLU:CG	8:7:491:HIS:HE1	1.72	1.02
2:2:501:VAL:CG1	2:2:504:PHE:HZ	1.71	1.02
1:3:65:LYS:HG2	1:3:66:ASN:H	1.23	1.02
3:0:715:SER:HA	3:0:718:LYS:CE	1.89	1.02
6:6:322:MET:HA	6:6:368:LEU:HD21	1.42	1.02
6:6:224:VAL:CG1	6:6:230:ARG:HE	1.72	1.01
2:2:380:ARG:NH1	2:2:440:GLN:O	1.91	1.01
6:6:145:ARG:O	6:6:149:ILE:HD12	1.58	1.01
2:2:43:ALA:O	2:2:47:ILE:HD12	1.60	1.01
3:0:633:ARG:O	3:0:636:LYS:HG2	1.60	1.01
6:6:166:ILE:HD11	6:6:375:HIS:HB3	1.39	1.01
8:7:754:ARG:HB2	8:7:757:ARG:CZ	1.88	1.01
3:0:109:THR:CG2	3:0:113:ASN:HD21	1.74	1.01
3:0:339:ILE:HG12	3:0:343:LYS:NZ	1.75	1.00
8:7:346:ASP:HB3	8:7:405:LYS:HE2	1.38	1.00
8:7:446:PHE:HD2	8:7:447:GLN:HE21	1.04	1.00
3:0:334:PHE:HA	3:0:337:ARG:HD3	1.03	1.00
3:0:571:VAL:HG21	4:1:375:LEU:CD2	1.90	1.00
3:0:639:LEU:HD22	3:0:642:MET:HE1	1.41	1.00
6:6:197:LYS:HD3	6:6:200:ARG:HH21	1.06	1.00
8:7:755:GLU:N	8:7:757:ARG:HH11	1.58	1.00
3:0:571:VAL:HG21	4:1:375:LEU:HD22	1.04	1.00
3:0:670:LEU:HA	3:0:675:ASP:OD2	1.61	1.00
8:7:489:GLU:HG3	8:7:491:HIS:HE1	0.95	1.00
3:0:639:LEU:HD13	3:0:642:MET:HE3	1.39	1.00
5:4:133:PHE:O	5:4:136:GLU:CD	1.99	1.00
5:4:133:PHE:O	5:4:136:GLU:OE2	1.79	1.00
3:0:639:LEU:HA	3:0:642:MET:HE3	1.43	1.00
6:6:381:HIS:HE1	6:6:449:HIS:CD2	1.73	1.00
8:7:631:THR:HG22	8:7:632:PRO:O	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:471:GLN:HA	8:7:474:MET:HE2	1.44	0.99
2:2:56:GLU:HG2	2:2:97:MET:CG	1.91	0.99
6:6:130:LEU:HB2	6:6:173:ILE:HG22	1.44	0.99
3:0:155:LEU:HD11	3:0:160:GLU:CG	1.93	0.99
6:6:159:GLU:O	6:6:163:GLN:NE2	1.96	0.99
1:3:114:GLU:O	3:0:330:HIS:HE1	1.43	0.99
3:0:83:LEU:HD21	3:0:207:ILE:HD11	1.44	0.99
3:0:571:VAL:CG2	4:1:375:LEU:HD22	1.93	0.99
6:6:322:MET:HE1	6:6:323:GLY:O	1.63	0.99
1:3:32:PRO:CD	1:3:69:LYS:HZ3	1.74	0.98
8:7:583:MET:HE1	8:7:763:VAL:HB	1.45	0.98
8:7:613:TYR:HB2	8:7:766:LYS:HG2	1.42	0.98
3:0:104:ARG:CZ	3:0:173:LYS:HA	1.94	0.98
9:N:59:DA:H2"	9:N:60:DT:C6	1.98	0.98
3:0:715:SER:HA	3:0:718:LYS:HE2	1.41	0.98
4:1:206:PRO:HB3	4:1:210:TRP:CZ3	1.99	0.98
9:N:53:DT:H2"	9:N:54:DT:C5	1.97	0.98
1:3:114:GLU:C	3:0:330:HIS:CE1	2.37	0.98
3:0:633:ARG:HB2	3:0:636:LYS:CD	1.94	0.98
4:1:206:PRO:CB	4:1:210:TRP:CZ3	2.47	0.98
8:7:754:ARG:HA	8:7:757:ARG:CD	1.94	0.98
8:7:571:ARG:HH11	8:7:572:GLU:HB3	1.28	0.98
9:N:67:DT:H2"	9:N:68:DT:C5	1.97	0.98
3:0:334:PHE:CA	3:0:337:ARG:HD3	1.92	0.98
2:2:431:GLN:OE1	2:2:434:PRO:CA	2.12	0.97
8:7:425:LEU:HB3	8:7:430:LEU:HD21	1.46	0.97
3:0:577:GLN:HE22	3:0:578:GLU:HG2	1.28	0.97
3:0:251:ASP:HA	3:0:436:ARG:HA	1.43	0.97
5:4:239:GLU:OE2	5:4:242:GLU:HB2	1.64	0.97
9:N:73:DA:H2"	9:N:74:DT:C6	1.98	0.97
8:7:442:ASN:HB2	8:7:444:GLU:HG2	1.45	0.97
5:4:150:ALA:HA	5:4:153:MET:CE	1.95	0.97
8:7:568:GLU:CD	8:7:571:ARG:NE	2.17	0.97
3:0:109:THR:HG21	3:0:113:ASN:ND2	1.80	0.96
3:0:166:GLU:HG3	3:0:198:ARG:NH1	1.79	0.96
3:0:643:ARG:HH12	3:0:647:ARG:HA	1.27	0.96
3:0:614:HIS:CE1	3:0:674:ASP:O	2.19	0.96
8:7:465:ASN:CB	8:7:471:GLN:NE2	2.27	0.96
8:7:677:TYR:CE2	8:7:682:GLN:HG2	2.01	0.96
1:3:67:LYS:O	1:3:69:LYS:NZ	1.99	0.96
3:0:135:ARG:HH22	3:0:392:GLU:HA	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:73:DA:H2"	9:N:74:DT:C5	2.01	0.96
3:0:633:ARG:HB2	3:0:636:LYS:HE3	1.43	0.96
3:0:304:GLU:OE1	3:0:386:ARG:NH1	1.97	0.96
3:0:310:PRO:HB3	3:0:404:THR:HG23	1.45	0.96
9:N:59:DA:H2"	9:N:60:DT:C5	2.01	0.96
6:6:351:ASN:O	6:6:353:HIS:ND1	1.98	0.96
3:0:50:VAL:HG22	3:0:85:GLU:OE2	1.66	0.96
8:7:548:HIS:CE1	8:7:695:ARG:HH22	1.83	0.96
2:2:471:LEU:HD13	2:2:501:VAL:HG21	1.48	0.95
8:7:625:PRO:HD2	8:7:649:ILE:HG12	1.48	0.95
4:1:593:LEU:HD21	4:1:597:PHE:HE2	1.30	0.95
7:5:42:VAL:HG11	7:5:47:VAL:HG22	1.48	0.95
3:0:339:ILE:C	3:0:343:LYS:NZ	2.20	0.95
2:2:15:GLU:HB3	2:2:84:LEU:CD1	1.95	0.95
2:2:501:VAL:HA	2:2:504:PHE:HE2	1.27	0.95
8:7:341:TYR:CE1	8:7:509:ALA:HB2	2.01	0.95
8:7:471:GLN:HA	8:7:474:MET:CE	1.97	0.94
8:7:491:HIS:CA	8:7:519:ARG:NH2	2.29	0.94
6:6:426:ARG:NH2	6:6:435:GLU:CB	2.30	0.94
6:6:132:CYS:SG	6:6:146:HIS:HE1	1.91	0.94
2:2:13:TYR:O	2:2:16:GLU:HG3	1.66	0.94
8:7:439:THR:HG21	8:7:456:THR:H	1.31	0.94
2:2:136:ASP:C	2:2:286:ARG:NH1	2.21	0.94
2:2:501:VAL:CG1	2:2:504:PHE:CZ	2.47	0.94
3:0:531:LYS:HG2	3:0:566:HIS:CE1	2.02	0.94
8:7:464:ARG:HD2	10:T:106:DA:H5"	1.46	0.94
3:0:104:ARG:NE	3:0:173:LYS:HA	1.83	0.93
2:2:504:PHE:CZ	2:2:504:PHE:CE1	0.93	0.93
3:0:469:TYR:CD2	3:0:472:MET:HE1	2.03	0.93
8:7:485:ILE:HD13	8:7:510:LYS:HG3	1.49	0.93
5:4:193:TYR:HB2	5:4:223:PHE:CE1	2.03	0.93
2:2:19:GLN:NE2	2:2:85:HIS:CB	2.25	0.93
3:0:224:ASN:HA	3:0:227:SER:OG	1.68	0.93
3:0:507:SER:HB2	3:0:683:ASP:OD1	1.68	0.93
5:4:290:SER:O	5:4:293:LEU:HD22	1.67	0.93
3:0:104:ARG:NH2	3:0:173:LYS:HA	1.82	0.93
3:0:312:LEU:HD23	3:0:315:ASP:OD2	1.68	0.93
2:2:497:GLY:HA2	2:2:500:GLN:HE22	1.32	0.93
8:7:664:LEU:HD23	8:7:689:ARG:HD2	1.49	0.92
8:7:447:GLN:HG3	8:7:476:PHE:CE1	2.03	0.92
8:7:469:ASP:CA	8:7:472:LYS:HE2	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:291:GLN:HE22	3:0:294:HIS:HA	1.32	0.92
4:1:596:LEU:O	4:1:600:VAL:HG23	1.68	0.92
8:7:356:LEU:HD12	8:7:404:LYS:NZ	1.83	0.92
8:7:571:ARG:CZ	8:7:572:GLU:CD	2.38	0.92
5:4:273:ARG:HH12	6:6:372:LEU:HB3	1.35	0.92
3:0:281:LYS:O	3:0:285:GLU:OE1	1.87	0.92
3:0:340:GLU:OE1	3:0:343:LYS:HD2	1.69	0.92
1:3:27:LYS:HZ3	1:3:29:LEU:HA	1.35	0.92
3:0:532:ILE:HD11	3:0:718:LYS:HG2	1.51	0.92
3:0:715:SER:HA	3:0:718:LYS:NZ	1.84	0.92
8:7:433:GLU:OE2	8:7:434:ASN:ND2	2.03	0.92
2:2:19:GLN:HA	2:2:22:GLN:OE1	1.69	0.91
3:0:639:LEU:HA	3:0:642:MET:HE2	1.50	0.91
6:6:178:LEU:HD22	6:6:180:GLN:HE21	1.35	0.91
3:0:83:LEU:HD21	3:0:207:ILE:CD1	2.00	0.91
8:7:467:SER:HB2	8:7:469:ASP:OD1	1.70	0.91
8:7:641:GLN:OE1	8:7:644:GLN:NE2	2.03	0.91
3:0:77:SER:HA	3:0:80:GLU:CD	1.89	0.91
2:2:504:PHE:CZ	2:2:504:PHE:HE1	1.63	0.91
4:1:237:UNK:CB	4:1:259:ILE:HD11	2.01	0.91
5:4:255:ASP:C	5:4:259:ARG:HH11	1.74	0.91
8:7:447:GLN:OE1	8:7:476:PHE:CG	2.24	0.91
2:2:360:LEU:O	2:2:364:VAL:HG12	1.70	0.91
3:0:195:ILE:O	3:0:199:MET:HG2	1.71	0.91
3:0:356:PRO:CA	3:0:359:PHE:CE2	2.52	0.91
4:1:222:LEU:HD11	6:6:216:MET:HA	1.50	0.91
8:7:411:CYS:HB3	8:7:417:VAL:HG22	1.53	0.90
8:7:478:THR:HG22	8:7:504:THR:HG22	1.51	0.90
3:0:135:ARG:NH1	3:0:391:THR:O	2.05	0.90
3:0:255:ASP:O	3:0:258:ARG:HG2	1.70	0.90
2:2:353:SER:N	2:2:356:GLN:HE21	1.68	0.90
2:2:197:ASN:O	2:2:201:TRP:HD1	1.54	0.90
3:0:135:ARG:NH2	3:0:392:GLU:HA	1.85	0.90
3:0:161:ASN:OD1	3:0:190:LEU:HD13	1.71	0.90
3:0:621:LEU:HG	3:0:680:VAL:HG21	1.54	0.90
3:0:703:ASP:HA	3:0:706:LEU:HD23	1.51	0.90
6:6:116:THR:CG2	6:6:385:PRO:HG2	2.00	0.90
2:2:501:VAL:CA	2:2:504:PHE:CD2	2.41	0.90
2:2:502:LEU:HD21	2:2:506:LYS:NZ	1.87	0.90
2:2:468:TYR:CD2	2:2:486:ASP:OD2	2.25	0.90
6:6:124:ARG:NH2	6:6:305:VAL:O	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:17:ILE:HG12	2:2:21:VAL:CG2	2.00	0.89
5:4:139:GLN:NE2	5:4:140:ILE:HG12	1.85	0.89
5:4:225:GLN:HE22	5:4:269:SER:CB	1.85	0.89
5:4:273:ARG:NH2	6:6:372:LEU:C	2.24	0.89
8:7:478:THR:CG2	8:7:504:THR:HG22	2.02	0.89
8:7:754:ARG:C	8:7:757:ARG:HH11	1.74	0.89
2:2:408:MET:HE1	2:2:411:LEU:HD13	1.53	0.89
3:0:374:LEU:CD2	3:0:410:SER:HB2	2.03	0.89
5:4:276:CYS:SG	5:4:296:LEU:HA	2.13	0.89
8:7:589:GLN:HB3	8:7:745:ILE:HD11	1.53	0.89
8:7:754:ARG:CB	8:7:757:ARG:NH1	2.35	0.89
1:3:34:CYS:HA	1:3:61:LYS:HE2	1.54	0.89
3:0:48:LYS:O	3:0:52:LEU:HG	1.72	0.89
3:0:275:ARG:HD2	3:0:276:LYS:HE3	1.55	0.89
3:0:109:THR:HG21	3:0:113:ASN:HD21	1.37	0.89
3:0:251:ASP:HB3	4:1:350:ARG:CZ	2.03	0.89
8:7:408:ILE:HD12	8:7:410:LEU:HD11	1.52	0.89
6:6:116:THR:N	6:6:117:PRO:HD2	1.88	0.89
8:7:754:ARG:C	8:7:757:ARG:HD3	1.93	0.89
6:6:171:ILE:O	6:6:181:LEU:HD12	1.73	0.88
6:6:386:LEU:HD13	6:6:451:CYS:HB2	1.56	0.88
3:0:633:ARG:HB2	3:0:636:LYS:CE	2.02	0.88
8:7:468:HIS:HA	8:7:471:GLN:OE1	1.73	0.88
9:N:64:DA:H2	10:T:102:DT:H3	1.21	0.88
3:0:287:GLU:HA	3:0:290:VAL:HG12	1.53	0.88
3:0:725:ALA:CB	6:6:290:ILE:HD11	2.04	0.88
8:7:406:SER:OG	8:7:480:ARG:NE	2.07	0.88
3:0:135:ARG:CA	3:0:138:ASN:ND2	2.34	0.88
8:7:447:GLN:OE1	8:7:476:PHE:CB	2.22	0.88
8:7:641:GLN:NE2	8:7:645:TYR:CD1	2.41	0.88
8:7:491:HIS:HA	8:7:519:ARG:CZ	2.04	0.88
6:6:132:CYS:SG	6:6:146:HIS:CE1	2.66	0.88
6:6:166:ILE:CD1	6:6:375:HIS:HB3	2.02	0.88
8:7:477:LEU:HA	8:7:482:TRP:HE1	1.39	0.88
3:0:104:ARG:HH21	3:0:173:LYS:HD2	1.38	0.87
8:7:383:ILE:HG21	8:7:528:ASN:ND2	1.89	0.87
3:0:198:ARG:NH1	3:0:199:MET:HE1	1.90	0.87
3:0:327:ARG:CB	3:0:330:HIS:HD2	1.85	0.87
8:7:552:VAL:CG1	8:7:731:TYR:CD1	2.58	0.87
8:7:604:LYS:NZ	8:7:694:LYS:HE3	1.89	0.87
3:0:102:ASP:HA	3:0:173:LYS:HZ2	1.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:341:TYR:CE1	3:0:363:LEU:HD13	2.09	0.87
6:6:199:ILE:O	6:6:202:GLN:HG3	1.74	0.87
8:7:710:SER:O	8:7:716:MET:HE3	1.72	0.87
3:0:135:ARG:HA	3:0:138:ASN:HD21	1.07	0.87
3:0:424:GLU:HB2	3:0:432:ASN:ND2	1.89	0.87
5:4:194:ILE:HA	5:4:197:MET:HE2	1.55	0.87
8:7:341:TYR:CD1	8:7:509:ALA:HB2	2.09	0.87
2:2:504:PHE:CE1	2:2:504:PHE:HZ	1.63	0.86
3:0:356:PRO:O	3:0:360:LEU:HB2	1.74	0.86
3:0:519:VAL:HG13	3:0:554:TRP:HE1	1.37	0.86
6:6:349:CYS:CB	6:6:352:CYS:SG	2.62	0.86
9:N:64:DA:H2"	9:N:65:DC:C5	2.10	0.86
6:6:126:LEU:O	6:6:169:MET:SD	2.32	0.86
2:2:56:GLU:C	2:2:97:MET:HE2	1.96	0.86
2:2:367:LYS:CB	2:2:375:LEU:HD23	2.05	0.86
8:7:383:ILE:HG13	8:7:528:ASN:HA	1.55	0.86
3:0:16:LYS:HB3	3:0:741:TYR:HE1	1.37	0.86
3:0:156:CYS:HB3	3:0:158:TYR:HD2	1.40	0.86
3:0:424:GLU:H	3:0:432:ASN:CG	1.78	0.86
6:6:426:ARG:CZ	6:6:435:GLU:CB	2.54	0.86
7:5:51:LYS:NZ	7:5:54:LEU:CD2	2.36	0.86
2:2:354:PRO:HA	2:2:357:ILE:CG1	2.03	0.86
3:0:301:ASP:HB3	3:0:304:GLU:HB2	1.55	0.86
8:7:693:ALA:HB1	8:7:695:ARG:NH1	1.91	0.86
3:0:104:ARG:NH1	3:0:171:LEU:O	2.08	0.86
9:N:75:DG:H2'	9:N:76:DT:H72	1.58	0.86
8:7:613:TYR:HB2	8:7:766:LYS:NZ	1.90	0.86
8:7:683:GLU:HG2	8:7:686:ARG:NH2	1.90	0.86
3:0:217:LYS:HB2	3:0:308:GLU:HG3	1.55	0.85
8:7:342:ASP:HB2	8:7:345:ASN:HB3	1.57	0.85
3:0:639:LEU:CA	3:0:642:MET:CE	2.54	0.85
6:6:429:CYS:HB3	6:6:432:CYS:SG	2.15	0.85
8:7:385:VAL:HG12	8:7:514:THR:HB	1.59	0.85
2:2:410:ARG:HA	2:2:413:GLU:HG2	1.59	0.85
3:0:275:ARG:NH1	3:0:276:LYS:CE	2.39	0.85
7:5:61:ASN:O	8:7:573:THR:OG1	1.93	0.85
3:0:39:ILE:CG2	3:0:480:GLN:HG3	2.06	0.85
3:0:136:MET:HE1	3:0:156:CYS:SG	2.16	0.85
3:0:198:ARG:NH1	3:0:199:MET:CE	2.40	0.85
3:0:424:GLU:HB2	3:0:432:ASN:HD21	1.40	0.85
8:7:754:ARG:C	8:7:757:ARG:NH1	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:127:GLU:OE1	5:4:131:LYS:HE3	1.77	0.85
8:7:357:LYS:HB2	8:7:429:THR:HB	1.59	0.85
3:0:104:ARG:NH2	3:0:172:PRO:C	2.29	0.85
4:1:197:GLU:HA	4:1:201:ASN:OD1	1.77	0.85
3:0:639:LEU:CD1	3:0:642:MET:HE3	2.07	0.84
8:7:408:ILE:HG23	8:7:482:TRP:CE3	2.11	0.84
8:7:469:ASP:HA	8:7:472:LYS:CE	2.04	0.84
8:7:571:ARG:NH1	8:7:572:GLU:HB3	1.90	0.84
8:7:664:LEU:HD23	8:7:689:ARG:HH11	1.42	0.84
6:6:199:ILE:CG2	6:6:202:GLN:HE21	1.90	0.84
1:3:42:CYS:O	1:3:45:ARG:HG3	1.77	0.84
2:2:365:HIS:HB3	2:2:385:ARG:HH22	1.41	0.84
3:0:312:LEU:CG	3:0:313:PRO:HD2	2.06	0.84
2:2:471:LEU:HD13	2:2:501:VAL:CG2	2.07	0.84
2:2:56:GLU:O	2:2:97:MET:CE	2.25	0.84
6:6:310:VAL:HG13	6:6:311:ASN:H	1.42	0.84
9:N:61:DG:H2'	9:N:62:DT:H72	1.57	0.84
3:0:135:ARG:CA	3:0:138:ASN:HD21	1.89	0.84
3:0:251:ASP:CB	3:0:436:ARG:HD3	2.06	0.84
8:7:445:MET:HE1	8:7:448:THR:C	1.98	0.84
8:7:568:GLU:OE1	8:7:571:ARG:NE	2.09	0.84
5:4:39:THR:O	5:4:43:GLU:OE1	1.95	0.84
8:7:443:LYS:HG3	8:7:469:ASP:OD2	1.77	0.84
6:6:134:GLU:OE1	6:6:206:GLY:O	1.94	0.84
2:2:452:ILE:HG22	7:5:11:GLN:O	1.78	0.84
4:1:206:PRO:O	4:1:210:TRP:CE3	2.31	0.84
7:5:19:LEU:HD23	7:5:22:GLN:CD	1.98	0.84
2:2:492:PHE:HB3	7:5:9:LEU:HD22	1.59	0.83
3:0:633:ARG:HB2	3:0:636:LYS:HD3	1.58	0.83
5:4:150:ALA:HA	5:4:153:MET:HE3	1.59	0.83
7:5:19:LEU:HD13	8:7:566:TYR:OH	1.77	0.83
8:7:496:ALA:O	8:7:499:ARG:HG3	1.77	0.83
1:3:27:LYS:NZ	1:3:29:LEU:HD23	1.92	0.83
6:6:299:GLU:O	6:6:303:GLU:OE1	1.96	0.83
7:5:25:ALA:N	7:5:29:ASP:OD1	2.10	0.83
1:3:68:PHE:C	1:3:69:LYS:HD3	1.99	0.83
6:6:269:GLN:HG3	6:6:288:TYR:CE2	2.13	0.83
8:7:437:VAL:O	8:7:442:ASN:ND2	2.11	0.83
4:1:206:PRO:HB3	4:1:210:TRP:CH2	2.13	0.83
5:4:124:THR:O	5:4:128:GLU:OE1	1.96	0.83
3:0:60:GLN:O	3:0:67:ARG:NH1	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:270:VAL:HG12	6:6:272:ILE:HG22	1.58	0.83
3:0:289:LEU:HD11	3:0:380:ARG:NH1	1.93	0.83
3:0:510:PHE:O	3:0:511:GLU:HG3	1.76	0.83
3:0:516:PRO:HA	3:0:519:VAL:HB	1.57	0.83
6:6:178:LEU:HD22	6:6:180:GLN:NE2	1.92	0.83
6:6:426:ARG:HH12	6:6:435:GLU:CA	1.91	0.83
5:4:60:PHE:CE2	5:4:253:PHE:CE1	2.66	0.83
5:4:273:ARG:HH22	6:6:373:SER:N	1.77	0.83
3:0:253:THR:HA	3:0:346:MET:HE1	1.61	0.83
9:N:67:DT:H2"	9:N:68:DT:C7	2.08	0.83
3:0:649:ARG:NH1	3:0:652:ASP:OD2	2.11	0.83
6:6:321:LYS:O	6:6:368:LEU:HD11	1.79	0.83
8:7:442:ASN:CB	8:7:444:GLU:HG2	2.08	0.83
3:0:372:LYS:O	3:0:375:ARG:HG2	1.79	0.83
8:7:641:GLN:O	8:7:645:TYR:N	2.11	0.83
3:0:625:ILE:HD13	3:0:686:PHE:HE1	1.44	0.82
5:4:150:ALA:HA	5:4:153:MET:HE2	1.61	0.82
8:7:548:HIS:ND1	8:7:695:ARG:NH2	2.25	0.82
8:7:571:ARG:HH12	8:7:572:GLU:CD	1.75	0.82
3:0:155:LEU:HD11	3:0:160:GLU:HG2	1.58	0.82
5:4:276:CYS:SG	5:4:297:SER:N	2.52	0.82
2:2:451:VAL:CG2	7:5:54:LEU:CD1	2.57	0.82
3:0:217:LYS:HB2	3:0:308:GLU:CG	2.08	0.82
3:0:714:ILE:O	3:0:718:LYS:HG3	1.78	0.82
1:3:34:CYS:HA	1:3:61:LYS:CE	2.09	0.82
8:7:544:SER:HB3	8:7:549:ILE:HB	1.60	0.82
3:0:264:ALA:HB3	3:0:336:LYS:HZ2	1.43	0.82
8:7:675:SER:CB	8:7:722:ARG:NH2	2.43	0.82
2:2:451:VAL:HG21	7:5:54:LEU:HD13	1.60	0.82
3:0:492:PHE:HB2	3:0:679:MET:CE	2.09	0.82
6:6:381:HIS:CE1	6:6:449:HIS:NE2	2.48	0.82
8:7:604:LYS:HZ1	8:7:694:LYS:CE	1.93	0.82
8:7:675:SER:HA	8:7:722:ARG:NH2	1.95	0.82
3:0:109:THR:HG23	3:0:110:SER:H	1.44	0.82
7:5:23:ILE:HG12	7:5:57:LEU:HD21	1.59	0.82
8:7:356:LEU:HB2	8:7:404:LYS:CE	2.10	0.82
8:7:575:ARG:O	8:7:578:MET:HG2	1.80	0.82
2:2:451:VAL:HG21	7:5:54:LEU:CD1	2.09	0.82
3:0:416:PHE:CD1	3:0:439:CYS:HA	2.15	0.82
3:0:471:ARG:HH22	3:0:647:ARG:HB2	1.45	0.82
1:3:27:LYS:CE	1:3:29:LEU:HD23	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:136:MET:CE	3:0:156:CYS:SG	2.68	0.81
3:0:670:LEU:HA	3:0:675:ASP:CG	2.00	0.81
3:0:109:THR:CB	3:0:113:ASN:HD21	1.92	0.81
3:0:334:PHE:HA	3:0:337:ARG:CD	1.99	0.81
3:0:633:ARG:HD3	3:0:636:LYS:HE3	1.62	0.81
6:6:136:MET:HE2	6:6:136:MET:HA	1.61	0.81
9:N:53:DT:H2"	9:N:54:DT:C7	2.08	0.81
2:2:380:ARG:HG3	2:2:384:ARG:HH12	1.46	0.81
2:2:468:TYR:CE2	2:2:486:ASP:CG	2.54	0.81
1:3:30:VAL:HB	1:3:71:GLN:HE22	1.43	0.81
1:3:34:CYS:CB	1:3:61:LYS:NZ	2.42	0.81
3:0:190:LEU:HB3	3:0:195:ILE:HD11	1.60	0.81
3:0:237:ALA:O	3:0:240:ILE:HG12	1.81	0.81
3:0:710:THR:O	3:0:714:ILE:HG12	1.80	0.81
3:0:715:SER:CA	3:0:718:LYS:NZ	2.42	0.81
4:1:194:VAL:HA	4:1:197:GLU:OE2	1.80	0.81
5:4:304:LYS:HG3	5:4:309:ASP:HA	1.63	0.81
2:2:201:TRP:HZ2	2:2:278:LEU:O	1.62	0.81
8:7:622:MET:HE2	8:7:624:LYS:HG3	1.60	0.81
2:2:17:ILE:CG1	2:2:21:VAL:HG21	2.10	0.81
3:0:689:LYS:HG3	3:0:692:GLN:NE2	1.95	0.81
4:1:218:ARG:NH1	6:6:222:LEU:HD12	1.95	0.81
5:4:163:ILE:HA	5:4:166:GLU:HG3	1.62	0.81
1:3:27:LYS:HZ2	1:3:29:LEU:HA	1.44	0.81
5:4:271:ASP:O	5:4:273:ARG:HD2	1.80	0.81
6:6:138:GLU:OE2	6:6:145:ARG:NE	2.14	0.80
8:7:411:CYS:SG	8:7:420:TRP:CZ3	2.74	0.80
2:2:468:TYR:CD2	2:2:486:ASP:CG	2.54	0.80
2:2:496:GLU:O	2:2:500:GLN:OE1	2.00	0.80
3:0:251:ASP:HB3	4:1:350:ARG:NH1	1.97	0.80
6:6:155:ASP:HB3	6:6:298:LYS:NZ	1.96	0.80
8:7:580:LEU:CA	8:7:583:MET:HE3	2.08	0.80
2:2:197:ASN:O	2:2:201:TRP:CD1	2.34	0.80
2:2:466:GLN:O	2:2:470:LEU:HD13	1.82	0.80
4:1:206:PRO:HB2	4:1:210:TRP:HZ3	1.46	0.80
3:0:643:ARG:NH1	3:0:647:ARG:HA	1.96	0.80
3:0:675:ASP:OD1	3:0:676:TYR:N	2.14	0.80
8:7:497:MET:SD	8:7:500:ARG:NH2	2.55	0.80
8:7:583:MET:SD	8:7:760:LEU:HA	2.22	0.80
3:0:521:ASN:C	3:0:525:MET:HE1	2.02	0.80
5:4:30:ILE:HD12	5:4:179:LEU:HB3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:754:ARG:HB3	8:7:757:ARG:CZ	2.11	0.80
8:7:755:GLU:N	8:7:757:ARG:NH1	2.29	0.80
2:2:13:TYR:CZ	2:2:208:LEU:HD21	2.17	0.80
2:2:454:TYR:CE2	7:5:11:GLN:CD	2.54	0.80
3:0:145:LEU:HD13	3:0:153:VAL:HB	1.64	0.80
8:7:370:LEU:HD21	8:7:395:VAL:HB	1.63	0.80
3:0:140:GLN:HA	3:0:143:ARG:HE	1.47	0.80
3:0:374:LEU:HD22	3:0:410:SER:CB	2.07	0.80
4:1:593:LEU:CD2	4:1:620:LEU:HD21	2.12	0.80
6:6:168:GLN:OE1	6:6:186:SER:O	1.99	0.80
2:2:352:ASN:C	2:2:356:GLN:HE21	1.83	0.80
3:0:478:VAL:HG12	3:0:479:LEU:HD12	1.62	0.80
6:6:322:MET:HA	6:6:368:LEU:CD2	2.12	0.80
3:0:741:TYR:C	3:0:742:GLU:OE1	2.20	0.80
4:1:222:LEU:CD2	6:6:216:MET:HG2	2.12	0.80
6:6:176:ASN:HA	6:6:206:GLY:HA3	1.63	0.80
8:7:411:CYS:SG	8:7:412:THR:N	2.54	0.80
8:7:445:MET:SD	8:7:449:GLU:HG3	2.21	0.80
8:7:571:ARG:NH2	8:7:572:GLU:CD	2.33	0.80
8:7:754:ARG:C	8:7:757:ARG:CD	2.48	0.80
3:0:708:LEU:HD22	3:0:712:MET:CE	2.12	0.80
6:6:349:CYS:HB3	6:6:352:CYS:SG	2.22	0.80
8:7:471:GLN:HG3	8:7:474:MET:CE	2.12	0.80
8:7:699:GLU:O	8:7:702:ASN:ND2	2.14	0.79
3:0:144:LYS:HA	3:0:147:GLU:CD	2.02	0.79
4:1:375:LEU:CA	4:1:378:MET:SD	2.69	0.79
3:0:275:ARG:CD	3:0:276:LYS:HE3	2.11	0.79
1:3:45:ARG:NH1	1:3:46:ILE:HG12	1.97	0.79
4:1:337:ILE:O	4:1:339:LEU:HD22	1.81	0.79
4:1:629:LYS:NZ	6:6:351:ASN:HD21	1.80	0.79
5:4:30:ILE:CD1	5:4:179:LEU:HB3	2.13	0.79
5:4:193:TYR:HB2	5:4:223:PHE:HE1	1.47	0.79
8:7:631:THR:HB	8:7:633:GLN:HE22	1.47	0.79
2:2:136:ASP:CA	2:2:286:ARG:NH1	2.44	0.79
3:0:341:TYR:CD1	3:0:363:LEU:HD13	2.17	0.79
3:0:371:ARG:NE	3:0:410:SER:O	2.15	0.79
4:1:343:ILE:O	4:1:345:ASP:N	2.15	0.79
8:7:754:ARG:C	8:7:757:ARG:CZ	2.51	0.79
6:6:383:LEU:HD22	6:6:384:MET:HE3	1.65	0.79
8:7:197:LEU:O	8:7:201:SER:N	2.12	0.79
8:7:447:GLN:CG	8:7:476:PHE:CD1	2.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:633:ARG:CB	3:0:636:LYS:HE3	2.12	0.79
4:1:511:ALA:HB2	5:4:264:LYS:HE3	1.64	0.79
2:2:78:ILE:HA	2:2:81:MET:SD	2.22	0.79
3:0:340:GLU:OE1	3:0:343:LYS:CD	2.30	0.79
3:0:41:GLU:OE2	3:0:696:TRP:CH2	2.35	0.79
8:7:571:ARG:HD2	8:7:572:GLU:N	1.98	0.79
3:0:537:MET:HG3	3:0:619:THR:OG1	1.83	0.79
6:6:197:LYS:CD	6:6:200:ARG:NH2	2.42	0.79
1:3:68:PHE:O	1:3:69:LYS:HD3	1.82	0.78
3:0:405:PHE:CE1	3:0:409:ILE:HD13	2.18	0.78
3:0:577:GLN:NE2	3:0:578:GLU:CG	2.43	0.78
8:7:459:MET:HE3	8:7:470:SER:CA	2.14	0.78
8:7:495:ALA:HB3	8:7:523:LYS:HE2	1.65	0.78
1:3:34:CYS:N	1:3:61:LYS:HZ3	1.82	0.78
5:4:273:ARG:NH1	6:6:372:LEU:HB3	1.99	0.78
3:0:79:ILE:HG23	3:0:207:ILE:CD1	2.11	0.78
3:0:371:ARG:CZ	3:0:410:SER:O	2.32	0.78
3:0:740:SER:OG	3:0:744:LEU:HD13	1.82	0.78
8:7:662:ILE:O	8:7:664:LEU:HD22	1.82	0.78
8:7:686:ARG:HG2	8:7:687:LEU:HD22	1.66	0.78
2:2:134:LEU:C	2:2:136:ASP:H	1.86	0.78
8:7:471:GLN:HG3	8:7:474:MET:HE1	1.65	0.78
2:2:10:VAL:HG12	2:2:205:LEU:HD11	1.64	0.78
2:2:353:SER:O	2:2:356:GLN:HG2	1.83	0.78
3:0:657:ASP:O	3:0:661:HIS:ND1	2.15	0.78
5:4:163:ILE:HA	5:4:166:GLU:CG	2.12	0.78
5:4:293:LEU:HD12	6:6:376:LEU:HD22	1.64	0.78
3:0:69:ILE:HG23	3:0:231:ILE:CG1	2.11	0.78
3:0:306:PHE:CE2	3:0:385:VAL:HG11	2.18	0.78
3:0:355:THR:O	3:0:359:PHE:CD2	2.36	0.78
3:0:614:HIS:HE1	3:0:675:ASP:HA	0.98	0.78
6:6:152:TYR:HE2	6:6:298:LYS:HB2	1.49	0.78
8:7:376:ASN:H	8:7:380:ARG:HH22	1.32	0.78
8:7:403:ILE:HD11	8:7:484:PHE:HB2	1.64	0.78
2:2:354:PRO:CA	2:2:357:ILE:HG12	2.09	0.78
8:7:438:PHE:HB2	8:7:442:ASN:HB2	1.64	0.78
3:0:276:LYS:HE2	3:0:276:LYS:HA	1.64	0.78
8:7:498:PHE:HA	8:7:501:VAL:HG22	1.66	0.78
8:7:693:ALA:HB1	8:7:695:ARG:HH12	1.48	0.78
1:3:30:VAL:HB	1:3:71:GLN:NE2	1.98	0.77
2:2:11:THR:OG1	2:2:12:GLN:OE1	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:454:TYR:HE2	7:5:11:GLN:HB2	1.48	0.77
3:0:250:LEU:HA	4:1:350:ARG:CG	2.12	0.77
2:2:502:LEU:HD21	2:2:506:LYS:HZ2	1.47	0.77
3:0:522:TYR:HA	3:0:525:MET:HE2	1.66	0.77
3:0:572:GLU:CD	3:0:600:SER:HB2	2.05	0.77
8:7:491:HIS:HA	8:7:519:ARG:HH21	1.46	0.77
3:0:251:ASP:O	4:1:350:ARG:NE	2.15	0.77
5:4:194:ILE:HA	5:4:197:MET:CE	2.12	0.77
3:0:468:MET:HE2	3:0:653:PHE:CE2	2.19	0.77
6:6:132:CYS:HB3	6:6:175:ARG:HG2	1.67	0.77
8:7:554:CYS:HB3	8:7:705:PHE:CD2	2.19	0.77
9:N:64:DA:H2"	9:N:65:DC:C6	2.19	0.77
3:0:569:ILE:HA	3:0:597:ILE:HG22	1.65	0.77
6:6:426:ARG:HH12	6:6:435:GLU:HA	1.46	0.77
7:5:25:ALA:CA	7:5:29:ASP:OD1	2.33	0.77
8:7:666:GLU:OE2	8:7:693:ALA:O	2.02	0.77
2:2:431:GLN:OE1	2:2:435:PRO:HD2	1.85	0.77
3:0:297:ASP:OD1	3:0:301:ASP:OD1	2.03	0.77
5:4:176:LEU:CD1	5:4:210:ILE:HG23	2.11	0.77
8:7:457:TYR:CZ	8:7:490:VAL:HG22	2.20	0.77
3:0:468:MET:HE2	3:0:653:PHE:HE2	1.48	0.77
5:4:163:ILE:O	5:4:167:SER:N	2.13	0.77
6:6:126:LEU:HD23	6:6:169:MET:CE	2.13	0.77
6:6:269:GLN:HG3	6:6:288:TYR:HE2	1.49	0.77
8:7:411:CYS:SG	8:7:420:TRP:CH2	2.78	0.77
8:7:599:GLU:HG2	8:7:650:ASN:HD22	1.48	0.77
8:7:612:VAL:HG23	8:7:766:LYS:HZ3	1.50	0.77
2:2:367:LYS:HB2	2:2:375:LEU:CD2	2.07	0.77
3:0:569:ILE:HA	3:0:597:ILE:CG2	2.15	0.77
4:1:175:LEU:O	4:1:181:GLN:NE2	2.18	0.77
6:6:224:VAL:HG12	6:6:230:ARG:HE	1.49	0.77
8:7:401:CYS:C	8:7:404:LYS:NZ	2.25	0.77
2:2:19:GLN:HE22	2:2:85:HIS:HB3	0.70	0.77
2:2:56:GLU:OE2	2:2:97:MET:CE	2.33	0.77
2:2:462:PHE:HB2	2:2:489:LYS:HD2	1.67	0.77
3:0:104:ARG:HE	3:0:173:LYS:HA	1.49	0.77
8:7:446:PHE:CD1	8:7:472:LYS:HE3	2.19	0.77
8:7:457:TYR:CE2	8:7:490:VAL:HG22	2.20	0.77
5:4:179:LEU:HD13	5:4:213:VAL:HB	1.67	0.77
8:7:554:CYS:HB3	8:7:705:PHE:HD2	1.48	0.77
2:2:468:TYR:OH	2:2:484:LYS:CD	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:501:VAL:HG13	2:2:504:PHE:HZ	0.75	0.76
3:0:353:SER:HA	3:0:419:ILE:HA	1.66	0.76
6:6:199:ILE:HG23	6:6:202:GLN:HE21	1.50	0.76
8:7:447:GLN:OE1	8:7:476:PHE:HB2	1.82	0.76
1:3:54:CYS:HB3	1:3:63:LEU:HD12	1.67	0.76
3:0:177:SER:O	3:0:181:LEU:N	2.15	0.76
2:2:481:LEU:HD23	2:2:493:ILE:HD13	1.65	0.76
3:0:109:THR:CG2	3:0:113:ASN:ND2	2.40	0.76
3:0:528:GLU:HG3	3:0:714:ILE:HD11	1.66	0.76
3:0:577:GLN:HE22	3:0:578:GLU:CG	1.97	0.76
5:4:192:GLN:HG2	5:4:196:ILE:HD11	1.65	0.76
8:7:666:GLU:OE1	8:7:694:LYS:HA	1.86	0.76
6:6:199:ILE:HG23	6:6:202:GLN:NE2	2.01	0.76
3:0:339:ILE:HG12	3:0:343:LYS:CE	2.15	0.76
3:0:708:LEU:HD22	3:0:712:MET:HE1	1.68	0.76
5:4:52:LYS:NZ	5:4:240:SER:O	2.19	0.76
7:5:23:ILE:CG1	7:5:57:LEU:HD21	2.14	0.76
3:0:748:GLN:O	3:0:752:LYS:N	2.18	0.76
8:7:434:ASN:O	8:7:449:GLU:HG3	1.85	0.76
1:3:33:GLU:O	1:3:61:LYS:HE2	1.85	0.76
2:2:408:MET:HE3	2:2:411:LEU:HB2	1.68	0.76
2:2:389:ASN:HB3	2:2:391:ILE:HG12	1.67	0.76
2:2:408:MET:CE	2:2:411:LEU:CD1	2.64	0.76
3:0:287:GLU:CA	3:0:290:VAL:HG12	2.16	0.76
2:2:502:LEU:O	2:2:506:LYS:HG2	1.86	0.76
4:1:185:LEU:HD11	4:1:195:PHE:CD2	2.21	0.76
8:7:554:CYS:HA	8:7:705:PHE:HB3	1.66	0.76
1:3:27:LYS:HZ2	1:3:29:LEU:CA	1.98	0.76
8:7:612:VAL:HG23	8:7:766:LYS:NZ	2.01	0.76
2:2:25:LEU:HD22	2:2:222:LEU:HD13	1.68	0.75
2:2:51:VAL:O	2:2:109:ARG:NH2	2.17	0.75
2:2:136:ASP:C	2:2:286:ARG:HH22	1.73	0.75
3:0:271:ILE:HD12	3:0:329:GLU:OE1	1.87	0.75
8:7:376:ASN:N	8:7:380:ARG:NH2	2.33	0.75
3:0:446:ILE:O	3:0:449:VAL:HG22	1.86	0.75
8:7:754:ARG:CA	8:7:757:ARG:CZ	2.64	0.75
3:0:287:GLU:O	3:0:290:VAL:HG12	1.85	0.75
3:0:423:TYR:HE1	3:0:425:ILE:CG1	1.99	0.75
4:1:235:UNK:O	4:1:238:UNK:N	2.20	0.75
4:1:383:GLU:O	4:1:387:MET:HG2	1.87	0.75
8:7:562:THR:HG21	8:7:564:GLU:OE2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:757:ARG:NE	8:7:758:GLU:OE2	2.19	0.75
2:2:100:LEU:HD12	2:2:101:ASN:C	2.06	0.75
5:4:64:HIS:CE1	5:4:71:ASN:ND2	2.54	0.75
7:5:19:LEU:HD11	8:7:566:TYR:CZ	2.20	0.75
8:7:421:ARG:NH2	8:7:432:PRO:HB3	2.02	0.75
8:7:465:ASN:ND2	8:7:474:MET:CE	2.50	0.75
3:0:291:GLN:NE2	3:0:294:HIS:HA	2.01	0.75
1:3:75:ASP:O	1:3:78:VAL:N	2.18	0.75
3:0:275:ARG:HH11	3:0:276:LYS:CE	1.99	0.75
6:6:165:PRO:HG2	6:6:375:HIS:HD2	1.52	0.75
6:6:322:MET:CA	6:6:368:LEU:HD21	2.15	0.75
8:7:352:LEU:HB2	8:7:406:SER:HA	1.69	0.75
3:0:63:TYR:O	3:0:67:ARG:NH2	2.19	0.75
3:0:1:MET:N	3:0:92:TYR:OH	2.19	0.75
3:0:188:LYS:HB2	3:0:190:LEU:HD23	1.67	0.75
5:4:137:LYS:H	5:4:140:ILE:HB	1.51	0.75
8:7:460:VAL:HG23	8:7:461:ALA:H	1.51	0.75
3:0:257:LEU:HD23	3:0:343:LYS:HG3	1.69	0.75
3:0:259:ARG:CG	3:0:262:ARG:NH2	2.49	0.75
5:4:289:CYS:SG	5:4:294:CYS:N	2.59	0.75
3:0:109:THR:HG23	3:0:110:SER:N	1.99	0.74
8:7:350:PRO:O	8:7:480:ARG:NH2	2.20	0.74
8:7:571:ARG:NH2	8:7:580:LEU:HD12	2.01	0.74
2:2:31:THR:HG22	2:2:226:PHE:HD2	1.51	0.74
2:2:66:VAL:HG12	2:2:67:ASN:O	1.87	0.74
3:0:263:GLY:O	3:0:267:LEU:HD23	1.86	0.74
3:0:264:ALA:HB3	3:0:336:LYS:NZ	2.02	0.74
3:0:287:GLU:HA	3:0:290:VAL:CG1	2.16	0.74
4:1:383:GLU:HA	4:1:386:ILE:HG22	1.69	0.74
8:7:376:ASN:H	8:7:380:ARG:NH2	1.84	0.74
8:7:625:PRO:HG2	8:7:649:ILE:CD1	2.17	0.74
8:7:675:SER:CA	8:7:722:ARG:NH2	2.51	0.74
1:3:45:ARG:NH2	1:3:46:ILE:HD11	2.01	0.74
2:2:501:VAL:HG22	2:2:504:PHE:HE2	1.51	0.74
3:0:519:VAL:HG11	3:0:553:MET:HE3	1.69	0.74
5:4:255:ASP:HA	5:4:259:ARG:HD3	1.67	0.74
6:6:224:VAL:C	6:6:230:ARG:HH21	1.89	0.74
6:6:281:ASN:ND2	6:6:287:PHE:CD2	2.55	0.74
2:2:485:ASP:HB2	2:2:487:LYS:HG2	1.68	0.74
8:7:754:ARG:CA	8:7:757:ARG:NH1	2.50	0.74
2:2:56:GLU:CG	2:2:97:MET:CG	2.58	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:26:LEU:HB3	5:4:73:VAL:HG12	1.69	0.74
