



## Full wwPDB EM Validation Report ⓘ

Nov 1, 2022 – 06:03 PM EDT

PDB ID : 5IY7  
EMDB ID : EMD-8132  
Title : Human holo-PIC in the open state  
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.  
Deposited on : 2016-03-24  
Resolution : 8.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

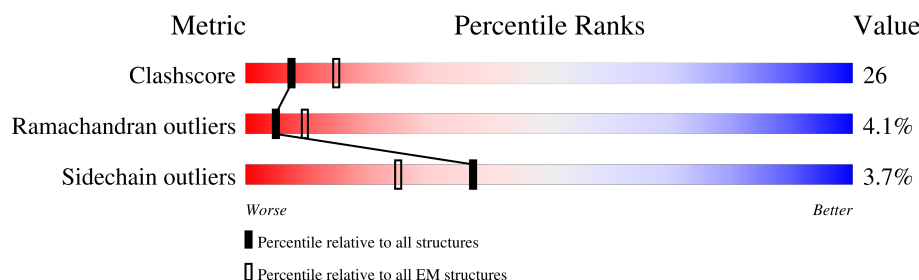
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.60 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	U	301	
22	V	782	
23	W	760	
24	0	395	
25	1	71	
26	2	462	
27	3	308	
28	X	77	
29	Y	77	

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 62705 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1454	Total	C	N	O	S	0	0
			11515	7234	2058	2150	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1165	Total	C	N	O	S	0	0
			9317	5878	1637	1738	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	275	Total	C	N	O	S	0	0
			2213	1386	380	440	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	129	Total	C	N	O	S	0	0
			1062	665	179	214	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1723	1088	301	325	9		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	86	Total	C	N	O	S	0	0
			689	437	120	127	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	310	Total	C	N	O	S	0	0
			2391	1490	426	457	18		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 21 is a protein called Transcription elongation factor TFIIS.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

- Molecule 22 is a protein called TFIIF basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	475	Total	C	N	O	S	0	0
			3855	2454	663	712	26		

- Molecule 23 is a protein called TFIIF basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	665	Total	C	N	O	S	0	0
			5348	3415	932	975	26		

- Molecule 24 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	0	188	Total	C	N	O	S	0	0
			1479	935	258	276	10		

- Molecule 25 is a protein called General transcription factor IIF subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	62	Total	C	N	O	S	0	0
			491	317	77	93	4		

- Molecule 26 is a protein called General transcription factor IIF subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	274	Total	C	N	O	S	0	0
			2196	1417	377	392	10		

- Molecule 27 is a protein called General transcription factor IIF subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	193	Total	C	N	O	S	0	0
			1526	978	252	284	12		

- Molecule 28 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	77	Total	C	N	O	P	0	0
			1591	753	303	459	76		

- Molecule 29 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	77	Total	C	N	O	P	0	0
			1561	741	279	465	76		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Mg	0
			1	1	
30	B	1	Total	Mg	0
			1	1	

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

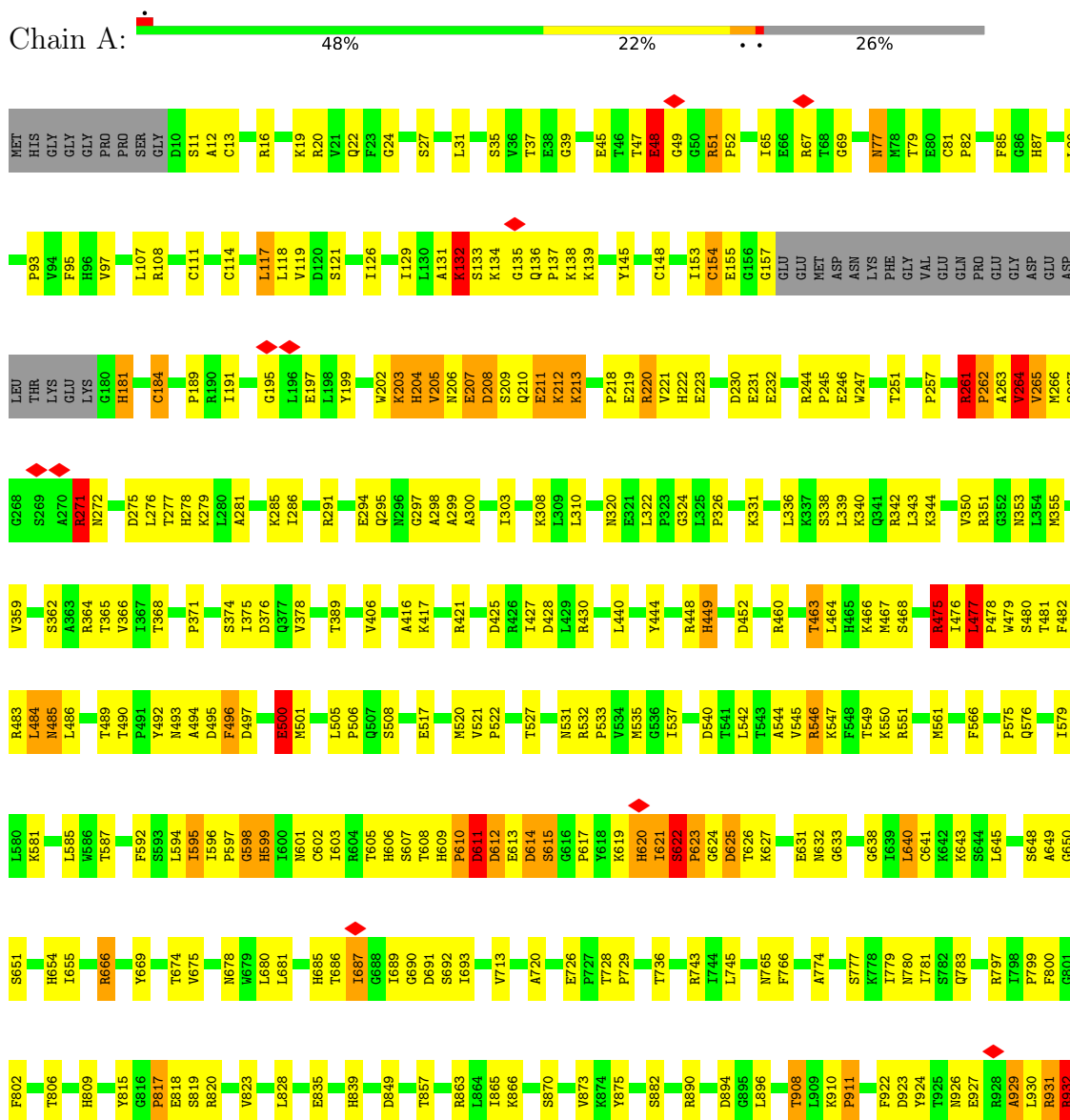
Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Zn	0
			2	2	
31	B	2	Total	Zn	0
			2	2	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	
31	Q	1	Total	Zn	0
			1	1	
31	U	1	Total	Zn	0
			1	1	