8:7:563:ALA:C	8:7:567:GLN:HE22	1.90	0.74
2:2:454:TYR:CE2	7:5:11:GLN:OE1	2.41	0.74
3:0:469:TYR:CD2	3:0:472:MET:CE	2.70	0.74
6:6:224:VAL:CB	6:6:230:ARG:HE	2.00	0.74
2:2:56:GLU:O	2:2:97:MET:HE3	1.88	0.74
6:6:298:LYS:HE3	6:6:302:ASN:HD21	1.52	0.74
8:7:594:LEU:O	8:7:598:HIS:ND1	2.19	0.74
4:1:206:PRO:O	4:1:210:TRP:HE3	1.68	0.74
5:4:255:ASP:HA	5:4:259:ARG:CD	2.18	0.74
6:6:224:VAL:HG13	6:6:228:CYS:HB2	1.70	0.74
8:7:343:PHE:HE2	8:7:379:ALA:H	1.36	0.74
6:6:166:ILE:CG1	6:6:375:HIS:HB3	2.18	0.74
6:6:281:ASN:OD1	6:6:287:PHE:HE2	1.69	0.74
9:N:66:DA:H1'	9:N:67:DT:H5'	1.69	0.74
3:0:7:ASP:HB3	3:0:8:LEU:HD12	1.68	0.73
6:6:363:CYS:HB3	6:6:368:LEU:H	1.53	0.73
7:5:42:VAL:CG1	7:5:47:VAL:HG22	2.17	0.73
3:0:339:ILE:HG12	3:0:343:LYS:HZ1	1.52	0.73
3:0:353:SER:HB3	3:0:419:ILE:CD1	2.17	0.73
3:0:460:SER:HB2	3:0:463:ILE:HG13	1.70	0.73
4:1:270:TYR:OH	4:1:279:LYS:HD2	1.88	0.73
7:5:27:MET:SD	7:5:30:ILE:HG13	2.28	0.73
8:7:544:SER:HA	8:7:549:ILE:C	2.07	0.73
2:2:201:TRP:CZ2	2:2:278:LEU:O	2.41	0.73
3:0:532:ILE:CD1	3:0:718:LYS:HG2	2.17	0.73
3:0:541:PHE:HE2	3:0:599:LEU:HB2	1.53	0.73
3:0:655:SER:O	3:0:659:MET:HG2	1.88	0.73
4:1:193:LYS:O	4:1:197:GLU:OE1	2.06	0.73
6:6:383:LEU:HD22	6:6:384:MET:CE	2.18	0.73
8:7:568:GLU:HA	8:7:571:ARG:CG	2.17	0.73
2:2:454:TYR:HB2	7:5:9:LEU:HB3	1.70	0.73
3:0:24:TYR:HD2	3:0:25:MET:CE	2.00	0.73
3:0:43:PRO:HG3	3:0:696:TRP:CE3	2.23	0.73
3:0:625:ILE:HD13	3:0:686:PHE:CE1	2.22	0.73
5:4:163:ILE:CA	5:4:166:GLU:HG3	2.18	0.73
5:4:235:TYR:CD2	5:4:266:ASN:HB2	2.23	0.73
7:5:42:VAL:HG12	7:5:43:ASN:N	2.02	0.73
3:0:140:GLN:HB3	3:0:144:LYS:HZ2	1.53	0.73
3:0:224:ASN:O	3:0:228:LYS:N	2.15	0.73
3:0:506:ILE:HG21	3:0:521:ASN:ND2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:197:GLU:CA	4:1:201:ASN:OD1	2.37	0.73
5:4:133:PHE:O	5:4:136:GLU:OE1	2.06	0.73
8:7:356:LEU:HD12	8:7:404:LYS:CE	2.19	0.73
8:7:411:CYS:HA	8:7:488:ASP:HB2	1.70	0.73
9:N:52:DA:H1'	9:N:53:DT:H5'	1.69	0.73
3:0:279:SER:OG	3:0:283:GLN:NE2	2.22	0.73
4:1:593:LEU:HD21	4:1:597:PHE:CE2	2.21	0.73
6:6:127:ILE:HD13	6:6:221:LEU:HD11	1.71	0.73
2:2:353:SER:HB2	2:2:356:GLN:HG2	1.70	0.73
3:0:427:ASN:O	3:0:430:VAL:HG22	1.88	0.73
7:5:36:ASP:OD1	7:5:39:HIS:ND1	2.18	0.73
8:7:571:ARG:NH1	8:7:572:GLU:CB	2.51	0.73
3:0:76:MET:O	3:0:80:GLU:OE1	2.07	0.73
3:0:259:ARG:HA	3:0:262:ARG:CZ	2.19	0.73
3:0:416:PHE:CE1	3:0:439:CYS:SG	2.82	0.73
3:0:492:PHE:HB2	3:0:679:MET:HE1	1.71	0.73
6:6:381:HIS:HE1	6:6:449:HIS:NE2	1.83	0.73
2:2:56:GLU:C	2:2:97:MET:CE	2.58	0.73
4:1:593:LEU:CD2	4:1:597:PHE:HE2	2.00	0.73
5:4:64:HIS:CE1	5:4:71:ASN:HD21	2.07	0.73
2:2:273:LYS:HE2	2:2:277:MET:CE	2.19	0.72
3:0:167:VAL:HA	3:0:198:ARG:HH21	1.48	0.72
3:0:250:LEU:CA	4:1:350:ARG:HG2	2.13	0.72
3:0:275:ARG:NH1	3:0:276:LYS:HE3	2.03	0.72
4:1:273:ASN:HD22	4:1:283:PHE:HE2	1.37	0.72
7:5:23:ILE:CD1	7:5:57:LEU:HD21	2.18	0.72
8:7:579:LEU:HA	8:7:582:ILE:HB	1.71	0.72
2:2:24:ARG:HB3	2:2:219:VAL:HG21	1.70	0.72
2:2:501:VAL:CB	2:2:504:PHE:CE2	2.72	0.72
5:4:180:THR:OG1	5:4:214:LYS:HG3	1.88	0.72
8:7:370:LEU:CD2	8:7:395:VAL:HB	2.19	0.72
2:2:43:ALA:O	2:2:47:ILE:CD1	2.36	0.72
3:0:143:ARG:O	3:0:147:GLU:OE1	2.07	0.72
3:0:416:PHE:HE1	3:0:439:CYS:SG	2.12	0.72
3:0:506:ILE:HD12	3:0:522:TYR:CE1	2.24	0.72
6:6:268:ALA:O	6:6:290:ILE:CD1	2.38	0.72
3:0:424:GLU:CB	3:0:432:ASN:ND2	2.53	0.72
8:7:403:ILE:CD1	8:7:484:PHE:HB2	2.18	0.72
8:7:552:VAL:HG12	8:7:731:TYR:HB3	1.72	0.72
8:7:568:GLU:CD	8:7:571:ARG:HH21	1.92	0.72
8:7:678:GLY:O	8:7:682:GLN:OE1	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:27:LYS:HZ2	1:3:29:LEU:CB	2.03	0.72
3:0:634:ILE:HG13	3:0:635:LEU:HD12	1.72	0.72
6:6:145:ARG:O	6:6:149:ILE:CD1	2.37	0.72
6:6:281:ASN:OD1	6:6:287:PHE:CE2	2.42	0.72
8:7:559:CYS:HB2	8:7:710:SER:HA	1.72	0.72
3:0:25:MET:HE3	3:0:51:SER:HB2	1.71	0.72
3:0:528:GLU:OE2	3:0:710:THR:OG1	2.07	0.72
3:0:614:HIS:HE1	3:0:675:ASP:CA	1.77	0.72
4:1:389:LEU:HD23	4:1:389:LEU:O	1.90	0.72
6:6:150:ILE:CG2	6:6:200:ARG:HG2	2.16	0.72
8:7:571:ARG:NH1	8:7:572:GLU:CG	2.52	0.72
8:7:666:GLU:OE2	8:7:692:ARG:NH1	2.23	0.72
3:0:396:PHE:HA	3:0:399:LEU:HD13	1.71	0.72
3:0:590:CYS:SG	3:0:596:ALA:HB3	2.29	0.72
3:0:633:ARG:HH11	3:0:636:LYS:HE2	1.54	0.72
8:7:393:THR:O	8:7:397:ILE:HG13	1.90	0.72
3:0:83:LEU:O	3:0:86:LEU:HG	1.90	0.71
3:0:220:GLU:CD	3:0:221:ARG:HG3	2.11	0.71
3:0:270:ARG:NH2	3:0:388:LEU:O	2.23	0.71
3:0:506:ILE:HD12	3:0:522:TYR:HE1	1.53	0.71
4:1:375:LEU:O	4:1:378:MET:SD	2.48	0.71
2:2:15:GLU:HA	2:2:84:LEU:HG	1.72	0.71
2:2:19:GLN:CA	2:2:22:GLN:OE1	2.37	0.71
3:0:117:HIS:HE1	3:0:119:GLU:HB3	1.55	0.71
5:4:258:LEU:HB3	5:4:260:PRO:HD3	1.71	0.71
6:6:155:ASP:HB3	6:6:298:LYS:HZ1	1.51	0.71
8:7:641:GLN:HA	8:7:644:GLN:HG2	1.72	0.71
2:2:56:GLU:OE2	2:2:97:MET:HE1	1.89	0.71
2:2:193:LEU:CA	2:2:395:GLN:NE2	2.53	0.71
1:3:27:LYS:NZ	1:3:29:LEU:CA	2.51	0.71
8:7:498:PHE:CE1	8:7:502:VAL:HG11	2.24	0.71
9:N:77:DG:H2"	9:N:78:DA:C8	2.25	0.71
2:2:18:PRO:O	2:2:22:GLN:OE1	2.07	0.71
3:0:2:LYS:HB2	3:0:96:GLU:OE2	1.91	0.71
7:5:27:MET:SD	7:5:27:MET:O	2.48	0.71
8:7:568:GLU:HA	8:7:571:ARG:HG3	1.71	0.71
8:7:571:ARG:NH2	8:7:580:LEU:CD1	2.53	0.71
2:2:475:ALA:CB	2:2:481:LEU:HG	2.14	0.71
3:0:741:TYR:CB	3:0:742:GLU:OE1	2.39	0.71
4:1:334:LYS:CD	4:1:336:ILE:HD12	2.21	0.71
2:2:11:THR:HG22	2:2:38:ILE:HG21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:41:GLU:HB3	3:0:482:SER:HA	1.71	0.71
3:0:633:ARG:HD3	3:0:636:LYS:CE	2.20	0.71
8:7:490:VAL:C	8:7:519:ARG:HH22	1.93	0.71
8:7:491:HIS:CA	8:7:519:ARG:CZ	2.67	0.71
8:7:675:SER:HB3	8:7:715:GLU:OE2	1.90	0.71
1:3:44:ASP:HA	1:3:47:PHE:CZ	2.24	0.71
2:2:364:VAL:HA	2:2:382:SER:HB3	1.72	0.71
3:0:275:ARG:NH1	3:0:276:LYS:NZ	2.39	0.71
4:1:255:LYS:O	4:1:259:ILE:HG12	1.89	0.71
8:7:459:MET:HE3	8:7:470:SER:C	2.11	0.71
9:N:61:DG:H2"	9:N:62:DT:C6	2.26	0.71
3:0:715:SER:CA	3:0:718:LYS:HZ1	2.04	0.71
8:7:754:ARG:O	8:7:757:ARG:NE	2.23	0.71
3:0:519:VAL:HG11	3:0:553:MET:CE	2.21	0.71
3:0:607:SER:O	3:0:668:ARG:NH2	2.24	0.71
6:6:268:ALA:O	6:6:290:ILE:HD13	1.89	0.71
7:5:25:ALA:HA	7:5:29:ASP:OD1	1.91	0.71
8:7:664:LEU:CD2	8:7:689:ARG:HH11	2.03	0.71
3:0:275:ARG:HH11	3:0:276:LYS:NZ	1.89	0.70
3:0:570:LEU:N	3:0:597:ILE:O	2.24	0.70
3:0:741:TYR:HB3	3:0:742:GLU:OE1	1.91	0.70
4:1:510:ASN:HB3	5:4:264:LYS:HD2	1.73	0.70
5:4:60:PHE:CZ	5:4:253:PHE:CE1	2.79	0.70
6:6:154:ILE:HD11	6:6:196:LEU:HB2	1.72	0.70
6:6:224:VAL:CA	6:6:230:ARG:HH21	2.03	0.70
6:6:426:ARG:NH1	6:6:435:GLU:CA	2.54	0.70
8:7:341:TYR:CE1	8:7:509:ALA:CB	2.74	0.70
1:3:32:PRO:CD	1:3:69:LYS:NZ	2.45	0.70
2:2:56:GLU:CD	2:2:97:MET:HE2	2.11	0.70
3:0:166:GLU:O	3:0:198:ARG:NH1	2.25	0.70
3:0:188:LYS:O	3:0:190:LEU:HD22	1.91	0.70
4:1:334:LYS:HD2	4:1:336:ILE:HD12	1.73	0.70
1:3:114:GLU:O	3:0:330:HIS:CE1	2.36	0.70
3:0:395:ASP:OD2	3:0:396:PHE:CZ	2.44	0.70
6:6:270:VAL:N	6:6:288:TYR:OH	2.24	0.70
6:6:426:ARG:NH1	6:6:435:GLU:CB	2.54	0.70
1:3:53:GLN:HA	1:3:63:LEU:H	1.56	0.70
2:2:399:TYR:O	2:2:403:HIS:N	2.22	0.70
6:6:165:PRO:HB2	6:6:375:HIS:CD2	2.26	0.70
8:7:617:GLU:OE2	8:7:621:LYS:NZ	2.22	0.70
6:6:172:ILE:HA	6:6:181:LEU:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:66:DA:H2'	9:N:67:DT:H72	1.73	0.70
3:0:155:LEU:CD1	3:0:160:GLU:HG2	2.22	0.70
3:0:310:PRO:HG3	3:0:404:THR:HA	1.73	0.70
3:0:443:SER:HB3	3:0:473:LEU:HA	1.72	0.70
6:6:174:MET:HE3	6:6:208:PRO:HB3	1.73	0.70
3:0:625:ILE:HG23	3:0:627:PHE:CD1	2.26	0.70
6:6:281:ASN:HD21	6:6:287:PHE:HD2	1.39	0.70
5:4:154:SER:HA	5:4:157:LEU:HD12	1.74	0.70
8:7:406:SER:HG	8:7:480:ARG:HE	1.38	0.70
3:0:614:HIS:HE1	3:0:674:ASP:O	1.69	0.70
6:6:126:LEU:HD23	6:6:169:MET:HE1	1.73	0.70
2:2:454:TYR:N	7:5:9:LEU:O	2.25	0.70
5:4:176:LEU:HG	5:4:210:ILE:HG12	1.72	0.70
6:6:168:GLN:OE1	6:6:186:SER:C	2.30	0.70
8:7:385:VAL:HG12	8:7:514:THR:CB	2.22	0.70
9:N:75:DG:H2"	9:N:76:DT:C6	2.26	0.70
2:2:56:GLU:CD	2:2:97:MET:CE	2.60	0.69
2:2:386:ALA:HB1	2:2:391:ILE:HB	1.75	0.69
3:0:43:PRO:HG3	3:0:696:TRP:CZ3	2.27	0.69
3:0:104:ARG:HH21	3:0:173:LYS:HA	1.55	0.69
3:0:286:TYR:O	3:0:326:ARG:NH1	2.24	0.69
8:7:465:ASN:ND2	8:7:474:MET:HE2	2.07	0.69
8:7:754:ARG:CA	8:7:757:ARG:CD	2.68	0.69
2:2:185:THR:O	2:2:189:PHE:N	2.19	0.69
2:2:414:GLU:HG3	2:2:415:LYS:HG3	1.72	0.69
2:2:431:GLN:OE1	2:2:435:PRO:CD	2.40	0.69
3:0:405:PHE:HE1	3:0:409:ILE:HD13	1.54	0.69
3:0:519:VAL:HG21	3:0:553:MET:HE3	1.74	0.69
3:0:633:ARG:CG	3:0:636:LYS:HE3	2.23	0.69
3:0:275:ARG:HH11	3:0:276:LYS:HE3	1.58	0.69
3:0:188:LYS:CB	3:0:190:LEU:HD23	2.21	0.69
3:0:333:SER:O	3:0:337:ARG:HD2	1.92	0.69
8:7:647:ASP:O	8:7:650:ASN:ND2	2.25	0.69
1:3:38:ILE:HD11	1:3:42:CYS:HB3	1.74	0.69
2:2:353:SER:HB2	2:2:356:GLN:CG	2.22	0.69
6:6:363:CYS:N	6:6:368:LEU:O	2.22	0.69
7:5:19:LEU:CD1	8:7:566:TYR:OH	2.39	0.69
8:7:599:GLU:OE2	8:7:624:LYS:NZ	2.24	0.69
1:3:45:ARG:CZ	1:3:46:ILE:CG1	2.70	0.69
2:2:365:HIS:NE2	2:2:377:GLN:O	2.26	0.69
2:2:490:LYS:HD3	7:5:35:LEU:HD22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:341:TYR:CZ	3:0:363:LEU:HD13	2.27	0.69
3:0:711:ASP:OD1	3:0:712:MET:N	2.26	0.69
8:7:339:GLU:O	8:7:380:ARG:NH1	2.25	0.69
8:7:494:PRO:HG2	8:7:497:MET:HE3	1.70	0.69
8:7:568:GLU:O	8:7:571:ARG:HG3	1.92	0.69
3:0:472:MET:HG3	3:0:473:LEU:CG	2.18	0.69
4:1:511:ALA:HB2	5:4:264:LYS:CE	2.23	0.69
4:1:606:GLU:HA	4:1:609:SER:OG	1.91	0.69
5:4:255:ASP:OD1	5:4:259:ARG:HD2	1.92	0.69
8:7:369:SER:HA	8:7:372:LYS:HD2	1.74	0.69
1:3:65:LYS:HG2	1:3:66:ASN:N	2.05	0.69
2:2:54:GLU:OE2	2:2:109:ARG:NH2	2.25	0.69
3:0:11:LEU:HD21	3:0:97:LEU:HG	1.74	0.69
3:0:569:ILE:C	3:0:570:LEU:HD12	2.12	0.69
4:1:204:LEU:HD12	4:1:205:PRO:HD2	1.74	0.69
5:4:249:ALA:HA	5:4:253:PHE:CE2	2.27	0.69
5:4:273:ARG:HH12	6:6:372:LEU:CB	2.03	0.69
6:6:432:CYS:HB3	6:6:454:CYS:SG	2.33	0.69
8:7:376:ASN:N	8:7:380:ARG:HH22	1.91	0.69
8:7:639:ILE:O	8:7:643:PHE:HB2	1.93	0.69
8:7:692:ARG:HG2	8:7:692:ARG:HH11	1.58	0.69
9:N:52:DA:H2'	9:N:53:DT:H72	1.73	0.69
3:0:670:LEU:CA	3:0:675:ASP:OD2	2.38	0.69
5:4:60:PHE:CZ	5:4:253:PHE:HE1	2.10	0.69
8:7:567:GLN:HA	8:7:570:LEU:HB3	1.74	0.69
8:7:675:SER:CB	8:7:722:ARG:HH22	2.04	0.69
2:2:468:TYR:CE2	2:2:486:ASP:OD2	2.45	0.69
2:2:468:TYR:CG	2:2:486:ASP:OD1	2.46	0.69
3:0:25:MET:SD	3:0:55:LEU:HB2	2.33	0.69
8:7:356:LEU:CG	8:7:404:LYS:NZ	2.55	0.69
8:7:465:ASN:HB3	8:7:471:GLN:HE22	1.56	0.69
2:2:56:GLU:HG2	2:2:97:MET:SD	2.32	0.68
3:0:525:MET:O	3:0:528:GLU:HG2	1.93	0.68
8:7:418:MET:CE	8:7:441:ASP:OD2	2.41	0.68
8:7:445:MET:HE1	8:7:449:GLU:N	2.08	0.68
8:7:625:PRO:HG2	8:7:649:ILE:HD11	1.75	0.68
2:2:62:LEU:HA	2:2:65:TRP:HD1	1.58	0.68
2:2:176:VAL:O	2:2:181:GLU:N	2.25	0.68
2:2:346:LYS:NZ	2:2:376:GLY:O	2.26	0.68
3:0:469:TYR:HA	3:0:472:MET:HG2	1.75	0.68
8:7:215:GLY:O	8:7:219:SER:N	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:376:ASN:OD1	8:7:380:ARG:NH2	2.26	0.68
3:0:117:HIS:HD2	3:0:156:CYS:HA	1.59	0.68
3:0:528:GLU:HG3	3:0:714:ILE:CD1	2.24	0.68
5:4:28:VAL:HB	5:4:75:VAL:HG22	1.75	0.68
5:4:40:PHE:HA	5:4:43:GLU:OE2	1.93	0.68
6:6:336:CYS:HB3	6:6:341:LYS:H	1.58	0.68
8:7:354:ILE:HG12	8:7:452:LEU:HD21	1.76	0.68
2:2:346:LYS:NZ	2:2:347:ILE:O	2.22	0.68
2:2:353:SER:N	2:2:356:GLN:NE2	2.42	0.68
3:0:208:TYR:HE1	3:0:213:LEU:HB2	1.57	0.68
3:0:633:ARG:CD	3:0:636:LYS:HE3	2.24	0.68
8:7:351:ASP:OD1	8:7:405:LYS:HE3	1.93	0.68
2:2:468:TYR:CE1	2:2:486:ASP:OD1	2.47	0.68
2:2:500:GLN:O	2:2:504:PHE:HD2	1.75	0.68
3:0:112:LYS:HG2	4:1:345:ASP:HB3	1.73	0.68
3:0:279:SER:O	3:0:283:GLN:OE1	2.11	0.68
6:6:165:PRO:HG2	6:6:375:HIS:CD2	2.28	0.68
3:0:522:TYR:HA	3:0:525:MET:CE	2.22	0.68
4:1:479:UNK:O	4:1:483:UNK:N	2.27	0.68
4:1:510:ASN:ND2	5:4:265:PRO:O	2.20	0.68
8:7:491:HIS:N	8:7:519:ARG:NH2	2.41	0.68
8:7:544:SER:CB	8:7:549:ILE:HB	2.23	0.68
8:7:548:HIS:CE1	8:7:695:ARG:NH2	2.59	0.68
2:2:67:ASN:ND2	5:4:260:PRO:O	2.26	0.68
3:0:237:ALA:HA	3:0:240:ILE:HD11	1.76	0.68
3:0:742:GLU:OE1	3:0:742:GLU:N	2.26	0.68
8:7:403:ILE:HD11	8:7:484:PHE:CB	2.24	0.68
8:7:425:LEU:HD12	8:7:430:LEU:HD23	1.76	0.68
8:7:459:MET:CE	8:7:470:SER:C	2.62	0.68
10:T:89:DC:H2"	10:T:90:DA:C8	2.29	0.68
2:2:75:GLN:HA	2:2:78:ILE:HG12	1.75	0.68
3:0:90:MET:CE	3:0:101:GLU:HG3	2.24	0.68
2:2:468:TYR:CZ	2:2:486:ASP:OD1	2.47	0.68
5:4:162:ARG:O	5:4:166:GLU:HG3	1.94	0.68
8:7:589:GLN:CB	8:7:745:ILE:HD11	2.24	0.68
8:7:641:GLN:NE2	8:7:645:TYR:CG	2.61	0.68
2:2:484:LYS:HA	2:2:491:PHE:HB3	1.76	0.68
3:0:625:ILE:HD12	3:0:626:PRO:HD2	1.76	0.68
7:5:19:LEU:HD23	7:5:22:GLN:NE2	2.09	0.68
8:7:446:PHE:CD2	8:7:472:LYS:HD2	2.29	0.68
8:7:598:HIS:HB2	8:7:605:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:103:DC:H2"	10:T:104:DA:C8	2.29	0.68
2:2:15:GLU:CA	2:2:84:LEU:HG	2.24	0.67
3:0:102:ASP:HA	3:0:173:LYS:NZ	2.09	0.67
3:0:625:ILE:HG23	3:0:627:PHE:HD1	1.57	0.67
6:6:144:ASN:OD1	6:6:147:ALA:N	2.26	0.67
8:7:356:LEU:CG	8:7:404:LYS:HZ3	2.08	0.67
2:2:56:GLU:O	2:2:97:MET:HE2	1.91	0.67
3:0:90:MET:HE2	3:0:101:GLU:OE2	1.94	0.67
3:0:714:ILE:C	3:0:718:LYS:HZ3	1.97	0.67
8:7:707:SER:OG	8:7:722:ARG:NH1	2.27	0.67
2:2:410:ARG:HA	2:2:413:GLU:CG	2.23	0.67
5:4:201:PHE:HE1	6:6:374:THR:HB	1.59	0.67
6:6:310:VAL:HG13	6:6:311:ASN:N	2.09	0.67
8:7:410:LEU:N	8:7:486:ILE:O	2.24	0.67
8:7:551:ASN:HB3	8:7:701:PHE:HA	1.75	0.67
8:7:641:GLN:CD	8:7:644:GLN:HE21	1.98	0.67
2:2:468:TYR:HH	2:2:484:LYS:HD3	1.60	0.67
4:1:195:PHE:CZ	4:1:210:TRP:CH2	2.83	0.67
6:6:452:PRO:O	6:6:456:SER:N	2.24	0.67
8:7:675:SER:HB3	8:7:715:GLU:CD	2.15	0.67
3:0:342:LEU:HD11	3:0:402:ILE:HD11	1.77	0.67
3:0:424:GLU:N	3:0:432:ASN:OD1	2.26	0.67
8:7:457:TYR:CZ	8:7:490:VAL:CG2	2.77	0.67
9:N:70:DA:C2'	9:N:71:DT:H71	2.25	0.67
9:N:77:DG:H2"	9:N:78:DA:H8	1.60	0.67
7:5:9:LEU:HD21	7:5:11:GLN:NE2	2.09	0.67
8:7:598:HIS:HB3	8:7:603:ASP:HB2	1.77	0.67
3:0:16:LYS:HB3	3:0:741:TYR:CE1	2.25	0.67
3:0:310:PRO:CB	3:0:404:THR:HG23	2.23	0.67
3:0:259:ARG:CG	3:0:262:ARG:HH22	2.04	0.67
3:0:318:THR:HG23	3:0:376:PHE:HZ	1.60	0.67
5:4:163:ILE:HG23	5:4:166:GLU:OE2	1.94	0.67
8:7:356:LEU:CD1	8:7:404:LYS:NZ	2.50	0.67
8:7:383:ILE:HG21	8:7:528:ASN:HD21	1.56	0.67
8:7:446:PHE:CG	8:7:472:LYS:HE3	2.28	0.67
8:7:613:TYR:HB3	8:7:766:LYS:HG2	1.74	0.67
1:3:72:ILE:HD11	1:3:74:ASP:OD2	1.94	0.67
2:2:408:MET:HE3	2:2:411:LEU:CB	2.25	0.67
3:0:24:TYR:HD2	3:0:25:MET:HE3	1.59	0.67
3:0:251:ASP:H	4:1:350:ARG:CG	2.07	0.67
3:0:356:PRO:HG2	3:0:413:GLU:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:492:PHE:CE2	3:0:700:GLY:HA3	2.29	0.67
5:4:249:ALA:HA	5:4:253:PHE:CZ	2.30	0.67
8:7:754:ARG:C	8:7:757:ARG:NE	2.48	0.67
3:0:133:CYS:SG	12:0:801:SF4:FE3	1.87	0.66
3:0:493:LEU:CD2	3:0:495:MET:HE1	2.10	0.66
5:4:271:ASP:OD2	5:4:273:ARG:NH1	2.27	0.66
6:6:224:VAL:HG13	6:6:228:CYS:CB	2.24	0.66
7:5:32:LEU:HB3	7:5:41:LEU:HG	1.77	0.66
2:2:75:GLN:CD	2:2:78:ILE:HD11	2.16	0.66
2:2:468:TYR:HE2	2:2:484:LYS:HZ3	1.44	0.66
3:0:101:GLU:CG	3:0:103:PHE:HB3	2.25	0.66
3:0:155:LEU:HD11	3:0:160:GLU:CD	2.16	0.66
3:0:504:VAL:O	3:0:506:ILE:HG23	1.95	0.66
3:0:725:ALA:HB1	6:6:290:ILE:HD11	1.76	0.66
5:4:235:TYR:CE2	5:4:237:HIS:HB2	2.29	0.66
6:6:234:ILE:HB	6:6:263:VAL:HG23	1.77	0.66
2:2:75:GLN:OE1	2:2:78:ILE:HD11	1.94	0.66
3:0:334:PHE:HD1	3:0:337:ARG:HE	1.43	0.66
7:5:51:LYS:HZ3	7:5:54:LEU:CD2	2.06	0.66
8:7:568:GLU:CD	8:7:571:ARG:NH2	2.48	0.66
9:N:53:DT:H2"	9:N:54:DT:C6	2.30	0.66
1:3:45:ARG:NE	1:3:46:ILE:HG13	2.11	0.66
5:4:213:VAL:HA	5:4:236:LEU:HB2	1.77	0.66
7:5:42:VAL:HG11	7:5:47:VAL:CG2	2.25	0.66
3:0:619:THR:HA	3:0:678:VAL:HB	1.78	0.66
4:1:558:CYS:SG	4:1:559:GLU:N	2.69	0.66
8:7:446:PHE:CE1	8:7:472:LYS:NZ	2.63	0.66
8:7:447:GLN:HA	8:7:476:PHE:CE1	2.28	0.66
2:2:468:TYR:CD1	2:2:486:ASP:OD1	2.49	0.66
3:0:77:SER:CA	3:0:80:GLU:OE1	2.38	0.66
3:0:167:VAL:CA	3:0:198:ARG:CZ	2.71	0.66
3:0:521:ASN:O	3:0:525:MET:SD	2.54	0.66
4:1:204:LEU:HD23	4:1:209:PHE:HB2	1.77	0.66
5:4:79:TYR:N	5:4:82:GLY:O	2.28	0.66
5:4:137:LYS:HG3	5:4:139:GLN:HG3	1.77	0.66
6:6:310:VAL:CG1	6:6:311:ASN:H	2.08	0.66
8:7:469:ASP:HA	8:7:472:LYS:HB3	1.77	0.66
8:7:752:SER:OG	8:7:755:GLU:HG3	1.96	0.66
9:N:56:DA:C2'	9:N:57:DT:H71	2.25	0.66
2:2:56:GLU:HG3	2:2:97:MET:HG3	1.78	0.66
2:2:137:GLU:N	2:2:286:ARG:NH1	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:243:SER:O	2:2:247:ARG:N	2.25	0.66
6:6:178:LEU:CD2	6:6:180:GLN:NE2	2.59	0.66
7:5:66:MET:HA	8:7:717:TYR:HE2	1.60	0.66
8:7:670:LEU:O	8:7:706:TYR:N	2.28	0.66
2:2:86:LEU:O	2:2:101:ASN:N	2.25	0.66
3:0:33:ASP:OD1	3:0:34:VAL:N	2.28	0.66
3:0:117:HIS:CE1	3:0:119:GLU:HB3	2.30	0.66
3:0:722:ARG:HH21	6:6:292:LEU:HB2	1.59	0.66
4:1:280:GLU:O	4:1:284:TRP:HB2	1.94	0.66
9:N:67:DT:H2"	9:N:68:DT:C6	2.30	0.66
2:2:475:ALA:HB3	2:2:481:LEU:CD1	2.25	0.66
3:0:371:ARG:NH1	3:0:375:ARG:HH12	1.94	0.66
3:0:703:ASP:CA	3:0:706:LEU:HD23	2.26	0.66
6:6:166:ILE:HD11	6:6:375:HIS:CB	2.22	0.66
8:7:576:LYS:HZ1	8:7:764:LEU:HA	1.61	0.66
1:3:102:ASP:O	1:3:106:TYR:N	2.29	0.65
3:0:49:THR:O	3:0:53:LEU:HG	1.96	0.65
3:0:492:PHE:HD2	3:0:494:PRO:HD3	1.60	0.65
3:0:534:PRO:HA	6:6:239:LEU:HD12	1.77	0.65
4:1:204:LEU:HG	4:1:205:PRO:O	1.95	0.65
5:4:125:LEU:HA	5:4:128:GLU:OE1	1.95	0.65
6:6:211:GLN:HB3	6:6:244:PRO:HD2	1.75	0.65
8:7:362:ILE:HD11	8:7:367:GLU:HB3	1.78	0.65
8:7:567:GLN:O	8:7:571:ARG:N	2.29	0.65
2:2:496:GLU:O	2:2:499:SER:N	2.29	0.65
3:0:16:LYS:CB	3:0:741:TYR:HE1	2.10	0.65
3:0:614:HIS:CE1	3:0:674:ASP:C	2.68	0.65
6:6:281:ASN:ND2	6:6:287:PHE:HD2	1.93	0.65
8:7:341:TYR:N	8:7:379:ALA:O	2.29	0.65
8:7:356:LEU:HB2	8:7:404:LYS:HE3	1.77	0.65
8:7:675:SER:CA	8:7:722:ARG:HH22	2.07	0.65
7:5:25:ALA:HA	7:5:29:ASP:CG	2.16	0.65
9:N:56:DA:H2'	9:N:57:DT:H71	1.78	0.65
8:7:754:ARG:CA	8:7:757:ARG:HH11	2.08	0.65
1:3:72:ILE:HG13	1:3:74:ASP:OD1	1.95	0.65
2:2:56:GLU:CG	2:2:97:MET:HE2	2.26	0.65
3:0:104:ARG:NH1	3:0:170:TYR:HD2	1.94	0.65
3:0:537:MET:CG	3:0:619:THR:OG1	2.44	0.65
3:0:572:GLU:OE2	3:0:600:SER:CB	2.31	0.65
8:7:428:CYS:SG	8:7:429:THR:N	2.69	0.65
8:7:592:GLN:HE22	8:7:747:ASN:HB3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:354:GLU:HB3	3:0:359:PHE:CD2	2.32	0.65
3:0:539:VAL:HG12	3:0:621:LEU:HB2	1.77	0.65
3:0:541:PHE:N	3:0:600:SER:O	2.30	0.65
3:0:692:GLN:OE1	3:0:692:GLN:N	2.29	0.65
8:7:580:LEU:HD23	8:7:583:MET:CE	2.27	0.65
3:0:143:ARG:O	3:0:146:GLU:HG2	1.97	0.65
3:0:254:THR:HA	3:0:257:LEU:CD1	2.23	0.65
4:1:181:GLN:O	4:1:185:LEU:HD23	1.97	0.65
4:1:561:LEU:O	4:1:565:ALA:N	2.22	0.65
5:4:40:PHE:HA	5:4:43:GLU:OE1	1.96	0.65
8:7:587:LYS:HD3	8:7:673:ILE:HD12	1.78	0.65
3:0:24:TYR:CD2	3:0:25:MET:CE	2.80	0.65
3:0:256:ALA:HA	3:0:259:ARG:HD3	1.79	0.65
5:4:58:ILE:O	5:4:62:ASN:ND2	2.30	0.65
5:4:293:LEU:HD12	6:6:376:LEU:CD2	2.26	0.65
6:6:175:ARG:NH2	6:6:203:GLU:O	2.30	0.65
6:6:426:ARG:HH22	6:6:435:GLU:CB	2.10	0.65
2:2:62:LEU:HA	2:2:65:TRP:CD1	2.32	0.65
3:0:52:LEU:O	3:0:56:THR:HG23	1.97	0.65
5:4:162:ARG:O	5:4:166:GLU:CG	2.45	0.65
5:4:193:TYR:O	5:4:197:MET:SD	2.55	0.65
5:4:292:CYS:HB2	5:4:308:CYS:SG	2.35	0.65
8:7:356:LEU:O	8:7:356:LEU:HD23	1.97	0.65
9:N:64:DA:H61	10:T:102:DT:H73	1.60	0.65
2:2:475:ALA:HB1	2:2:481:LEU:CG	2.17	0.65
3:0:101:GLU:HG2	3:0:103:PHE:HB3	1.79	0.65
3:0:162:LEU:HD11	3:0:198:ARG:CD	2.26	0.65
3:0:492:PHE:HE2	3:0:700:GLY:HA3	1.62	0.65
5:4:193:TYR:CE1	5:4:197:MET:SD	2.90	0.65
8:7:445:MET:SD	8:7:445:MET:O	2.55	0.65
3:0:313:PRO:O	3:0:314:GLN:HG2	1.97	0.64
3:0:502:ASP:CG	3:0:504:VAL:HG23	2.17	0.64
3:0:730:PRO:HB2	3:0:732:ASP:OD1	1.97	0.64
4:1:214:ILE:HG23	4:1:215:PRO:HD3	1.79	0.64
8:7:556:GLU:HG2	8:7:707:SER:HB3	1.80	0.64
8:7:668:THR:OG1	8:7:694:LYS:NZ	2.22	0.64
3:0:42:MET:HB3	3:0:48:LYS:CE	2.27	0.64
3:0:553:MET:SD	3:0:554:TRP:CD1	2.91	0.64
8:7:465:ASN:CB	8:7:471:GLN:HE21	2.06	0.64
8:7:577:ARG:HH11	8:7:714:GLN:HB2	1.62	0.64
9:N:70:DA:H2'	9:N:71:DT:H71	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:401:GLU:HG3	2:2:433:LEU:HD13	1.78	0.64
3:0:539:VAL:CG1	3:0:621:LEU:HB2	2.26	0.64
3:0:611:ASP:HA	3:0:668:ARG:HD2	1.79	0.64
7:5:51:LYS:HZ3	7:5:54:LEU:HD21	1.62	0.64
8:7:408:ILE:CD1	8:7:410:LEU:HD11	2.25	0.64
8:7:631:THR:HB	8:7:633:GLN:NE2	2.13	0.64
8:7:631:THR:C	8:7:633:GLN:NE2	2.51	0.64
3:0:252:LEU:HB2	3:0:435:MET:HB2	1.78	0.64
3:0:295:SER:HA	3:0:298:ILE:HG22	1.80	0.64
3:0:639:LEU:HD22	3:0:642:MET:CE	2.22	0.64
5:4:29:ILE:O	5:4:179:LEU:N	2.30	0.64
5:4:40:PHE:HA	5:4:43:GLU:CD	2.17	0.64
10:T:88:DT:H2'	10:T:89:DC:C6	2.32	0.64
10:T:93:DT:H2"	10:T:94:DC:C6	2.32	0.64
10:T:110:DT:H2"	10:T:111:DC:C5	2.32	0.64
1:3:114:GLU:CB	3:0:330:HIS:CE1	2.81	0.64
3:0:339:ILE:C	3:0:343:LYS:HZ3	2.01	0.64
4:1:325:UNK:C	4:1:329:LEU:HD23	2.27	0.64
4:1:510:ASN:OD1	4:1:513:GLN:NE2	2.30	0.64
2:2:108:LEU:O	2:2:112:LEU:HD23	1.97	0.64
3:0:113:ASN:OD1	3:0:114:LEU:HG	1.97	0.64
3:0:715:SER:N	3:0:718:LYS:NZ	2.46	0.64
5:4:235:TYR:HD2	5:4:266:ASN:HB2	1.62	0.64
6:6:247:ILE:HG23	6:6:248:HIS:ND1	2.13	0.64
6:6:303:GLU:OE1	6:6:303:GLU:N	2.31	0.64
10:T:96:DT:H2"	10:T:97:DC:C5	2.32	0.64
3:0:11:LEU:HD21	3:0:97:LEU:CD1	2.28	0.64
3:0:41:GLU:OE2	3:0:696:TRP:CZ3	2.50	0.64
3:0:351:VAL:HG23	3:0:421:GLU:HG2	1.78	0.64
8:7:477:LEU:HB3	8:7:505:ILE:HD12	1.80	0.64
8:7:664:LEU:CG	8:7:689:ARG:CG	2.68	0.64
2:2:31:THR:O	2:2:35:ILE:HG12	1.98	0.64
3:0:30:LYS:O	3:0:33:ASP:OD1	2.16	0.64
3:0:287:GLU:C	3:0:290:VAL:HG12	2.18	0.64
6:6:286:SER:O	6:6:289:LYS:NZ	2.29	0.64
8:7:664:LEU:CD2	8:7:689:ARG:HD2	2.26	0.64
8:7:754:ARG:CA	8:7:757:ARG:NE	2.60	0.64
2:2:72:LEU:HD12	2:2:73:GLN:HG3	1.80	0.64
3:0:5:ILE:HD13	3:0:22:TYR:CZ	2.33	0.64
6:6:133:SER:HB2	6:6:206:GLY:O	1.98	0.64
6:6:236:PHE:CZ	6:6:238:SER:OG	2.51	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:552:VAL:HG11	8:7:731:TYR:CG	2.33	0.64
10:T:86:DC:H2"	10:T:87:DA:C8	2.33	0.64
1:3:32:PRO:HG3	1:3:69:LYS:HZ1	1.62	0.64
3:0:104:ARG:NH2	3:0:173:LYS:HD2	2.09	0.64
3:0:294:HIS:CE1	3:0:297:ASP:HB3	2.32	0.64
3:0:621:LEU:HG	3:0:680:VAL:HG22	1.77	0.64
3:0:745:ILE:HG13	3:0:746:LYS:N	2.13	0.64
5:4:193:TYR:HA	5:4:196:ILE:HD12	1.80	0.64
8:7:461:ALA:HB3	8:7:497:MET:HB3	1.80	0.64
8:7:699:GLU:HG3	8:7:701:PHE:H	1.62	0.64
2:2:273:LYS:HE2	2:2:277:MET:HE2	1.80	0.63
3:0:79:ILE:CG2	3:0:207:ILE:HD12	2.15	0.63
3:0:109:THR:HG23	3:0:113:ASN:OD1	1.98	0.63
3:0:622:MET:HE1	3:0:662:ALA:HA	1.80	0.63
3:0:638:ARG:O	3:0:642:MET:HG3	1.98	0.63
6:6:163:GLN:HE21	6:6:305:VAL:HG11	1.63	0.63
6:6:199:ILE:HG22	6:6:202:GLN:HE21	1.63	0.63
8:7:375:GLY:HA3	8:7:380:ARG:CZ	2.29	0.63
8:7:571:ARG:HD2	8:7:572:GLU:HB3	1.78	0.63
9:N:68:DT:H1'	9:N:69:DG:C8	2.33	0.63
3:0:144:LYS:CA	3:0:147:GLU:OE2	2.40	0.63
3:0:571:VAL:HG22	3:0:572:GLU:N	2.12	0.63
3:0:572:GLU:CD	3:0:600:SER:HA	2.18	0.63
5:4:136:GLU:OE1	5:4:136:GLU:N	2.30	0.63
8:7:447:GLN:HA	8:7:476:PHE:CE2	2.34	0.63
8:7:568:GLU:HG3	8:7:577:ARG:HG3	1.80	0.63
8:7:613:TYR:HB2	8:7:766:LYS:CG	2.22	0.63
1:3:31:ASN:ND2	1:3:64:ARG:H	1.95	0.63
4:1:283:PHE:HD1	4:1:284:TRP:CD1	2.16	0.63
6:6:224:VAL:HB	6:6:230:ARG:HE	1.62	0.63
8:7:666:GLU:CD	8:7:693:ALA:O	2.37	0.63
10:T:107:DT:H2"	10:T:108:DC:C6	2.33	0.63
1:3:52:ALA:O	1:3:63:LEU:N	2.32	0.63
2:2:454:TYR:HE2	7:5:11:GLN:CB	2.11	0.63
3:0:314:GLN:HA	3:0:317:LEU:HD13	1.81	0.63
8:7:458:SER:O	8:7:462:ASN:HB2	1.98	0.63
8:7:490:VAL:C	8:7:519:ARG:NH2	2.52	0.63
8:7:544:SER:CA	8:7:549:ILE:O	2.46	0.63
8:7:605:ILE:HD12	8:7:650:ASN:O	1.98	0.63
1:3:27:LYS:HZ2	1:3:29:LEU:HD23	1.63	0.63
3:0:188:LYS:O	3:0:190:LEU:CD2	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:519:VAL:HG13	3:0:554:TRP:NE1	2.12	0.63
3:0:572:GLU:HG3	3:0:599:LEU:O	1.99	0.63
6:6:178:LEU:HD23	6:6:179:ALA:N	2.14	0.63
1:3:13:CYS:SG	1:3:38:ILE:HG13	2.38	0.63
3:0:663:ALA:HA	3:0:666:LEU:HD12	1.81	0.63
8:7:433:GLU:OE2	8:7:434:ASN:CG	2.37	0.63
8:7:562:THR:HB	8:7:756:ARG:HH11	1.63	0.63
8:7:591:CYS:HA	8:7:594:LEU:HD12	1.80	0.63
2:2:39:LEU:HD13	2:2:47:ILE:HD13	1.81	0.63
3:0:336:LYS:HA	3:0:339:ILE:HG22	1.81	0.63
3:0:703:ASP:HA	3:0:706:LEU:CD2	2.28	0.63
6:6:116:THR:H	6:6:117:PRO:HD3	1.61	0.63
7:5:9:LEU:HD21	7:5:11:GLN:HE21	1.64	0.63
8:7:356:LEU:HD12	8:7:404:LYS:HE2	1.81	0.63
8:7:585:PRO:HG2	8:7:756:ARG:HG2	1.80	0.63
8:7:675:SER:HA	8:7:722:ARG:HH22	1.64	0.63
8:7:683:GLU:HG2	8:7:686:ARG:HH21	1.64	0.63
3:0:24:TYR:HE2	3:0:52:LEU:HD23	1.64	0.63
5:4:25:LEU:HA	5:4:72:LYS:O	1.99	0.63
6:6:282:TYR:CZ	6:6:313:ILE:HD13	2.33	0.63
1:3:45:ARG:HD2	1:3:46:ILE:N	2.13	0.62
3:0:339:ILE:HG12	3:0:343:LYS:HZ3	1.59	0.62
3:0:569:ILE:O	3:0:570:LEU:HD12	1.99	0.62
3:0:696:TRP:CD1	3:0:697:ILE:CD1	2.82	0.62
5:4:79:TYR:OH	5:4:84:LYS:HB2	1.99	0.62
5:4:225:GLN:OE1	5:4:226:GLN:HG3	1.98	0.62
6:6:445:HIS:O	6:6:449:HIS:CE1	2.52	0.62
7:5:23:ILE:HD11	7:5:57:LEU:HD21	1.81	0.62
9:N:54:DT:H1'	9:N:55:DG:C8	2.33	0.62
3:0:145:LEU:HB2	3:0:153:VAL:HG11	1.81	0.62
3:0:480:GLN:N	3:0:480:GLN:OE1	2.32	0.62
5:4:125:LEU:CA	5:4:128:GLU:OE1	2.47	0.62
6:6:322:MET:HA	6:6:368:LEU:CG	2.29	0.62
6:6:448:LEU:HD12	6:6:448:LEU:O	1.99	0.62
7:5:49:PHE:CA	7:5:52:HIS:ND1	2.54	0.62