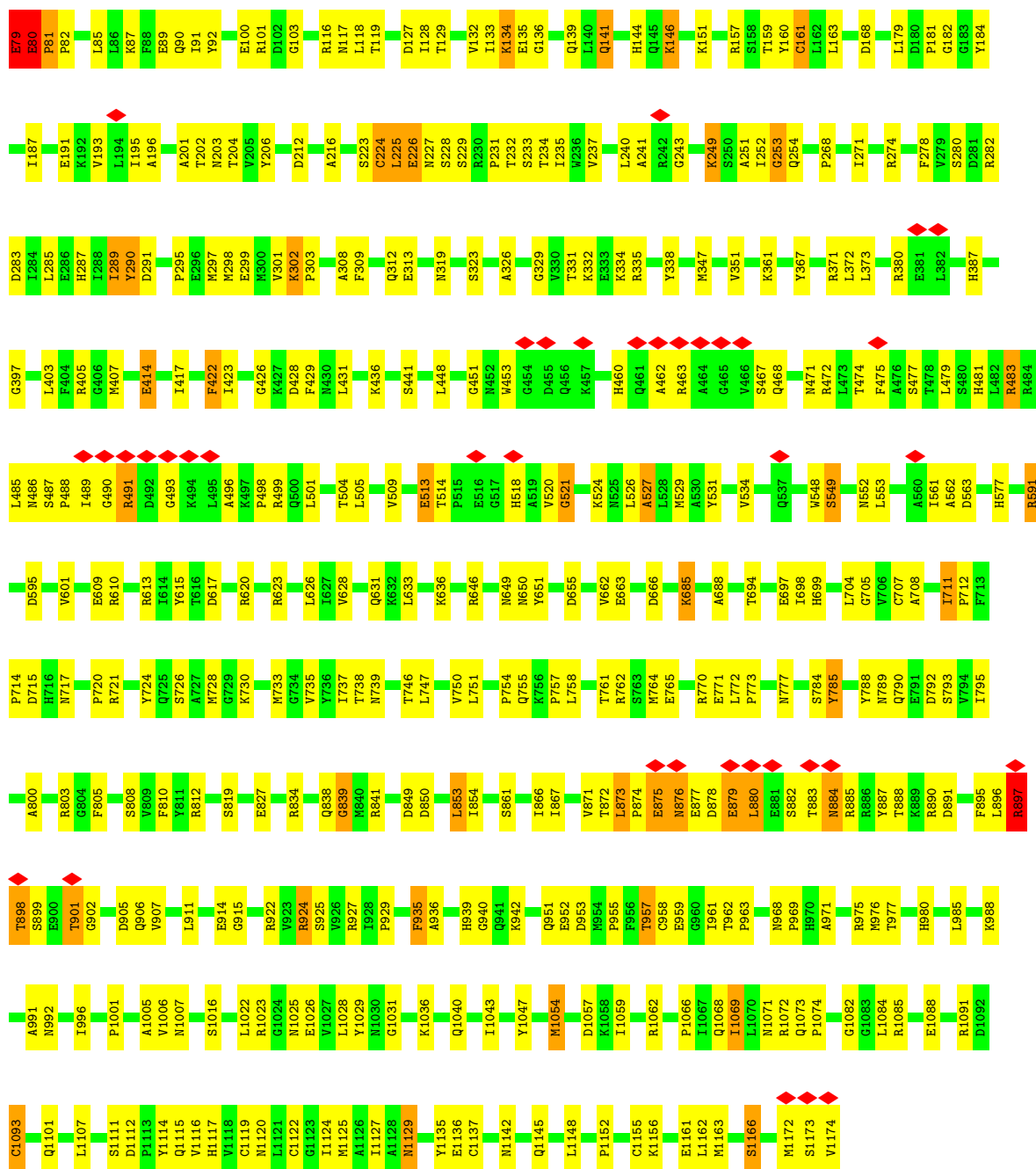
### 3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

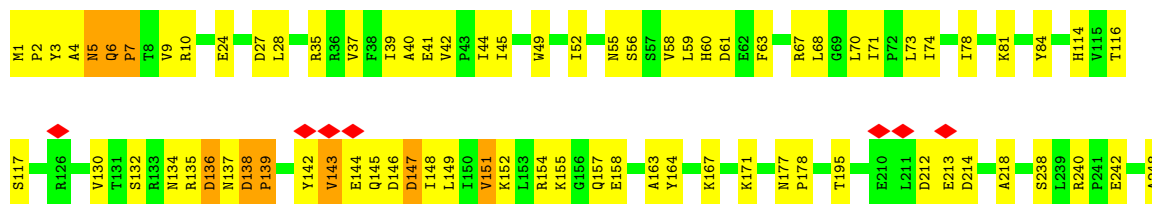






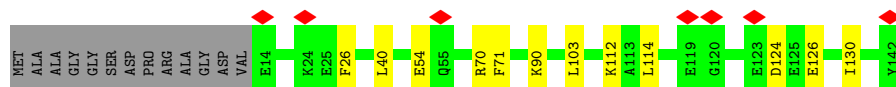
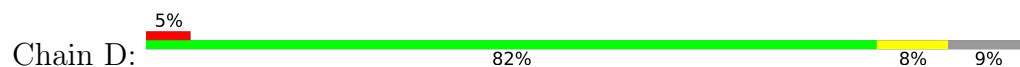
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 69% 28%





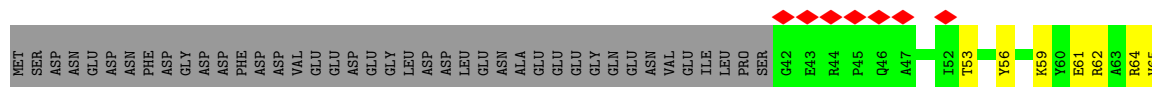
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



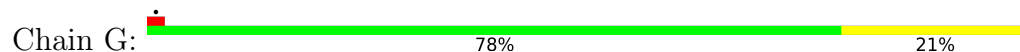
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5



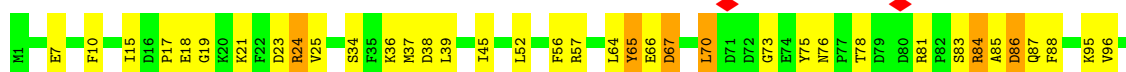
- Molecule 6: DNA-directed RNA polymerase II subunit RPB6



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

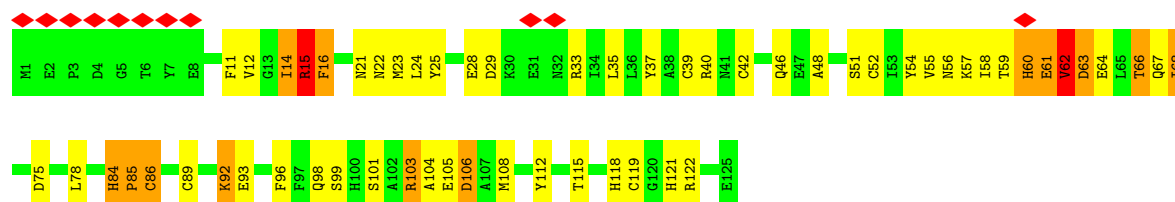


- Molecule 8: DNA-directed RNA polymerase II subunit RPB8

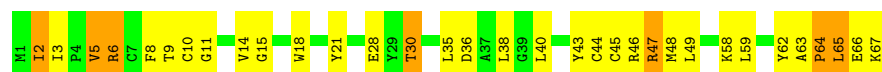




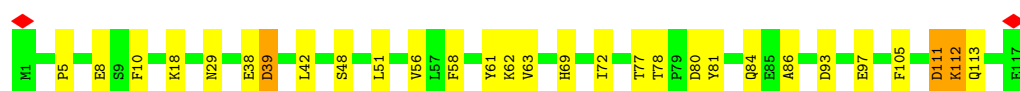
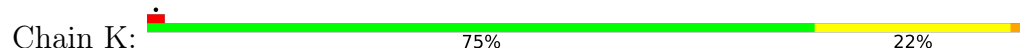
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



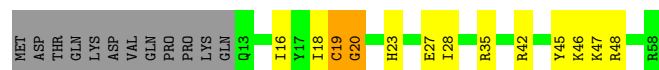
- Molecule 10: DNA-directed RNA polymerase II subunit RPB10



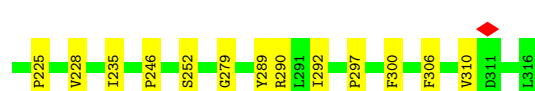
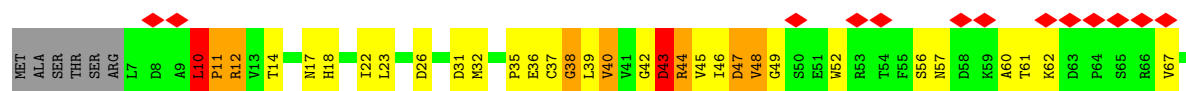
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



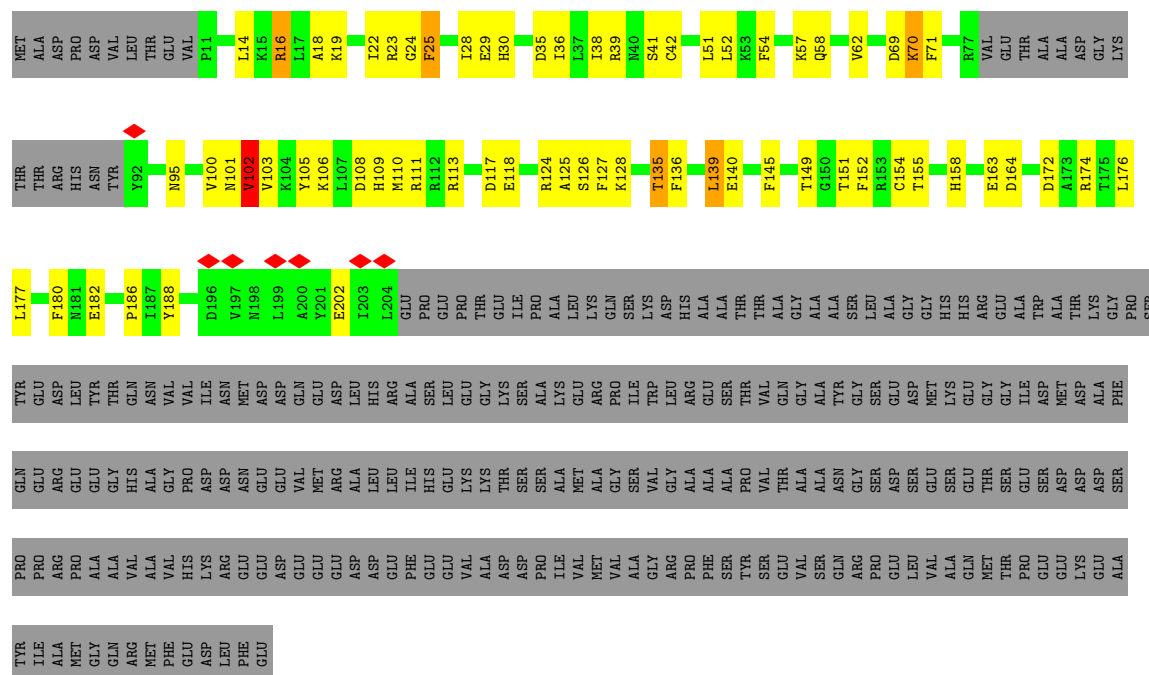
- Molecule 12: DNA-directed RNA polymerase II subunit RPB12



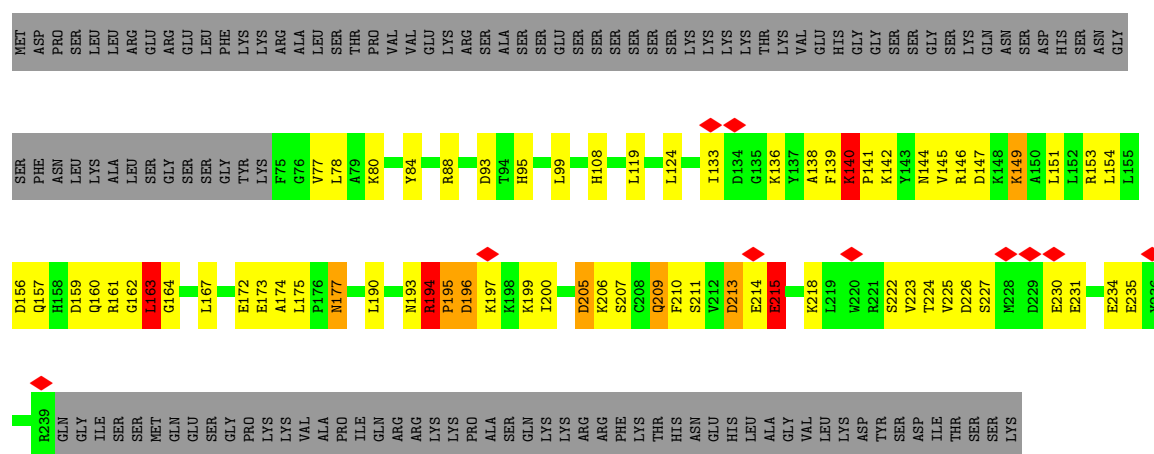
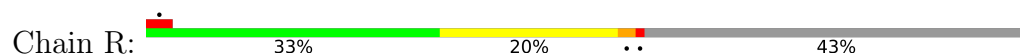
- Molecule 13: Transcription initiation factor IIB