3:0:592:ASN:OD1	3:0:593:GLY:N	2.28	0.62
6:6:119:GLN:OE1	6:6:312:LYS:HG3	1.98	0.62
6:6:195:ALA:O	6:6:199:ILE:HG12	1.99	0.62
6:6:319:LEU:HD23	6:6:320:VAL:N	2.14	0.62
7:5:48:GLU:O	7:5:52:HIS:ND1	2.32	0.62
8:7:414:SER:O	8:7:418:MET:CE	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:466:ARG:HB2	10:T:107:DT:H5'	1.80	0.62
3:0:156:CYS:HB3	3:0:158:TYR:CD2	2.30	0.62
3:0:251:ASP:C	4:1:350:ARG:NH2	2.52	0.62
3:0:353:SER:CA	3:0:419:ILE:HD12	2.29	0.62
4:1:210:TRP:HA	4:1:213:ARG:HB2	1.81	0.62
8:7:442:ASN:HD22	8:7:444:GLU:HG3	1.64	0.62
9:N:53:DT:C2'	9:N:54:DT:C5	2.79	0.62
3:0:69:ILE:HB	3:0:205:ILE:HG13	1.80	0.62
6:6:325:PRO:HB2	6:6:348:PHE:H	1.64	0.62
8:7:468:HIS:O	8:7:472:LYS:N	2.30	0.62
9:N:67:DT:C2'	9:N:68:DT:C5	2.79	0.62
2:2:7:LYS:HZ2	2:2:9:SER:CB	2.13	0.62
3:0:371:ARG:NH1	3:0:375:ARG:NH1	2.47	0.62
3:0:639:LEU:CG	3:0:642:MET:HE3	2.30	0.62
5:4:78:ALA:HB1	5:4:148:THR:OG1	2.00	0.62
5:4:235:TYR:CZ	5:4:237:HIS:HB2	2.35	0.62
6:6:234:ILE:CG2	6:6:263:VAL:HG23	2.29	0.62
7:5:32:LEU:N	7:5:41:LEU:O	2.33	0.62
8:7:412:THR:O	8:7:456:THR:OG1	2.18	0.62
8:7:544:SER:HB2	8:7:549:ILE:O	2.00	0.62
9:N:73:DA:C2'	9:N:74:DT:C5	2.81	0.62
2:2:25:LEU:HD22	2:2:222:LEU:CD1	2.29	0.62
2:2:81:MET:HG3	2:2:87:LEU:HD22	1.80	0.62
3:0:50:VAL:CG2	3:0:85:GLU:OE2	2.46	0.62
3:0:162:LEU:HD11	3:0:198:ARG:HD3	1.81	0.62
3:0:340:GLU:OE1	3:0:343:LYS:CE	2.47	0.62
3:0:423:TYR:HE1	3:0:425:ILE:HG12	1.64	0.62
3:0:522:TYR:HD1	3:0:525:MET:CE	2.13	0.62
3:0:571:VAL:HG12	4:1:379:ASN:OD1	1.99	0.62
5:4:85:TYR:HD2	5:4:88:PRO:HG2	1.62	0.62
5:4:192:GLN:O	5:4:196:ILE:HG13	1.99	0.62
5:4:271:ASP:O	5:4:273:ARG:CD	2.47	0.62
5:4:288:ILE:HG12	6:6:320:VAL:O	1.99	0.62
8:7:463:THR:OG1	9:N:64:DA:OP1	2.17	0.62
2:2:90:ASN:OD1	2:2:99:ASN:OD1	2.16	0.62
2:2:350:TYR:O	2:2:372:ASN:HB2	1.99	0.62
2:2:416:LEU:HD12	2:2:432:VAL:HG21	1.79	0.62
3:0:25:MET:CE	3:0:51:SER:HB2	2.30	0.62
3:0:53:LEU:HD13	3:0:86:LEU:HB3	1.82	0.62
3:0:312:LEU:O	3:0:314:GLN:N	2.33	0.62
3:0:578:GLU:OE2	4:1:330:LEU:HD21	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:683:ASP:HB3	3:0:686:PHE:CE2	2.35	0.62
7:5:14:PRO:HB3	7:5:37:ASP:HB3	1.80	0.62
8:7:365:TYR:OH	8:7:390:ALA:O	2.16	0.62
8:7:421:ARG:HH22	8:7:432:PRO:HB3	1.64	0.62
8:7:457:TYR:HA	8:7:460:VAL:CG2	2.29	0.62
8:7:572:GLU:OE2	8:7:577:ARG:N	2.33	0.62
1:3:18:THR:HG23	1:3:18:THR:O	1.99	0.62
2:2:501:VAL:CG2	2:2:504:PHE:HE2	2.13	0.62
3:0:749:ASN:HA	3:0:752:LYS:HB3	1.81	0.62
4:1:181:GLN:HB3	4:1:210:TRP:NE1	2.15	0.62
5:4:76:ILE:HG12	5:4:85:TYR:HA	1.82	0.62
5:4:271:ASP:HB3	5:4:273:ARG:NE	2.15	0.62
6:6:107:LYS:HD2	6:6:107:LYS:O	2.00	0.62
8:7:446:PHE:CZ	8:7:472:LYS:HD2	2.33	0.62
8:7:604:LYS:NZ	8:7:694:LYS:CE	2.58	0.62
9:N:53:DT:H2"	9:N:54:DT:H71	1.81	0.62
1:3:34:CYS:CA	1:3:61:LYS:HZ3	2.12	0.62
3:0:210:TYR:CE2	3:0:240:ILE:HD11	2.34	0.62
5:4:85:TYR:OH	6:6:405:SER:O	2.18	0.62
5:4:201:PHE:CE1	6:6:374:THR:HB	2.33	0.62
9:N:64:DA:C2	10:T:102:DT:N3	2.57	0.62
2:2:468:TYR:CZ	2:2:484:LYS:HD3	2.35	0.61
4:1:228:UNK:C	6:6:244:PRO:HB3	2.30	0.61
10:T:94:DC:H2"	10:T:95:DA:C8	2.34	0.61
3:0:41:GLU:CD	3:0:696:TRP:CZ3	2.73	0.61
3:0:157:GLU:OE1	3:0:160:GLU:HB2	1.98	0.61
3:0:198:ARG:NH1	3:0:199:MET:HE3	2.13	0.61
3:0:277:VAL:O	3:0:278:ASP:OD1	2.18	0.61
3:0:331:PHE:O	3:0:335:LEU:CD1	2.48	0.61
3:0:354:GLU:HB3	3:0:359:PHE:HD2	1.66	0.61
3:0:492:PHE:HB2	3:0:679:MET:HE2	1.80	0.61
4:1:188:ASN:HD22	4:1:191:LEU:HG	1.65	0.61
8:7:372:LYS:HB3	8:7:535:LEU:HD12	1.80	0.61
2:2:352:ASN:C	2:2:356:GLN:NE2	2.53	0.61
2:2:416:LEU:HD12	2:2:432:VAL:CG2	2.29	0.61
3:0:696:TRP:CD1	3:0:697:ILE:HD13	2.35	0.61
5:4:279:THR:HG22	5:4:281:ARG:H	1.63	0.61
8:7:597:TYR:HA	8:7:600:ARG:HE	1.65	0.61
10:T:108:DC:H2"	10:T:109:DA:C8	2.34	0.61
2:2:369:ARG:HA	2:2:374:VAL:HG13	1.80	0.61
3:0:251:ASP:C	4:1:350:ARG:HH21	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:258:LEU:C	5:4:260:PRO:HD3	2.20	0.61
8:7:418:MET:HE1	8:7:441:ASP:OD2	2.00	0.61
8:7:616:GLN:O	8:7:620:LEU:HD23	2.01	0.61
1:3:34:CYS:CA	1:3:61:LYS:CE	2.77	0.61
3:0:298:ILE:HG23	3:0:299:LEU:HG	1.82	0.61
3:0:332:VAL:HA	3:0:335:LEU:HD13	1.81	0.61
3:0:642:MET:O	3:0:646:TYR:N	2.22	0.61
8:7:421:ARG:CZ	8:7:426:GLN:HE21	2.14	0.61
8:7:723:GLN:HA	8:7:726:LEU:HD12	1.82	0.61
2:2:481:LEU:HD23	2:2:493:ILE:CD1	2.30	0.61
3:0:140:GLN:HB3	3:0:144:LYS:NZ	2.15	0.61
3:0:619:THR:HG22	3:0:678:VAL:CG2	2.31	0.61
5:4:156:GLY:O	5:4:160:VAL:HG23	2.01	0.61
5:4:226:GLN:HA	5:4:229:ASP:HB3	1.82	0.61
1:3:34:CYS:CA	1:3:61:LYS:NZ	2.63	0.61
3:0:258:ARG:HH11	3:0:262:ARG:HH12	1.47	0.61
3:0:562:GLU:OE2	3:0:566:HIS:NE2	2.33	0.61
3:0:614:HIS:HB3	3:0:618:ARG:NH2	2.16	0.61
4:1:503:VAL:O	4:1:507:ILE:HG12	2.00	0.61
7:5:33:GLU:HG2	7:5:34:GLU:H	1.64	0.61
8:7:562:THR:CG2	8:7:564:GLU:OE2	2.48	0.61
9:N:67:DT:H2”	9:N:68:DT:H71	1.81	0.61
8:7:622:MET:SD	8:7:623:GLY:N	2.74	0.61
2:2:201:TRP:CZ2	2:2:278:LEU:HG	2.36	0.61
3:0:494:PRO:HA	3:0:679:MET:O	2.01	0.61
6:6:273:CYS:HB2	6:6:288:TYR:CE1	2.35	0.61
9:N:78:DA:H2’	9:N:79:DT:H72	1.82	0.61
1:3:119:LYS:O	1:3:123:GLY:N	2.29	0.61
3:0:671:ARG:N	3:0:675:ASP:OD2	2.34	0.61
4:1:560:PHE:O	4:1:564:PHE:CD2	2.54	0.61
8:7:589:GLN:HB3	8:7:745:ILE:CD1	2.28	0.61
3:0:423:TYR:HE1	3:0:425:ILE:HG13	1.66	0.60
6:6:247:ILE:HG23	6:6:248:HIS:N	2.16	0.60
8:7:457:TYR:HA	8:7:460:VAL:HG21	1.82	0.60
8:7:618:TYR:HA	8:7:621:LYS:HB2	1.83	0.60
3:0:260:ALA:HB3	3:0:339:ILE:HD11	1.84	0.60
4:1:197:GLU:C	4:1:201:ASN:OD1	2.39	0.60
5:4:61:LEU:HD11	5:4:73:VAL:HG21	1.82	0.60
5:4:273:ARG:HH12	6:6:372:LEU:CG	2.14	0.60
5:4:286:GLY:N	6:6:322:MET:O	2.33	0.60
6:6:266:LEU:HD22	6:6:291:LEU:HD21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:571:ARG:CZ	8:7:572:GLU:CG	2.78	0.60
8:7:675:SER:OG	8:7:722:ARG:NH2	2.34	0.60
3:0:355:THR:O	3:0:359:PHE:HD2	1.84	0.60
4:1:339:LEU:HA	4:1:342:ASN:HB3	1.83	0.60
6:6:199:ILE:HA	6:6:202:GLN:HG3	1.83	0.60
6:6:291:LEU:HD23	6:6:291:LEU:H	1.67	0.60
3:0:104:ARG:NH2	3:0:173:LYS:CA	2.63	0.60
3:0:472:MET:CG	3:0:473:LEU:HG	2.24	0.60
5:4:276:CYS:SG	5:4:296:LEU:CA	2.87	0.60
6:6:126:LEU:HD23	6:6:169:MET:HE3	1.81	0.60
6:6:165:PRO:CG	6:6:375:HIS:HD2	2.14	0.60
3:0:123:GLU:OE1	3:0:125:LYS:N	2.35	0.60
3:0:331:PHE:CD1	3:0:380:ARG:HG2	2.36	0.60
3:0:339:ILE:HG23	3:0:340:GLU:CD	2.22	0.60
4:1:491:UNK:O	4:1:493:UNK:N	2.34	0.60
5:4:211:ASP:OD2	5:4:234:VAL:HG22	2.02	0.60
6:6:224:VAL:HB	6:6:230:ARG:NE	2.16	0.60
8:7:425:LEU:CB	8:7:430:LEU:HD21	2.26	0.60
8:7:549:ILE:O	8:7:549:ILE:HG22	2.02	0.60
3:0:7:ASP:OD2	3:0:63:TYR:OH	2.19	0.60
3:0:251:ASP:CB	4:1:350:ARG:CZ	2.76	0.60
4:1:195:PHE:CZ	4:1:210:TRP:HH2	2.17	0.60
6:6:116:THR:N	6:6:117:PRO:CD	2.37	0.60
6:6:325:PRO:HB2	6:6:347:TYR:HB3	1.84	0.60
8:7:471:GLN:HA	8:7:474:MET:HE3	1.80	0.60
6:6:126:LEU:HD11	6:6:233:LEU:HB2	1.83	0.60
6:6:319:LEU:HD23	6:6:320:VAL:C	2.22	0.60
8:7:516:THR:OG1	8:7:681:ARG:NH2	2.35	0.60
8:7:554:CYS:HB2	8:7:733:PHE:HD1	1.67	0.60
2:2:100:LEU:HD13	2:2:105:LYS:H	1.66	0.60
2:2:410:ARG:CA	2:2:413:GLU:HG2	2.30	0.60
6:6:282:TYR:CE1	6:6:313:ILE:HD13	2.37	0.60
1:3:27:LYS:HD2	1:3:29:LEU:HG	1.83	0.60
3:0:568:LEU:O	3:0:597:ILE:HG22	2.01	0.60
5:4:175:ARG:HD3	5:4:255:ASP:HB2	1.84	0.60
6:6:154:ILE:HD11	6:6:196:LEU:CB	2.32	0.60
8:7:591:CYS:SG	8:7:671:ILE:HD13	2.42	0.60
2:2:134:LEU:C	2:2:136:ASP:N	2.54	0.60
3:0:341:TYR:CE1	3:0:363:LEU:CD1	2.84	0.60
3:0:538:VAL:O	3:0:620:VAL:HA	2.02	0.60
5:4:273:ARG:HH22	6:6:372:LEU:HB3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:260:ARG:HA	6:6:280:THR:HB	1.83	0.60
7:5:17:LYS:HD3	7:5:37:ASP:O	2.01	0.60
8:7:445:MET:O	8:7:449:GLU:OE2	2.20	0.60
8:7:459:MET:HE1	8:7:474:MET:HG3	1.82	0.60
2:2:25:LEU:CD1	2:2:219:VAL:HG13	2.32	0.59
3:0:331:PHE:O	3:0:335:LEU:HD13	2.02	0.59
3:0:439:CYS:SG	3:0:440:LEU:N	2.75	0.59
5:4:270:VAL:HG22	5:4:272:PHE:H	1.67	0.59
5:4:273:ARG:CZ	6:6:372:LEU:HB3	2.32	0.59
8:7:761:GLN:O	8:7:765:LEU:HG	2.02	0.59
3:0:264:ALA:CB	3:0:336:LYS:NZ	2.65	0.59
3:0:468:MET:HE1	3:0:653:PHE:CD2	2.37	0.59
3:0:601:VAL:HG12	3:0:603:ARG:H	1.67	0.59
5:4:293:LEU:CD1	6:6:376:LEU:HD22	2.31	0.59
5:4:311:GLN:NE2	5:4:312:PHE:O	2.34	0.59
6:6:126:LEU:HB3	6:6:169:MET:HE1	1.83	0.59
8:7:352:LEU:HD23	8:7:452:LEU:HD23	1.82	0.59
8:7:370:LEU:HD21	8:7:395:VAL:CB	2.30	0.59
8:7:457:TYR:OH	8:7:490:VAL:CG2	2.49	0.59
8:7:466:ARG:HD2	10:T:107:DT:C4'	2.33	0.59
9:N:61:DG:H2'	9:N:62:DT:C7	2.31	0.59
9:N:75:DG:H2'	9:N:76:DT:C7	2.31	0.59
2:2:468:TYR:CE2	2:2:486:ASP:OD1	2.55	0.59
3:0:568:LEU:O	3:0:597:ILE:N	2.29	0.59
7:5:19:LEU:CD1	8:7:566:TYR:CZ	2.86	0.59
1:3:43:VAL:O	1:3:47:PHE:CD2	2.55	0.59
3:0:340:GLU:HA	3:0:343:LYS:HZ2	1.66	0.59
3:0:722:ARG:HG2	6:6:267:SER:OG	2.01	0.59
3:0:725:ALA:HB3	6:6:290:ILE:HD11	1.81	0.59
6:6:174:MET:HA	6:6:179:ALA:HA	1.83	0.59
1:3:27:LYS:HZ2	1:3:29:LEU:CD2	2.15	0.59
3:0:105:GLY:HA3	3:0:205:ILE:HG22	1.85	0.59
3:0:468:MET:CE	3:0:653:PHE:CE2	2.85	0.59
3:0:575:ASP:OD2	3:0:578:GLU:HB2	2.02	0.59
4:1:206:PRO:CA	4:1:210:TRP:HZ3	2.15	0.59
1:3:62:ILE:HG22	1:3:64:ARG:HD2	1.85	0.59
2:2:378:ILE:HD12	2:2:382:SER:CB	2.32	0.59
3:0:380:ARG:O	3:0:383:LEU:HG	2.02	0.59
4:1:206:PRO:HB2	4:1:210:TRP:CZ3	2.30	0.59
5:4:136:GLU:HG2	5:4:136:GLU:O	2.02	0.59
7:5:42:VAL:CG1	7:5:47:VAL:CG2	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:354:ILE:HD12	8:7:404:LYS:HA	1.84	0.59
3:0:515:ASP:O	3:0:517:SER:N	2.36	0.59
3:0:575:ASP:CG	3:0:578:GLU:HB2	2.23	0.59
3:0:614:HIS:CE1	3:0:675:ASP:N	2.70	0.59
5:4:273:ARG:NH1	6:6:372:LEU:CG	2.65	0.59
8:7:458:SER:CA	8:7:462:ASN:OD1	2.25	0.59
2:2:136:ASP:CA	2:2:286:ARG:HH12	2.14	0.59
3:0:1:MET:HE3	3:0:745:ILE:HD13	1.83	0.59
3:0:627:PHE:HE2	3:0:654:LEU:HB3	1.68	0.59
3:0:681:LEU:HB3	3:0:686:PHE:CE2	2.38	0.59
4:1:487:UNK:O	4:1:491:UNK:N	2.35	0.59
5:4:87:TYR:HA	5:4:125:LEU:HD21	1.85	0.59
6:6:271:ALA:O	6:6:274:LYS:HG3	2.03	0.59
8:7:469:ASP:OD1	8:7:469:ASP:N	2.35	0.59
8:7:577:ARG:HA	8:7:580:LEU:HD12	1.83	0.59
9:N:79:DT:H2"	9:N:80:DG:N7	2.17	0.59
1:3:45:ARG:CZ	1:3:46:ILE:HG13	2.31	0.59
2:2:468:TYR:CD2	2:2:486:ASP:OD1	2.55	0.59
5:4:182:GLY:N	5:4:215:ILE:O	2.34	0.59
5:4:288:ILE:HD11	6:6:320:VAL:HG13	1.85	0.59
5:4:297:SER:C	5:4:299:ILE:H	2.06	0.59
7:5:46:LYS:O	7:5:50:VAL:HG23	2.02	0.59
2:2:12:GLN:OE1	2:2:12:GLN:N	2.36	0.59
2:2:386:ALA:O	2:2:391:ILE:N	2.31	0.59
2:2:454:TYR:CE2	7:5:11:GLN:CG	2.85	0.59
3:0:383:LEU:HD12	3:0:384:LEU:N	2.18	0.59
4:1:511:ALA:HB2	5:4:264:LYS:NZ	2.18	0.59
7:5:35:LEU:HB2	7:5:39:HIS:HB2	1.83	0.59
7:5:42:VAL:HG12	7:5:43:ASN:H	1.67	0.59
8:7:478:THR:CG2	8:7:504:THR:CG2	2.80	0.59
1:3:45:ARG:NH1	1:3:46:ILE:CG1	2.66	0.58
2:2:20:GLN:NE2	2:2:21:VAL:HG13	2.18	0.58
2:2:31:THR:HG22	2:2:226:PHE:CD2	2.36	0.58
3:0:571:VAL:HG12	4:1:379:ASN:CG	2.23	0.58
3:0:622:MET:CE	3:0:662:ALA:HA	2.33	0.58
6:6:130:LEU:CB	6:6:173:ILE:HG22	2.28	0.58
6:6:168:GLN:HG2	6:6:185:VAL:CG2	2.33	0.58
6:6:215:GLU:OE1	6:6:218:ARG:NE	2.27	0.58
6:6:296:HIS:O	6:6:300:LEU:HG	2.03	0.58
6:6:336:CYS:SG	6:6:337:SER:N	2.76	0.58
7:5:32:LEU:HD23	7:5:41:LEU:HD21	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:351:ASP:OD1	8:7:405:LYS:CD	2.51	0.58
8:7:445:MET:SD	8:7:449:GLU:CG	2.91	0.58
8:7:622:MET:HE1	8:7:624:LYS:HB2	1.85	0.58
8:7:664:LEU:HD23	8:7:689:ARG:CD	2.30	0.58
1:3:39:CYS:SG	1:3:41:SER:OG	2.62	0.58
3:0:250:LEU:HD21	3:0:405:PHE:HB2	1.83	0.58
3:0:251:ASP:CB	4:1:350:ARG:NH2	2.66	0.58
4:1:375:LEU:C	4:1:378:MET:SD	2.82	0.58
4:1:606:GLU:O	4:1:610:ASN:N	2.28	0.58
8:7:406:SER:O	8:7:483:GLY:N	2.36	0.58
8:7:568:GLU:HA	8:7:571:ARG:HG2	1.84	0.58
8:7:580:LEU:HD23	8:7:583:MET:HE1	1.85	0.58
8:7:606:ILE:O	8:7:671:ILE:N	2.33	0.58
8:7:613:TYR:CG	8:7:766:LYS:HG2	2.37	0.58
1:3:32:PRO:CG	1:3:69:LYS:HZ1	2.15	0.58
2:2:451:VAL:CG2	7:5:54:LEU:HD11	2.31	0.58
2:2:454:TYR:HE2	7:5:11:GLN:CG	2.16	0.58
2:2:458:LEU:HD11	2:2:490:LYS:HB3	1.85	0.58
3:0:304:GLU:CD	3:0:386:ARG:NH1	2.56	0.58
3:0:354:GLU:N	3:0:418:LEU:O	2.28	0.58
5:4:288:ILE:HD11	6:6:320:VAL:CG1	2.33	0.58
8:7:407:VAL:HG13	8:7:484:PHE:HB3	1.85	0.58
8:7:597:TYR:O	8:7:601:ARG:N	2.35	0.58
9:N:59:DA:C2'	9:N:60:DT:C5	2.81	0.58
2:2:102:PRO:O	2:2:106:ILE:HG22	2.02	0.58
2:2:366:LEU:HD23	2:2:367:LYS:N	2.18	0.58
3:0:86:LEU:HD12	3:0:87:GLU:N	2.19	0.58
3:0:615:GLN:OE1	3:0:615:GLN:N	2.29	0.58
5:4:24:SER:H	5:4:71:ASN:HB2	1.68	0.58
8:7:583:MET:O	8:7:618:TYR:OH	2.21	0.58
8:7:590:ALA:O	8:7:594:LEU:HG	2.03	0.58
8:7:613:TYR:HB2	8:7:766:LYS:HZ2	1.67	0.58
2:2:47:ILE:O	2:2:51:VAL:HG23	2.02	0.58
2:2:253:MET:O	2:2:258:LEU:N	2.37	0.58
2:2:473:LYS:NZ	2:2:477:ASP:OD1	2.28	0.58
3:0:301:ASP:HB2	3:0:305:PRO:HG3	1.84	0.58
8:7:409:VAL:HG22	8:7:486:ILE:HD12	1.85	0.58
8:7:499:ARG:HD2	8:7:500:ARG:N	2.18	0.58
1:3:30:VAL:HG22	1:3:36:HIS:O	2.03	0.58
2:2:360:LEU:HA	2:2:363:PHE:CZ	2.38	0.58
2:2:468:TYR:HE2	2:2:484:LYS:NZ	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:11:LEU:HD21	3:0:97:LEU:CG	2.33	0.58
3:0:396:PHE:O	3:0:400:LYS:NZ	2.36	0.58
4:1:560:PHE:O	4:1:564:PHE:HD2	1.86	0.58
8:7:386:LEU:HD12	8:7:392:LYS:HG3	1.84	0.58
8:7:613:TYR:HB2	8:7:766:LYS:HZ3	1.67	0.58
8:7:754:ARG:HB3	8:7:757:ARG:NE	2.18	0.58
2:2:497:GLY:HA2	2:2:500:GLN:CD	2.23	0.58
3:0:270:ARG:HG2	3:0:388:LEU:HD13	1.84	0.58
6:6:168:GLN:CG	6:6:185:VAL:CG2	2.82	0.58
8:7:343:PHE:CD2	8:7:403:ILE:HG22	2.38	0.58
2:2:25:LEU:HD13	2:2:219:VAL:HG13	1.86	0.58
2:2:419:LYS:NZ	2:2:426:CYS:O	2.37	0.58
3:0:39:ILE:O	3:0:480:GLN:HA	2.04	0.58
3:0:117:HIS:CD2	3:0:156:CYS:HA	2.38	0.58
3:0:539:VAL:HG12	3:0:621:LEU:HD13	1.85	0.58
5:4:225:GLN:HE22	5:4:269:SER:CA	2.17	0.58
8:7:742:MET:HG3	8:7:743:GLU:OE2	2.03	0.58
5:4:124:THR:C	5:4:128:GLU:OE1	2.42	0.58
8:7:465:ASN:HB3	8:7:471:GLN:HE21	1.56	0.58
8:7:527:LEU:HD22	8:7:530:LEU:HD22	1.86	0.58
3:0:73:SER:OG	3:0:79:ILE:HG12	2.04	0.58
3:0:468:MET:HE1	3:0:653:PHE:HD2	1.67	0.58
3:0:659:MET:HE3	3:0:693:LEU:HD21	1.86	0.58
8:7:498:PHE:CE1	8:7:502:VAL:CG1	2.86	0.58
3:0:53:LEU:O	3:0:57:ILE:HG12	2.04	0.57
3:0:257:LEU:HB3	3:0:343:LYS:HE3	1.86	0.57
4:1:593:LEU:CD2	4:1:597:PHE:CE2	2.82	0.57
5:4:40:PHE:CA	5:4:43:GLU:OE1	2.52	0.57
5:4:163:ILE:O	5:4:166:GLU:HG3	2.03	0.57
5:4:239:GLU:OE2	5:4:242:GLU:CB	2.46	0.57
6:6:199:ILE:CG2	6:6:202:GLN:NE2	2.61	0.57
7:5:27:MET:SD	7:5:30:ILE:CG1	2.92	0.57
8:7:409:VAL:O	8:7:455:SER:N	2.37	0.57
8:7:491:HIS:HB3	8:7:519:ARG:CZ	2.34	0.57
8:7:622:MET:CE	8:7:624:LYS:HG3	2.31	0.57
8:7:622:MET:HG2	8:7:653:PHE:HZ	1.68	0.57
8:7:672:GLN:HE22	8:7:687:LEU:HD21	1.67	0.57
2:2:90:ASN:HB2	2:2:97:MET:HB3	1.85	0.57
2:2:408:MET:HB3	2:2:411:LEU:HB3	1.85	0.57
3:0:255:ASP:O	3:0:259:ARG:HG3	2.03	0.57
3:0:471:ARG:O	3:0:646:TYR:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:185:LEU:HD11	4:1:195:PHE:HD2	1.69	0.57
6:6:168:GLN:HG3	6:6:185:VAL:HG23	1.86	0.57
6:6:371:ILE:HD12	6:6:375:HIS:HB2	1.86	0.57
8:7:592:GLN:NE2	8:7:746:PRO:O	2.37	0.57
3:0:135:ARG:NH2	3:0:392:GLU:CA	2.63	0.57
3:0:196:VAL:O	3:0:200:ILE:HG12	2.04	0.57
5:4:197:MET:HA	5:4:200:ILE:HD12	1.87	0.57
6:6:175:ARG:HH21	6:6:205:LYS:HG2	1.68	0.57
8:7:189:GLU:O	8:7:193:ILE:N	2.23	0.57
8:7:406:SER:OG	8:7:480:ARG:CZ	2.51	0.57
8:7:501:VAL:O	8:7:505:ILE:HG12	2.04	0.57
3:0:336:LYS:HA	3:0:336:LYS:HE2	1.87	0.57
3:0:341:TYR:CD1	3:0:363:LEU:CD1	2.86	0.57
8:7:579:LEU:HD21	8:7:611:ASN:HB3	1.86	0.57
8:7:639:ILE:O	8:7:643:PHE:CB	2.52	0.57
6:6:360:PRO:O	6:6:369:MET:CE	2.53	0.57
8:7:498:PHE:O	8:7:502:VAL:HG22	2.03	0.57
8:7:754:ARG:HB2	8:7:757:ARG:NH2	2.19	0.57
2:2:55:ASN:O	2:2:55:ASN:OD1	2.21	0.57
2:2:87:LEU:HA	2:2:100:LEU:HA	1.87	0.57
3:0:108:LEU:HB3	3:0:196:VAL:HG21	1.86	0.57
3:0:117:HIS:HB2	3:0:156:CYS:SG	2.45	0.57
3:0:220:GLU:OE2	3:0:221:ARG:CG	2.38	0.57
3:0:311:VAL:HG11	3:0:317:LEU:HD11	1.86	0.57
4:1:374:ILE:O	4:1:378:MET:CE	2.52	0.57
6:6:224:VAL:CG1	6:6:230:ARG:NE	2.56	0.57
6:6:360:PRO:O	6:6:369:MET:HE3	2.04	0.57
7:5:54:LEU:HD23	7:5:55:ASN:N	2.19	0.57
8:7:544:SER:CB	8:7:549:ILE:O	2.53	0.57
1:3:127:ALA:O	1:3:131:GLU:N	2.24	0.57
2:2:351:SER:N	2:2:407:GLN:OE1	2.35	0.57
3:0:143:ARG:O	3:0:146:GLU:N	2.37	0.57
3:0:627:PHE:CE2	3:0:654:LEU:HB3	2.38	0.57
3:0:745:ILE:HG13	3:0:746:LYS:H	1.69	0.57
6:6:297:LEU:O	6:6:301:PHE:HD1	1.87	0.57
6:6:381:HIS:HE1	6:6:449:HIS:CG	2.19	0.57
8:7:392:LYS:HG2	8:7:513:LEU:HD13	1.85	0.57
1:3:32:PRO:CG	1:3:69:LYS:NZ	2.68	0.57
3:0:294:HIS:O	3:0:298:ILE:N	2.36	0.57
3:0:363:LEU:O	3:0:367:THR:N	2.20	0.57
3:0:610:ILE:O	3:0:668:ARG:NH1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:199:VAL:HG21	4:1:206:PRO:HG3	1.85	0.57
4:1:383:GLU:HA	4:1:386:ILE:CG2	2.35	0.57
8:7:416:SER:HB3	8:7:420:TRP:CZ2	2.39	0.57
3:0:237:ALA:O	3:0:240:ILE:CG1	2.52	0.57
6:6:274:LYS:HD2	6:6:275:GLU:N	2.20	0.57
8:7:464:ARG:NH1	10:T:105:DC:O2	2.38	0.57
8:7:669:CYS:SG	8:7:706:TYR:CE2	2.98	0.57
3:0:41:GLU:CG	3:0:696:TRP:HZ3	2.18	0.56
3:0:639:LEU:HD13	3:0:642:MET:CE	2.24	0.56
7:5:19:LEU:HD23	7:5:22:GLN:OE1	2.04	0.56
8:7:351:ASP:OD1	8:7:405:LYS:HD3	2.05	0.56
3:0:111:ARG:HD2	3:0:130:ASP:HA	1.87	0.56
3:0:271:ILE:O	3:0:275:ARG:HG3	2.05	0.56
3:0:641:PHE:CD1	3:0:644:GLU:OE2	2.57	0.56
4:1:239:PRO:O	4:1:241:UNK:N	2.38	0.56
7:5:19:LEU:CD2	7:5:22:GLN:NE2	2.68	0.56
8:7:526:ASP:O	8:7:530:LEU:HD13	2.04	0.56
9:N:56:DA:H2"	9:N:57:DT:C6	2.40	0.56
2:2:9:SER:O	2:2:12:GLN:N	2.35	0.56
2:2:17:ILE:C	2:2:22:GLN:NE2	2.55	0.56
2:2:357:ILE:HA	2:2:360:LEU:HD12	1.87	0.56
3:0:61:MET:HE1	3:0:101:GLU:O	2.05	0.56
3:0:155:LEU:CD1	3:0:160:GLU:OE2	2.53	0.56
3:0:297:ASP:OD1	3:0:304:GLU:OE1	2.24	0.56
3:0:352:ILE:O	3:0:420:ILE:N	2.35	0.56
3:0:353:SER:N	3:0:419:ILE:HD12	2.20	0.56
3:0:603:ARG:NH2	3:0:628:GLN:HG2	2.20	0.56
4:1:193:LYS:O	4:1:196:GLN:HG3	2.04	0.56
4:1:214:ILE:CG2	4:1:215:PRO:HD3	2.35	0.56
4:1:236:UNK:HA	4:1:239:PRO:HG2	1.87	0.56
5:4:234:VAL:HG12	5:4:263:VAL:HG13	1.88	0.56
5:4:273:ARG:NH2	6:6:372:LEU:HB3	2.21	0.56
6:6:172:ILE:HD11	6:6:220:LEU:CD1	2.35	0.56
8:7:416:SER:O	8:7:420:TRP:CD1	2.58	0.56
8:7:438:PHE:HA	8:7:442:ASN:H	1.70	0.56
8:7:646:ASN:OD1	8:7:648:GLN:OE1	2.23	0.56
1:3:34:CYS:HB3	1:3:61:LYS:HZ3	1.61	0.56
2:2:18:PRO:O	2:2:22:GLN:CD	2.44	0.56
2:2:454:TYR:CE2	7:5:11:GLN:HB2	2.37	0.56
2:2:501:VAL:HG22	2:2:504:PHE:CE2	2.36	0.56
3:0:234:PHE:HB3	3:0:237:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:500:GLY:O	3:0:503:GLN:NE2	2.39	0.56
3:0:614:HIS:HE1	3:0:674:ASP:C	2.08	0.56
5:4:114:UNK:C	5:4:116:ARG:H	2.17	0.56
5:4:149:LEU:O	5:4:153:MET:HG3	2.05	0.56
8:7:568:GLU:CD	8:7:571:ARG:CZ	2.64	0.56
1:3:38:ILE:CG2	1:3:43:VAL:HB	2.35	0.56
2:2:18:PRO:C	2:2:22:GLN:OE1	2.43	0.56
3:0:166:GLU:CG	3:0:198:ARG:HH11	1.98	0.56
3:0:167:VAL:CA	3:0:198:ARG:NH2	2.46	0.56
5:4:149:LEU:HD21	5:4:192:GLN:HG3	1.86	0.56
6:6:224:VAL:HG12	6:6:230:ARG:NE	2.19	0.56
6:6:391:GLU:HA	6:6:427:TYR:HA	1.86	0.56
8:7:425:LEU:HD12	8:7:430:LEU:CD2	2.35	0.56
2:2:7:LYS:HG2	2:2:9:SER:H	1.71	0.56
3:0:135:ARG:HH22	3:0:392:GLU:CA	2.11	0.56
3:0:327:ARG:CB	3:0:330:HIS:CD2	2.72	0.56
3:0:423:TYR:CE1	3:0:425:ILE:HG13	2.39	0.56
3:0:473:LEU:HB2	3:0:475:PHE:CE1	2.41	0.56
3:0:639:LEU:CA	3:0:642:MET:HE3	2.25	0.56
4:1:194:VAL:CA	4:1:197:GLU:OE2	2.52	0.56
6:6:224:VAL:CG1	6:6:228:CYS:HB2	2.36	0.56
6:6:269:GLN:HA	6:6:288:TYR:OH	2.05	0.56
6:6:426:ARG:HH22	6:6:435:GLU:N	2.03	0.56
8:7:489:GLU:O	8:7:489:GLU:HG2	2.05	0.56
8:7:594:LEU:HD13	8:7:706:TYR:CD2	2.40	0.56
8:7:641:GLN:O	8:7:644:GLN:N	2.39	0.56
8:7:675:SER:HB2	8:7:722:ARG:HH22	1.71	0.56
2:2:7:LYS:HZ2	2:2:9:SER:HB2	1.71	0.56
3:0:493:LEU:CD2	3:0:495:MET:CE	2.76	0.56
3:0:506:ILE:HG22	3:0:518:ILE:HD12	1.88	0.56
3:0:507:SER:OG	3:0:685:ARG:NH2	2.33	0.56
5:4:30:ILE:CD1	5:4:179:LEU:CB	2.82	0.56
1:3:66:ASN:O	1:3:67:LYS:HB2	2.05	0.56
2:2:160:SER:O	2:2:164:LEU:N	2.22	0.56
2:2:497:GLY:CA	2:2:500:GLN:NE2	2.52	0.56
3:0:37:ASN:ND2	3:0:476:LYS:O	2.39	0.56
5:4:273:ARG:NH2	6:6:372:LEU:O	2.39	0.56
6:6:134:GLU:CD	6:6:206:GLY:O	2.44	0.56
8:7:460:VAL:HG23	8:7:461:ALA:N	2.16	0.56
8:7:494:PRO:CG	8:7:497:MET:HE1	2.15	0.56
8:7:666:GLU:HA	8:7:692:ARG:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:70:DA:H2"	9:N:71:DT:C6	2.40	0.56
1:3:53:GLN:HB3	1:3:62:ILE:HD13	1.87	0.56
3:0:104:ARG:HH21	3:0:173:LYS:CD	2.15	0.56
3:0:312:LEU:H	3:0:412:TYR:HH	1.51	0.56
3:0:378:SER:OG	3:0:407:THR:OG1	2.21	0.56
3:0:729:ASP:O	3:0:731:LYS:NZ	2.26	0.56
3:0:741:TYR:CA	3:0:742:GLU:OE1	2.53	0.56
8:7:608:PHE:N	8:7:671:ILE:O	2.29	0.56
8:7:625:PRO:HG2	8:7:649:ILE:HD13	1.87	0.56
1:3:27:LYS:HD3	1:3:28:PHE:N	2.21	0.56
2:2:21:VAL:HA	2:2:24:ARG:HB2	1.87	0.56
3:0:37:ASN:HA	3:0:456:VAL:O	2.06	0.56
3:0:237:ALA:C	3:0:240:ILE:HG12	2.25	0.56
3:0:280:GLN:HA	3:0:283:GLN:OE1	2.05	0.56
3:0:506:ILE:CD1	3:0:522:TYR:HE1	2.19	0.56
7:5:24:ASP:OD2	7:5:31:VAL:HG23	2.06	0.56
7:5:27:MET:HE1	7:5:46:LYS:HB3	1.88	0.56
8:7:417:VAL:HG21	8:7:456:THR:HB	1.87	0.56
8:7:573:THR:HA	8:7:577:ARG:NH2	2.21	0.56
8:7:754:ARG:O	8:7:758:GLU:HG2	2.06	0.56
3:0:258:ARG:O	3:0:261:THR:OG1	2.22	0.55
3:0:275:ARG:CZ	3:0:276:LYS:HE3	2.36	0.55
3:0:312:LEU:HG	3:0:313:PRO:CD	2.23	0.55
3:0:715:SER:N	3:0:718:LYS:HZ3	2.03	0.55
5:4:25:LEU:HB3	5:4:174:SER:HB2	1.87	0.55
6:6:128:LEU:HD21	6:6:130:LEU:CD2	2.36	0.55
8:7:409:VAL:HA	8:7:486:ILE:HB	1.87	0.55
2:2:382:SER:HA	2:2:385:ARG:HH11	1.71	0.55
3:0:68:LYS:HA	3:0:204:ASN:O	2.06	0.55
3:0:155:LEU:HD11	3:0:160:GLU:OE2	2.06	0.55
3:0:354:GLU:HB2	3:0:418:LEU:HB3	1.88	0.55
6:6:173:ILE:O	6:6:180:GLN:N	2.21	0.55
7:5:47:VAL:O	7:5:50:VAL:HB	2.05	0.55
8:7:340:GLU:HA	8:7:380:ARG:HB3	1.88	0.55
2:2:475:ALA:HB3	2:2:481:LEU:HD11	1.89	0.55
3:0:271:ILE:O	3:0:275:ARG:CG	2.54	0.55
3:0:747:HIS:O	3:0:751:ARG:HG2	2.06	0.55
4:1:465:UNK:O	4:1:470:UNK:N	2.39	0.55
8:7:582:ILE:HG23	8:7:673:ILE:CG2	2.36	0.55
1:3:45:ARG:O	1:3:49:LEU:HG	2.06	0.55
1:3:98:ASP:HA	1:3:101:GLY:HA2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:176:PHE:O	3:0:181:LEU:HB2	2.06	0.55
4:1:511:ALA:CB	5:4:264:LYS:HE3	2.37	0.55
5:4:30:ILE:HD12	5:4:179:LEU:CB	2.35	0.55
6:6:153:ALA:O	6:6:157:VAL:HG23	2.06	0.55
8:7:447:GLN:OE1	8:7:476:PHE:CD2	2.60	0.55
8:7:459:MET:CE	8:7:470:SER:O	2.54	0.55
8:7:467:SER:CB	8:7:469:ASP:OD1	2.49	0.55
3:0:468:MET:CE	3:0:648:ILE:HD13	2.35	0.55
3:0:618:ARG:O	3:0:678:VAL:N	2.23	0.55
5:4:133:PHE:C	5:4:136:GLU:OE1	2.45	0.55
5:4:215:ILE:HG13	5:4:238:VAL:CG2	2.36	0.55
6:6:271:ALA:HA	6:6:274:LYS:HG3	1.88	0.55
7:5:54:LEU:HD23	7:5:54:LEU:C	2.27	0.55
2:2:238:LYS:H	2:2:269:PHE:N	2.04	0.55
3:0:108:LEU:HD12	3:0:108:LEU:O	2.06	0.55
3:0:116:LEU:HD23	3:0:158:TYR:CD1	2.41	0.55
3:0:140:GLN:HE22	3:0:389:GLU:HB3	1.71	0.55
3:0:215:ASP:HB2	3:0:218:ILE:HG12	1.89	0.55
3:0:250:LEU:N	3:0:437:PHE:O	2.35	0.55
3:0:318:THR:CG2	3:0:376:PHE:HZ	2.18	0.55
3:0:378:SER:HA	3:0:403:ALA:HB1	1.88	0.55
4:1:194:VAL:HA	4:1:197:GLU:CD	2.26	0.55
4:1:483:UNK:O	4:1:485:UNK:N	2.39	0.55
5:4:249:ALA:O	5:4:253:PHE:CD2	2.60	0.55
5:4:288:ILE:O	6:6:319:LEU:HG	2.07	0.55
6:6:251:ILE:O	6:6:255:VAL:HG12	2.07	0.55
8:7:409:VAL:C	8:7:410:LEU:HD12	2.27	0.55
8:7:467:SER:OG	8:7:470:SER:HB3	2.06	0.55
8:7:527:LEU:HA	8:7:530:LEU:HD13	1.89	0.55
2:2:353:SER:O	2:2:356:GLN:N	2.39	0.55
3:0:34:VAL:O	3:0:34:VAL:HG23	2.07	0.55
3:0:333:SER:O	3:0:337:ARG:CD	2.55	0.55
3:0:641:PHE:CZ	3:0:645:ASN:ND2	2.70	0.55
7:5:24:ASP:OD1	7:5:30:ILE:N	2.39	0.55
8:7:162:GLU:O	8:7:174:LYS:N	2.40	0.55
8:7:459:MET:HE3	8:7:470:SER:HB2	1.89	0.55
8:7:477:LEU:HB3	8:7:505:ILE:CD1	2.36	0.55
9:N:75:DG:C2'	9:N:76:DT:H72	2.34	0.55
3:0:134:ARG:C	3:0:138:ASN:OD1	2.45	0.55
3:0:375:ARG:HG3	3:0:376:PHE:CD1	2.41	0.55
3:0:471:ARG:NH2	3:0:647:ARG:H	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:26:LEU:HB3	5:4:73:VAL:CG1	2.37	0.55
5:4:189:GLU:O	5:4:192:GLN:NE2	2.33	0.55
5:4:193:TYR:CD1	5:4:197:MET:SD	3.00	0.55
5:4:193:TYR:HD1	5:4:223:PHE:HD1	1.53	0.55
5:4:217:GLY:O	5:4:237:HIS:HE1	1.89	0.55
6:6:168:GLN:HG3	6:6:169:MET:H	1.72	0.55
8:7:410:LEU:HB2	8:7:487:LEU:HD23	1.88	0.55
1:3:128:LYS:O	1:3:132:LYS:CB	2.55	0.55
2:2:87:LEU:HD23	2:2:87:LEU:H	1.70	0.55
2:2:419:LYS:HB3	2:2:432:VAL:HG11	1.88	0.55
3:0:110:SER:O	3:0:113:ASN:OD1	2.24	0.55
3:0:120:VAL:HG22	3:0:132:LYS:HD2	1.88	0.55
3:0:131:GLU:HA	3:0:134:ARG:HD3	1.89	0.55
3:0:140:GLN:HA	3:0:143:ARG:NE	2.20	0.55
3:0:251:ASP:HB2	3:0:436:ARG:CD	2.17	0.55
3:0:348:VAL:O	3:0:422:PRO:HB3	2.05	0.55
3:0:366:LEU:HD23	3:0:367:THR:OG1	2.07	0.55
3:0:424:GLU:H	3:0:432:ASN:ND2	2.04	0.55
5:4:175:ARG:HA	5:4:208:CYS:SG	2.47	0.55
6:6:126:LEU:C	6:6:169:MET:SD	2.85	0.55
8:7:414:SER:O	8:7:418:MET:SD	2.65	0.55
8:7:593:PHE:HA	8:7:596:GLN:HG2	1.89	0.55
4:1:181:GLN:HG2	4:1:210:TRP:CD1	2.42	0.55
4:1:348:VAL:HG23	4:1:348:VAL:O	2.07	0.55
6:6:175:ARG:NH2	6:6:205:LYS:HG2	2.22	0.55
8:7:498:PHE:CZ	8:7:502:VAL:HG11	2.41	0.55
8:7:522:ASP:OD1	8:7:526:ASP:OD2	2.24	0.55
2:2:13:TYR:CE2	2:2:208:LEU:HD21	2.42	0.54
3:0:79:ILE:HD12	3:0:207:ILE:HB	1.89	0.54
3:0:537:MET:HG3	3:0:619:THR:O	2.07	0.54
6:6:426:ARG:HH22	6:6:435:GLU:CA	2.20	0.54
7:5:33:GLU:HG2	7:5:34:GLU:N	2.22	0.54
8:7:401:CYS:O	8:7:404:LYS:HG2	2.07	0.54
8:7:683:GLU:CG	8:7:686:ARG:HH21	2.19	0.54
1:3:34:CYS:CB	1:3:61:LYS:HZ1	2.01	0.54
3:0:42:MET:HB3	3:0:48:LYS:HE2	1.88	0.54
3:0:250:LEU:O	3:0:437:PHE:N	2.40	0.54
3:0:276:LYS:CE	3:0:276:LYS:HA	2.35	0.54
5:4:234:VAL:HG12	5:4:263:VAL:CG1	2.37	0.54
5:4:286:GLY:O	5:4:287:PHE:HD1	1.89	0.54
6:6:178:LEU:HD23	6:6:179:ALA:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:271:ALA:HB1	6:6:274:LYS:HE3	1.89	0.54
8:7:471:GLN:CA	8:7:474:MET:HE2	2.27	0.54
8:7:692:ARG:NH1	8:7:692:ARG:HG2	2.19	0.54
4:1:325:UNK:O	4:1:329:LEU:CD2	2.44	0.54
5:4:222:THR:HA	5:4:225:GLN:HB3	1.88	0.54
5:4:273:ARG:HH12	6:6:372:LEU:HD23	1.72	0.54
8:7:411:CYS:HB2	8:7:420:TRP:CE3	2.43	0.54
9:N:61:DG:H2"	9:N:62:DT:H6	1.72	0.54
1:3:107:ASN:CB	3:0:323:GLY:HA2	2.37	0.54
2:2:457:SER:OG	7:5:6:LYS:HA	2.07	0.54
3:0:101:GLU:HG2	3:0:103:PHE:CB	2.37	0.54
3:0:553:MET:SD	3:0:554:TRP:HD1	2.31	0.54
3:0:573:THR:O	3:0:579:THR:OG1	2.25	0.54
3:0:639:LEU:HD12	3:0:650:GLU:HA	1.89	0.54
5:4:258:LEU:HB3	5:4:260:PRO:CD	2.37	0.54
6:6:270:VAL:CG1	6:6:272:ILE:HG22	2.34	0.54
7:5:19:LEU:HD11	8:7:566:TYR:CE2	2.41	0.54
8:7:597:TYR:O	8:7:601:ARG:HG2	2.06	0.54
1:3:27:LYS:HD2	1:3:29:LEU:CD2	2.37	0.54
2:2:100:LEU:CD1	2:2:101:ASN:O	2.56	0.54
4:1:206:PRO:C	4:1:210:TRP:CE3	2.80	0.54
4:1:344:UNK:C	4:1:347:PRO:HD2	2.38	0.54
6:6:299:GLU:O	6:6:303:GLU:CD	2.45	0.54
8:7:391:GLY:CA	8:7:394:LEU:HD13	2.37	0.54
8:7:496:ALA:C	8:7:499:ARG:HG3	2.27	0.54
8:7:583:MET:HE1	8:7:763:VAL:CB	2.29	0.54
1:3:115:ASP:N	3:0:330:HIS:CE1	2.75	0.54
2:2:501:VAL:CA	2:2:504:PHE:CZ	2.84	0.54
3:0:5:ILE:HD13	3:0:22:TYR:OH	2.08	0.54
3:0:334:PHE:HD1	3:0:337:ARG:NE	2.05	0.54
3:0:395:ASP:N	3:0:395:ASP:OD1	2.41	0.54
3:0:416:PHE:CE1	3:0:439:CYS:CB	2.91	0.54
6:6:128:LEU:HD23	6:6:129:THR:N	2.23	0.54
6:6:384:MET:O	6:6:384:MET:HG2	2.07	0.54
8:7:356:LEU:HG	8:7:404:LYS:NZ	2.23	0.54
8:7:401:CYS:O	8:7:404:LYS:CE	2.54	0.54
8:7:607:VAL:HG22	8:7:671:ILE:HD12	1.89	0.54
9:N:67:DT:C2'	9:N:68:DT:C7	2.84	0.54
2:2:353:SER:CB	2:2:356:GLN:HG2	2.37	0.54
3:0:15:PRO:C	3:0:741:TYR:CD1	2.80	0.54
3:0:171:LEU:HB3	3:0:172:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:312:LEU:CD1	3:0:313:PRO:HD2	2.37	0.54
3:0:519:VAL:CG1	3:0:553:MET:HE3	2.37	0.54
3:0:619:THR:HG22	3:0:678:VAL:HB	1.89	0.54
4:1:235:UNK:C	4:1:239:PRO:HD2	2.38	0.54
8:7:349:ASN:ND2	8:7:406:SER:H	2.05	0.54
8:7:459:MET:CE	8:7:470:SER:HB2	2.37	0.54
3:0:17:ILE:HG13	3:0:18:TYR:N	2.23	0.54
3:0:116:LEU:HD23	3:0:158:TYR:CE1	2.43	0.54
3:0:339:ILE:CG1	3:0:343:LYS:NZ	2.62	0.54
3:0:506:ILE:CG2	3:0:521:ASN:ND2	2.69	0.54
3:0:708:LEU:HD22	3:0:712:MET:HE3	1.89	0.54
6:6:156:PHE:HE2	6:6:304:ALA:HB3	1.72	0.54
8:7:425:LEU:O	8:7:430:LEU:HG	2.08	0.54
8:7:434:ASN:O	8:7:449:GLU:CG	2.55	0.54
8:7:466:ARG:HD2	10:T:107:DT:H4'	1.90	0.54
3:0:104:ARG:HH12	3:0:171:LEU:C	2.06	0.54
3:0:198:ARG:HG3	3:0:199:MET:CE	2.37	0.54
8:7:351:ASP:OD1	8:7:405:LYS:CE	2.55	0.54
8:7:420:TRP:CD1	8:7:420:TRP:N	2.71	0.54
8:7:474:MET:O	8:7:478:THR:HG23	2.07	0.54
8:7:666:GLU:HB3	8:7:694:LYS:HB2	1.90	0.54
8:7:710:SER:O	8:7:716:MET:CE	2.53	0.54
10:T:113:DA:H2"	10:T:114:DT:C6	2.43	0.54
3:0:30:LYS:HD3	3:0:479:LEU:HD21	1.90	0.54
4:1:383:GLU:CA	4:1:386:ILE:HG22	2.37	0.54
5:4:155:ALA:O	5:4:158:THR:OG1	2.22	0.54
5:4:163:ILE:CG2	5:4:166:GLU:OE2	2.55	0.54
6:6:172:ILE:HG12	6:6:181:LEU:CD1	2.38	0.54
8:7:394:LEU:HA	8:7:397:ILE:HD12	1.91	0.54
8:7:460:VAL:CG2	8:7:461:ALA:H	2.20	0.54
9:N:64:DA:C2'	9:N:65:DC:C5	2.88	0.54
10:T:99:DA:H2"	10:T:100:DT:C6	2.43	0.54
2:2:72:LEU:HD12	2:2:73:GLN:N	2.22	0.53
2:2:338:SER:CA	2:2:351:SER:OG	2.57	0.53
2:2:378:ILE:HD12	2:2:382:SER:HB2	1.90	0.53
3:0:135:ARG:HH21	3:0:393:VAL:HG23	1.73	0.53
3:0:633:ARG:C	3:0:636:LYS:HG2	2.27	0.53
5:4:25:LEU:HD12	5:4:73:VAL:HA	1.89	0.53
6:6:150:ILE:HG21	6:6:200:ARG:CD	2.36	0.53
6:6:165:PRO:CB	6:6:375:HIS:HD2	2.21	0.53
8:7:411:CYS:SG	8:7:420:TRP:CE3	3.01	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:548:HIS:HA	8:7:695:ARG:NH1	2.23	0.53
8:7:606:ILE:N	8:7:669:CYS:O	2.32	0.53
8:7:628:TYR:CD2	8:7:629:GLY:O	2.61	0.53
8:7:683:GLU:O	8:7:687:LEU:HD23	2.07	0.53
8:7:710:SER:O	8:7:713:THR:OG1	2.18	0.53
3:0:72:CYS:HB2	3:0:234:PHE:CD1	2.43	0.53
3:0:178:PHE:O	3:0:182:LEU:HB2	2.07	0.53
3:0:294:HIS:C	3:0:298:ILE:HG22	2.29	0.53
3:0:416:PHE:CE1	3:0:439:CYS:HB2	2.43	0.53
6:6:291:LEU:HB3	6:6:300:LEU:HD11	1.91	0.53
8:7:401:CYS:O	8:7:404:LYS:CD	2.56	0.53
8:7:411:CYS:CB	8:7:420:TRP:CZ3	2.91	0.53
8:7:445:MET:SD	8:7:449:GLU:CD	2.87	0.53
8:7:739:LEU:HB2	8:7:742:MET:HB2	1.89	0.53
9:N:66:DA:C2'	9:N:67:DT:H72	2.37	0.53
4:1:347:PRO:HB2	4:1:349:VAL:HG13	1.89	0.53
4:1:510:ASN:O	4:1:513:GLN:NE2	2.41	0.53
5:4:273:ARG:NH1	6:6:372:LEU:CB	2.68	0.53
6:6:234:ILE:CB	6:6:263:VAL:HG23	2.39	0.53
9:N:56:DA:H2'	9:N:57:DT:C7	2.39	0.53
2:2:419:LYS:HE3	2:2:430:LEU:HG	1.91	0.53
3:0:41:GLU:HG2	3:0:696:TRP:HZ3	1.73	0.53
3:0:434:ILE:HG13	3:0:434:ILE:O	2.09	0.53
3:0:507:SER:HG	3:0:509:ARG:H	1.56	0.53
3:0:510:PHE:HZ	3:0:513:ARG:O	1.90	0.53
4:1:383:GLU:O	4:1:386:ILE:HG22	2.07	0.53
5:4:255:ASP:HA	5:4:259:ARG:HD2	1.91	0.53
5:4:262:ILE:HD12	5:4:262:ILE:H	1.72	0.53
7:5:55:ASN:HA	7:5:58:LEU:HG	1.90	0.53
8:7:412:THR:HG22	8:7:489:GLU:HB3	1.90	0.53
2:2:356:GLN:HB2	2:2:403:HIS:CE1	2.43	0.53
3:0:5:ILE:O	3:0:5:ILE:HG22	2.07	0.53
3:0:341:TYR:CG	3:0:363:LEU:HD13	2.43	0.53
3:0:422:PRO:HG2	3:0:423:TYR:CE2	2.43	0.53
3:0:712:MET:SD	3:0:713:ALA:N	2.82	0.53
6:6:386:LEU:CD1	6:6:451:CYS:HB2	2.34	0.53
6:6:403:CYS:H	6:6:408:SER:H	1.57	0.53
7:5:21:LEU:HD11	7:5:40:LEU:HD21	1.89	0.53
8:7:445:MET:HE3	8:7:449:GLU:HA	1.90	0.53
8:7:562:THR:HG23	8:7:564:GLU:CD	2.28	0.53
3:0:166:GLU:C	3:0:198:ARG:NH1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:407:THR:O	3:0:411:THR:OG1	2.18	0.53
5:4:176:LEU:CG	5:4:210:ILE:HG12	2.39	0.53
5:4:197:MET:O	5:4:200:ILE:HB	2.08	0.53
5:4:273:ARG:NH1	6:6:372:LEU:HG	2.24	0.53
6:6:362:VAL:HA	6:6:369:MET:HA	1.91	0.53
8:7:600:ARG:HB3	8:7:601:ARG:NH2	2.23	0.53
2:2:72:LEU:CD1	2:2:73:GLN:HG3	2.37	0.53
2:2:78:ILE:O	2:2:81:MET:HG2	2.09	0.53
2:2:222:LEU:HA	2:2:225:ILE:HD12	1.90	0.53
3:0:3:PHE:O	3:0:10:VAL:N	2.41	0.53
3:0:161:ASN:ND2	3:0:189:THR:O	2.42	0.53
3:0:465:PRO:HG2	3:0:467:ASP:OD1	2.09	0.53
3:0:485:MET:HA	3:0:485:MET:CE	2.38	0.53
3:0:487:LEU:HG	3:0:489:LYS:H	1.74	0.53
3:0:522:TYR:N	3:0:525:MET:HE1	2.24	0.53
7:5:21:LEU:HD21	7:5:40:LEU:HD22	1.90	0.53
8:7:478:THR:HA	8:7:505:ILE:HA	1.90	0.53
8:7:578:MET:HA	8:7:581:TYR:CE2	2.43	0.53
2:2:410:ARG:HA	2:2:413:GLU:CD	2.29	0.53
4:1:218:ARG:NH1	6:6:222:LEU:CD1	2.70	0.53
4:1:334:LYS:HD3	4:1:336:ILE:HD12	1.89	0.53
8:7:383:ILE:HG21	8:7:528:ASN:HD22	1.73	0.53
8:7:465:ASN:HB3	8:7:471:GLN:CD	2.22	0.53
8:7:569:TYR:CD1	8:7:577:ARG:NH1	2.77	0.53
8:7:681:ARG:O	8:7:681:ARG:HD3	2.09	0.53
2:2:136:ASP:O	2:2:286:ARG:NE	2.37	0.53
2:2:454:TYR:HE2	7:5:11:GLN:CD	2.12	0.53
2:2:454:TYR:CG	7:5:9:LEU:HD23	2.44	0.53
3:0:167:VAL:HG13	3:0:167:VAL:O	2.07	0.53
5:4:120:ASN:OD1	5:4:121:VAL:N	2.41	0.53
6:6:191:ASP:O	6:6:194:ASP:OD1	2.27	0.53
8:7:416:SER:HA	8:7:419:GLN:OE1	2.09	0.53
8:7:436:ALA:HB3	8:7:449:GLU:OE2	2.09	0.53
8:7:438:PHE:HE2	8:7:469:ASP:HB2	1.74	0.53
8:7:464:ARG:O	8:7:466:ARG:HG3	2.09	0.53
8:7:523:LYS:NZ	8:7:527:LEU:HD21	2.24	0.53
8:7:752:SER:OG	8:7:755:GLU:CG	2.56	0.53
8:7:761:GLN:HA	8:7:764:LEU:HD12	1.91	0.53
2:2:497:GLY:CA	2:2:500:GLN:HE22	2.14	0.53
3:0:191:CYS:O	3:0:195:ILE:HG13	2.08	0.53
3:0:489:LYS:NZ	3:0:728:THR:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:743:ASP:O	3:0:747:HIS:N	2.23	0.53
3:0:744:LEU:HB3	3:0:748:GLN:NE2	2.24	0.53
5:4:200:ILE:O	5:4:204:THR:HG23	2.09	0.53
5:4:213:VAL:HG12	5:4:215:ILE:HD11	1.90	0.53
6:6:186:SER:HB2	6:6:192:HIS:NE2	2.24	0.53
6:6:189:PRO:O	6:6:193:ILE:HG12	2.09	0.53
6:6:216:MET:O	6:6:220:LEU:HG	2.09	0.53
6:6:426:ARG:HH22	6:6:435:GLU:H	1.55	0.53
8:7:339:GLU:HG2	8:7:380:ARG:HD3	1.91	0.53
8:7:471:GLN:CA	8:7:474:MET:CE	2.82	0.53
2:2:408:MET:HE3	2:2:411:LEU:CD1	2.38	0.52
3:0:83:LEU:HA	3:0:86:LEU:CD2	2.39	0.52
3:0:334:PHE:CD1	3:0:337:ARG:NE	2.75	0.52
3:0:472:MET:O	3:0:646:TYR:OH	2.17	0.52
4:1:235:UNK:O	4:1:237:UNK:N	2.42	0.52
5:4:194:ILE:H	5:4:194:ILE:HD12	1.74	0.52
8:7:496:ALA:HA	8:7:499:ARG:CG	2.39	0.52
9:N:51:DC:O2	9:N:52:DA:C5	2.62	0.52
2:2:419:LYS:HZ2	2:2:423:ASP:HA	1.75	0.52
3:0:77:SER:HA	3:0:80:GLU:OE2	2.09	0.52
3:0:312:LEU:CD1	3:0:448:PRO:HG3	2.17	0.52
3:0:328:ALA:O	3:0:331:PHE:HB3	2.09	0.52
3:0:469:TYR:CE2	3:0:472:MET:HE1	2.45	0.52
3:0:669:VAL:O	3:0:675:ASP:OD2	2.27	0.52
4:1:288:PHE:O	4:1:292:LEU:HG	2.10	0.52
5:4:87:TYR:HA	5:4:125:LEU:CD2	2.39	0.52
5:4:161:ASN:HD21	5:4:165:LYS:NZ	2.07	0.52
5:4:303:ASN:HB3	5:4:311:GLN:HE21	1.74	0.52
6:6:232:VAL:HG12	6:6:233:LEU:N	2.24	0.52
8:7:383:ILE:O	8:7:534:LYS:HA	2.09	0.52
8:7:459:MET:HE3	8:7:470:SER:CB	2.38	0.52
3:0:210:TYR:OH	3:0:235:ASP:O	2.24	0.52
3:0:322:PRO:HB3	3:0:376:PHE:HD2	1.74	0.52
3:0:521:ASN:O	3:0:524:SER:OG	2.22	0.52
3:0:537:MET:O	3:0:597:ILE:HG13	2.09	0.52
3:0:720:PHE:O	3:0:723:THR:OG1	2.19	0.52
5:4:273:ARG:HH22	6:6:372:LEU:CA	2.21	0.52
5:4:290:SER:OG	5:4:291:VAL:N	2.42	0.52
6:6:155:ASP:HB3	6:6:298:LYS:HZ3	1.75	0.52
6:6:315:LYS:HG3	6:6:316:GLY:H	1.75	0.52
8:7:344:ARG:HB2	8:7:378:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:457:TYR:O	8:7:462:ASN:OD1	2.27	0.52
8:7:463:THR:O	9:N:63:DG:H4'	2.09	0.52
8:7:499:ARG:CZ	8:7:500:ARG:HG3	2.39	0.52
8:7:583:MET:SD	8:7:760:LEU:CA	2.95	0.52
8:7:678:GLY:C	8:7:682:GLN:OE1	2.48	0.52
9:N:52:DA:H2'	9:N:53:DT:C7	2.39	0.52
9:N:52:DA:C2'	9:N:53:DT:H72	2.37	0.52
2:2:354:PRO:HA	2:2:357:ILE:CD1	2.39	0.52
3:0:185:CYS:O	3:0:189:THR:N	2.43	0.52
3:0:235:ASP:HA	3:0:459:THR:O	2.09	0.52
3:0:416:PHE:CD1	3:0:439:CYS:CA	2.90	0.52
4:1:253:ARG:HG2	4:1:257:LEU:HD23	1.90	0.52
5:4:117:ARG:HA	5:4:120:ASN:ND2	2.24	0.52
8:7:640:LEU:O	8:7:644:GLN:HG2	2.10	0.52
1:3:70:THR:HG23	1:3:70:THR:O	2.10	0.52
3:0:264:ALA:HB1	3:0:336:LYS:HE3	1.92	0.52
3:0:306:PHE:HZ	3:0:393:VAL:HG22	1.75	0.52
5:4:150:ALA:CA	5:4:153:MET:HE2	2.35	0.52
8:7:621:LYS:O	8:7:747:ASN:ND2	2.43	0.52
1:3:45:ARG:CZ	1:3:46:ILE:HD11	2.40	0.52
2:2:501:VAL:C	2:2:504:PHE:CE2	2.80	0.52
3:0:514:ASN:CG	3:0:553:MET:HG2	2.30	0.52
3:0:721:LEU:HD12	3:0:722:ARG:N	2.25	0.52
4:1:386:ILE:HG23	4:1:387:MET:HE3	1.92	0.52
4:1:466:UNK:O	4:1:468:UNK:N	2.43	0.52
5:4:33:ALA:O	5:4:37:TRP:N	2.26	0.52
5:4:193:TYR:CD1	5:4:223:PHE:CD1	2.97	0.52
5:4:271:ASP:C	5:4:273:ARG:HD2	2.29	0.52
8:7:752:SER:HG	8:7:755:GLU:CG	2.23	0.52
2:2:468:TYR:OH	2:2:486:ASP:N	2.42	0.52
3:0:367:THR:HG22	3:0:369:ILE:HG12	1.90	0.52
5:4:292:CYS:SG	5:4:308:CYS:HB3	2.49	0.52
8:7:569:TYR:HD1	8:7:577:ARG:NH1	2.08	0.52
8:7:583:MET:CE	8:7:763:VAL:HB	2.29	0.52
8:7:668:THR:HG1	8:7:694:LYS:HZ2	1.52	0.52
9:N:61:DG:C2'	9:N:62:DT:C7	2.87	0.52
9:N:75:DG:C2'	9:N:76:DT:C7	2.88	0.52
2:2:234:GLY:N	2:2:269:PHE:O	2.43	0.52
2:2:501:VAL:O	2:2:504:PHE:CZ	2.62	0.52
3:0:41:GLU:CG	3:0:696:TRP:CZ3	2.93	0.52
3:0:171:LEU:HD22	3:0:184:TYR:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:238:UNK:O	4:1:296:LEU:HD11	2.10	0.52
8:7:544:SER:HA	8:7:549:ILE:O	2.09	0.52
3:0:192:PRO:HA	3:0:195:ILE:HD12	1.91	0.52
3:0:331:PHE:CE2	3:0:335:LEU:HD11	2.45	0.52
3:0:440:LEU:HD22	3:0:638:ARG:HA	1.91	0.52
4:1:265:ILE:HG13	4:1:266:VAL:N	2.25	0.52
4:1:503:VAL:HG22	5:4:247:TYR:CZ	2.45	0.52
5:4:70:ALA:HA	5:4:117:ARG:HH22	1.75	0.52
5:4:163:ILE:C	5:4:166:GLU:HG3	2.29	0.52
5:4:303:ASN:HB2	5:4:311:GLN:HG2	1.92	0.52
8:7:143:LEU:H	8:7:171:HIS:H	1.58	0.52
2:2:110:ASN:O	2:2:115:GLY:N	2.42	0.52
3:0:24:TYR:CE2	3:0:52:LEU:HD23	2.45	0.52
3:0:68:LYS:HE3	3:0:225:GLU:OE2	2.09	0.52
3:0:548:GLU:HA	3:0:551:VAL:HG12	1.92	0.52
5:4:273:ARG:NH2	6:6:373:SER:N	2.52	0.52
6:6:130:LEU:N	6:6:172:ILE:O	2.36	0.52
6:6:165:PRO:CB	6:6:375:HIS:CD2	2.93	0.52
8:7:363:ARG:CD	8:7:366:GLN:NE2	2.73	0.52
8:7:382:GLY:HA2	8:7:532:GLY:HA3	1.92	0.52
3:0:258:ARG:HH11	3:0:262:ARG:NH1	2.08	0.51
6:6:128:LEU:HA	6:6:233:LEU:HB3	1.90	0.51
6:6:168:GLN:HG3	6:6:169:MET:N	2.25	0.51
6:6:281:ASN:CG	6:6:287:PHE:CD2	2.84	0.51
8:7:459:MET:HE3	8:7:470:SER:HA	1.92	0.51
8:7:465:ASN:HD22	8:7:474:MET:HE2	1.76	0.51
2:2:33:LEU:O	2:2:37:ARG:HG2	2.09	0.51
2:2:100:LEU:HD11	2:2:102:PRO:HA	1.91	0.51
2:2:360:LEU:HD23	2:2:363:PHE:HZ	1.75	0.51
3:0:39:ILE:HG23	3:0:480:GLN:CG	2.24	0.51
3:0:134:ARG:O	3:0:138:ASN:CG	2.49	0.51
3:0:473:LEU:HB2	3:0:475:PHE:CD1	2.45	0.51
4:1:291:LYS:O	4:1:295:LYS:N	2.43	0.51
6:6:128:LEU:HG	6:6:233:LEU:HD22	1.91	0.51
8:7:341:TYR:O	8:7:378:ARG:HB3	2.11	0.51
8:7:469:ASP:HB3	8:7:472:LYS:NZ	2.25	0.51
8:7:522:ASP:OD1	8:7:526:ASP:CG	2.48	0.51
8:7:555:ALA:HA	8:7:734:LYS:O	2.10	0.51
8:7:713:THR:OG1	8:7:716:MET:HE3	2.10	0.51
1:3:27:LYS:HZ2	1:3:29:LEU:CG	2.23	0.51
1:3:75:ASP:O	1:3:77:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:350:TYR:H	2:2:407:GLN:CD	2.13	0.51
2:2:500:GLN:O	2:2:504:PHE:CD2	2.61	0.51
3:0:42:MET:CG	3:0:48:LYS:HE3	2.41	0.51
3:0:331:PHE:C	3:0:335:LEU:HD13	2.30	0.51
3:0:654:LEU:O	3:0:657:ASP:OD1	2.28	0.51
8:7:568:GLU:CA	8:7:571:ARG:HG3	2.39	0.51
8:7:635:GLU:O	8:7:639:ILE:HG13	2.10	0.51
3:0:176:PHE:HB3	3:0:181:LEU:HA	1.91	0.51
3:0:425:ILE:HA	3:0:428:ALA:HB2	1.91	0.51
5:4:192:GLN:HG2	5:4:196:ILE:CD1	2.39	0.51
6:6:172:ILE:HG12	6:6:181:LEU:HD13	1.92	0.51
8:7:554:CYS:SG	8:7:726:LEU:HD22	2.51	0.51
9:N:56:DA:H2"	9:N:57:DT:H71	1.92	0.51
1:3:31:ASN:HD21	1:3:64:ARG:H	1.57	0.51
2:2:184:ILE:O	2:2:389:ASN:ND2	2.43	0.51
3:0:361:GLN:O	3:0:365:GLN:HG2	2.10	0.51
3:0:573:THR:HG23	3:0:575:ASP:OD1	2.10	0.51
3:0:649:ARG:HG3	3:0:651:ASN:OD1	2.11	0.51
4:1:283:PHE:CD1	4:1:284:TRP:CD1	2.98	0.51
5:4:193:TYR:CB	5:4:223:PHE:HE1	2.19	0.51
7:5:28:SER:OG	7:5:30:ILE:HD11	2.10	0.51
8:7:447:GLN:CD	8:7:476:PHE:CG	2.82	0.51
2:2:12:GLN:O	2:2:15:GLU:HG3	2.11	0.51
3:0:15:PRO:O	3:0:741:TYR:HD1	1.94	0.51
3:0:238:HIS:CD2	3:0:664:GLN:HE21	2.28	0.51
4:1:597:PHE:CZ	4:1:620:LEU:HD11	2.45	0.51
6:6:293:ASP:O	6:6:296:HIS:HB3	2.10	0.51
8:7:401:CYS:HB3	8:7:404:LYS:HZ1	1.74	0.51
8:7:439:THR:OG1	8:7:455:SER:HA	2.11	0.51
8:7:464:ARG:NH1	10:T:105:DC:H1'	2.25	0.51
8:7:469:ASP:O	8:7:473:VAL:HG23	2.10	0.51
8:7:558:TRP:HB3	8:7:711:LYS:HB3	1.91	0.51
8:7:564:GLU:HG2	8:7:565:PHE:N	2.25	0.51
9:N:70:DA:H2'	9:N:71:DT:C7	2.39	0.51
1:3:45:ARG:CD	1:3:46:ILE:HG13	2.40	0.51
1:3:72:ILE:CG1	1:3:74:ASP:OD1	2.58	0.51
2:2:405:HIS:HA	2:2:408:MET:HB2	1.93	0.51
3:0:394:GLU:HG2	3:0:395:ASP:N	2.25	0.51
3:0:422:PRO:HG2	3:0:423:TYR:CD2	2.46	0.51
3:0:536:GLY:O	3:0:618:ARG:HB2	2.10	0.51
6:6:286:SER:OG	6:6:289:LYS:NZ	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:571:ARG:HD2	8:7:572:GLU:CB	2.41	0.51
2:2:28:SER:OG	2:2:31:THR:CG2	2.58	0.51
3:0:83:LEU:HD21	3:0:207:ILE:HD13	1.87	0.51
3:0:339:ILE:C	3:0:343:LYS:HZ2	2.01	0.51
3:0:341:TYR:HA	3:0:344:THR:HG22	1.92	0.51
3:0:572:GLU:CD	3:0:600:SER:CB	2.76	0.51
3:0:639:LEU:CD2	3:0:642:MET:HE1	2.28	0.51
4:1:188:ASN:ND2	4:1:191:LEU:HG	2.25	0.51
6:6:231:GLU:HG3	6:6:260:ARG:O	2.09	0.51
8:7:596:GLN:HG3	8:7:600:ARG:NH2	2.26	0.51
8:7:618:TYR:HD1	8:7:621:LYS:HD2	1.75	0.51
2:2:380:ARG:CD	2:2:444:TRP:CB	2.88	0.51
3:0:395:ASP:OD2	3:0:396:PHE:CE1	2.63	0.51
3:0:468:MET:HG2	3:0:656:PHE:CZ	2.46	0.51
3:0:469:TYR:CG	3:0:472:MET:HE1	2.46	0.51
5:4:163:ILE:HA	5:4:166:GLU:OE2	2.11	0.51
5:4:193:TYR:O	5:4:196:ILE:HB	2.11	0.51
5:4:200:ILE:HG12	5:4:227:THR:HG23	1.93	0.51
6:6:165:PRO:HB2	6:6:375:HIS:HD2	1.76	0.51
8:7:440:SER:HB3	8:7:459:MET:HG3	1.91	0.51
8:7:591:CYS:HB2	8:7:708:LEU:HD11	1.91	0.51
2:2:340:ILE:O	2:2:347:ILE:HA	2.11	0.51
2:2:366:LEU:HD11	2:2:374:VAL:HG11	1.93	0.51
2:2:463:GLU:HG2	2:2:464:THR:N	2.26	0.51
3:0:36:GLY:O	3:0:456:VAL:N	2.44	0.51
3:0:254:THR:HB	3:0:346:MET:SD	2.51	0.51
3:0:279:SER:CB	3:0:283:GLN:HE22	2.23	0.51
3:0:371:ARG:NH2	3:0:411:THR:O	2.43	0.51
3:0:521:ASN:OD1	3:0:525:MET:SD	2.69	0.51
3:0:586:TYR:CE1	3:0:596:ALA:C	2.85	0.51
3:0:681:LEU:HB3	3:0:686:PHE:CD2	2.46	0.51
5:4:30:ILE:HD13	5:4:179:LEU:HB3	1.92	0.51
5:4:176:LEU:CD2	5:4:210:ILE:HG12	2.41	0.51
5:4:246:GLN:O	5:4:250:THR:HG23	2.10	0.51
5:4:293:LEU:HB2	6:6:380:TYR:HE1	1.75	0.51
6:6:426:ARG:NH2	6:6:435:GLU:CA	2.74	0.51
8:7:408:ILE:HG23	8:7:482:TRP:CD2	2.45	0.51
8:7:410:LEU:HG	8:7:455:SER:OG	2.11	0.51
8:7:604:LYS:NZ	8:7:694:LYS:NZ	2.59	0.51
9:N:70:DA:H2"	9:N:71:DT:H71	1.92	0.51
10:T:99:DA:H2'	10:T:100:DT:H71	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:5:ILE:CD1	3:0:22:TYR:CZ	2.94	0.50
3:0:74:ARG:HG2	3:0:75:THR:HG23	1.92	0.50
3:0:471:ARG:O	3:0:646:TYR:CE1	2.63	0.50
3:0:519:VAL:CG2	3:0:553:MET:HE3	2.40	0.50
3:0:752:LYS:HG3	3:0:752:LYS:O	2.12	0.50
5:4:124:THR:O	5:4:128:GLU:CD	2.48	0.50
5:4:177:LEU:HD12	5:4:211:ASP:O	2.11	0.50
6:6:132:CYS:SG	6:6:204:PRO:HB3	2.51	0.50
6:6:154:ILE:HD13	6:6:196:LEU:CD1	2.41	0.50
8:7:340:GLU:HB2	8:7:378:ARG:HB2	1.93	0.50
8:7:544:SER:CA	8:7:549:ILE:HB	2.41	0.50
8:7:576:LYS:NZ	8:7:764:LEU:HA	2.26	0.50
8:7:641:GLN:HA	8:7:644:GLN:CG	2.39	0.50
8:7:759:LEU:O	8:7:763:VAL:HG23	2.12	0.50
9:N:61:DG:C2'	9:N:62:DT:H72	2.34	0.50
1:3:27:LYS:HD2	1:3:29:LEU:CG	2.41	0.50
1:3:72:ILE:CD1	1:3:74:ASP:OD2	2.58	0.50
2:2:19:GLN:NE2	2:2:85:HIS:CG	2.78	0.50
3:0:285:GLU:HG2	3:0:387:THR:HG21	1.92	0.50
3:0:412:TYR:CB	3:0:416:PHE:CE2	2.94	0.50
6:6:156:PHE:CE2	6:6:304:ALA:HB3	2.46	0.50
6:6:322:MET:HE3	6:6:324:PHE:CE1	2.47	0.50
8:7:459:MET:HE1	8:7:470:SER:O	2.11	0.50
3:0:614:HIS:CE1	3:0:675:ASP:CB	2.94	0.50
3:0:643:ARG:HD3	3:0:649:ARG:HA	1.92	0.50
4:1:375:LEU:HA	4:1:378:MET:CE	2.40	0.50
6:6:144:ASN:CG	6:6:147:ALA:H	2.14	0.50
6:6:236:PHE:CE2	6:6:238:SER:OG	2.54	0.50
8:7:599:GLU:HG2	8:7:650:ASN:HB2	1.93	0.50
1:3:27:LYS:HB3	1:3:40:GLU:HG2	1.93	0.50
2:2:345:PHE:CZ	2:2:437:VAL:HA	2.46	0.50
2:2:365:HIS:HB3	2:2:385:ARG:NH2	2.19	0.50
3:0:83:LEU:HA	3:0:86:LEU:HD21	1.93	0.50
3:0:352:ILE:C	3:0:419:ILE:HD12	2.31	0.50
3:0:568:LEU:HB2	3:0:596:ALA:HA	1.93	0.50
3:0:696:TRP:HD1	3:0:697:ILE:HD13	1.75	0.50
5:4:138:LYS:O	5:4:138:LYS:NZ	2.36	0.50
5:4:203:ALA:HB2	5:4:210:ILE:HD11	1.94	0.50
6:6:451:CYS:SG	6:6:454:CYS:HB2	2.51	0.50
7:5:18:ALA:O	7:5:22:GLN:HG3	2.11	0.50
7:5:42:VAL:CG1	7:5:43:ASN:N	2.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:342:ASP:OD1	8:7:342:ASP:N	2.45	0.50
8:7:457:TYR:OH	8:7:490:VAL:HG21	2.11	0.50
8:7:581:TYR:CE1	8:7:582:ILE:HG13	2.46	0.50
2:2:174:GLU:N	2:2:183:LYS:O	2.45	0.50
3:0:356:PRO:CG	3:0:413:GLU:HA	2.42	0.50
3:0:484:ALA:HB2	3:0:695:LYS:HE3	1.92	0.50
5:4:217:GLY:O	5:4:219:LYS:N	2.45	0.50
6:6:322:MET:CE	6:6:323:GLY:O	2.47	0.50
8:7:683:GLU:CG	8:7:686:ARG:NH2	2.68	0.50
8:7:754:ARG:CB	8:7:757:ARG:NE	2.73	0.50
2:2:50:MET:CE	2:2:56:GLU:HA	2.41	0.50
3:0:120:VAL:HG12	3:0:129:VAL:HG13	1.93	0.50
3:0:254:THR:HB	3:0:346:MET:HG2	1.94	0.50
3:0:380:ARG:HD2	3:0:383:LEU:HD11	1.94	0.50
5:4:159:TYR:O	5:4:163:ILE:HG13	2.11	0.50
6:6:150:ILE:HG21	6:6:200:ARG:HG3	1.83	0.50
6:6:168:GLN:OE1	6:6:186:SER:N	2.45	0.50
8:7:490:VAL:O	8:7:490:VAL:HG12	2.12	0.50
8:7:494:PRO:CG	8:7:497:MET:CE	2.70	0.50
1:3:45:ARG:HD2	1:3:46:ILE:HG13	1.94	0.50
2:2:197:ASN:C	2:2:201:TRP:HD1	2.13	0.50
3:0:66:HIS:N	3:0:67:ARG:HH21	2.09	0.50
3:0:191:CYS:SG	3:0:194:PHE:HB2	2.52	0.50
3:0:293:LEU:O	3:0:298:ILE:HG21	2.12	0.50
3:0:339:ILE:HG23	3:0:340:GLU:OE2	2.12	0.50
3:0:356:PRO:CA	3:0:359:PHE:CZ	2.69	0.50
3:0:380:ARG:HA	3:0:383:LEU:CD2	2.41	0.50
3:0:564:TRP:CZ2	3:0:569:ILE:HB	2.47	0.50
5:4:136:GLU:HA	5:4:140:ILE:HG13	1.94	0.50
6:6:128:LEU:HD23	6:6:128:LEU:C	2.32	0.50
7:5:23:ILE:HA	7:5:26:LYS:HD2	1.94	0.50
7:5:24:ASP:O	7:5:27:MET:N	2.45	0.50
8:7:636:ARG:HH22	8:7:657:VAL:HG11	1.76	0.50
10:T:107:DT:H2"	10:T:108:DC:C5	2.47	0.50
3:0:720:PHE:O	3:0:724:MET:HG2	2.12	0.50
6:6:281:ASN:CG	6:6:287:PHE:CE2	2.84	0.50
8:7:355:ASP:CG	8:7:357:LYS:HZ3	2.15	0.50
8:7:413:SER:O	8:7:417:VAL:HG23	2.12	0.50
8:7:447:GLN:CD	8:7:476:PHE:HB2	2.31	0.50
8:7:499:ARG:HD2	8:7:500:ARG:HG3	1.94	0.50
9:N:53:DT:C2'	9:N:54:DT:C7	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:104:DA:H2"	10:T:105:DC:C6	2.46	0.50
2:2:39:LEU:HD13	2:2:47:ILE:CD1	2.42	0.50
2:2:349:SER:HA	2:2:407:GLN:HE22	1.76	0.50
2:2:380:ARG:HD2	2:2:444:TRP:CB	2.40	0.50
2:2:473:LYS:HD2	2:2:476:GLN:HB3	1.94	0.50
3:0:11:LEU:N	3:0:11:LEU:HD12	2.26	0.50
3:0:135:ARG:CZ	3:0:392:GLU:HA	2.40	0.50
3:0:238:HIS:HE2	3:0:664:GLN:HG3	1.76	0.50
3:0:306:PHE:CZ	3:0:385:VAL:HG11	2.47	0.50
3:0:383:LEU:O	3:0:387:THR:HG23	2.12	0.50
3:0:515:ASP:N	3:0:515:ASP:OD1	2.45	0.50
3:0:544:TYR:OH	3:0:574:PRO:HD3	2.12	0.50
3:0:575:ASP:OD1	3:0:575:ASP:O	2.30	0.50
4:1:206:PRO:C	4:1:210:TRP:CZ3	2.85	0.50
5:4:62:ASN:OD1	5:4:118:PHE:HB3	2.11	0.50
6:6:145:ARG:C	6:6:149:ILE:CD1	2.81	0.50
7:5:11:GLN:NE2	7:5:39:HIS:CD2	2.80	0.50
8:7:425:LEU:HB3	8:7:430:LEU:CD2	2.30	0.50
9:N:75:DG:H2"	9:N:76:DT:H6	1.72	0.50
2:2:475:ALA:CB	2:2:481:LEU:CD1	2.90	0.49
3:0:163:TYR:HA	3:0:167:VAL:HG12	1.93	0.49
3:0:241:ASP:O	3:0:245:ILE:HG12	2.11	0.49
3:0:356:PRO:O	3:0:360:LEU:CB	2.54	0.49
3:0:424:GLU:CB	3:0:432:ASN:HD21	2.16	0.49
3:0:510:PHE:O	3:0:511:GLU:CG	2.55	0.49
3:0:721:LEU:HD13	6:6:268:ALA:HA	1.93	0.49
4:1:273:ASN:HA	4:1:276:LYS:O	2.12	0.49
5:4:34:PRO:O	5:4:38:THR:CB	2.60	0.49
8:7:372:LYS:HE3	8:7:536:TYR:CD1	2.47	0.49
8:7:447:GLN:CG	8:7:476:PHE:CE1	2.89	0.49
8:7:561:MET:H	8:7:711:LYS:HE2	1.77	0.49
8:7:562:THR:CG2	8:7:564:GLU:CD	2.80	0.49
8:7:571:ARG:HH21	8:7:580:LEU:HD12	1.74	0.49
8:7:588:PHE:CZ	8:7:621:LYS:HB3	2.47	0.49
8:7:664:LEU:HG	8:7:689:ARG:CD	2.40	0.49
10:T:90:DA:H2"	10:T:91:DC:C6	2.46	0.49
10:T:93:DT:H2"	10:T:94:DC:C5	2.46	0.49
10:T:104:DA:H2"	10:T:105:DC:C5	2.47	0.49
10:T:113:DA:H2'	10:T:114:DT:H71	1.92	0.49
3:0:128:VAL:O	3:0:131:GLU:HG3	2.12	0.49
3:0:134:ARG:O	3:0:138:ASN:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:136:MET:HE3	3:0:156:CYS:SG	2.50	0.49
3:0:157:GLU:CD	3:0:160:GLU:HB2	2.32	0.49
3:0:208:TYR:CE1	3:0:213:LEU:HB2	2.43	0.49
3:0:272:SER:HA	3:0:275:ARG:HE	1.78	0.49
4:1:258:ASN:O	4:1:262:ASN:HB2	2.13	0.49
8:7:418:MET:HE3	8:7:441:ASP:OD2	2.12	0.49
8:7:544:SER:HA	8:7:549:ILE:HB	1.95	0.49
2:2:15:GLU:HB3	2:2:84:LEU:CG	2.41	0.49
2:2:56:GLU:OE2	2:2:97:MET:SD	2.71	0.49
2:2:417:GLU:O	2:2:417:GLU:CD	2.50	0.49
3:0:31:THR:O	3:0:34:VAL:N	2.46	0.49
3:0:251:ASP:H	4:1:350:ARG:HG2	1.75	0.49
3:0:257:LEU:O	3:0:261:THR:HG23	2.13	0.49
3:0:258:ARG:HG3	3:0:262:ARG:HH12	1.77	0.49
3:0:572:GLU:CD	3:0:600:SER:CA	2.80	0.49
3:0:577:GLN:HE22	3:0:578:GLU:CD	2.16	0.49
5:4:225:GLN:NE2	5:4:269:SER:CB	2.66	0.49
6:6:166:ILE:HG12	6:6:375:HIS:HB3	1.93	0.49
6:6:282:TYR:OH	6:6:313:ILE:CD1	2.59	0.49
7:5:21:LEU:HD23	7:5:31:VAL:HG21	1.93	0.49
2:2:143:TRP:O	2:2:146:ILE:HG22	2.12	0.49
2:2:397:ILE:O	2:2:401:GLU:HG2	2.12	0.49
3:0:353:SER:HA	3:0:419:ILE:HD12	1.94	0.49
3:0:354:GLU:HB2	3:0:418:LEU:HD23	1.94	0.49
5:4:255:ASP:O	5:4:257:SER:N	2.46	0.49
7:5:54:LEU:HD23	7:5:58:LEU:HD21	1.94	0.49
2:2:353:SER:CA	2:2:356:GLN:HG2	2.42	0.49
2:2:365:HIS:CE1	2:2:377:GLN:H	2.30	0.49
3:0:17:ILE:HG21	3:0:745:ILE:CG2	2.43	0.49
3:0:156:CYS:C	3:0:158:TYR:H	2.16	0.49
3:0:167:VAL:HG23	3:0:198:ARG:HE	1.76	0.49
3:0:354:GLU:O	3:0:418:LEU:N	2.45	0.49
3:0:632:SER:OG	3:0:633:ARG:N	2.45	0.49
5:4:30:ILE:O	5:4:30:ILE:HG23	2.12	0.49
8:7:496:ALA:HA	8:7:499:ARG:HG2	1.95	0.49
1:3:65:LYS:CG	1:3:66:ASN:H	2.05	0.49
3:0:15:PRO:C	3:0:741:TYR:HD1	2.15	0.49
3:0:175:VAL:O	3:0:175:VAL:HG23	2.13	0.49
3:0:423:TYR:CE1	3:0:425:ILE:CG1	2.88	0.49
5:4:30:ILE:HA	5:4:179:LEU:HB2	1.94	0.49
5:4:154:SER:O	5:4:158:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:193:TYR:CB	5:4:223:PHE:CE1	2.89	0.49
8:7:365:TYR:O	8:7:368:LYS:HG2	2.13	0.49
1:3:38:ILE:HG21	1:3:43:VAL:HB	1.94	0.49
2:2:14:LEU:O	2:2:17:ILE:HG22	2.12	0.49
3:0:23:ASN:ND2	3:0:483:TYR:CE1	2.80	0.49
3:0:143:ARG:C	3:0:147:GLU:OE1	2.51	0.49
3:0:297:ASP:OD2	3:0:386:ARG:NH1	2.45	0.49
3:0:467:ASP:OD1	3:0:468:MET:N	2.46	0.49
3:0:510:PHE:CZ	3:0:513:ARG:O	2.65	0.49
3:0:659:MET:CE	3:0:689:LYS:HB3	2.43	0.49
4:1:306:UNK:O	4:1:308:UNK:N	2.46	0.49
8:7:343:PHE:O	8:7:405:LYS:NZ	2.37	0.49
8:7:436:ALA:HB2	8:7:445:MET:HG3	1.94	0.49
8:7:516:THR:OG1	8:7:681:ARG:CZ	2.61	0.49
8:7:619:ALA:HB1	8:7:626:PHE:CG	2.47	0.49
10:T:90:DA:H2"	10:T:91:DC:C5	2.47	0.49
2:2:50:MET:HE1	2:2:57:VAL:HG23	1.94	0.49
2:2:431:GLN:CD	2:2:435:PRO:HD2	2.33	0.49
3:0:130:ASP:O	3:0:134:ARG:HG3	2.12	0.49
3:0:251:ASP:N	4:1:350:ARG:HG2	2.28	0.49
3:0:441:ASP:OD1	3:0:443:SER:OG	2.20	0.49
3:0:633:ARG:HH11	3:0:636:LYS:CE	2.24	0.49
5:4:177:LEU:HD11	5:4:213:VAL:HG23	1.95	0.49
8:7:411:CYS:HB2	8:7:420:TRP:CZ3	2.47	0.49
8:7:425:LEU:HA	8:7:428:CYS:HB3	1.93	0.49