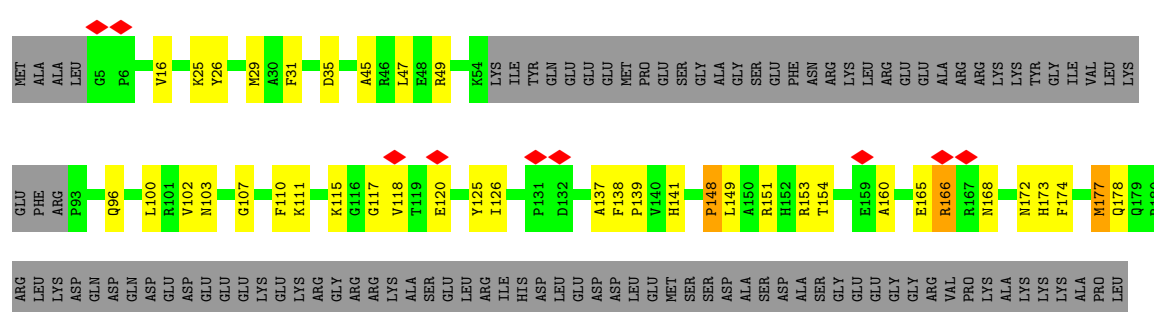


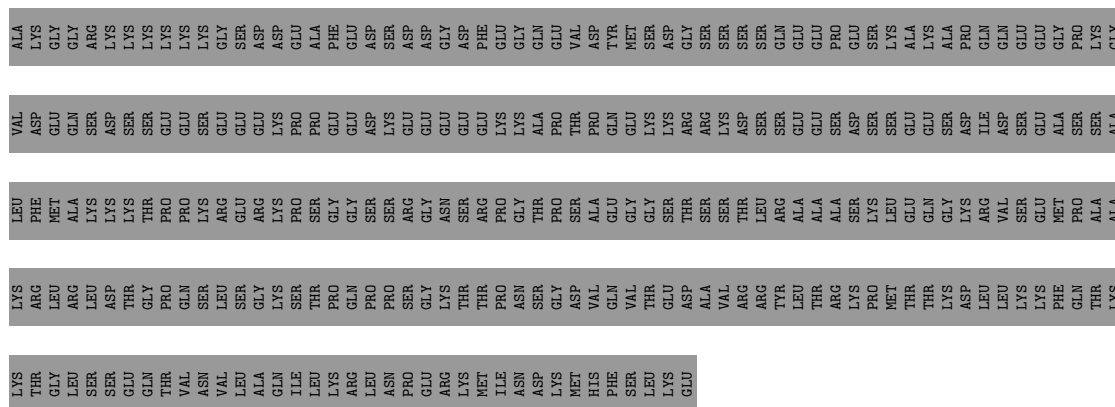


• Molecule 18: Transcription initiation factor IIE subunit beta

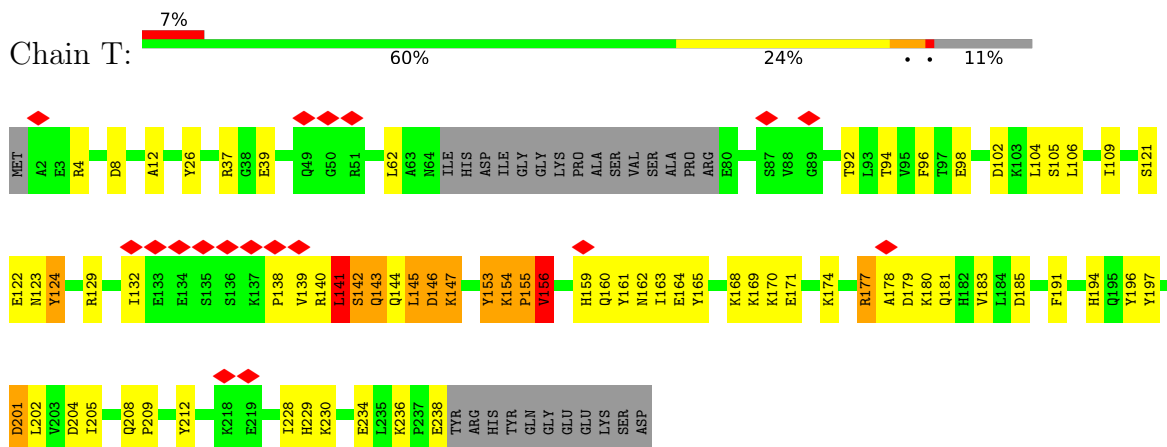


• Molecule 19: General transcription factor IIF subunit 1

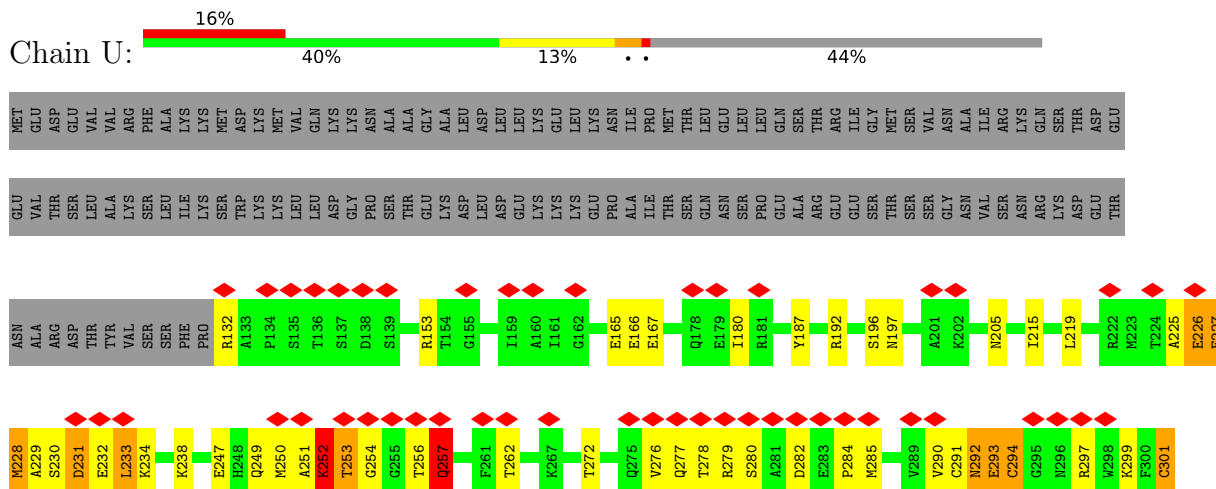




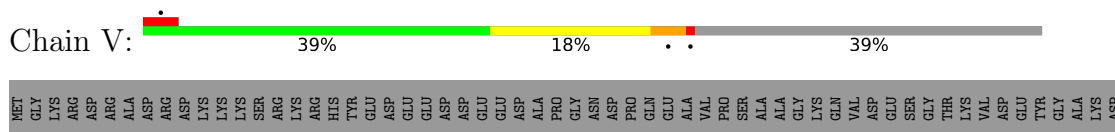
- Molecule 20: General transcription factor IIF subunit 2



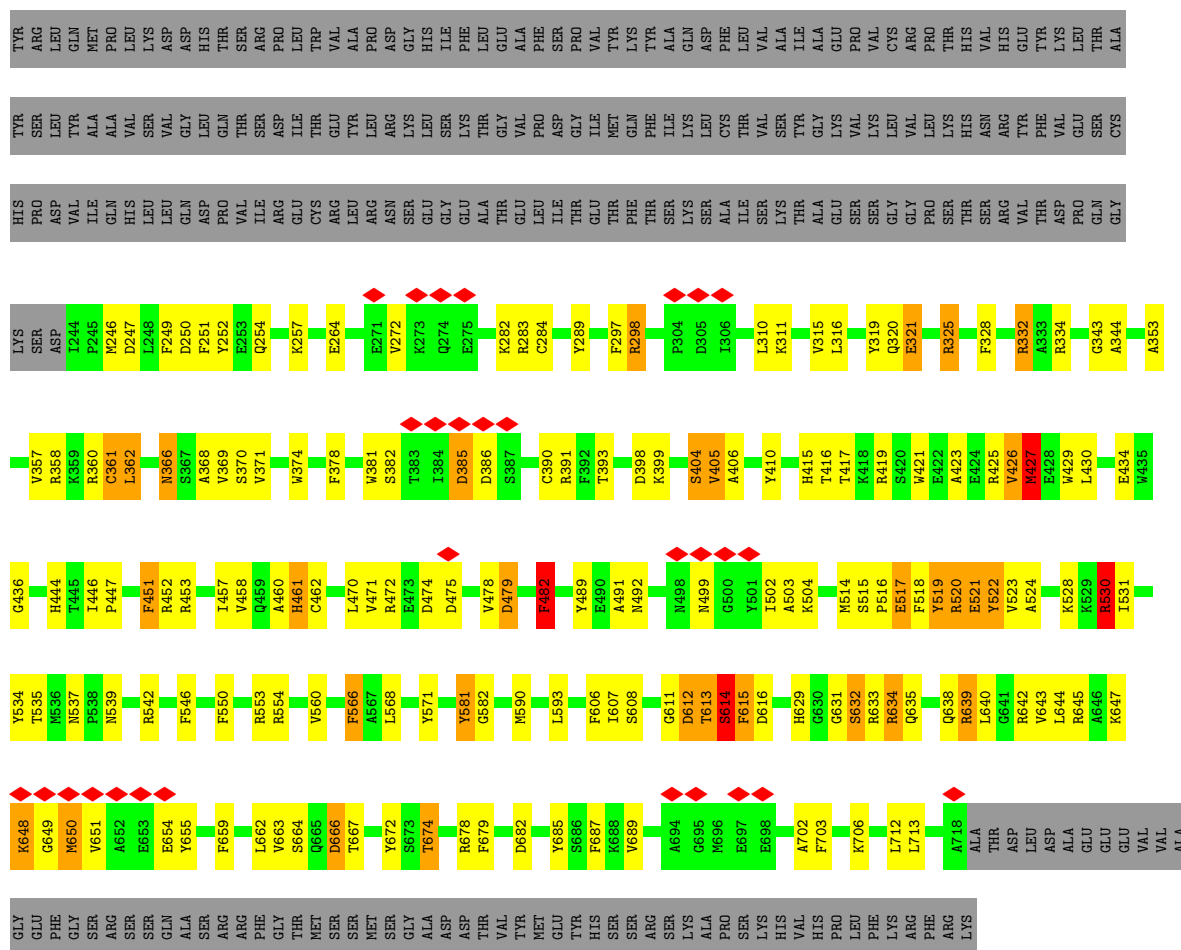
- Molecule 21: Transcription elongation factor TFIIS



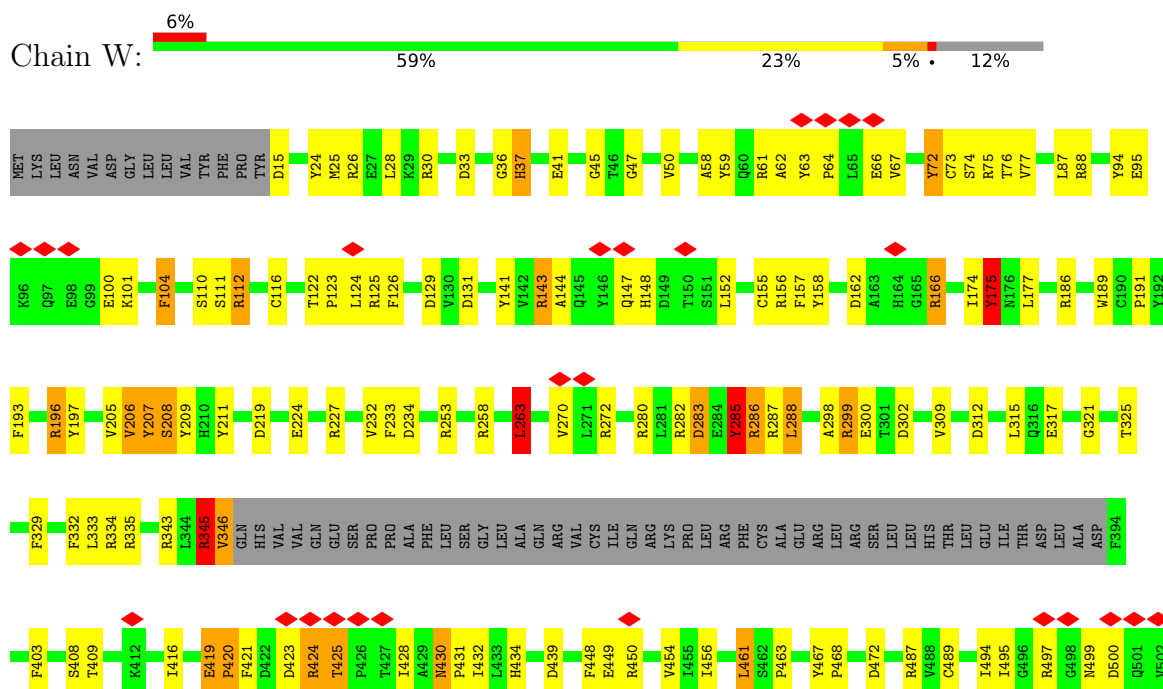
● Molecule 22: TFIIF basal transcription factor complex helicase XPB subunit