8:7:754:ARG:HA	8:7:757:ARG:NE	2.27	0.49
2:2:26:TYR:CD2	2:2:104:PHE:HB2	2.48	0.49
3:0:18:TYR:HD2	3:0:21:GLN:HE21	1.59	0.49
3:0:70:ILE:N	3:0:231:ILE:O	2.27	0.49
3:0:252:LEU:N	4:1:350:ARG:HH21	2.10	0.49
4:1:218:ARG:HH21	6:6:223:PRO:HG3	1.78	0.49
6:6:130:LEU:O	6:6:174:MET:N	2.45	0.49
7:5:54:LEU:CD2	7:5:58:LEU:HD21	2.42	0.49
8:7:752:SER:HG	8:7:755:GLU:HB2	1.78	0.49
2:2:284:THR:O	2:2:284:THR:HG22	2.12	0.49
3:0:107:GLY:CA	3:0:207:ILE:HG13	2.42	0.49
3:0:222:VAL:HG11	3:0:452:ARG:NH1	2.28	0.49
3:0:257:LEU:HD23	3:0:343:LYS:CG	2.40	0.49
3:0:478:VAL:C	3:0:480:GLN:OE1	2.51	0.49
5:4:31:GLU:OE2	5:4:181:CYS:N	2.41	0.49
6:6:159:GLU:C	6:6:163:GLN:NE2	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:361:GLN:O	8:7:394:LEU:HD23	2.12	0.49
8:7:459:MET:HE1	8:7:470:SER:C	2.34	0.49
8:7:491:HIS:CB	8:7:519:ARG:CZ	2.91	0.49
1:3:28:PHE:HA	1:3:38:ILE:O	2.13	0.48
2:2:75:GLN:NE2	2:2:78:ILE:HD11	2.28	0.48
3:0:136:MET:HE3	12:0:801:SF4:S1	2.53	0.48
3:0:326:ARG:O	3:0:380:ARG:NH2	2.45	0.48
3:0:659:MET:HE1	3:0:689:LYS:CB	2.43	0.48
5:4:26:LEU:HD11	5:4:28:VAL:HG23	1.95	0.48
7:5:11:GLN:HE21	7:5:39:HIS:HD2	1.60	0.48
7:5:23:ILE:HG12	7:5:57:LEU:CD2	2.38	0.48
8:7:411:CYS:O	8:7:456:THR:HA	2.12	0.48
8:7:754:ARG:CB	8:7:757:ARG:NH2	2.74	0.48
9:N:66:DA:H2'	9:N:67:DT:C7	2.40	0.48
3:0:17:ILE:HG13	3:0:18:TYR:H	1.78	0.48
3:0:19:PRO:HG3	3:0:739:TRP:CG	2.48	0.48
3:0:90:MET:CE	3:0:101:GLU:OE2	2.62	0.48
3:0:104:ARG:NE	3:0:173:LYS:CA	2.65	0.48
3:0:109:THR:HG21	3:0:113:ASN:CG	2.32	0.48
3:0:575:ASP:OD1	3:0:578:GLU:HB2	2.12	0.48
5:4:27:THR:HG21	5:4:160:VAL:CG2	2.43	0.48
6:6:129:THR:OG1	6:6:234:ILE:HA	2.14	0.48
7:5:47:VAL:HA	7:5:50:VAL:CG2	2.43	0.48
8:7:461:ALA:O	8:7:497:MET:HG2	2.13	0.48
1:3:54:CYS:O	1:3:59:CYS:HB3	2.12	0.48
2:2:389:ASN:CB	2:2:391:ILE:HG12	2.41	0.48
2:2:496:GLU:C	2:2:500:GLN:OE1	2.51	0.48
3:0:39:ILE:CG2	3:0:480:GLN:CG	2.85	0.48
3:0:136:MET:O	3:0:155:LEU:HA	2.13	0.48
3:0:255:ASP:OD1	3:0:255:ASP:N	2.45	0.48
3:0:468:MET:CE	3:0:653:PHE:CD2	2.96	0.48
3:0:487:LEU:HD23	3:0:489:LYS:O	2.12	0.48
3:0:633:ARG:HB2	3:0:636:LYS:CG	2.42	0.48
4:1:386:ILE:HG23	4:1:387:MET:CE	2.43	0.48
5:4:183:SER:O	5:4:219:LYS:NZ	2.35	0.48
5:4:273:ARG:NH1	6:6:372:LEU:HD23	2.29	0.48
6:6:224:VAL:HB	6:6:230:ARG:NH2	2.29	0.48
8:7:442:ASN:HD22	8:7:444:GLU:CG	2.27	0.48
8:7:478:THR:HG21	8:7:504:THR:CG2	2.43	0.48
8:7:662:ILE:O	8:7:664:LEU:CD2	2.56	0.48
2:2:137:GLU:N	2:2:286:ARG:HH12	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:74:ARG:HA	3:0:210:TYR:CD2	2.48	0.48
3:0:133:CYS:HB2	12:0:801:SF4:S4	2.53	0.48
3:0:143:ARG:HA	3:0:146:GLU:HG2	1.95	0.48
3:0:529:PHE:CE2	3:0:621:LEU:HD21	2.49	0.48
3:0:586:TYR:HE1	3:0:596:ALA:C	2.16	0.48
4:1:195:PHE:CE1	4:1:210:TRP:CH2	3.01	0.48
4:1:275:PRO:O	4:1:278:PHE:HE1	1.96	0.48
4:1:283:PHE:CD1	4:1:284:TRP:HD1	2.32	0.48
5:4:85:TYR:CD2	5:4:88:PRO:HG2	2.46	0.48
6:6:134:GLU:OE2	6:6:207:ASN:ND2	2.46	0.48
6:6:168:GLN:CG	6:6:185:VAL:HG23	2.43	0.48
6:6:196:LEU:O	6:6:200:ARG:HG3	2.13	0.48
7:5:52:HIS:O	7:5:56:ARG:HG3	2.13	0.48
7:5:53:GLU:HB2	7:5:56:ARG:HH21	1.78	0.48
8:7:410:LEU:HD22	8:7:487:LEU:CD2	2.44	0.48
8:7:465:ASN:HD21	8:7:474:MET:CE	2.25	0.48
8:7:605:ILE:HA	8:7:669:CYS:HB3	1.96	0.48
3:0:128:VAL:HA	3:0:131:GLU:HG3	1.94	0.48
3:0:238:HIS:CB	3:0:462:THR:OG1	2.61	0.48
3:0:258:ARG:NH1	3:0:262:ARG:HH12	2.09	0.48
3:0:259:ARG:HA	3:0:262:ARG:NH2	2.28	0.48
3:0:402:ILE:HD12	3:0:405:PHE:HB3	1.95	0.48
3:0:712:MET:O	3:0:715:SER:OG	2.24	0.48
5:4:25:LEU:HD12	5:4:72:LYS:C	2.34	0.48
5:4:192:GLN:O	5:4:195:PRO:HD2	2.13	0.48
8:7:446:PHE:CD2	8:7:472:LYS:CD	2.95	0.48
8:7:466:ARG:HD2	10:T:107:DT:H5'	1.95	0.48
8:7:647:ASP:OD1	8:7:648:GLN:NE2	2.46	0.48
2:2:343:THR:HG22	2:2:343:THR:O	2.14	0.48
2:2:467:GLU:HA	2:2:470:LEU:HB2	1.96	0.48
3:0:39:ILE:HD11	3:0:463:ILE:HG21	1.96	0.48
3:0:635:LEU:HA	3:0:638:ARG:HB3	1.95	0.48
4:1:337:ILE:O	4:1:338:UNK:C	2.60	0.48
5:4:30:ILE:HD13	5:4:179:LEU:HG	1.93	0.48
5:4:225:GLN:HE22	5:4:269:SER:HA	1.78	0.48
6:6:150:ILE:CG2	6:6:200:ARG:HD3	2.43	0.48
6:6:334:THR:HA	6:6:343:VAL:O	2.13	0.48
6:6:377:ALA:HA	6:6:380:TYR:CD2	2.48	0.48
8:7:579:LEU:HD23	8:7:582:ILE:HD12	1.96	0.48
3:0:353:SER:CB	3:0:419:ILE:HD13	2.30	0.48
3:0:399:LEU:HA	3:0:402:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:121:GLY:O	6:6:307:PRO:HB3	2.13	0.48
8:7:438:PHE:CD2	8:7:443:LYS:HA	2.49	0.48
8:7:589:GLN:HB2	8:7:742:MET:CE	2.44	0.48
8:7:607:VAL:O	8:7:654:LEU:N	2.23	0.48
3:0:86:LEU:O	3:0:90:MET:HG2	2.14	0.48
3:0:162:LEU:HD11	3:0:198:ARG:HD2	1.95	0.48
3:0:255:ASP:O	3:0:258:ARG:CG	2.54	0.48
7:5:17:LYS:HG3	7:5:40:LEU:HD11	1.95	0.48
8:7:349:ASN:OD1	8:7:480:ARG:NH2	2.47	0.48
2:2:41:PRO:HA	2:2:44:LYS:HB2	1.96	0.48
2:2:100:LEU:HD13	2:2:105:LYS:N	2.28	0.48
2:2:388:THR:C	2:2:390:GLY:H	2.17	0.48
2:2:454:TYR:CB	7:5:9:LEU:HD23	2.43	0.48
2:2:475:ALA:CB	2:2:481:LEU:CG	2.84	0.48
3:0:80:GLU:HG2	3:0:81:LYS:N	2.29	0.48
3:0:158:TYR:HB3	3:0:191:CYS:N	2.28	0.48
3:0:331:PHE:O	3:0:335:LEU:HD12	2.14	0.48
3:0:341:TYR:OH	3:0:362:HIS:ND1	2.47	0.48
3:0:478:VAL:HG12	3:0:479:LEU:CD1	2.40	0.48
3:0:506:ILE:HG22	3:0:518:ILE:CD1	2.43	0.48
4:1:337:ILE:O	4:1:339:LEU:N	2.47	0.48
6:6:132:CYS:SG	6:6:204:PRO:HA	2.53	0.48
6:6:282:TYR:CE1	6:6:313:ILE:HG21	2.48	0.48
8:7:592:GLN:NE2	8:7:747:ASN:HB3	2.26	0.48
2:2:18:PRO:O	2:2:21:VAL:CG2	2.62	0.48
2:2:60:LEU:O	2:2:60:LEU:HD23	2.14	0.48
2:2:193:LEU:CA	2:2:395:GLN:HE22	2.26	0.48
3:0:107:GLY:HA3	3:0:207:ILE:HG13	1.96	0.48
3:0:109:THR:CG2	3:0:113:ASN:CG	2.82	0.48
3:0:510:PHE:CE2	3:0:515:ASP:CG	2.87	0.48
3:0:535:ASP:OD1	3:0:535:ASP:N	2.46	0.48
4:1:502:ARG:HA	4:1:502:ARG:HD2	1.62	0.48
4:1:635:ASN:O	4:1:639:ASN:N	2.35	0.48
6:6:260:ARG:HB2	6:6:281:ASN:OD1	2.13	0.48
6:6:426:ARG:CZ	6:6:435:GLU:CA	2.92	0.48
8:7:375:GLY:HA3	8:7:380:ARG:NH2	2.29	0.48
8:7:498:PHE:CA	8:7:501:VAL:HG22	2.42	0.48
8:7:584:ASN:O	8:7:587:LYS:HB3	2.14	0.48
1:3:26:VAL:HG23	1:3:26:VAL:O	2.14	0.47
2:2:18:PRO:O	2:2:21:VAL:HG22	2.14	0.47
2:2:419:LYS:NZ	2:2:423:ASP:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:454:TYR:CZ	7:5:11:GLN:OE1	2.67	0.47
3:0:24:TYR:OH	3:0:52:LEU:HD21	2.14	0.47
3:0:295:SER:CA	3:0:298:ILE:HG22	2.43	0.47
4:1:593:LEU:HD23	4:1:593:LEU:C	2.33	0.47
6:6:173:ILE:HG13	6:6:180:GLN:HB2	1.96	0.47
8:7:442:ASN:HB2	8:7:444:GLU:CG	2.32	0.47
8:7:446:PHE:CE2	8:7:472:LYS:CD	2.77	0.47
8:7:464:ARG:CD	10:T:106:DA:H5"	2.31	0.47
8:7:555:ALA:N	8:7:705:PHE:O	2.47	0.47
8:7:624:LYS:NZ	8:7:648:GLN:O	2.35	0.47
9:N:69:DG:H2"	9:N:70:DA:N7	2.29	0.47
2:2:451:VAL:O	2:2:451:VAL:HG12	2.13	0.47
2:2:488:LYS:HE2	7:5:35:LEU:O	2.14	0.47
2:2:495:LYS:O	2:2:499:SER:N	2.46	0.47
2:2:501:VAL:C	2:2:504:PHE:CD2	2.87	0.47
3:0:199:MET:HE2	3:0:199:MET:HA	1.95	0.47
3:0:705:ASP:HA	3:0:708:LEU:HD21	1.94	0.47
4:1:374:ILE:O	4:1:378:MET:SD	2.72	0.47
6:6:172:ILE:CG1	6:6:181:LEU:HD13	2.44	0.47
8:7:439:THR:HG21	8:7:456:THR:N	2.13	0.47
8:7:528:ASN:O	8:7:532:GLY:N	2.47	0.47
8:7:647:ASP:OD1	8:7:648:GLN:OE1	2.32	0.47
2:2:468:TYR:CE2	2:2:484:LYS:NZ	2.81	0.47
3:0:58:ALA:O	3:0:62:HIS:CB	2.62	0.47
3:0:65:GLU:OE1	3:0:65:GLU:N	2.45	0.47
3:0:104:ARG:HH12	3:0:170:TYR:HD2	1.60	0.47
3:0:281:LYS:O	3:0:284:ASP:HB3	2.13	0.47
3:0:657:ASP:OD1	3:0:658:ALA:N	2.48	0.47
6:6:224:VAL:CB	6:6:230:ARG:HH21	2.25	0.47
8:7:133:TRP:O	8:7:142:ILE:N	2.46	0.47
8:7:412:THR:CG2	8:7:489:GLU:HB3	2.44	0.47
8:7:571:ARG:HH21	8:7:580:LEU:CD1	2.26	0.47
9:N:51:DC:O2	9:N:52:DA:N7	2.46	0.47
9:N:55:DG:H2"	9:N:56:DA:N7	2.29	0.47
1:3:42:CYS:O	1:3:45:ARG:CG	2.57	0.47
2:2:24:ARG:O	2:2:219:VAL:HG11	2.14	0.47
2:2:100:LEU:CD1	2:2:102:PRO:HA	2.44	0.47
3:0:24:TYR:CD2	3:0:25:MET:HE2	2.47	0.47
3:0:352:ILE:HG22	3:0:420:ILE:HB	1.96	0.47
3:0:472:MET:CE	3:0:473:LEU:HD11	2.44	0.47
3:0:512:ILE:O	3:0:512:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:188:ASN:OD1	4:1:189:LYS:N	2.48	0.47
5:4:213:VAL:HG22	5:4:236:LEU:HG	1.96	0.47
6:6:291:LEU:HD13	6:6:297:LEU:HD13	1.96	0.47
7:5:23:ILE:O	7:5:26:LYS:HB2	2.14	0.47
8:7:437:VAL:O	8:7:437:VAL:HG23	2.13	0.47
8:7:495:ALA:HB3	8:7:523:LYS:CE	2.38	0.47
3:0:42:MET:HB3	3:0:48:LYS:HE3	1.94	0.47
3:0:90:MET:HE3	3:0:101:GLU:HG3	1.96	0.47
3:0:90:MET:HE1	3:0:101:GLU:HG3	1.94	0.47
3:0:111:ARG:O	3:0:115:CYS:N	2.45	0.47
4:1:222:LEU:HD23	4:1:222:LEU:C	2.35	0.47
5:4:114:UNK:C	5:4:116:ARG:N	2.78	0.47
5:4:255:ASP:CB	5:4:259:ARG:HD2	2.45	0.47
6:6:224:VAL:HB	6:6:230:ARG:CZ	2.45	0.47
8:7:551:ASN:CB	8:7:702:ASN:H	2.27	0.47
8:7:568:GLU:HG2	8:7:580:LEU:HB3	1.97	0.47
8:7:613:TYR:HB2	8:7:766:LYS:CE	2.44	0.47
8:7:715:GLU:HG3	8:7:718:TYR:HD2	1.79	0.47
1:3:13:CYS:HA	1:3:37:ARG:O	2.15	0.47
3:0:18:TYR:CE1	3:0:673:LYS:HD2	2.50	0.47
3:0:109:THR:OG1	4:1:346:ASP:OD2	2.31	0.47
3:0:222:VAL:CG1	3:0:452:ARG:HH12	2.27	0.47
4:1:327:UNK:C	4:1:329:LEU:H	2.26	0.47
4:1:374:ILE:C	4:1:378:MET:CE	2.83	0.47
6:6:152:TYR:CE2	6:6:298:LYS:HB2	2.40	0.47
6:6:197:LYS:HA	6:6:200:ARG:HE	1.80	0.47
6:6:384:MET:SD	6:6:384:MET:N	2.87	0.47
8:7:552:VAL:CG1	8:7:731:TYR:HD1	2.18	0.47
3:0:19:PRO:HG3	3:0:739:TRP:CD2	2.50	0.47
3:0:80:GLU:HB3	3:0:178:PHE:CD2	2.49	0.47
3:0:148:ASP:CG	3:0:150:GLU:OE1	2.52	0.47
3:0:166:GLU:HG3	3:0:198:ARG:HD3	1.96	0.47
3:0:244:CYS:O	3:0:247:SER:OG	2.21	0.47
3:0:307:VAL:H	3:0:382:SER:HB3	1.79	0.47
3:0:312:LEU:CG	3:0:313:PRO:CD	2.88	0.47
3:0:318:THR:HG23	3:0:376:PHE:CZ	2.47	0.47
3:0:377:CYS:SG	3:0:407:THR:OG1	2.64	0.47
3:0:695:LYS:O	3:0:699:GLN:HG2	2.14	0.47
5:4:273:ARG:HH12	6:6:372:LEU:CD2	2.27	0.47
5:4:290:SER:O	5:4:293:LEU:N	2.46	0.47
6:6:225:PRO:HD2	6:6:228:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:322:MET:SD	6:6:324:PHE:CE1	3.08	0.47
8:7:349:ASN:ND2	8:7:351:ASP:HA	2.30	0.47
8:7:381:SER:O	8:7:532:GLY:HA3	2.14	0.47
8:7:478:THR:HG22	8:7:504:THR:CG2	2.34	0.47
8:7:499:ARG:NE	8:7:500:ARG:HG3	2.29	0.47
8:7:571:ARG:CZ	8:7:572:GLU:OE1	2.49	0.47
8:7:579:LEU:HD23	8:7:582:ILE:CD1	2.45	0.47
8:7:613:TYR:N	8:7:766:LYS:HZ3	2.13	0.47
2:2:451:VAL:HG23	7:5:54:LEU:HD11	1.97	0.47
3:0:291:GLN:HE22	3:0:294:HIS:CA	2.15	0.47
5:4:138:LYS:HA	5:4:141:GLU:HB2	1.97	0.47
5:4:179:LEU:HA	5:4:213:VAL:O	2.14	0.47
5:4:271:ASP:HB3	5:4:273:ARG:CZ	2.45	0.47
6:6:182:VAL:HG11	6:6:199:ILE:HD11	1.96	0.47
7:5:42:VAL:CG1	7:5:43:ASN:H	2.28	0.47
7:5:57:LEU:HA	7:5:60:LYS:HD3	1.96	0.47
8:7:383:ILE:HG13	8:7:528:ASN:HD22	1.79	0.47
8:7:406:SER:OG	8:7:480:ARG:NH2	2.48	0.47
8:7:465:ASN:ND2	8:7:474:MET:HE1	2.26	0.47
3:0:147:GLU:HG2	3:0:148:ASP:N	2.30	0.47
3:0:499:LYS:HB3	3:0:503:GLN:HA	1.97	0.47
5:4:30:ILE:HD13	5:4:179:LEU:CB	2.44	0.47
6:6:224:VAL:HB	6:6:230:ARG:HH21	1.80	0.47
7:5:66:MET:HA	8:7:717:TYR:CE2	2.45	0.47
8:7:363:ARG:HG3	8:7:366:GLN:CD	2.35	0.47
8:7:464:ARG:HD2	10:T:106:DA:C5'	2.33	0.47
8:7:523:LYS:HG2	8:7:525:GLY:O	2.14	0.47
2:2:136:ASP:C	2:2:138:TYR:N	2.66	0.47
2:2:480:VAL:HG21	2:2:497:GLY:H	1.79	0.47
3:0:90:MET:CE	3:0:101:GLU:CG	2.93	0.47
3:0:568:LEU:N	3:0:595:GLY:O	2.47	0.47
5:4:79:TYR:CD2	5:4:82:GLY:C	2.88	0.47
5:4:244:LEU:O	5:4:248:LEU:HG	2.15	0.47
6:6:403:CYS:SG	6:6:436:PHE:HA	2.55	0.47
8:7:349:ASN:HD21	8:7:406:SER:H	1.62	0.47
2:2:410:ARG:HA	2:2:413:GLU:OE2	2.14	0.46
3:0:12:PHE:HE2	3:0:14:TYR:HB2	1.79	0.46
3:0:399:LEU:O	3:0:402:ILE:HG22	2.15	0.46
5:4:225:GLN:NE2	5:4:269:SER:HA	2.31	0.46
6:6:124:ARG:NH1	6:6:306:THR:O	2.48	0.46
6:6:165:PRO:CG	6:6:375:HIS:CD2	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:32:PRO:HB3	1:3:69:LYS:HE3	1.96	0.46
2:2:50:MET:HE3	2:2:55:ASN:O	2.15	0.46
2:2:454:TYR:CD2	7:5:9:LEU:HD23	2.50	0.46
3:0:140:GLN:C	3:0:144:LYS:HZ3	2.17	0.46
3:0:198:ARG:HG3	3:0:199:MET:HE3	1.97	0.46
3:0:198:ARG:HH12	3:0:199:MET:HE1	1.77	0.46
7:5:24:ASP:O	7:5:29:ASP:N	2.42	0.46
8:7:604:LYS:CE	8:7:694:LYS:HE3	2.45	0.46
2:2:396:ILE:HA	2:2:399:TYR:HB3	1.97	0.46
3:0:1:MET:O	3:0:11:LEU:HA	2.15	0.46
3:0:210:TYR:CE2	3:0:240:ILE:CD1	2.98	0.46
3:0:251:ASP:CG	4:1:350:ARG:NH2	2.69	0.46
3:0:275:ARG:HD2	3:0:276:LYS:N	2.31	0.46
3:0:331:PHE:CE1	3:0:380:ARG:HG2	2.51	0.46
3:0:339:ILE:HG23	3:0:343:LYS:HZ3	1.80	0.46
3:0:372:LYS:HA	3:0:375:ARG:HE	1.81	0.46
3:0:442:ALA:O	3:0:446:ILE:HG12	2.16	0.46
4:1:492:UNK:C	4:1:494:UNK:H	2.28	0.46
5:4:139:GLN:NE2	5:4:140:ILE:CG1	2.70	0.46
8:7:499:ARG:CZ	8:7:500:ARG:CG	2.93	0.46
8:7:675:SER:HA	8:7:722:ARG:HH21	1.75	0.46
2:2:40:PRO:HG2	2:2:43:ALA:HB3	1.97	0.46
2:2:91:LYS:HA	2:2:95:THR:O	2.15	0.46
2:2:501:VAL:CG2	2:2:504:PHE:CE2	2.93	0.46
3:0:162:LEU:HD12	3:0:166:GLU:HG2	1.97	0.46
3:0:493:LEU:HD22	3:0:495:MET:SD	2.55	0.46
3:0:639:LEU:CD2	3:0:642:MET:CE	2.92	0.46
4:1:593:LEU:CD2	4:1:620:LEU:CD2	2.89	0.46
5:4:193:TYR:CG	5:4:223:PHE:HE1	2.34	0.46
5:4:217:GLY:O	5:4:237:HIS:CE1	2.68	0.46
2:2:501:VAL:O	2:2:504:PHE:CE2	2.69	0.46
3:0:17:ILE:HG21	3:0:745:ILE:HG21	1.98	0.46
3:0:69:ILE:HG12	3:0:231:ILE:HD11	1.97	0.46
3:0:472:MET:HE3	3:0:473:LEU:HD11	1.97	0.46
3:0:528:GLU:O	3:0:532:ILE:HG22	2.15	0.46
4:1:182:GLN:HA	4:1:185:LEU:HB2	1.97	0.46
5:4:154:SER:OG	5:4:199:CYS:SG	2.68	0.46
6:6:136:MET:HE1	6:6:145:ARG:HD3	1.97	0.46
6:6:199:ILE:C	6:6:202:GLN:HG3	2.34	0.46
8:7:385:VAL:CG2	8:7:537:GLU:HA	2.46	0.46
8:7:465:ASN:HB2	8:7:471:GLN:HE21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:625:PRO:CG	8:7:649:ILE:HD13	2.46	0.46
9:N:52:DA:C2'	9:N:53:DT:C7	2.93	0.46
1:3:38:ILE:HG23	1:3:43:VAL:HB	1.98	0.46
2:2:7:LYS:NZ	2:2:9:SER:CB	2.78	0.46
3:0:116:LEU:HG	3:0:116:LEU:O	2.15	0.46
3:0:304:GLU:CD	3:0:386:ARG:HH11	2.18	0.46
3:0:338:LEU:O	3:0:339:ILE:C	2.53	0.46
5:4:25:LEU:HD12	5:4:72:LYS:O	2.16	0.46
6:6:247:ILE:CG2	6:6:248:HIS:ND1	2.78	0.46
7:5:49:PHE:HA	7:5:52:HIS:CG	2.47	0.46
8:7:436:ALA:HB2	8:7:445:MET:SD	2.56	0.46
8:7:571:ARG:HD2	8:7:571:ARG:C	2.35	0.46
2:2:498:ASN:O	2:2:502:LEU:HB2	2.16	0.46
3:0:60:GLN:OE1	3:0:69:ILE:HG13	2.15	0.46
3:0:371:ARG:HH12	3:0:375:ARG:HH12	1.61	0.46
3:0:537:MET:SD	3:0:619:THR:OG1	2.72	0.46
3:0:722:ARG:CG	6:6:267:SER:OG	2.63	0.46
6:6:282:TYR:OH	6:6:313:ILE:HD13	2.16	0.46
8:7:356:LEU:HG	8:7:404:LYS:HZ1	1.80	0.46
8:7:363:ARG:HD2	8:7:366:GLN:NE2	2.30	0.46
8:7:373:MET:HA	8:7:535:LEU:HG	1.97	0.46
8:7:478:THR:HG23	8:7:478:THR:H	1.51	0.46
8:7:551:ASN:HB3	8:7:702:ASN:H	1.80	0.46
8:7:582:ILE:HG23	8:7:673:ILE:HG22	1.98	0.46
3:0:162:LEU:HD22	3:0:194:PHE:CB	2.46	0.46
3:0:353:SER:CB	3:0:419:ILE:CD1	2.92	0.46
3:0:424:GLU:CG	3:0:432:ASN:ND2	2.79	0.46
3:0:528:GLU:CG	3:0:714:ILE:HD11	2.42	0.46
3:0:538:VAL:HG22	3:0:598:LEU:H	1.81	0.46
3:0:638:ARG:O	3:0:642:MET:HE2	2.16	0.46
4:1:222:LEU:HD21	6:6:216:MET:CG	2.21	0.46
6:6:136:MET:HA	6:6:136:MET:CE	2.37	0.46
8:7:412:THR:HG23	8:7:420:TRP:HH2	1.79	0.46
8:7:469:ASP:HB3	8:7:472:LYS:HZ1	1.79	0.46
8:7:672:GLN:HE22	8:7:687:LEU:CD2	2.27	0.46
9:N:63:DG:H2"	9:N:64:DA:C8	2.51	0.46
2:2:392:THR:HG22	2:2:394:ASP:N	2.30	0.46
3:0:162:LEU:HD12	3:0:166:GLU:HB3	1.97	0.46
3:0:285:GLU:HA	3:0:288:LYS:HB2	1.98	0.46
3:0:310:PRO:HB2	3:0:408:LEU:HD21	1.98	0.46
3:0:380:ARG:HA	3:0:383:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:465:PRO:CG	3:0:467:ASP:OD1	2.64	0.46
3:0:471:ARG:NH2	3:0:647:ARG:HB2	2.24	0.46
3:0:514:ASN:OD1	3:0:553:MET:HG2	2.16	0.46
3:0:614:HIS:HE1	3:0:675:ASP:N	2.10	0.46
5:4:273:ARG:HH22	6:6:372:LEU:CB	2.29	0.46
6:6:118:TYR:HB3	6:6:119:GLN:H	1.50	0.46
6:6:176:ASN:HD21	6:6:205:LYS:HB2	1.80	0.46
7:5:33:GLU:O	7:5:41:LEU:N	2.41	0.46
8:7:349:ASN:HD21	8:7:406:SER:N	2.14	0.46
8:7:427:TRP:H	8:7:427:TRP:HE3	1.61	0.46
8:7:445:MET:HB2	8:7:448:THR:OG1	2.15	0.46
9:N:55:DG:H2"	9:N:56:DA:C8	2.51	0.46
9:N:66:DA:C2'	9:N:67:DT:C7	2.93	0.46
1:3:42:CYS:C	1:3:45:ARG:HG3	2.34	0.46
2:2:28:SER:O	2:2:31:THR:OG1	2.25	0.46
3:0:232:VAL:O	3:0:457:ILE:N	2.49	0.46
3:0:293:LEU:HD13	3:0:319:GLU:HA	1.98	0.46
3:0:485:MET:HA	3:0:485:MET:HE1	1.98	0.46
4:1:505:THR:HA	4:1:508:LYS:HG2	1.97	0.46
8:7:477:LEU:HA	8:7:482:TRP:NE1	2.21	0.46
2:2:346:LYS:HD2	2:2:377:GLN:HA	1.98	0.45
2:2:452:ILE:HD12	2:2:453:THR:H	1.81	0.45
3:0:197:ARG:HG2	3:0:221:ARG:HH12	1.81	0.45
3:0:210:TYR:O	3:0:214:LEU:HG	2.16	0.45
4:1:214:ILE:HG23	4:1:215:PRO:CD	2.46	0.45
4:1:229:GLY:HA3	6:6:242:THR:HG22	1.98	0.45
6:6:132:CYS:SG	6:6:204:PRO:CA	3.04	0.45
8:7:694:LYS:HZ1	8:7:696:ARG:HD3	1.81	0.45
3:0:236:GLU:HB3	3:0:238:HIS:HE1	1.82	0.45
3:0:659:MET:HE1	3:0:689:LYS:HB2	1.98	0.45
4:1:181:GLN:HB3	4:1:210:TRP:CE2	2.51	0.45
6:6:199:ILE:HA	6:6:202:GLN:CG	2.44	0.45
6:6:313:ILE:HG13	6:6:313:ILE:O	2.17	0.45
8:7:563:ALA:C	8:7:567:GLN:NE2	2.57	0.45
2:2:405:HIS:CD2	2:2:412:ALA:HB3	2.52	0.45
3:0:294:HIS:O	3:0:298:ILE:HG22	2.16	0.45
3:0:539:VAL:O	3:0:599:LEU:HA	2.15	0.45
5:4:60:PHE:CD2	5:4:248:LEU:HB3	2.51	0.45
5:4:271:ASP:CB	5:4:273:ARG:HE	2.29	0.45
6:6:115:ILE:H	6:6:115:ILE:HG12	1.45	0.45
6:6:133:SER:O	6:6:204:PRO:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:19:LEU:CD2	7:5:22:GLN:OE1	2.64	0.45
8:7:385:VAL:HG12	8:7:514:THR:CG2	2.46	0.45
8:7:411:CYS:CB	8:7:417:VAL:HG22	2.35	0.45
8:7:478:THR:HG21	8:7:504:THR:HG22	1.91	0.45
8:7:544:SER:HA	8:7:549:ILE:CA	2.46	0.45
8:7:595:ILE:HA	8:7:605:ILE:HD13	1.96	0.45
8:7:604:LYS:HZ3	8:7:694:LYS:NZ	2.15	0.45
8:7:619:ALA:HB1	8:7:626:PHE:CD2	2.52	0.45
8:7:625:PRO:CG	8:7:649:ILE:CD1	2.92	0.45
8:7:760:LEU:HD23	8:7:760:LEU:O	2.15	0.45
9:N:61:DG:N1	10:T:106:DA:C2	2.85	0.45
2:2:350:TYR:H	2:2:407:GLN:NE2	2.14	0.45
3:0:18:TYR:HE1	3:0:738:VAL:HG22	1.82	0.45
3:0:315:ASP:N	3:0:315:ASP:OD1	2.48	0.45
3:0:617:GLY:O	3:0:618:ARG:HD3	2.16	0.45
4:1:385:MET:HG3	4:1:386:ILE:N	2.31	0.45
4:1:482:UNK:O	4:1:484:UNK:N	2.49	0.45
8:7:446:PHE:CD1	8:7:472:LYS:CE	2.97	0.45
8:7:497:MET:N	8:7:500:ARG:HH21	2.14	0.45
8:7:752:SER:O	8:7:756:ARG:HG3	2.15	0.45
2:2:11:THR:CG2	2:2:38:ILE:HG21	2.44	0.45
2:2:492:PHE:CG	7:5:9:LEU:HB2	2.51	0.45
3:0:104:ARG:CZ	3:0:173:LYS:CA	2.81	0.45
3:0:312:LEU:HD12	3:0:313:PRO:HD3	1.98	0.45
3:0:405:PHE:O	3:0:409:ILE:HG12	2.17	0.45
3:0:418:LEU:HD12	3:0:437:PHE:HB2	1.99	0.45
3:0:468:MET:HE1	3:0:648:ILE:HD13	1.99	0.45
3:0:570:LEU:O	3:0:598:LEU:HA	2.16	0.45
3:0:586:TYR:CE1	3:0:596:ALA:O	2.69	0.45
3:0:636:LYS:HG3	3:0:637:ALA:N	2.31	0.45
3:0:731:LYS:HE2	3:0:731:LYS:HB2	1.73	0.45
5:4:193:TYR:CD2	5:4:197:MET:HE1	2.50	0.45
6:6:156:PHE:HD2	6:6:301:PHE:HD2	1.63	0.45
6:6:172:ILE:CG1	6:6:181:LEU:CD1	2.94	0.45
6:6:175:ARG:N	6:6:178:LEU:O	2.41	0.45
7:5:54:LEU:HD23	7:5:58:LEU:CD2	2.47	0.45
8:7:356:LEU:HA	8:7:401:CYS:HB3	1.99	0.45
8:7:378:ARG:HA	8:7:378:ARG:HD3	1.79	0.45
8:7:742:MET:O	8:7:745:ILE:HG12	2.17	0.45
3:0:331:PHE:CE1	3:0:380:ARG:CG	3.00	0.45
3:0:508:SER:HB2	3:0:546:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:564:TRP:CE3	3:0:564:TRP:HA	2.50	0.45
4:1:374:ILE:O	4:1:378:MET:HE3	2.16	0.45
4:1:378:MET:SD	4:1:378:MET:N	2.88	0.45
5:4:300:PRO:O	5:4:302:GLY:N	2.50	0.45
8:7:420:TRP:HA	8:7:423:GLN:CD	2.36	0.45
8:7:465:ASN:HD22	8:7:474:MET:CE	2.26	0.45
1:3:54:CYS:HB3	1:3:63:LEU:CD1	2.43	0.45
2:2:29:PRO:HB3	2:2:107:SER:O	2.16	0.45
2:2:53:ASN:O	2:2:55:ASN:N	2.47	0.45
2:2:100:LEU:HD13	2:2:101:ASN:O	2.16	0.45
3:0:166:GLU:O	3:0:198:ARG:CZ	2.64	0.45
3:0:468:MET:HG2	3:0:656:PHE:CE1	2.51	0.45
3:0:584:GLU:OE1	3:0:588:LYS:HE3	2.17	0.45
3:0:672:GLY:O	3:0:675:ASP:N	2.49	0.45
5:4:271:ASP:CG	5:4:273:ARG:HH11	2.18	0.45
6:6:126:LEU:CD2	6:6:169:MET:HE3	2.45	0.45
6:6:156:PHE:HD2	6:6:301:PHE:CD2	2.34	0.45
6:6:247:ILE:HG23	6:6:248:HIS:H	1.81	0.45
6:6:326:THR:O	6:6:347:TYR:HA	2.16	0.45
6:6:426:ARG:HG3	6:6:426:ARG:O	2.16	0.45
7:5:53:GLU:HA	7:5:56:ARG:HD2	1.99	0.45
8:7:516:THR:OG1	8:7:681:ARG:NE	2.49	0.45
8:7:621:LYS:HE3	8:7:749:ALA:HB1	1.98	0.45
2:2:364:VAL:HG22	2:2:365:HIS:N	2.32	0.45
2:2:454:TYR:HB2	7:5:9:LEU:CB	2.45	0.45
3:0:83:LEU:HD13	3:0:177:SER:HA	1.98	0.45
3:0:140:GLN:NE2	3:0:389:GLU:HB3	2.31	0.45
3:0:238:HIS:HB3	3:0:462:THR:OG1	2.16	0.45
3:0:249:SER:HB2	3:0:436:ARG:CZ	2.46	0.45
3:0:441:ASP:OD1	3:0:444:ILE:N	2.42	0.45
4:1:185:LEU:CD1	4:1:192:MET:HA	2.47	0.45
5:4:271:ASP:CB	5:4:273:ARG:NE	2.80	0.45
8:7:385:VAL:HA	8:7:514:THR:HB	1.99	0.45
8:7:580:LEU:HA	8:7:583:MET:HE2	1.90	0.45
8:7:587:LYS:HG3	8:7:708:LEU:HD13	1.99	0.45
8:7:647:ASP:OD1	8:7:648:GLN:CD	2.55	0.45
9:N:69:DG:H2"	9:N:70:DA:C8	2.51	0.45
10:T:113:DA:C2'	10:T:114:DT:H71	2.47	0.45
1:3:23:SER:C	1:3:25:ASP:H	2.21	0.45
2:2:63:ASP:HA	2:2:74:PHE:CE2	2.51	0.45
2:2:366:LEU:HA	2:2:375:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:419:LYS:HG2	2:2:430:LEU:H	1.82	0.45
3:0:136:MET:CE	12:0:801:SF4:S1	3.05	0.45
3:0:143:ARG:CZ	3:0:143:ARG:HB2	2.47	0.45
3:0:249:SER:OG	4:1:350:ARG:O	2.34	0.45
3:0:275:ARG:NH1	3:0:276:LYS:HZ2	2.15	0.45
3:0:312:LEU:HD12	3:0:313:PRO:CD	2.46	0.45
5:4:196:ILE:O	5:4:200:ILE:HG13	2.17	0.45
6:6:322:MET:SD	6:6:323:GLY:N	2.90	0.45
6:6:323:GLY:HA3	6:6:350:PRO:HG3	1.99	0.45
7:5:30:ILE:HG21	7:5:46:LYS:HG3	1.99	0.45
7:5:49:PHE:O	7:5:52:HIS:HB2	2.16	0.45
8:7:392:LYS:HD2	8:7:513:LEU:HB3	1.99	0.45
8:7:473:VAL:O	8:7:477:LEU:HG	2.16	0.45
8:7:544:SER:HG	8:7:731:TYR:HE1	1.64	0.45
2:2:378:ILE:HD12	2:2:382:SER:HB3	1.99	0.45
2:2:411:LEU:O	2:2:414:GLU:HG2	2.17	0.45
3:0:111:ARG:HD3	3:0:133:CYS:HB3	1.99	0.45
3:0:312:LEU:CD1	3:0:313:PRO:CD	2.95	0.45
3:0:328:ALA:O	3:0:332:VAL:HG23	2.17	0.45
3:0:472:MET:HG3	3:0:473:LEU:N	2.32	0.45
3:0:571:VAL:HG22	3:0:572:GLU:H	1.79	0.45
3:0:619:THR:HG22	3:0:678:VAL:CB	2.47	0.45
3:0:625:ILE:HG21	3:0:627:PHE:HE1	1.82	0.45
5:4:147:SER:O	5:4:149:LEU:HD23	2.17	0.45
6:6:296:HIS:O	6:6:299:GLU:HG3	2.17	0.45
6:6:363:CYS:O	6:6:367:ASP:HA	2.16	0.45
8:7:417:VAL:CG2	8:7:456:THR:HB	2.46	0.45
9:N:70:DA:C2'	9:N:71:DT:C7	2.94	0.45
2:2:136:ASP:O	2:2:139:SER:N	2.49	0.44
2:2:432:VAL:HG13	2:2:432:VAL:O	2.17	0.44
3:0:83:LEU:CD2	3:0:207:ILE:CD1	2.85	0.44
3:0:90:MET:CE	3:0:101:GLU:CD	2.85	0.44
3:0:227:SER:HB2	3:0:453:PHE:HE1	1.82	0.44
6:6:199:ILE:CA	6:6:202:GLN:HG3	2.46	0.44
6:6:247:ILE:CG2	6:6:248:HIS:N	2.80	0.44
7:5:27:MET:CE	7:5:30:ILE:HG13	2.47	0.44
7:5:51:LYS:HD2	7:5:54:LEU:HD13	1.98	0.44
8:7:552:VAL:HA	8:7:703:ALA:HB3	1.99	0.44
10:T:92:DA:H2"	10:T:93:DT:C5	2.52	0.44
2:2:445:GLN:O	2:2:449:ASP:N	2.50	0.44
2:2:468:TYR:CD2	2:2:468:TYR:C	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:188:LYS:HA	3:0:188:LYS:HD3	1.82	0.44
3:0:297:ASP:OD1	3:0:297:ASP:O	2.35	0.44
3:0:297:ASP:CG	3:0:386:ARG:HH22	2.20	0.44
3:0:669:VAL:HG13	3:0:670:LEU:HG	1.98	0.44
5:4:27:THR:OG1	5:4:176:LEU:CB	2.66	0.44
5:4:203:ALA:CB	5:4:210:ILE:HD11	2.46	0.44
5:4:276:CYS:HB3	5:4:279:THR:HB	1.98	0.44
5:4:293:LEU:CD1	6:6:376:LEU:CD2	2.92	0.44
7:5:11:GLN:NE2	7:5:39:HIS:HD2	2.16	0.44
8:7:554:CYS:N	8:7:732:ALA:O	2.41	0.44
3:0:251:ASP:N	3:0:436:ARG:HH11	2.15	0.44
3:0:580:SER:OG	4:1:339:LEU:HB2	2.17	0.44
4:1:564:PHE:HA	4:1:567:HIS:O	2.18	0.44
4:1:629:LYS:HZ3	6:6:351:ASN:HD21	1.60	0.44
5:4:273:ARG:HD2	5:4:273:ARG:N	2.33	0.44
6:6:127:ILE:HG23	6:6:170:GLY:O	2.17	0.44
6:6:132:CYS:N	6:6:174:MET:O	2.43	0.44
6:6:136:MET:CE	6:6:145:ARG:HD3	2.46	0.44
6:6:383:LEU:HD22	6:6:384:MET:HE1	1.96	0.44
6:6:423:UNK:O	6:6:425:SER:N	2.50	0.44
8:7:431:GLN:N	8:7:431:GLN:OE1	2.51	0.44
8:7:499:ARG:NH1	8:7:500:ARG:HG2	2.33	0.44
8:7:590:ALA:N	8:7:742:MET:HE1	2.32	0.44
8:7:625:PRO:HB2	8:7:649:ILE:HD13	1.99	0.44
9:N:75:DG:N1	10:T:92:DA:C2	2.85	0.44
10:T:99:DA:C2'	10:T:100:DT:H71	2.47	0.44
2:2:20:GLN:OE1	2:2:20:GLN:N	2.48	0.44
3:0:4:TYR:HA	3:0:8:LEU:O	2.17	0.44
3:0:109:THR:CG2	3:0:113:ASN:OD1	2.64	0.44
3:0:397:THR:O	3:0:400:LYS:HG2	2.17	0.44
3:0:570:LEU:HD22	3:0:586:TYR:CB	2.30	0.44
4:1:383:GLU:C	4:1:386:ILE:HG22	2.37	0.44
6:6:159:GLU:C	6:6:163:GLN:HE22	2.20	0.44
8:7:446:PHE:CE1	8:7:472:LYS:CE	3.01	0.44
8:7:552:VAL:CG1	8:7:731:TYR:HB3	2.45	0.44
8:7:675:SER:HB2	8:7:722:ARG:NH2	2.26	0.44
8:7:725:PHE:O	8:7:728:ASP:HB2	2.17	0.44
8:7:752:SER:HB2	8:7:754:ARG:CZ	2.48	0.44
2:2:100:LEU:HD12	2:2:102:PRO:N	2.32	0.44
2:2:201:TRP:O	2:2:205:LEU:HG	2.18	0.44
2:2:471:LEU:HD13	2:2:501:VAL:HG23	1.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:525:MET:HA	3:0:528:GLU:CD	2.38	0.44
3:0:649:ARG:HG2	3:0:652:ASP:OD2	2.18	0.44
3:0:669:VAL:HG13	3:0:670:LEU:CD2	2.47	0.44
4:1:221:ALA:O	4:1:225:SER:OG	2.35	0.44
4:1:268:LYS:O	4:1:271:THR:OG1	2.30	0.44
6:6:131:ASP:O	6:6:136:MET:HG3	2.18	0.44
6:6:150:ILE:CB	6:6:200:ARG:HG2	2.48	0.44
8:7:387:PRO:HG2	8:7:390:ALA:HB3	1.99	0.44
8:7:589:GLN:HB2	8:7:742:MET:HE1	1.99	0.44
8:7:662:ILE:C	8:7:664:LEU:HD22	2.37	0.44
8:7:670:LEU:HD21	8:7:672:GLN:HE21	1.81	0.44
8:7:752:SER:HG	8:7:755:GLU:CB	2.30	0.44
2:2:13:TYR:O	2:2:16:GLU:CG	2.51	0.44
2:2:57:VAL:O	2:2:98:ILE:N	2.42	0.44
2:2:176:VAL:O	2:2:180:GLY:N	2.50	0.44
2:2:394:ASP:OD1	2:2:395:GLN:N	2.50	0.44
4:1:193:LYS:C	4:1:197:GLU:OE1	2.55	0.44
6:6:168:GLN:CG	6:6:185:VAL:HG22	2.47	0.44
6:6:182:VAL:CG1	6:6:199:ILE:HD11	2.48	0.44
8:7:697:ASN:HA	8:7:702:ASN:OD1	2.18	0.44
9:N:78:DA:H1'	9:N:79:DT:H5'	1.99	0.44