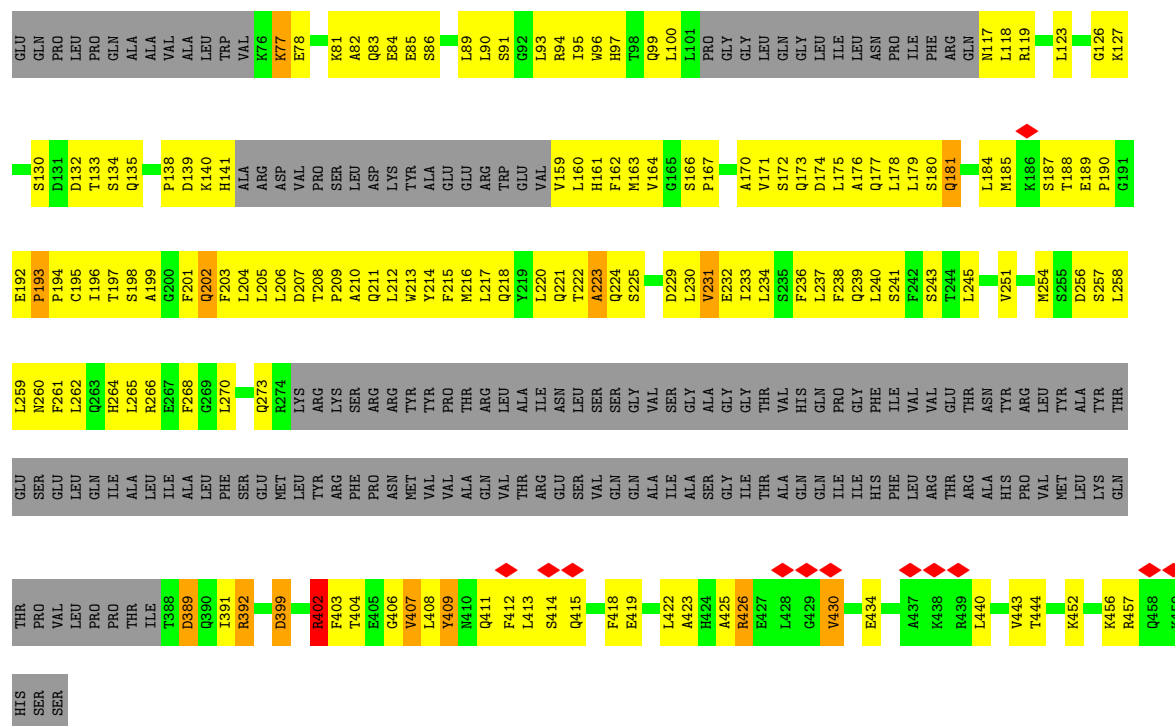




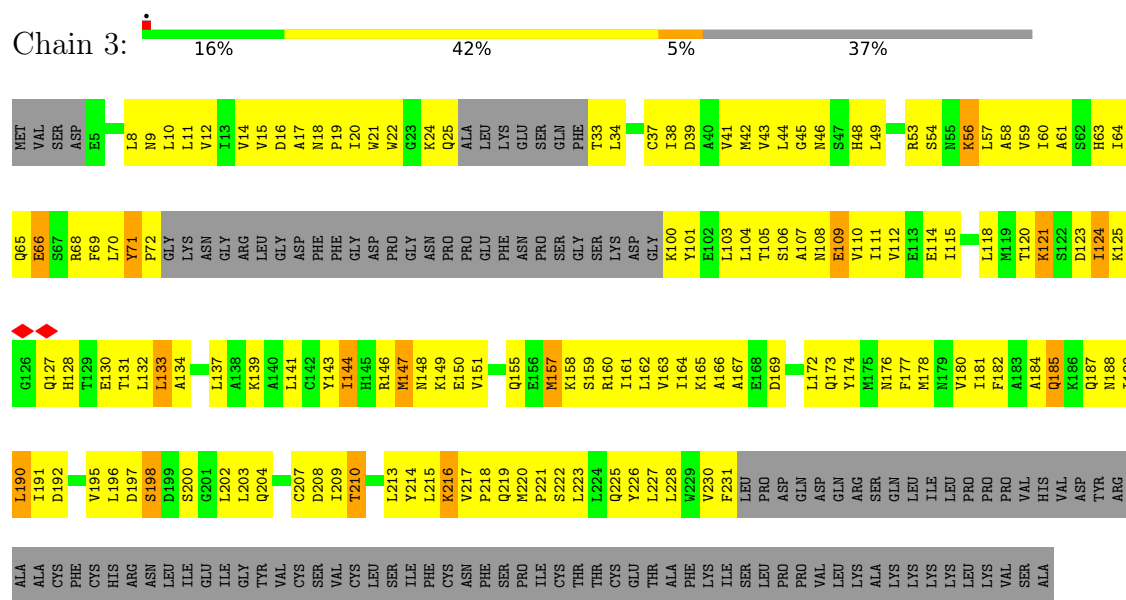
• Molecule 23: TFIID basal transcription factor complex helicase XPD subunit



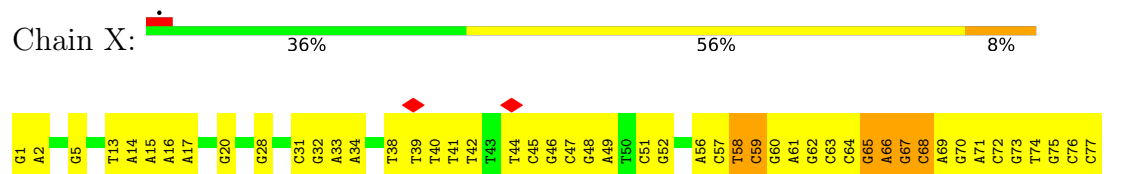




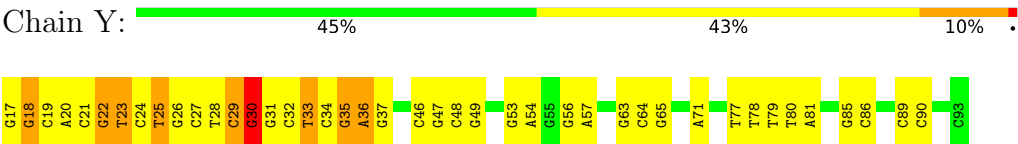
• Molecule 27: General transcription factor IIH subunit 3



• Molecule 28: SCP-X



• Molecule 29: SCP-Y



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59271	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 ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	503.03998, 503.03998, 503.03998	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.62, 2.62, 2.62	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.48	2/11727 (0.0%)	0.78	17/15833 (0.1%)
2	B	0.56	1/9503 (0.0%)	0.82	7/12831 (0.1%)
3	C	0.49	0/2259	0.93	5/3073 (0.2%)
4	D	0.26	0/1077	0.47	0/1446
5	E	0.39	0/1753	0.77	5/2368 (0.2%)
6	F	0.43	0/700	0.67	0/946
7	G	0.27	0/1382	0.55	0/1874
8	H	0.35	0/1227	0.66	0/1654
9	I	0.34	0/1038	0.99	3/1407 (0.2%)
10	J	0.55	0/542	0.89	0/730
11	K	0.39	0/956	0.63	0/1294
12	L	0.45	0/394	0.61	0/524
13	M	0.33	0/2429	0.66	3/3281 (0.1%)
14	N	0.26	0/945	0.59	1/1274 (0.1%)
15	O	0.24	0/816	0.48	0/1105
16	P	0.26	0/1489	0.75	1/2005 (0.0%)
17	Q	0.27	0/1507	0.63	1/2023 (0.0%)
18	R	0.45	0/1380	0.93	2/1854 (0.1%)
19	S	0.26	0/1167	0.51	0/1576
20	T	0.32	0/1817	0.67	2/2445 (0.1%)
21	U	0.32	0/1358	0.63	2/1820 (0.1%)
22	V	1.41	12/3931 (0.3%)	1.89	98/5298 (1.8%)
23	W	1.53	22/5460 (0.4%)	2.02	161/7390 (2.2%)
24	O	1.49	5/1506 (0.3%)	1.95	44/2038 (2.2%)
25	1	0.83	0/496	1.15	1/669 (0.1%)
26	2	0.88	0/2243	1.18	9/3024 (0.3%)
27	3	0.84	0/1548	1.13	2/2090 (0.1%)
28	X	1.16	17/1788 (1.0%)	1.45	39/2762 (1.4%)
29	Y	1.17	21/1746 (1.2%)	1.48	41/2690 (1.5%)
All	All	0.79	80/64184 (0.1%)	1.13	444/87324 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
5	E	0	1
8	H	0	1
14	N	0	3
18	R	0	6
19	S	0	1
20	T	0	1
22	V	0	8
23	W	0	14
24	O	0	1
25	1	0	1
26	2	0	8
28	X	0	2
29	Y	0	3
All	All	0	52

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X	65	DG	P-O5'	-9.90	1.49	1.59
29	Y	35	DG	C5'-C4'	9.12	1.61	1.51
28	X	73	DG	C5'-C4'	8.56	1.60	1.51
28	X	63	DC	C4'-C3'	8.47	1.61	1.53
29	Y	21	DC	C4'-C3'	8.12	1.61	1.53
23	W	158	TYR	CE1-CZ	8.00	1.49	1.38
29	Y	35	DG	P-O5'	8.00	1.67	1.59
29	Y	26	DG	P-O5'	7.97	1.67	1.59
29	Y	24	DC	O4'-C1'	-7.89	1.32	1.42
22	V	672	TYR	CE1-CZ	7.82	1.48	1.38
28	X	71	DA	C5'-C4'	7.79	1.59	1.51
28	X	56	DA	O3'-P	-7.46	1.52	1.61
28	X	75	DG	C5'-C4'	7.25	1.59	1.51
23	W	104	PHE	CG-CD1	7.18	1.49	1.38
29	Y	23	DT	P-O5'	-7.04	1.52	1.59
22	V	391	ARG	CZ-NH2	-6.97	1.24	1.33
29	Y	20	DA	C2'-C1'	6.84	1.59	1.52
28	X	74	DT	C4'-C3'	6.81	1.60	1.53
23	W	110	SER	CA-CB	6.76	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X	69	DA	C5'-C4'	6.65	1.58	1.51
1	A	500	GLU	CG-CD	6.64	1.61	1.51
22	V	325	ARG	CZ-NH1	-6.63	1.24	1.33
22	V	633	ARG	CZ-NH1	-6.60	1.24	1.33
29	Y	35	DG	C4'-C3'	6.56	1.59	1.53
29	Y	18	DG	C4'-O4'	-6.56	1.38	1.45
28	X	66	DA	C1'-N9	6.45	1.57	1.49
23	W	521	GLY	N-CA	6.44	1.55	1.46
24	O	122	GLY	N-CA	6.43	1.55	1.46
23	W	208	SER	CB-OG	-6.43	1.33	1.42
29	Y	36	DA	P-O5'	6.40	1.66	1.59
1	A	475	ARG	CG-CD	6.37	1.67	1.51
29	Y	35	DG	N7-C5	6.36	1.43	1.39
22	V	606	PHE	CG-CD1	6.30	1.48	1.38
28	X	65	DG	C3'-C2'	6.30	1.59	1.52
22	V	554	ARG	NE-CZ	6.26	1.41	1.33
29	Y	23	DT	O4'-C1'	-6.25	1.34	1.42
23	W	683	ARG	CZ-NH2	-6.24	1.25	1.33
28	X	69	DA	C4'-O4'	-6.22	1.38	1.45
22	V	453	ARG	CZ-NH2	-6.04	1.25	1.33
28	X	66	DA	C2'-C1'	5.99	1.58	1.52
29	Y	24	DC	C5'-C4'	5.98	1.57	1.51
28	X	65	DG	C4'-O4'	-5.96	1.39	1.45
29	Y	34	DC	P-O5'	5.94	1.65	1.59
28	X	75	DG	P-O5'	5.92	1.65	1.59
29	Y	34	DC	C5'-C4'	5.92	1.57	1.51
23	W	321	GLY	N-CA	5.78	1.54	1.46
28	X	77	DC	P-O5'	5.76	1.65	1.59
29	Y	24	DC	C4'-O4'	-5.72	1.39	1.45
29	Y	28	DT	C1'-N1	5.71	1.56	1.49
24	O	195	ARG	CZ-NH1	-5.69	1.25	1.33
23	W	286	ARG	CZ-NH1	-5.69	1.25	1.33
22	V	252	TYR	CE1-CZ	5.67	1.46	1.38
29	Y	24	DC	C1'-N1	5.64	1.56	1.49
23	W	47	GLY	N-CA	5.59	1.54	1.46
28	X	70	DG	O3'-P	5.44	1.67	1.61
23	W	334	ARG	CZ-NH2	-5.42	1.26	1.33
22	V	332	ARG	CZ-NH2	-5.41	1.26	1.33
23	W	610	PHE	CG-CD1	5.40	1.46	1.38
23	W	448	PHE	CE1-CZ	5.38	1.47	1.37
28	X	75	DG	C1'-N9	-5.36	1.39	1.47
23	W	674	TYR	CE1-CZ	5.35	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	606	GLU	CA-CB	5.33	1.65	1.53
23	W	286	ARG	CZ-NH2	-5.33	1.26	1.33
29	Y	35	DG	O3'-P	5.28	1.67	1.61
23	W	253	ARG	CZ-NH1	-5.27	1.26	1.33
22	V	659	PHE	CG-CD2	5.25	1.46	1.38
2	B	1093	CYS	CB-SG	-5.25	1.73	1.81
23	W	24	TYR	CE2-CZ	5.24	1.45	1.38
22	V	452	ARG	CZ-NH2	-5.22	1.26	1.33
29	Y	36	DA	C5'-C4'	5.20	1.57	1.51
24	O	112	LYS	N-CA	5.14	1.56	1.46
24	O	95	TYR	CG-CD1	5.13	1.45	1.39
23	W	345	ARG	CZ-NH1	-5.11	1.26	1.33
23	W	639	TYR	CZ-OH	-5.11	1.29	1.37
24	O	146	TYR	CD2-CE2	5.11	1.47	1.39
23	W	511	ARG	NE-CZ	-5.09	1.26	1.33
29	Y	18	DG	C5'-C4'	5.07	1.56	1.51
23	W	74	SER	CA-CB	-5.07	1.45	1.52
22	V	451	PHE	CG-CD2	5.04	1.46	1.38
23	W	520	TYR	CZ-OH	-5.03	1.29	1.37