2:2:88:ILE:O	2:2:88:ILE:HG23	2.17	0.44
3:0:12:PHE:CE2	3:0:14:TYR:HB2	2.52	0.44
3:0:104:ARG:HE	3:0:173:LYS:CA	2.25	0.44
3:0:139:GLY:N	3:0:303:GLU:OE1	2.50	0.44
3:0:166:GLU:O	3:0:198:ARG:NH2	2.51	0.44
3:0:251:ASP:OD1	3:0:252:LEU:N	2.50	0.44
3:0:346:MET:HE3	3:0:433:PRO:HB2	2.00	0.44
3:0:448:PRO:O	3:0:452:ARG:HG3	2.16	0.44
4:1:180:LEU:HD11	4:1:221:ALA:HB2	2.00	0.44
4:1:282:GLU:OE1	4:1:282:GLU:N	2.30	0.44
4:1:503:VAL:HG11	5:4:246:GLN:HG3	1.99	0.44
5:4:300:PRO:C	5:4:302:GLY:H	2.21	0.44
8:7:659:ASP:HA	8:7:660:THR:HA	1.80	0.44
8:7:755:GLU:H	8:7:757:ARG:HH11	1.54	0.44
1:3:43:VAL:O	1:3:47:PHE:HD2	2.01	0.44
3:0:8:LEU:CD2	3:0:59:TYR:HA	2.47	0.44
3:0:25:MET:HA	3:0:28:ILE:HG22	1.98	0.44
3:0:70:ILE:HB	3:0:232:VAL:HG22	1.99	0.44
3:0:311:VAL:HG23	3:0:411:THR:HG21	2.00	0.44
3:0:571:VAL:HG11	4:1:375:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:598:LEU:HG	3:0:599:LEU:N	2.33	0.44
5:4:39:THR:C	5:4:43:GLU:OE1	2.53	0.44
6:6:271:ALA:CA	6:6:274:LYS:HG3	2.47	0.44
8:7:466:ARG:CD	10:T:107:DT:H4'	2.47	0.44
8:7:485:ILE:O	8:7:511:LEU:HB3	2.18	0.44
8:7:750:TYR:HA	8:7:755:GLU:CB	2.48	0.44
1:3:13:CYS:H	1:3:17:LYS:HA	1.83	0.44
1:3:33:GLU:O	1:3:61:LYS:CE	2.63	0.44
2:2:144:GLU:CA	2:2:355:LEU:HD11	2.47	0.44
2:2:371:VAL:HG22	8:7:117:ASP:O	2.17	0.44
3:0:188:LYS:CB	3:0:190:LEU:CD2	2.94	0.44
3:0:487:LEU:CD2	3:0:491:SER:OG	2.66	0.44
3:0:541:PHE:CE2	3:0:599:LEU:HB2	2.43	0.44
3:0:626:PRO:HG2	3:0:658:ALA:O	2.18	0.44
5:4:273:ARG:NH2	6:6:372:LEU:CA	2.81	0.44
6:6:108:LYS:HD3	6:6:110:THR:OG1	2.18	0.44
6:6:126:LEU:CD2	6:6:169:MET:CE	2.90	0.44
6:6:211:GLN:NE2	6:6:247:ILE:HA	2.33	0.44
8:7:604:LYS:O	8:7:668:THR:HB	2.18	0.44
9:N:76:DT:H2"	9:N:77:DG:C8	2.53	0.44
10:T:106:DA:H2"	10:T:107:DT:C5	2.52	0.44
1:3:27:LYS:HD3	1:3:29:LEU:N	2.33	0.43
2:2:23:ASN:ND2	2:2:26:TYR:CE2	2.86	0.43
2:2:24:ARG:NH2	2:2:219:VAL:HB	2.33	0.43
2:2:346:LYS:HZ1	2:2:373:MET:HE2	1.83	0.43
3:0:318:THR:CG2	3:0:376:PHE:CZ	3.01	0.43
3:0:715:SER:N	3:0:718:LYS:HZ1	2.12	0.43
3:0:744:LEU:N	3:0:744:LEU:HD12	2.33	0.43
5:4:58:ILE:HG23	5:4:122:ASP:OD2	2.18	0.43
5:4:135:LEU:C	5:4:136:GLU:OE1	2.56	0.43
5:4:176:LEU:C	5:4:176:LEU:HD12	2.38	0.43
5:4:255:ASP:C	5:4:259:ARG:NH1	2.51	0.43
5:4:288:ILE:O	5:4:288:ILE:HG13	2.18	0.43
6:6:110:THR:O	6:6:112:LYS:HD3	2.17	0.43
6:6:145:ARG:HD3	6:6:266:LEU:HD12	2.00	0.43
7:5:19:LEU:HD23	7:5:19:LEU:HA	1.47	0.43
8:7:400:ALA:HB2	8:7:486:ILE:HD11	2.00	0.43
8:7:438:PHE:O	8:7:438:PHE:CG	2.70	0.43
9:N:56:DA:C2'	9:N:57:DT:C7	2.94	0.43
1:3:31:ASN:ND2	1:3:64:ARG:N	2.66	0.43
3:0:322:PRO:HB2	3:0:325:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:539:VAL:CB	3:0:621:LEU:HB2	2.48	0.43
3:0:715:SER:CB	3:0:718:LYS:HZ1	2.30	0.43
3:0:721:LEU:HD12	3:0:721:LEU:C	2.38	0.43
5:4:289:CYS:O	6:6:319:LEU:HA	2.17	0.43
6:6:266:LEU:O	6:6:268:ALA:N	2.50	0.43
6:6:347:TYR:HB2	6:6:356:VAL:CG1	2.49	0.43
8:7:373:MET:O	8:7:380:ARG:HG2	2.17	0.43
8:7:416:SER:O	8:7:420:TRP:CG	2.71	0.43
8:7:421:ARG:CZ	8:7:432:PRO:HB3	2.47	0.43
8:7:421:ARG:HA	8:7:425:LEU:HD23	2.00	0.43
8:7:527:LEU:CD2	8:7:530:LEU:HD22	2.47	0.43
2:2:134:LEU:O	2:2:136:ASP:N	2.51	0.43
2:2:273:LYS:HE2	2:2:277:MET:HE3	1.97	0.43
2:2:454:TYR:CD1	2:2:482:LEU:HD13	2.53	0.43
3:0:234:PHE:N	3:0:457:ILE:O	2.47	0.43
3:0:371:ARG:HG3	3:0:410:SER:OG	2.18	0.43
3:0:510:PHE:C	3:0:511:GLU:HG3	2.38	0.43
5:4:297:SER:C	5:4:299:ILE:N	2.71	0.43
6:6:386:LEU:HD13	6:6:451:CYS:CB	2.38	0.43
8:7:353:ASP:HB3	8:7:451:GLY:HA2	2.01	0.43
8:7:370:LEU:HD21	8:7:395:VAL:CA	2.48	0.43
8:7:604:LYS:H	8:7:668:THR:HB	1.83	0.43
8:7:642:ASN:O	8:7:646:ASN:HB3	2.18	0.43
1:3:13:CYS:HB3	1:3:16:CYS:C	2.38	0.43
2:2:382:SER:HA	2:2:385:ARG:NH1	2.34	0.43
2:2:462:PHE:HD2	2:2:489:LYS:HB3	1.82	0.43
3:0:115:CYS:SG	3:0:120:VAL:HB	2.58	0.43
3:0:140:GLN:HG2	3:0:143:ARG:HE	1.83	0.43
3:0:169:ASP:OD1	3:0:170:TYR:N	2.47	0.43
4:1:562:LYS:O	4:1:566:ILE:HG13	2.19	0.43
5:4:213:VAL:HG12	5:4:215:ILE:CD1	2.48	0.43
6:6:160:PHE:HA	6:6:305:VAL:HG13	2.00	0.43
8:7:366:GLN:HB3	8:7:395:VAL:CG1	2.48	0.43
8:7:462:ASN:O	8:7:464:ARG:N	2.40	0.43
8:7:527:LEU:HA	8:7:530:LEU:HB2	2.00	0.43
8:7:600:ARG:HB3	8:7:601:ARG:HH22	1.82	0.43
1:3:27:LYS:NZ	1:3:29:LEU:CD2	2.70	0.43
2:2:428:GLU:OE1	2:2:428:GLU:HA	2.19	0.43
2:2:484:LYS:HD2	2:2:484:LYS:C	2.39	0.43
3:0:8:LEU:HD23	3:0:62:HIS:HB3	2.00	0.43
3:0:66:HIS:ND1	3:0:231:ILE:HG23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:100:GLN:OE1	3:0:100:GLN:N	2.52	0.43
3:0:195:ILE:O	3:0:199:MET:CG	2.55	0.43
4:1:191:LEU:HA	4:1:194:VAL:HG22	2.00	0.43
4:1:511:ALA:N	5:4:264:LYS:HE3	2.34	0.43
5:4:27:THR:HG21	5:4:160:VAL:HG22	2.00	0.43
5:4:60:PHE:CE2	5:4:253:PHE:CZ	3.07	0.43
6:6:168:GLN:HG2	6:6:185:VAL:HG22	1.99	0.43
2:2:25:LEU:CD2	2:2:222:LEU:HD13	2.41	0.43
3:0:11:LEU:HD21	3:0:97:LEU:HD11	1.99	0.43
3:0:198:ARG:HG3	3:0:199:MET:HE2	1.99	0.43
3:0:325:ILE:O	3:0:325:ILE:HG22	2.18	0.43
3:0:332:VAL:O	3:0:335:LEU:HB2	2.19	0.43
3:0:340:GLU:OE1	3:0:343:LYS:HE2	2.18	0.43
5:4:53:VAL:O	5:4:57:LEU:HG	2.19	0.43
5:4:76:ILE:HG23	5:4:84:LYS:O	2.18	0.43
5:4:77:ALA:CB	5:4:86:LEU:HD11	2.49	0.43
6:6:426:ARG:NH1	6:6:435:GLU:HA	2.21	0.43
8:7:349:ASN:HD22	8:7:405:LYS:HD2	1.84	0.43
8:7:460:VAL:CG2	8:7:461:ALA:N	2.78	0.43
8:7:494:PRO:CG	8:7:497:MET:HE3	2.44	0.43
8:7:598:HIS:O	8:7:603:ASP:N	2.51	0.43
9:N:66:DA:C8	9:N:67:DT:H72	2.53	0.43
1:3:61:LYS:HE3	1:3:61:LYS:HB3	1.76	0.43
1:3:114:GLU:CA	3:0:330:HIS:CE1	3.02	0.43
2:2:24:ARG:O	2:2:27:THR:HG22	2.18	0.43
2:2:75:GLN:OE1	2:2:78:ILE:CD1	2.63	0.43
2:2:380:ARG:HH22	2:2:440:GLN:CB	2.31	0.43
3:0:18:TYR:HB2	3:0:21:GLN:HG3	1.99	0.43
3:0:58:ALA:O	3:0:62:HIS:HB3	2.19	0.43
3:0:79:ILE:O	3:0:83:LEU:HG	2.18	0.43
3:0:128:VAL:HA	3:0:131:GLU:CG	2.49	0.43
3:0:332:VAL:CA	3:0:335:LEU:HD13	2.49	0.43
3:0:571:VAL:H	4:1:379:ASN:HD21	1.66	0.43
3:0:683:ASP:HB3	3:0:686:PHE:CZ	2.52	0.43
5:4:121:VAL:O	5:4:124:THR:OG1	2.35	0.43
5:4:194:ILE:HA	5:4:197:MET:HE1	1.96	0.43
8:7:445:MET:CE	8:7:449:GLU:HA	2.49	0.43
8:7:568:GLU:C	8:7:571:ARG:HG3	2.39	0.43
8:7:611:ASN:HD22	8:7:614:ALA:HB3	1.83	0.43
9:N:62:DT:H2"	9:N:63:DG:C8	2.53	0.43
1:3:44:ASP:CA	1:3:47:PHE:CE2	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:380:ARG:HG3	2:2:384:ARG:NH1	2.25	0.43
3:0:123:GLU:CD	3:0:125:LYS:H	2.21	0.43
3:0:176:PHE:HB3	3:0:181:LEU:CA	2.48	0.43
3:0:570:LEU:N	3:0:570:LEU:HD12	2.34	0.43
4:1:374:ILE:C	4:1:378:MET:HE1	2.38	0.43
5:4:85:TYR:HB3	5:4:88:PRO:HD2	2.01	0.43
6:6:108:LYS:HB2	6:6:110:THR:HG23	2.01	0.43
8:7:351:ASP:CG	8:7:405:LYS:HD3	2.39	0.43
8:7:356:LEU:HG	8:7:401:CYS:HB3	2.00	0.43
2:2:12:GLN:HA	2:2:15:GLU:HG3	2.01	0.43
2:2:40:PRO:HG2	2:2:43:ALA:CB	2.49	0.43
3:0:224:ASN:CA	3:0:227:SER:OG	2.55	0.43
3:0:348:VAL:HG12	3:0:350:HIS:H	1.84	0.43
3:0:639:LEU:CD1	3:0:650:GLU:HA	2.48	0.43
3:0:671:ARG:H	3:0:675:ASP:CB	2.32	0.43
4:1:374:ILE:HG22	4:1:378:MET:CE	2.49	0.43
4:1:609:SER:HG	4:1:610:ASN:N	2.15	0.43
6:6:152:TYR:HB3	6:6:301:PHE:CZ	2.54	0.43
6:6:325:PRO:HD3	6:6:370:LEU:HD22	2.01	0.43
8:7:165:SER:O	8:7:172:GLU:N	2.51	0.43
8:7:405:LYS:O	8:7:407:VAL:HG23	2.19	0.43
8:7:571:ARG:HH22	8:7:580:LEU:HD12	1.81	0.43
8:7:581:TYR:CZ	8:7:715:GLU:HB2	2.54	0.43
8:7:757:ARG:HG2	8:7:758:GLU:N	2.34	0.43
9:N:79:DT:H2"	9:N:80:DG:C8	2.54	0.43
3:0:2:LYS:HE3	3:0:11:LEU:HD11	2.00	0.43
3:0:42:MET:CB	3:0:48:LYS:HE3	2.49	0.43
3:0:312:LEU:N	3:0:412:TYR:OH	2.39	0.43
3:0:334:PHE:O	3:0:337:ARG:HB2	2.19	0.43
3:0:538:VAL:HG13	3:0:598:LEU:C	2.39	0.43
6:6:116:THR:HG21	6:6:385:PRO:CG	2.26	0.43
6:6:172:ILE:HD11	6:6:220:LEU:HD11	1.99	0.43
8:7:421:ARG:C	8:7:426:GLN:HE22	2.22	0.43
8:7:467:SER:O	8:7:471:GLN:OE1	2.37	0.43
1:3:30:VAL:HG12	1:3:31:ASN:O	2.19	0.42
3:0:73:SER:HG	3:0:79:ILE:HG12	1.83	0.42
3:0:172:PRO:HD3	3:0:184:TYR:OH	2.19	0.42
3:0:293:LEU:HB2	3:0:319:GLU:HB3	2.01	0.42
3:0:321:ILE:HG13	3:0:323:GLY:H	1.82	0.42
3:0:412:TYR:HB3	3:0:416:PHE:CE2	2.54	0.42
3:0:416:PHE:CD1	3:0:439:CYS:CB	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:436:ARG:HD2	3:0:437:PHE:H	1.83	0.42
3:0:744:LEU:HB3	3:0:748:GLN:HE21	1.83	0.42
4:1:235:UNK:C	4:1:237:UNK:N	2.82	0.42
5:4:79:TYR:CD2	5:4:82:GLY:CA	3.02	0.42
7:5:7:GLY:HA3	7:5:41:LEU:HD11	2.00	0.42
8:7:438:PHE:HB3	8:7:444:GLU:HB2	1.99	0.42
8:7:666:GLU:HG2	8:7:692:ARG:C	2.39	0.42
9:N:61:DG:C6	10:T:106:DA:C2	3.07	0.42
1:3:98:ASP:C	1:3:101:GLY:H	2.22	0.42
2:2:43:ALA:C	2:2:47:ILE:HD12	2.34	0.42
2:2:56:GLU:CA	2:2:97:MET:HE2	2.47	0.42
2:2:502:LEU:HD21	2:2:506:LYS:CE	2.49	0.42
3:0:42:MET:HG2	3:0:48:LYS:HB3	2.01	0.42
3:0:162:LEU:HD22	3:0:194:PHE:HB3	2.01	0.42
3:0:250:LEU:HD12	4:1:350:ARG:HG2	2.01	0.42
3:0:331:PHE:CD2	3:0:335:LEU:HD11	2.54	0.42
3:0:539:VAL:HB	3:0:621:LEU:HB2	2.01	0.42
3:0:625:ILE:CD1	3:0:626:PRO:HD2	2.47	0.42
3:0:628:GLN:OE1	3:0:628:GLN:HA	2.19	0.42
4:1:197:GLU:O	4:1:201:ASN:OD1	2.36	0.42
4:1:597:PHE:CE2	4:1:620:LEU:HD11	2.53	0.42
8:7:339:GLU:OE2	8:7:533:PRO:HG3	2.18	0.42
8:7:343:PHE:CZ	8:7:378:ARG:HD3	2.54	0.42
8:7:363:ARG:HG3	8:7:366:GLN:OE1	2.19	0.42
8:7:372:LYS:HD3	8:7:535:LEU:O	2.19	0.42
8:7:572:GLU:OE1	8:7:576:LYS:HD3	2.19	0.42
8:7:622:MET:CE	8:7:651:THR:HB	2.48	0.42
8:7:677:TYR:CD2	8:7:682:GLN:HG2	2.51	0.42
10:T:91:DC:H2"	10:T:92:DA:C8	2.55	0.42
2:2:73:GLN:HA	2:2:76:ASN:HB2	2.01	0.42
3:0:215:ASP:OD1	3:0:247:SER:HB3	2.19	0.42
3:0:295:SER:N	3:0:298:ILE:HG22	2.34	0.42
3:0:715:SER:HB3	3:0:718:LYS:HZ1	1.84	0.42
4:1:266:VAL:HG21	4:1:287:PHE:CE1	2.54	0.42
5:4:175:ARG:HB3	5:4:209:PRO:HD2	2.02	0.42
5:4:289:CYS:SG	5:4:290:SER:N	2.91	0.42
6:6:134:GLU:OE1	6:6:134:GLU:N	2.46	0.42
6:6:154:ILE:HD13	6:6:196:LEU:HD12	2.01	0.42
6:6:276:LEU:HD12	6:6:277:CYS:N	2.34	0.42
6:6:403:CYS:HB3	6:6:408:SER:H	1.84	0.42
7:5:13:ASP:OD1	7:5:15:SER:OG	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:523:LYS:HG3	8:7:525:GLY:H	1.83	0.42
2:2:43:ALA:C	2:2:47:ILE:CD1	2.88	0.42
2:2:201:TRP:CE2	2:2:278:LEU:CD1	3.02	0.42
3:0:117:HIS:HA	3:0:158:TYR:CE2	2.54	0.42
3:0:371:ARG:NH2	3:0:410:SER:O	2.52	0.42
3:0:424:GLU:N	3:0:432:ASN:CG	2.60	0.42
3:0:643:ARG:HA	3:0:643:ARG:HD2	1.87	0.42
4:1:206:PRO:O	4:1:209:PHE:HB3	2.19	0.42
4:1:274:VAL:O	4:1:279:LYS:NZ	2.45	0.42
5:4:25:LEU:HD12	5:4:73:VAL:CA	2.50	0.42
5:4:194:ILE:HB	5:4:195:PRO:HD3	2.02	0.42
5:4:293:LEU:HB3	6:6:380:TYR:OH	2.19	0.42
6:6:154:ILE:HG12	6:6:196:LEU:HD13	2.00	0.42
6:6:221:LEU:HD23	6:6:230:ARG:HG3	2.01	0.42
6:6:291:LEU:HA	6:6:296:HIS:CE1	2.54	0.42
7:5:61:ASN:HA	8:7:573:THR:HB	2.01	0.42
8:7:608:PHE:CE2	8:7:674:SER:HB3	2.54	0.42
8:7:713:THR:H	8:7:716:MET:HG2	1.84	0.42
9:N:52:DA:C8	9:N:53:DT:H72	2.54	0.42
2:2:406:PRO:HA	2:2:409:ARG:CZ	2.49	0.42
3:0:24:TYR:CE2	3:0:52:LEU:CD2	3.02	0.42
3:0:148:ASP:C	3:0:148:ASP:OD1	2.58	0.42
3:0:325:ILE:CG2	3:0:331:PHE:HD1	2.33	0.42
4:1:218:ARG:HH12	6:6:222:LEU:CD1	2.31	0.42
5:4:121:VAL:O	5:4:125:LEU:HG	2.19	0.42
5:4:122:ASP:O	5:4:126:VAL:HG23	2.20	0.42
6:6:174:MET:CE	6:6:208:PRO:HB3	2.45	0.42
8:7:356:LEU:HB2	8:7:404:LYS:NZ	2.34	0.42
8:7:599:GLU:OE2	8:7:624:LYS:CE	2.67	0.42
2:2:457:SER:HB3	7:5:4:ALA:HB1	2.02	0.42
2:2:485:ASP:OD1	2:2:488:LYS:HB2	2.20	0.42
3:0:13:PRO:HA	3:0:92:TYR:CG	2.55	0.42
3:0:294:HIS:O	3:0:294:HIS:CG	2.72	0.42
6:6:146:HIS:NE2	6:6:204:PRO:HD3	2.34	0.42
6:6:237:GLY:HA2	6:6:266:LEU:HG	2.02	0.42
8:7:615:LEU:HD11	8:7:653:PHE:HB3	2.01	0.42
8:7:641:GLN:C	8:7:645:TYR:HB2	2.39	0.42
8:7:664:LEU:CG	8:7:689:ARG:HD2	2.49	0.42
10:T:105:DC:H2"	10:T:106:DA:C8	2.54	0.42
3:0:25:MET:HE1	3:0:51:SER:C	2.40	0.42
3:0:71:TYR:HD1	3:0:233:ILE:HB	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:200:ILE:HG22	3:0:226:VAL:HG11	2.02	0.42
5:4:304:LYS:H	5:4:311:GLN:HA	1.84	0.42
6:6:136:MET:HE1	6:6:266:LEU:HD12	2.02	0.42
8:7:407:VAL:HA	8:7:484:PHE:O	2.19	0.42
8:7:507:ALA:HB3	8:7:510:LYS:HE3	2.01	0.42
8:7:546:LYS:HD2	8:7:546:LYS:HA	1.38	0.42
8:7:641:GLN:O	8:7:643:PHE:N	2.52	0.42
8:7:660:THR:HA	8:7:661:SER:HA	1.92	0.42
9:N:75:DG:C6	10:T:92:DA:C2	3.07	0.42
1:3:27:LYS:CD	1:3:29:LEU:HD23	2.49	0.42
1:3:66:ASN:HA	1:3:68:PHE:CE2	2.55	0.42
1:3:74:ASP:HB2	1:3:79:GLU:CB	2.50	0.42
2:2:7:LYS:HG2	2:2:9:SER:N	2.33	0.42
2:2:350:TYR:N	2:2:407:GLN:OE1	2.47	0.42
2:2:382:SER:O	2:2:385:ARG:HB2	2.19	0.42
2:2:392:THR:HG22	2:2:394:ASP:H	1.85	0.42
2:2:432:VAL:HA	2:2:433:LEU:HA	1.80	0.42
2:2:452:ILE:O	7:5:10:VAL:HA	2.19	0.42
3:0:224:ASN:HA	3:0:227:SER:HG	1.77	0.42
3:0:416:PHE:CD1	3:0:439:CYS:SG	3.12	0.42
3:0:555:GLN:OE1	4:1:297:UNK:HA	2.20	0.42
3:0:575:ASP:OD2	3:0:578:GLU:CG	2.68	0.42
3:0:586:TYR:HE1	3:0:597:ILE:CA	2.32	0.42
5:4:163:ILE:HA	5:4:166:GLU:CD	2.40	0.42
5:4:203:ALA:O	5:4:207:LYS:N	2.53	0.42
6:6:255:VAL:HG21	6:6:279:ALA:O	2.19	0.42
7:5:14:PRO:HA	7:5:37:ASP:O	2.20	0.42
8:7:421:ARG:O	8:7:426:GLN:NE2	2.49	0.42
8:7:593:PHE:HB2	8:7:745:ILE:HG21	2.02	0.42
8:7:673:ILE:HD11	8:7:708:LEU:HD12	2.02	0.42
1:3:45:ARG:CZ	1:3:46:ILE:CD1	2.98	0.42
2:2:21:VAL:HG22	2:2:21:VAL:H	1.59	0.42
2:2:100:LEU:HD12	2:2:101:ASN:O	2.19	0.42
2:2:286:ARG:O	2:2:286:ARG:HD3	2.19	0.42
3:0:63:TYR:HB3	3:0:65:GLU:OE1	2.19	0.42
3:0:76:MET:SD	3:0:77:SER:N	2.93	0.42
3:0:418:LEU:N	3:0:437:PHE:HD1	2.17	0.42
3:0:506:ILE:O	3:0:683:ASP:HA	2.19	0.42
3:0:624:GLY:O	3:0:686:PHE:HZ	2.03	0.42
5:4:126:VAL:HA	5:4:129:ILE:HG12	2.02	0.42
5:4:206:MET:HG3	5:4:206:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:178:LEU:HB3	6:6:180:GLN:NE2	2.35	0.42
7:5:54:LEU:CD2	7:5:58:LEU:CD2	2.97	0.42
8:7:408:ILE:HG23	8:7:482:TRP:CZ3	2.54	0.42
2:2:50:MET:HE1	2:2:56:GLU:HA	2.02	0.42
2:2:71:LYS:O	2:2:74:PHE:HB3	2.19	0.42
3:0:11:LEU:CD2	3:0:97:LEU:HG	2.46	0.42
3:0:18:TYR:OH	3:0:673:LYS:HB2	2.19	0.42
4:1:325:UNK:O	4:1:326:UNK:C	2.67	0.42
4:1:556:THR:O	4:1:560:PHE:HD2	2.03	0.42
5:4:31:GLU:HG3	5:4:180:THR:HA	2.01	0.42
6:6:224:VAL:HG13	6:6:228:CYS:HB3	1.99	0.42
8:7:407:VAL:HB	8:7:452:LEU:HD22	2.01	0.42
8:7:544:SER:HB3	8:7:549:ILE:CB	2.41	0.42
2:2:218:LEU:O	2:2:222:LEU:HG	2.20	0.41
2:2:405:HIS:NE2	2:2:409:ARG:HA	2.36	0.41
3:0:13:PRO:HA	3:0:92:TYR:CD1	2.54	0.41
3:0:107:GLY:HA2	3:0:207:ILE:O	2.19	0.41
3:0:270:ARG:O	3:0:274:VAL:HG22	2.20	0.41
3:0:286:TYR:HB3	3:0:326:ARG:NH2	2.35	0.41
3:0:495:MET:HG3	3:0:497:ILE:HD11	2.02	0.41
3:0:668:ARG:HA	3:0:668:ARG:HD3	1.75	0.41
4:1:189:LYS:O	4:1:192:MET:HG3	2.20	0.41
4:1:606:GLU:CA	4:1:609:SER:OG	2.65	0.41
8:7:739:LEU:HG	8:7:742:MET:SD	2.59	0.41
2:2:345:PHE:CE2	2:2:437:VAL:HA	2.55	0.41
3:0:42:MET:HG3	3:0:48:LYS:HE3	2.02	0.41
3:0:66:HIS:ND1	3:0:229:ASP:O	2.53	0.41
3:0:251:ASP:C	4:1:350:ARG:CZ	2.89	0.41
3:0:288:LYS:O	3:0:291:GLN:HG3	2.20	0.41
3:0:478:VAL:O	3:0:480:GLN:OE1	2.38	0.41
3:0:586:TYR:HE1	3:0:597:ILE:N	2.17	0.41
3:0:588:LYS:HE3	3:0:588:LYS:HB2	1.72	0.41
4:1:235:UNK:O	4:1:239:PRO:HD2	2.21	0.41
5:4:79:TYR:HH	5:4:84:LYS:HB2	1.84	0.41
6:6:322:MET:C	6:6:368:LEU:HD21	2.40	0.41
6:6:383:LEU:HB3	6:6:384:MET:HE1	2.02	0.41
8:7:385:VAL:HG23	8:7:537:GLU:HA	2.00	0.41
8:7:410:LEU:N	8:7:410:LEU:HD12	2.35	0.41
8:7:495:ALA:HB2	8:7:521:ASP:CG	2.40	0.41
2:2:124:VAL:N	2:2:235:LYS:O	2.42	0.41
2:2:353:SER:HB2	2:2:356:GLN:CD	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:358:ALA:O	2:2:362:LEU:HG	2.20	0.41
3:0:90:MET:HE3	3:0:101:GLU:CD	2.40	0.41
3:0:134:ARG:NH2	3:0:306:PHE:HA	2.35	0.41
3:0:251:ASP:C	4:1:350:ARG:NE	2.73	0.41
3:0:297:ASP:CG	3:0:386:ARG:HH12	2.24	0.41
3:0:322:PRO:HG2	3:0:325:ILE:HB	2.02	0.41
3:0:346:MET:CE	3:0:433:PRO:HG2	2.51	0.41
3:0:544:TYR:OH	3:0:573:THR:HA	2.21	0.41
3:0:625:ILE:HG22	3:0:685:ARG:HH21	1.86	0.41
3:0:639:LEU:CG	3:0:642:MET:CE	2.98	0.41
6:6:294:GLU:H	6:6:294:GLU:CD	2.24	0.41
8:7:417:VAL:HG13	8:7:454:VAL:HG22	2.02	0.41
8:7:463:THR:HG1	9:N:64:DA:P	2.40	0.41
8:7:499:ARG:CD	8:7:500:ARG:HG3	2.49	0.41
8:7:562:THR:HB	8:7:756:ARG:NH1	2.33	0.41
8:7:664:LEU:O	8:7:692:ARG:HD3	2.20	0.41
9:N:72:DG:H1'	9:N:73:DA:H5'	2.02	0.41
2:2:457:SER:HA	2:2:492:PHE:CE2	2.56	0.41
2:2:467:GLU:HA	2:2:467:GLU:OE2	2.20	0.41
3:0:197:ARG:CG	3:0:221:ARG:NH1	2.83	0.41
3:0:264:ALA:CB	3:0:336:LYS:HE3	2.51	0.41
3:0:495:MET:HB2	3:0:708:LEU:HD12	2.02	0.41
3:0:521:ASN:C	3:0:525:MET:CE	2.82	0.41
3:0:521:ASN:O	3:0:525:MET:CE	2.68	0.41
3:0:553:MET:O	3:0:556:THR:HB	2.21	0.41
4:1:260:PHE:CG	4:1:267:LYS:HB2	2.55	0.41
4:1:273:ASN:HD21	4:1:310:UNK:CB	2.32	0.41
4:1:343:ILE:HG13	4:1:344:UNK:N	2.36	0.41
4:1:346:ASP:HB2	4:1:347:PRO:HD3	2.02	0.41
6:6:325:PRO:HA	6:6:348:PHE:O	2.19	0.41
6:6:384:MET:O	6:6:384:MET:CG	2.67	0.41
7:5:19:LEU:CD2	7:5:22:GLN:CD	2.81	0.41
7:5:61:ASN:O	8:7:573:THR:CB	2.68	0.41
8:7:750:TYR:HA	8:7:755:GLU:HB2	2.03	0.41
2:2:412:ALA:O	2:2:416:LEU:CB	2.68	0.41
3:0:124:ARG:O	3:0:124:ARG:HG2	2.20	0.41
3:0:251:ASP:HB3	4:1:350:ARG:NH2	2.27	0.41
3:0:263:GLY:O	3:0:267:LEU:CD2	2.62	0.41
3:0:339:ILE:CG1	3:0:343:LYS:HZ3	2.28	0.41
3:0:409:ILE:HG13	3:0:410:SER:N	2.35	0.41
4:1:551:ARG:NH2	4:1:615:TYR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:30:ILE:HD13	5:4:179:LEU:CG	2.50	0.41
5:4:252:MET:O	5:4:253:PHE:HD1	2.04	0.41
5:4:271:ASP:CA	5:4:273:ARG:HE	2.34	0.41
6:6:273:CYS:HB2	6:6:288:TYR:CD1	2.56	0.41
6:6:273:CYS:O	6:6:276:LEU:HG	2.21	0.41
6:6:288:TYR:CD2	6:6:288:TYR:O	2.74	0.41
8:7:588:PHE:HB2	8:7:618:TYR:CZ	2.55	0.41
8:7:603:ASP:OD1	8:7:696:ARG:NH2	2.43	0.41
8:7:697:ASN:O	8:7:697:ASN:OD1	2.37	0.41
1:3:34:CYS:CB	1:3:61:LYS:CE	2.99	0.41
2:2:339:LEU:O	2:2:407:GLN:NE2	2.54	0.41
2:2:488:LYS:HB3	2:2:490:LYS:HD2	2.03	0.41
3:0:270:ARG:NE	3:0:388:LEU:HB3	2.36	0.41
3:0:291:GLN:NE2	3:0:294:HIS:CA	2.80	0.41
3:0:319:GLU:OE1	3:0:319:GLU:N	2.54	0.41
3:0:534:PRO:CA	6:6:239:LEU:HD12	2.45	0.41
4:1:206:PRO:CA	4:1:210:TRP:CZ3	2.97	0.41
8:7:457:TYR:HA	8:7:460:VAL:HG22	2.01	0.41
8:7:491:HIS:HA	8:7:519:ARG:NE	2.32	0.41
8:7:526:ASP:O	8:7:530:LEU:CD1	2.67	0.41
9:N:63:DG:H2"	9:N:64:DA:H8	1.84	0.41
1:3:30:VAL:CB	1:3:71:GLN:NE2	2.77	0.41
2:2:455:GLU:HG2	2:2:456:GLY:N	2.36	0.41
3:0:117:HIS:ND1	3:0:120:VAL:HG23	2.35	0.41
3:0:198:ARG:HH11	3:0:199:MET:HE3	1.81	0.41
3:0:198:ARG:CZ	3:0:199:MET:CE	2.95	0.41
3:0:283:GLN:HA	3:0:286:TYR:CD2	2.56	0.41
3:0:393:VAL:O	3:0:393:VAL:HG12	2.21	0.41
3:0:416:PHE:HA	3:0:439:CYS:HA	2.03	0.41
5:4:55:GLU:O	5:4:59:VAL:HG23	2.21	0.41
5:4:79:TYR:CD2	5:4:83:ILE:N	2.89	0.41
5:4:225:GLN:HE22	5:4:269:SER:HB2	1.76	0.41
6:6:148:MET:HB2	6:6:148:MET:HE3	1.87	0.41
6:6:173:ILE:N	6:6:180:GLN:O	2.27	0.41
7:5:52:HIS:HB3	7:5:56:ARG:CZ	2.50	0.41
8:7:397:ILE:HD13	8:7:428:CYS:SG	2.61	0.41
8:7:612:VAL:HG23	8:7:613:TYR:N	2.35	0.41
1:3:72:ILE:HD13	1:3:72:ILE:HG21	1.69	0.41
3:0:171:LEU:HD22	3:0:184:TYR:CE2	2.55	0.41
3:0:270:ARG:CZ	3:0:390:VAL:HA	2.50	0.41
3:0:275:ARG:HD2	3:0:276:LYS:CE	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:325:ILE:O	3:0:380:ARG:NH2	2.54	0.41
3:0:340:GLU:HA	3:0:343:LYS:HD2	2.03	0.41
3:0:490:LYS:O	3:0:491:SER:OG	2.35	0.41
3:0:500:GLY:HA3	3:0:521:ASN:OD1	2.21	0.41
4:1:229:GLY:N	6:6:244:PRO:HB3	2.35	0.41
4:1:375:LEU:HA	4:1:378:MET:HE1	2.02	0.41
5:4:254:ILE:O	5:4:258:LEU:HB2	2.20	0.41
6:6:175:ARG:NH2	6:6:205:LYS:CG	2.84	0.41
6:6:232:VAL:CG1	6:6:233:LEU:N	2.84	0.41
6:6:236:PHE:O	6:6:266:LEU:HG	2.21	0.41
8:7:563:ALA:O	8:7:567:GLN:CD	2.53	0.41
8:7:572:GLU:HG3	8:7:574:ALA:H	1.85	0.41
8:7:626:PHE:HB2	8:7:653:PHE:CD2	2.56	0.41
8:7:760:LEU:HD23	8:7:760:LEU:C	2.40	0.41
1:3:26:VAL:HB	1:3:39:CYS:HB2	2.03	0.41
2:2:353:SER:C	2:2:356:GLN:HG2	2.38	0.41
2:2:405:HIS:CE1	2:2:409:ARG:HG2	2.56	0.41
3:0:11:LEU:N	3:0:11:LEU:CD1	2.84	0.41
3:0:71:TYR:HB3	3:0:207:ILE:HG22	2.03	0.41
3:0:288:LYS:HD3	3:0:294:HIS:NE2	2.36	0.41
3:0:406:ALA:HA	3:0:409:ILE:HG12	2.03	0.41
3:0:465:PRO:HB2	3:0:467:ASP:OD1	2.21	0.41
3:0:522:TYR:HD1	3:0:525:MET:HE1	1.84	0.41
3:0:571:VAL:CG2	3:0:572:GLU:N	2.82	0.41
3:0:633:ARG:O	3:0:636:LYS:CG	2.51	0.41
3:0:730:PRO:C	3:0:732:ASP:H	2.24	0.41
4:1:196:GLN:NE2	4:1:197:GLU:OE1	2.54	0.41
4:1:300:UNK:O	4:1:302:UNK:N	2.54	0.41
5:4:77:ALA:HB3	5:4:86:LEU:HD11	2.03	0.41
5:4:177:LEU:HD13	5:4:252:MET:HG2	2.02	0.41
6:6:171:ILE:HB	6:6:182:VAL:HG23	2.03	0.41
7:5:8:ALA:HB2	7:5:44:PRO:HG3	2.01	0.41
7:5:27:MET:CE	7:5:30:ILE:CG1	2.99	0.41
7:5:28:SER:HG	7:5:30:ILE:HD11	1.86	0.41
8:7:349:ASN:HB3	8:7:405:LYS:HD2	2.03	0.41
8:7:359:SER:HB2	8:7:429:THR:HG22	2.03	0.41
8:7:382:GLY:HA2	8:7:532:GLY:CA	2.51	0.41
8:7:416:SER:HB3	8:7:420:TRP:CE2	2.56	0.41
8:7:446:PHE:HB3	8:7:473:VAL:HG22	2.02	0.41
8:7:499:ARG:NH1	8:7:500:ARG:CG	2.84	0.41
8:7:581:TYR:CD1	8:7:582:ILE:HG13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:598:HIS:CB	8:7:603:ASP:HB2	2.49	0.41
8:7:678:GLY:HA2	8:7:679:SER:HA	1.77	0.41
1:3:25:ASP:O	1:3:25:ASP:OD1	2.39	0.41
2:2:406:PRO:O	2:2:409:ARG:NH1	2.53	0.41
2:2:473:LYS:HD2	2:2:473:LYS:HA	1.82	0.41
3:0:40:LEU:CD2	3:0:479:LEU:O	2.69	0.41
3:0:208:TYR:HD1	3:0:209:SER:O	2.04	0.41
3:0:222:VAL:HG11	3:0:452:ARG:HH12	1.86	0.41
3:0:275:ARG:NH1	3:0:276:LYS:CD	2.84	0.41
3:0:296:ALA:O	3:0:300:THR:HB	2.20	0.41
3:0:377:CYS:SG	3:0:378:SER:N	2.94	0.41
3:0:659:MET:HE2	3:0:689:LYS:HB3	2.03	0.41
6:6:264:LEU:HA	6:6:289:LYS:O	2.21	0.41
7:5:24:ASP:CG	7:5:31:VAL:HG23	2.41	0.41
8:7:573:THR:HA	8:7:577:ARG:HH21	1.86	0.41
9:N:58:DG:H1'	9:N:59:DA:H5'	2.02	0.41
3:0:76:MET:O	3:0:79:ILE:HB	2.21	0.40
3:0:625:ILE:CG2	3:0:627:PHE:CE1	3.03	0.40
8:7:569:TYR:HA	8:7:577:ARG:NE	2.36	0.40
8:7:598:HIS:O	8:7:602:GLY:N	2.54	0.40
2:2:346:LYS:HG2	2:2:348:TYR:CZ	2.55	0.40
2:2:381:GLU:HG2	2:2:384:ARG:HH21	1.87	0.40
3:0:206:ILE:HG22	3:0:207:ILE:N	2.36	0.40
3:0:267:LEU:CD2	3:0:396:PHE:CE1	3.05	0.40
3:0:287:GLU:O	3:0:290:VAL:CG1	2.64	0.40
3:0:423:TYR:CE1	3:0:425:ILE:HG12	2.50	0.40
3:0:506:ILE:HB	3:0:522:TYR:OH	2.21	0.40
5:4:60:PHE:CE2	5:4:253:PHE:HE1	2.24	0.40
5:4:79:TYR:HB2	5:4:81:GLN:H	1.86	0.40
5:4:193:TYR:C	5:4:197:MET:HE1	2.42	0.40
5:4:215:ILE:HG13	5:4:238:VAL:HG21	2.03	0.40
8:7:466:ARG:HD2	10:T:107:DT:C5'	2.51	0.40
8:7:490:VAL:O	8:7:490:VAL:CG1	2.69	0.40
8:7:514:THR:HG22	8:7:515:ALA:N	2.36	0.40
8:7:608:PHE:HB3	8:7:672:GLN:HA	2.02	0.40
8:7:754:ARG:O	8:7:757:ARG:CZ	2.69	0.40
1:3:71:GLN:HB3	1:3:73:PHE:H	1.86	0.40
2:2:201:TRP:CH2	2:2:278:LEU:HG	2.56	0.40
3:0:145:LEU:HB2	3:0:153:VAL:CG1	2.49	0.40
3:0:145:LEU:HD22	3:0:153:VAL:HG12	2.03	0.40
3:0:208:TYR:CD1	3:0:212:TYR:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:355:THR:HG1	3:0:358:SER:CB	2.34	0.40
3:0:544:TYR:HH	3:0:573:THR:HA	1.86	0.40
3:0:610:ILE:HD12	4:1:337:ILE:HD13	2.03	0.40
3:0:708:LEU:CB	3:0:712:MET:SD	2.85	0.40
4:1:496:UNK:O	4:1:500:UNK:N	2.55	0.40
5:4:59:VAL:HA	5:4:62:ASN:HD22	1.86	0.40
5:4:137:LYS:O	5:4:141:GLU:N	2.46	0.40
6:6:136:MET:HE2	6:6:145:ARG:CD	2.51	0.40
6:6:264:LEU:HD22	6:6:300:LEU:HD13	2.04	0.40
6:6:351:ASN:HA	6:6:353:HIS:CE1	2.56	0.40
6:6:381:HIS:HE1	6:6:449:HIS:CE1	2.39	0.40
7:5:30:ILE:HG21	7:5:46:LYS:HB2	2.03	0.40
8:7:421:ARG:NH2	8:7:426:GLN:HE21	2.19	0.40
3:0:16:LYS:H	3:0:16:LYS:HG2	1.58	0.40
3:0:40:LEU:HD23	3:0:479:LEU:O	2.21	0.40
3:0:197:ARG:HD3	3:0:197:ARG:HA	1.79	0.40
3:0:436:ARG:HD2	3:0:437:PHE:N	2.36	0.40
3:0:472:MET:HG3	3:0:473:LEU:CD2	2.51	0.40
3:0:572:GLU:OE1	3:0:600:SER:HA	2.21	0.40
3:0:620:VAL:C	3:0:621:LEU:HD12	2.42	0.40
3:0:635:LEU:HD12	3:0:635:LEU:H	1.87	0.40
3:0:643:ARG:NH1	3:0:646:TYR:O	2.55	0.40
4:1:237:UNK:CB	4:1:259:ILE:CD1	2.88	0.40
4:1:327:UNK:C	4:1:329:LEU:N	2.84	0.40
6:6:116:THR:OG1	6:6:385:PRO:CG	2.70	0.40
6:6:171:ILE:C	6:6:181:LEU:HD12	2.39	0.40
8:7:356:LEU:HA	8:7:401:CYS:SG	2.62	0.40
8:7:356:LEU:CB	8:7:404:LYS:NZ	2.83	0.40
8:7:484:PHE:CZ	8:7:511:LEU:HB2	2.56	0.40
8:7:751:ALA:O	8:7:756:ARG:NH2	2.49	0.40
8:7:757:ARG:CD	8:7:758:GLU:OE2	2.70	0.40
2:2:46:PHE:CE1	2:2:62:LEU:HG	2.57	0.40
3:0:35:GLY:HA3	3:0:455:SER:OG	2.22	0.40
3:0:156:CYS:O	3:0:157:GLU:HB3	2.21	0.40
3:0:216:PRO:O	3:0:220:GLU:HB3	2.21	0.40
3:0:233:ILE:O	3:0:234:PHE:HD1	2.04	0.40
3:0:279:SER:O	3:0:282:LEU:HB2	2.21	0.40
3:0:639:LEU:HD13	3:0:642:MET:SD	2.60	0.40
4:1:196:GLN:O	4:1:200:ILE:HB	2.22	0.40
6:6:142:ARG:HB2	6:6:143:PRO:CD	2.51	0.40
8:7:400:ALA:HB1	8:7:407:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:482:TRP:HD1	8:7:505:ILE:HG23	1.87	0.40
8:7:713:THR:OG1	8:7:716:MET:CE	2.70	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	3	136/321 (42%)	110 (81%)	24 (18%)	2 (2%)	10 46
2	2	456/513 (89%)	378 (83%)	78 (17%)	0	100 100
3	0	752/778 (97%)	657 (87%)	94 (12%)	1 (0%)	51 86
4	1	256/537 (48%)	223 (87%)	30 (12%)	3 (1%)	13 50
5	4	279/338 (82%)	218 (78%)	61 (22%)	0	100 100
6	6	336/461 (73%)	278 (83%)	55 (16%)	3 (1%)	17 57
7	5	64/72 (89%)	50 (78%)	14 (22%)	0	100 100
8	7	544/843 (64%)	469 (86%)	75 (14%)	0	100 100
All	All	2823/3863 (73%)	2383 (84%)	431 (15%)	9 (0%)	44 77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1	230	PRO
6	6	116	THR
6	6	411	PRO
4	1	389	LEU
4	1	239	PRO
6	6	118	TYR
1	3	66	ASN
3	0	172	PRO