All (444) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	84	HIS	C-N-CD	-25.39	64.75	120.60
3	C	6	GLN	C-N-CD	-24.88	65.87	120.60
2	B	80	GLU	C-N-CD	-22.45	71.22	120.60
16	P	206	GLU	C-N-CD	-22.24	71.67	120.60
18	R	194	ARG	C-N-CD	-22.19	71.78	120.60
1	A	261	ARG	C-N-CD	-21.71	72.84	120.60
24	O	77	LYS	C-N-CD	-21.64	72.99	120.60
27	3	71	TYR	C-N-CD	-20.76	74.94	120.60
3	C	138	ASP	C-N-CD	-20.36	75.81	120.60
23	W	335	ARG	NE-CZ-NH1	-19.54	110.53	120.30
29	Y	20	DA	O4'-C1'-N9	19.29	121.50	108.00
23	W	26	ARG	NE-CZ-NH2	18.69	129.64	120.30
22	V	358	ARG	NE-CZ-NH2	17.80	129.20	120.30
28	X	77	DC	O4'-C1'-N1	17.49	120.24	108.00
24	O	195	ARG	NE-CZ-NH1	17.02	128.81	120.30
23	W	186	ARG	NE-CZ-NH1	16.15	128.38	120.30
23	W	497	ARG	NE-CZ-NH1	15.91	128.25	120.30
23	W	287	ARG	NE-CZ-NH2	15.65	128.12	120.30
22	V	634	ARG	NE-CZ-NH2	14.88	127.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	0	206	ARG	NE-CZ-NH1	14.77	127.68	120.30
1	A	475	ARG	NE-CZ-NH1	-14.65	112.97	120.30
23	W	592	ARG	NE-CZ-NH1	14.29	127.44	120.30
23	W	335	ARG	NE-CZ-NH2	14.21	127.41	120.30
13	M	10	LEU	C-N-CD	-13.97	89.86	120.60
5	E	52	ARG	C-N-CD	-13.95	89.90	120.60
23	W	272	ARG	NE-CZ-NH1	13.91	127.26	120.30
23	W	112	ARG	NE-CZ-NH1	13.91	127.25	120.30
22	V	332	ARG	NE-CZ-NH1	13.88	127.24	120.30
23	W	669	ARG	NE-CZ-NH1	13.79	127.19	120.30
23	W	75	ARG	NE-CZ-NH1	13.27	126.93	120.30
29	Y	21	DC	O4'-C1'-N1	13.21	117.25	108.00
23	W	343	ARG	NE-CZ-NH2	13.03	126.81	120.30
22	V	633	ARG	NE-CZ-NH2	-12.84	113.88	120.30
29	Y	30	DG	O4'-C1'-N9	12.59	116.82	108.00
23	W	467	TYR	CB-CG-CD1	-12.38	113.57	121.00
23	W	627	TYR	CB-CG-CD2	-12.18	113.69	121.00
23	W	601	ARG	NE-CZ-NH2	-11.93	114.33	120.30
23	W	631	ARG	NE-CZ-NH1	11.90	126.25	120.30
22	V	452	ARG	NE-CZ-NH1	11.86	126.23	120.30
23	W	26	ARG	NH1-CZ-NH2	-11.66	106.58	119.40
23	W	636	ARG	NE-CZ-NH1	11.62	126.11	120.30
23	W	487	ARG	NE-CZ-NH1	11.49	126.05	120.30
22	V	283	ARG	NE-CZ-NH2	-11.47	114.56	120.30
23	W	343	ARG	NE-CZ-NH1	-11.31	114.65	120.30
23	W	88	ARG	NE-CZ-NH1	11.26	125.93	120.30
23	W	647	ARG	NE-CZ-NH1	11.16	125.88	120.30
23	W	419	GLU	C-N-CD	-11.12	96.14	120.60
23	W	683	ARG	NE-CZ-NH2	10.88	125.74	120.30
28	X	73	DG	O4'-C4'-C3'	10.74	112.44	106.00
23	W	690	ARG	NE-CZ-NH2	10.71	125.66	120.30
28	X	69	DA	O4'-C1'-N9	10.61	115.43	108.00
29	Y	34	DC	C2-N1-C1'	-10.34	107.42	118.80
23	W	88	ARG	NE-CZ-NH2	-10.25	115.18	120.30
22	V	391	ARG	NE-CZ-NH1	-10.17	115.21	120.30
22	V	427	MET	N-CA-C	10.06	138.18	111.00
22	V	687	PHE	CB-CG-CD2	-10.01	113.79	120.80
22	V	452	ARG	NE-CZ-NH2	-10.00	115.30	120.30
28	X	56	DA	O3'-P-O5'	-9.85	85.29	104.00
23	W	497	ARG	NE-CZ-NH2	-9.84	115.38	120.30
22	V	553	ARG	NE-CZ-NH2	9.82	125.21	120.30
22	V	283	ARG	NE-CZ-NH1	9.74	125.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	X	67	DG	O4'-C1'-C2'	9.67	113.63	105.90
24	O	59	ARG	NE-CZ-NH2	9.62	125.11	120.30
29	Y	17	DG	O4'-C1'-N9	9.56	114.69	108.00
22	V	520	ARG	CA-C-N	-9.55	96.20	117.20
29	Y	34	DC	C6-N1-C1'	9.54	132.25	120.80
22	V	334	ARG	CD-NE-CZ	9.49	136.88	123.60
23	W	658	ARG	NE-CZ-NH2	-9.44	115.58	120.30
29	Y	27	DC	O4'-C4'-C3'	9.35	111.61	106.00
23	W	227	ARG	NE-CZ-NH1	9.32	124.96	120.30
23	W	627	TYR	CG-CD2-CE2	-9.22	113.92	121.30
23	W	511	ARG	NE-CZ-NH2	9.19	124.90	120.30
22	V	645	ARG	NE-CZ-NH1	9.18	124.89	120.30
23	W	686	ARG	NE-CZ-NH1	9.18	124.89	120.30
22	V	264	GLU	OE1-CD-OE2	-9.12	112.35	123.30
23	W	666	ARG	NE-CZ-NH1	9.12	124.86	120.30
24	O	219	TYR	CB-CG-CD1	-9.12	115.53	121.00
23	W	286	ARG	NE-CZ-NH2	9.02	124.81	120.30
23	W	703	ASP	CB-CG-OD2	9.02	126.41	118.30
24	O	206	ARG	NH1-CZ-NH2	-8.85	109.66	119.40
22	V	550	PHE	CB-CG-CD1	-8.77	114.66	120.80
29	Y	27	DC	C2-N1-C1'	-8.76	109.17	118.80
1	A	666	ARG	CG-CD-NE	8.75	130.17	111.80
3	C	35	ARG	NE-CZ-NH1	8.72	124.66	120.30
28	X	73	DG	O4'-C1'-N9	8.72	114.10	108.00
28	X	64	DC	O4'-C1'-N1	8.62	114.03	108.00
29	Y	23	DT	O4'-C1'-N1	-8.61	101.98	108.00
28	X	73	DG	C4'-C3'-C2'	-8.49	95.46	103.10
22	V	581	TYR	CG-CD1-CE1	-8.47	114.53	121.30
23	W	654	PHE	CB-CG-CD2	-8.46	114.88	120.80
23	W	450	ARG	NE-CZ-NH1	8.45	124.53	120.30
22	V	419	ARG	NE-CZ-NH1	8.39	124.50	120.30
28	X	73	DG	C1'-O4'-C4'	-8.36	101.74	110.10
29	Y	27	DC	C1'-O4'-C4'	-8.31	101.79	110.10
24	O	213	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	475	ARG	CD-NE-CZ	8.27	135.18	123.60
22	V	520	ARG	C-N-CA	-8.24	101.10	121.70
23	W	497	ARG	CD-NE-CZ	8.22	135.11	123.60
23	W	332	PHE	CB-CG-CD2	-8.21	115.05	120.80
28	X	58	DT	C6-C5-C7	-8.20	117.98	122.90
22	V	685	TYR	CB-CG-CD2	8.19	125.91	121.00
22	V	634	ARG	NE-CZ-NH1	-8.17	116.21	120.30
29	Y	35	DG	C5'-C4'-C3'	8.17	128.81	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	29	DC	O4'-C1'-N1	-8.14	102.30	108.00
22	V	520	ARG	NE-CZ-NH2	8.10	124.35	120.30
29	Y	27	DC	C6-N1-C1'	8.06	130.48	120.80
29	Y	36	DA	C5-C6-N1	8.05	121.73	117.70
29	Y	35	DG	O5'-C5'-C4'	8.05	131.13	111.00
29	Y	35	DG	N3-C2-N2	-7.93	114.35	119.90
22	V	386	ASP	CB-CG-OD2	-7.92	111.17	118.30
29	Y	35	DG	O4'-C4'-C3'	-7.92	101.25	106.00
22	V	358	ARG	NH1-CZ-NH2	-7.92	110.69	119.40
5	E	64	HIS	N-CA-C	7.92	132.38	111.00
22	V	410	TYR	CB-CG-CD1	-7.91	116.25	121.00
22	V	520	ARG	O-C-N	7.89	135.33	122.70
23	W	601	ARG	NE-CZ-NH1	7.85	124.23	120.30
29	Y	26	DG	O4'-C4'-C3'	-7.83	101.30	106.00
23	W	75	ARG	NE-CZ-NH2	-7.80	116.40	120.30
29	Y	34	DC	O3'-P-O5'	7.78	118.78	104.00