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Mol	Chain	Res	Type
1	3	72	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	3	53/303 (18%)	52 (98%)	1 (2%)	57 75
2	2	258/468 (55%)	253 (98%)	5 (2%)	57 75
3	0	686/707 (97%)	685 (100%)	1 (0%)	93 97
4	1	169/395 (43%)	167 (99%)	2 (1%)	71 83
5	4	198/298 (66%)	198 (100%)	0	100 100
6	6	247/406 (61%)	241 (98%)	6 (2%)	49 69
7	5	53/66 (80%)	53 (100%)	0	100 100
8	7	379/737 (51%)	371 (98%)	8 (2%)	53 72
All	All	2043/3380 (60%)	2020 (99%)	23 (1%)	74 84

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	61	LYS
2	2	410	ARG
2	2	450	ARG
2	2	452	ILE
2	2	453	THR
2	2	484	LYS
3	0	649	ARG
4	1	189	LYS
4	1	276	LYS
6	6	108	LYS
6	6	113	LYS
6	6	115	ILE
6	6	118	TYR
6	6	274	LYS

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Mol	Chain	Res	Type
6	6	366	CYS
8	7	411	CYS
8	7	534	LYS
8	7	541	MET
8	7	546	LYS
8	7	553	GLN
8	7	625	PRO
8	7	754	ARG
8	7	757	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	36	HIS
2	2	19	GLN
2	2	23	ASN
2	2	356	GLN
2	2	395	GLN
3	0	211	HIS
3	0	291	GLN
3	0	330	HIS
3	0	566	HIS
3	0	577	GLN
3	0	614	HIS
5	4	62	ASN
5	4	64	HIS
5	4	139	GLN
5	4	161	ASN
5	4	225	GLN
5	4	237	HIS
5	4	311	GLN
6	6	146	HIS
6	6	163	GLN
6	6	202	GLN
6	6	302	ASN
6	6	351	ASN
6	6	375	HIS
6	6	381	HIS
6	6	449	HIS
8	7	366	GLN
8	7	426	GLN
8	7	442	ASN

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Mol	Chain	Res	Type
8	7	447	GLN
8	7	465	ASN
8	7	491	HIS
8	7	528	ASN
8	7	567	GLN
8	7	592	GLN
8	7	644	GLN
8	7	672	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	SF4	0	801	3	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SF4	0	801	3	-	-	0/6/5/5

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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	0	801	SF4	4	0

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
4	1	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	393:UNK	C	465:UNK	N	85.89
1	1	519:UNK	C	537:GLU	N	12.88
1	1	355:UNK	C	368:UNK	N	12.28
1	1	567:HIS	C	573:GLN	N	4.45

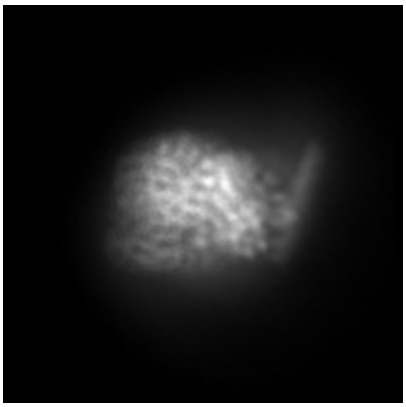
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23907. These allow visual inspection of the internal detail of the map and identification of artifacts.

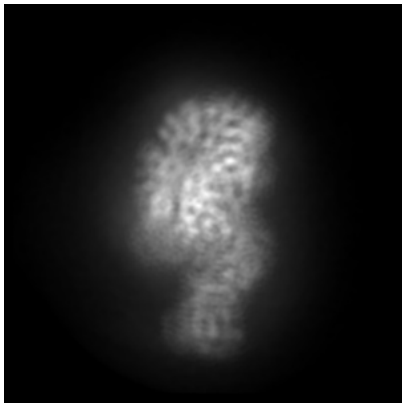
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

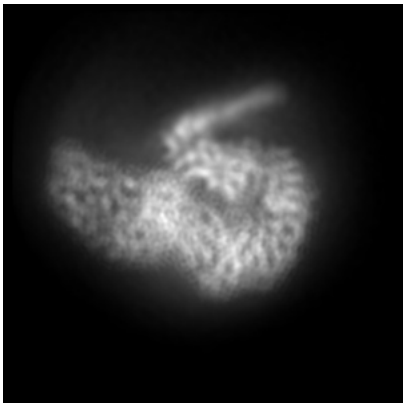
6.1.1 Primary map



X



Y

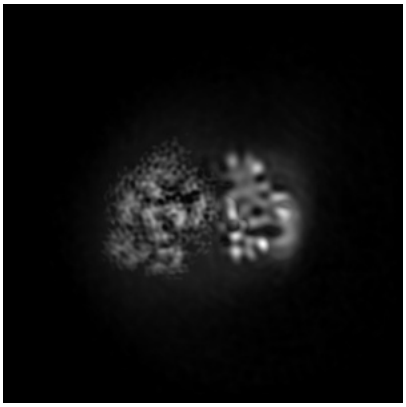


Z

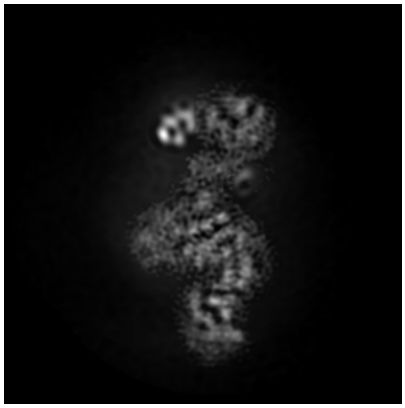
The images above show the map projected in three orthogonal directions.

6.2 Central slices

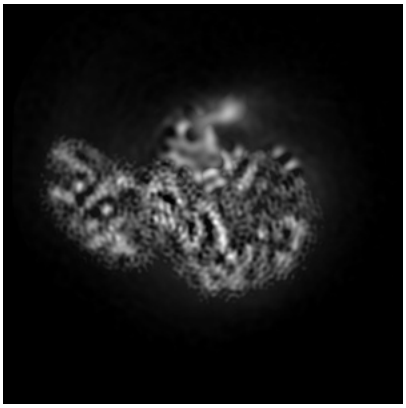
6.2.1 Primary map



X Index: 129



Y Index: 129

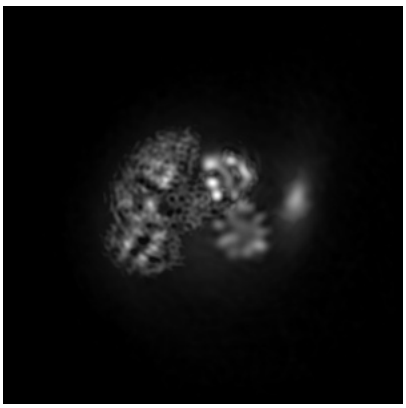


Z Index: 128

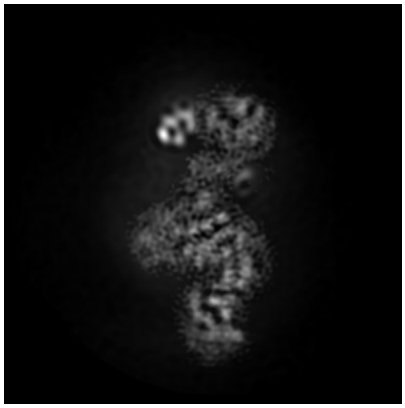
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

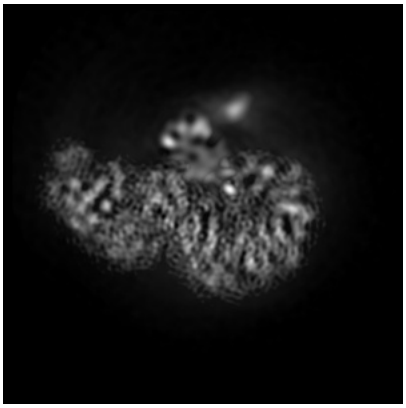
6.3.1 Primary map



X Index: 147



Y Index: 129

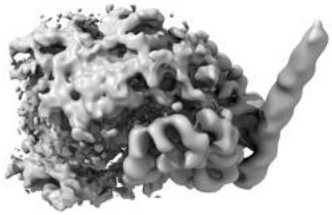


Z Index: 133

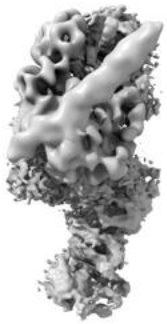
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

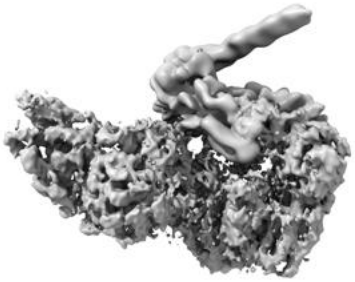
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

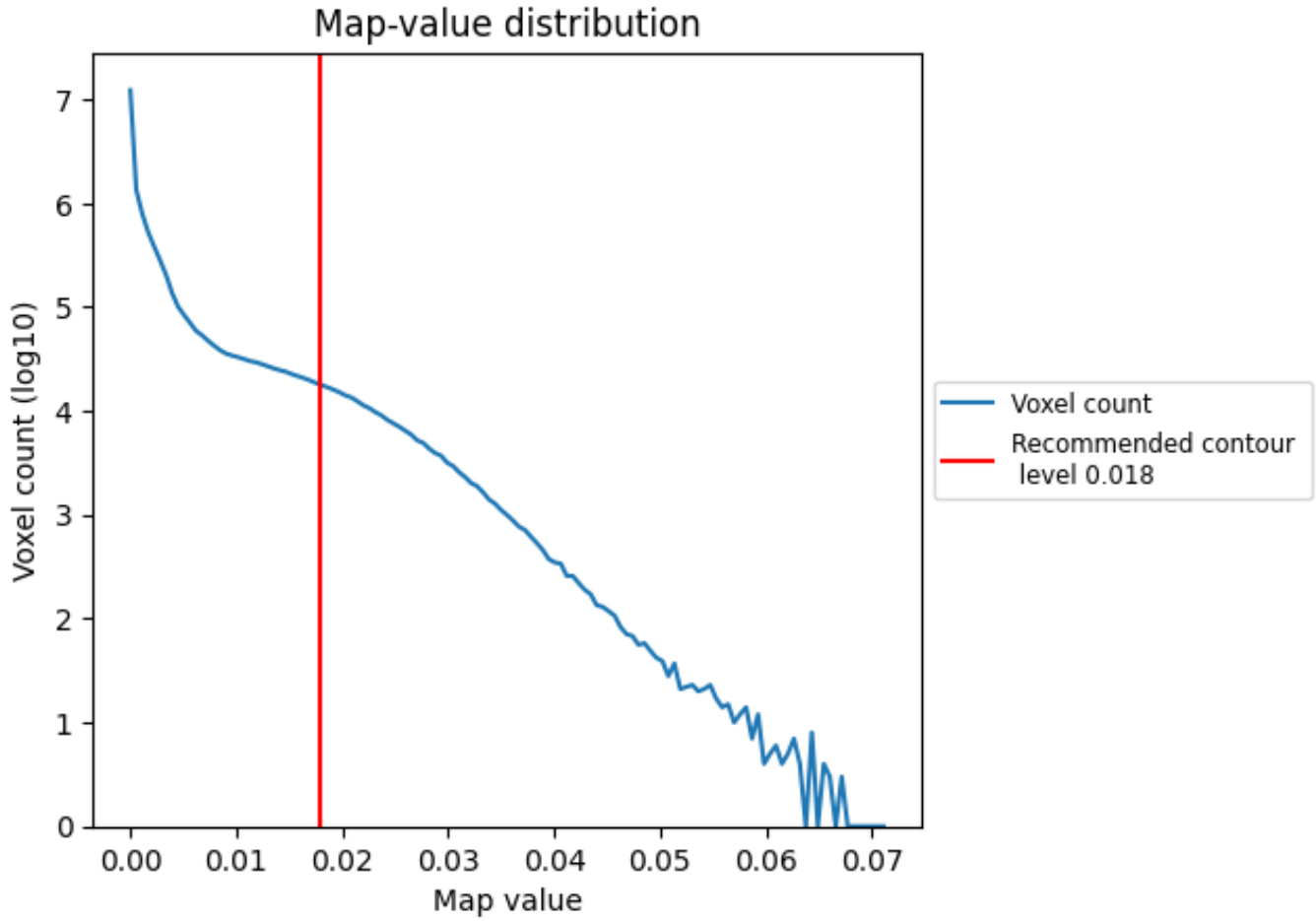
6.5 Mask visualisation (i)

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

7 Map analysis

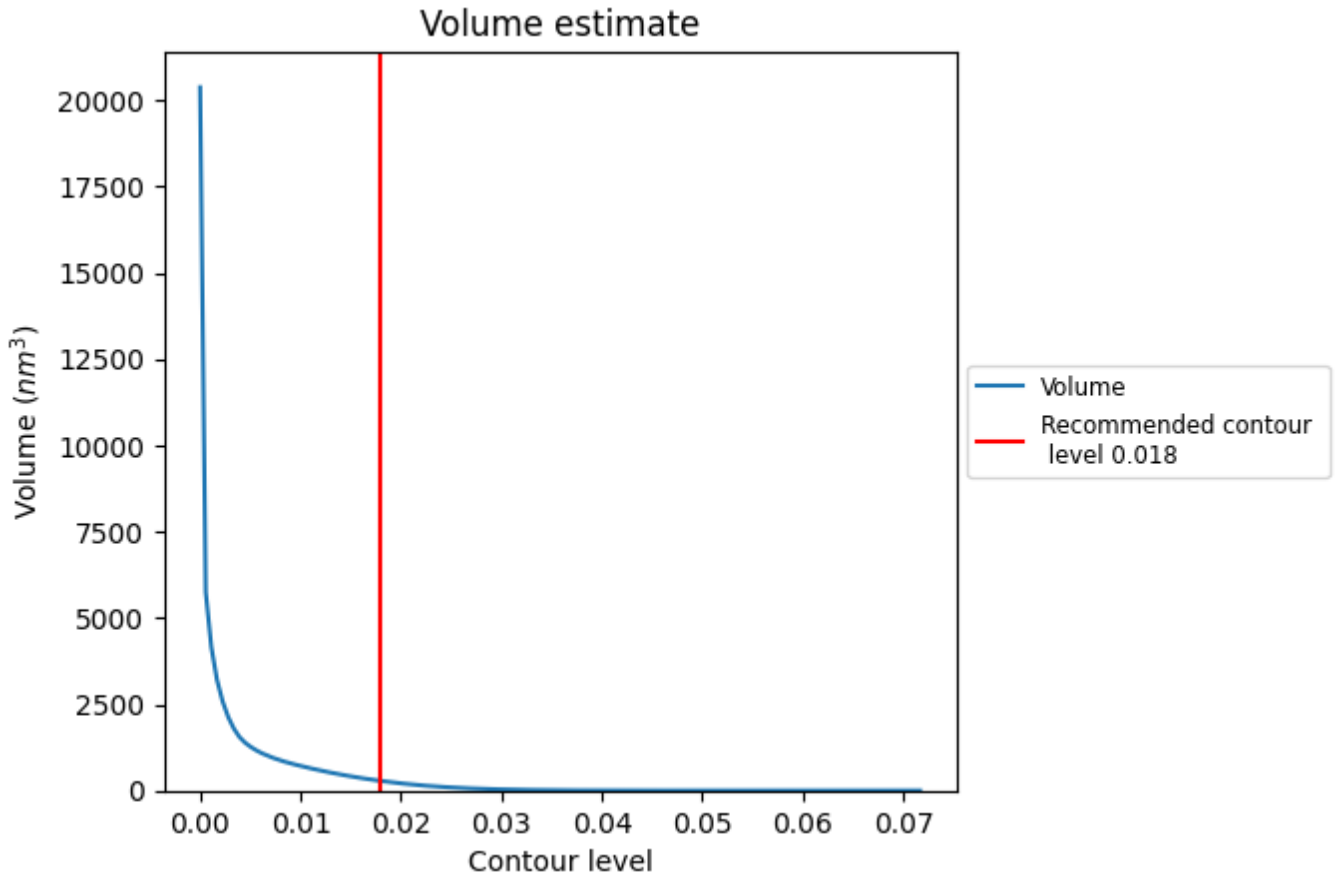
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 279 nm^3; this corresponds to an approximate mass of 252 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.

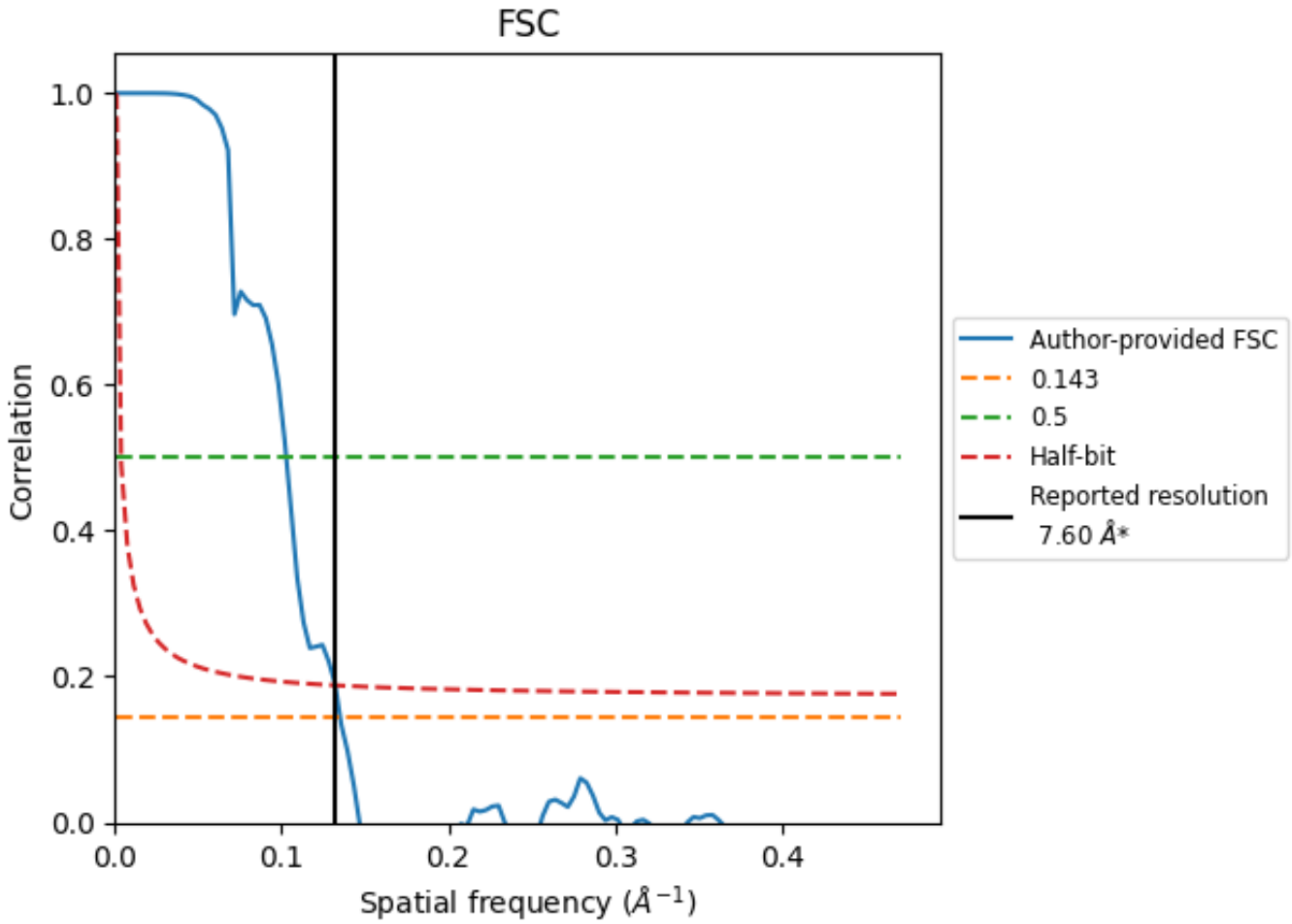
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.132 Å^{-1}

8.2 Resolution estimates (i)

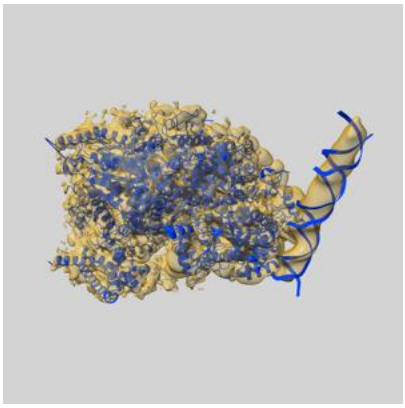
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.60	-	-
Author-provided FSC curve	7.40	9.73	7.56
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

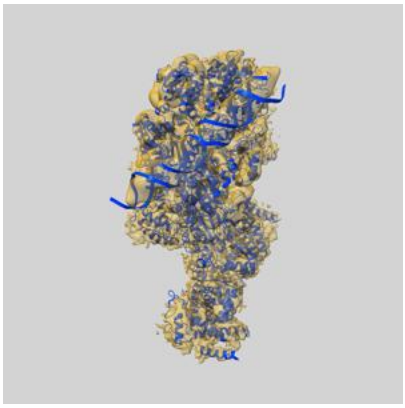
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23907 and PDB model 7ML3. Per-residue inclusion information can be found in section 3 on page 7.

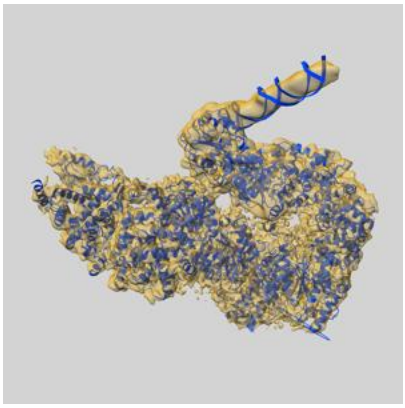
9.1 Map-model overlay



X



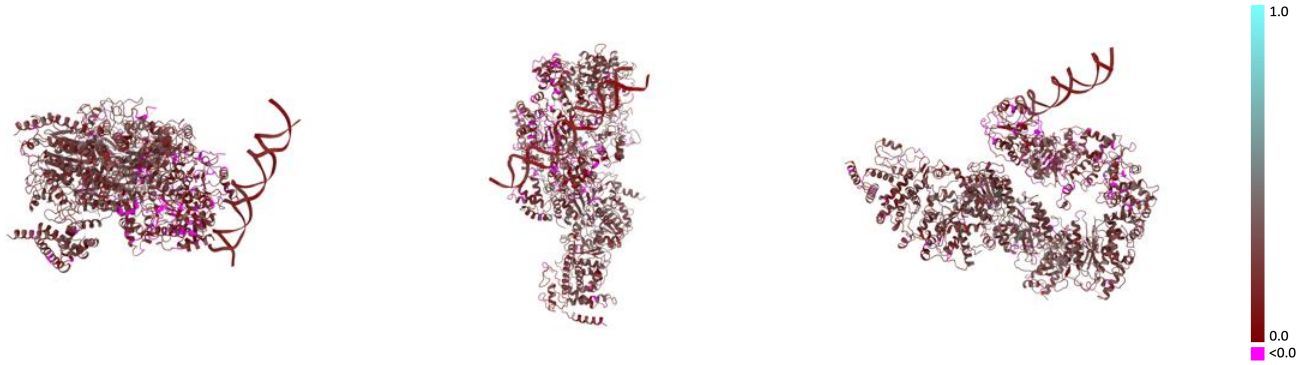
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

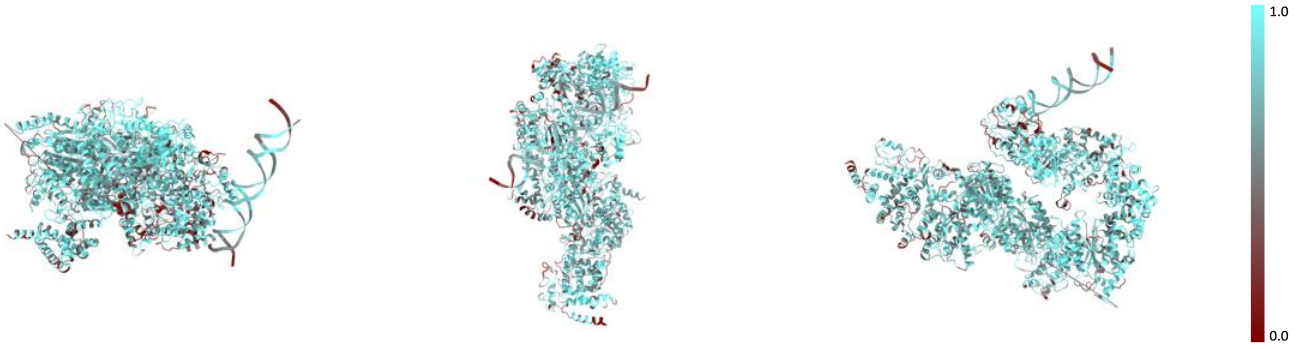
9.2 Q-score mapped to coordinate model



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.

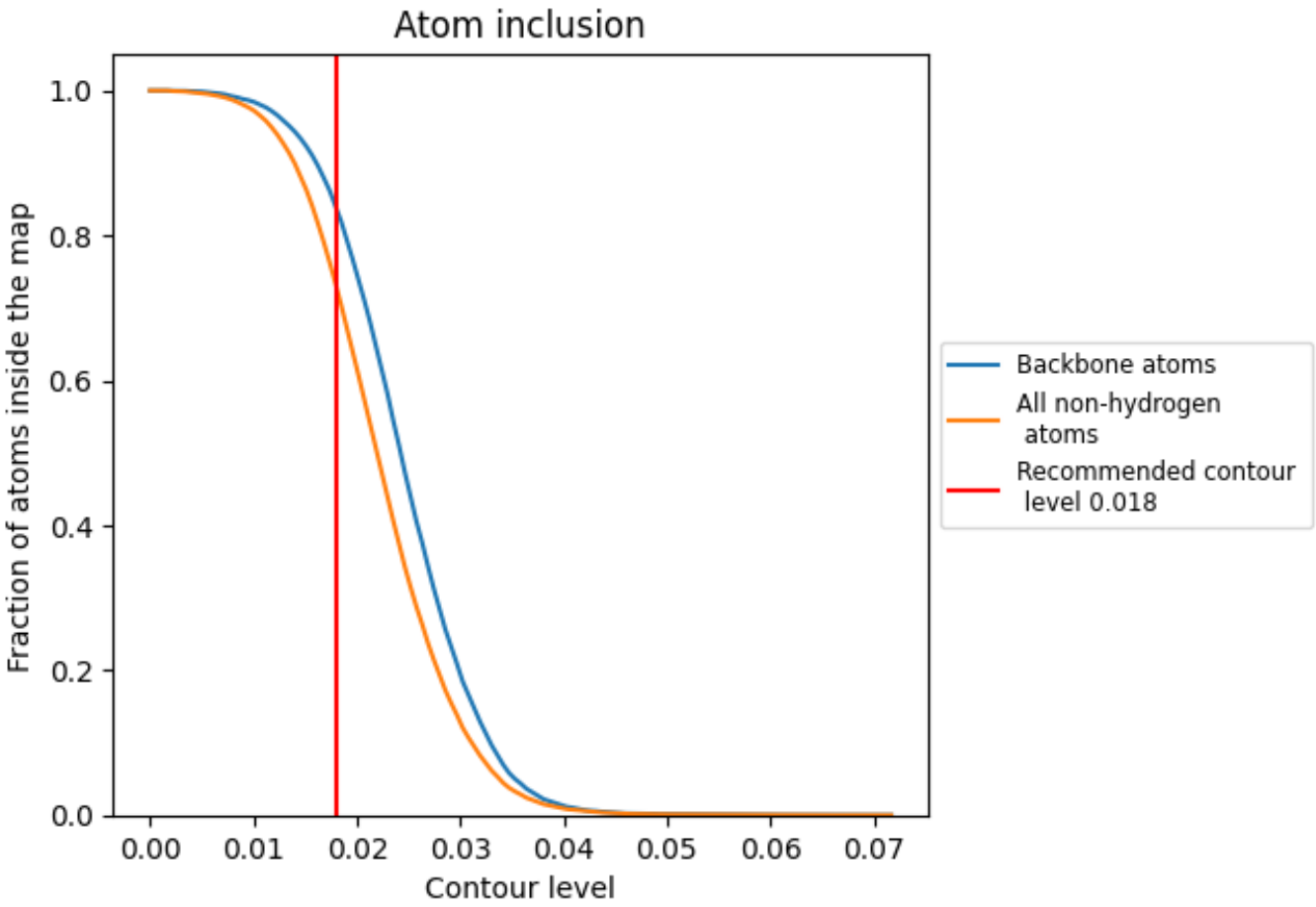
9.3 Atom inclusion mapped to coordinate model



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 73% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7303	0.2150
0	0.7489	0.2480
1	0.6626	0.2230
2	0.7397	0.1980
3	0.6569	0.2150
4	0.7357	0.2550
5	0.6951	0.1500
6	0.8229	0.2810
7	0.7284	0.1390
N	0.6554	0.1560
T	0.5875	0.1270