23	W	125	ARG	NE-CZ-NH1	7.77	124.19	120.30
28	X	60	DG	O4'-C1'-C2'	-7.77	99.68	105.90
29	Y	27	DC	O4'-C1'-C2'	7.76	112.11	105.90
23	W	467	TYR	CB-CG-CD2	7.73	125.64	121.00
29	Y	24	DC	O4'-C4'-C3'	7.71	110.63	106.00
23	W	644	PHE	CB-CG-CD1	7.71	126.19	120.80
23	W	126	PHE	CB-CG-CD2	7.70	126.19	120.80
1	A	475	ARG	CG-CD-NE	-7.69	95.66	111.80
23	W	448	PHE	CB-CG-CD2	7.67	126.17	120.80
23	W	582	GLU	OE1-CD-OE2	-7.66	114.11	123.30
23	W	143	ARG	NE-CZ-NH1	7.65	124.12	120.30
23	W	232	VAL	CA-CB-CG1	7.62	122.33	110.90
22	V	542	ARG	NE-CZ-NH2	7.59	124.09	120.30
24	0	90	TYR	CB-CG-CD2	-7.58	116.45	121.00
23	W	520	TYR	CG-CD1-CE1	-7.55	115.26	121.30
22	V	474	ASP	CB-CG-OD2	7.54	125.08	118.30
28	X	60	DG	O4'-C1'-N9	7.53	113.27	108.00
29	Y	24	DC	C4'-C3'-C2'	-7.52	96.33	103.10
23	W	193	PHE	CB-CG-CD1	-7.51	115.55	120.80
26	2	402	ARG	NE-CZ-NH1	7.50	124.05	120.30
23	W	272	ARG	NH1-CZ-NH2	-7.43	111.23	119.40
24	0	73	ASP	CB-CG-OD2	-7.42	111.62	118.30
22	V	522	TYR	CB-CG-CD2	-7.38	116.57	121.00
24	0	95	TYR	CB-CG-CD1	-7.38	116.57	121.00
23	W	592	ARG	NH1-CZ-NH2	-7.37	111.29	119.40
22	V	249	PHE	CB-CG-CD2	7.36	125.95	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	685	TYR	CB-CG-CD1	-7.35	116.59	121.00
13	M	43	ASP	N-CA-C	-7.31	91.26	111.00
28	X	59	DC	O4'-C4'-C3'	7.29	110.37	106.00
24	0	236	VAL	CA-CB-CG1	7.25	121.78	110.90
22	V	554	ARG	NE-CZ-NH1	7.25	123.92	120.30
29	Y	21	DC	O4'-C1'-C2'	-7.21	100.13	105.90
23	W	186	ARG	NE-CZ-NH2	-7.17	116.72	120.30
29	Y	36	DA	N1-C6-N6	-7.12	114.33	118.60
22	V	639	ARG	NE-CZ-NH2	7.08	123.84	120.30
28	X	63	DC	C2-N1-C1'	-7.07	111.03	118.80
24	0	89	GLU	OE1-CD-OE2	-7.06	114.83	123.30
23	W	317	GLU	OE1-CD-OE2	-7.05	114.84	123.30
21	U	257	GLN	C-N-CA	-7.03	104.13	121.70
23	W	166	ARG	CD-NE-CZ	7.02	133.43	123.60
28	X	57	DC	N3-C2-O2	-7.01	116.99	121.90
28	X	73	DG	P-O3'-C3'	6.97	128.07	119.70
23	W	627	TYR	CD1-CG-CD2	6.97	125.57	117.90
22	V	643	VAL	CA-CB-CG1	6.92	121.28	110.90
13	M	94	ASP	N-CA-C	-6.91	92.34	111.00
23	W	332	PHE	CB-CG-CD1	6.91	125.63	120.80
24	0	136	ASP	CB-CG-OD1	6.90	124.51	118.30
23	W	280	ARG	NE-CZ-NH1	-6.89	116.86	120.30
23	W	219	ASP	CB-CG-OD1	6.87	124.48	118.30
22	V	385	ASP	CB-CG-OD1	-6.86	112.13	118.30
24	0	195	ARG	NE-CZ-NH2	-6.85	116.87	120.30
26	2	35	TYR	CA-CB-CG	-6.82	100.45	113.40
29	Y	33	DT	O4'-C1'-N1	6.81	112.76	108.00
24	0	95	TYR	CD1-CE1-CZ	-6.78	113.70	119.80
23	W	345	ARG	CD-NE-CZ	6.78	133.09	123.60
23	W	644	PHE	CB-CG-CD2	-6.77	116.06	120.80
22	V	581	TYR	CD1-CE1-CZ	6.77	125.89	119.80
23	W	125	ARG	CD-NE-CZ	6.75	133.06	123.60
28	X	75	DG	C8-N9-C1'	6.75	135.78	127.00
22	V	530	ARG	NE-CZ-NH2	-6.75	116.93	120.30
23	W	654	PHE	CB-CG-CD1	6.74	125.52	120.80
23	W	566	LEU	CB-CG-CD1	6.72	122.43	111.00
22	V	655	TYR	CB-CG-CD2	-6.72	116.97	121.00
23	W	253	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	B	141	GLN	N-CA-C	-6.70	92.91	111.00
22	V	334	ARG	NE-CZ-NH1	6.70	123.65	120.30
23	W	616	ARG	NE-CZ-NH1	-6.70	116.95	120.30
23	W	26	ARG	NE-CZ-NH1	6.70	123.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	196	ARG	NE-CZ-NH1	6.70	123.65	120.30
28	X	67	DG	O4'-C1'-N9	6.70	112.69	108.00
23	W	50	VAL	CA-CB-CG1	6.70	120.94	110.90
28	X	75	DG	C4-N9-C1'	-6.69	117.80	126.50
26	2	61	PHE	CB-CA-C	-6.68	97.04	110.40
23	W	674	TYR	CB-CG-CD1	6.65	124.99	121.00
23	W	125	ARG	NE-CZ-NH2	-6.61	116.99	120.30
23	W	30	ARG	CD-NE-CZ	6.59	132.82	123.60
1	A	1311	LEU	CA-CB-CG	-6.58	100.16	115.30
24	0	219	TYR	CG-CD1-CE1	-6.54	116.07	121.30
29	Y	34	DC	C3'-C2'-C1'	-6.53	94.67	102.50
23	W	302	ASP	CB-CG-OD1	6.52	124.17	118.30
28	X	63	DC	C6-N1-C1'	6.50	128.60	120.80
23	W	487	ARG	NH1-CZ-NH2	-6.50	112.25	119.40
14	N	356	GLY	N-CA-C	6.50	129.34	113.10
23	W	76	THR	CA-CB-OG1	6.49	122.64	109.00
23	W	315	LEU	CB-CG-CD1	6.49	122.03	111.00
26	2	193	PRO	CA-N-CD	-6.48	102.43	111.50
22	V	404	SER	CB-CA-C	6.47	122.39	110.10
29	Y	35	DG	P-O3'-C3'	6.46	127.45	119.70
29	Y	26	DG	O4'-C1'-C2'	-6.44	100.75	105.90
22	V	298	ARG	NE-CZ-NH1	6.44	123.52	120.30
22	V	682	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	477	LEU	CB-CG-CD1	6.40	121.87	111.00
1	A	484	LEU	CB-CG-CD1	6.38	121.85	111.00
23	W	669	ARG	NH1-CZ-NH2	-6.37	112.39	119.40
23	W	722	ARG	CD-NE-CZ	6.37	132.51	123.60
28	X	59	DC	P-O3'-C3'	6.37	127.34	119.70
23	W	683	ARG	CD-NE-CZ	6.37	132.51	123.60
29	Y	28	DT	C4'-C3'-C2'	-6.36	97.37	103.10
28	X	77	DC	C4'-C3'-C2'	-6.35	97.38	103.10
23	W	641	ARG	NE-CZ-NH1	6.35	123.47	120.30
24	0	113	ARG	NE-CZ-NH1	6.35	123.47	120.30
23	W	639	TYR	CB-CG-CD2	-6.34	117.19	121.00
23	W	189	TRP	NE1-CE2-CD2	-6.34	100.96	107.30
22	V	332	ARG	NH1-CZ-NH2	-6.33	112.43	119.40
23	W	263	LEU	N-CA-CB	-6.33	97.74	110.40
9	I	15	ARG	N-CA-C	-6.33	93.92	111.00
20	T	234	GLU	CG-CD-OE2	-6.32	105.66	118.30
23	W	131	ASP	CB-CG-OD1	-6.31	112.62	118.30
24	0	59	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
22	V	521	GLU	OE1-CD-OE2	-6.31	115.73	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	36	DA	C4-C5-C6	-6.30	113.85	117.00
22	V	369	VAL	CA-CB-CG1	6.28	120.31	110.90
23	W	30	ARG	NE-CZ-NH1	6.25	123.42	120.30
22	V	344	ALA	N-CA-CB	-6.24	101.36	110.10
23	W	175	TYR	N-CA-C	6.21	127.78	111.00
23	W	206	VAL	CA-CB-CG1	6.19	120.18	110.90
1	A	1311	LEU	CB-CG-CD1	-6.16	100.52	111.00
22	V	522	TYR	CB-CG-CD1	6.16	124.70	121.00
24	O	137	MET	CG-SD-CE	6.15	110.04	100.20
22	V	410	TYR	CZ-CE2-CD2	-6.14	114.28	119.80
1	A	622	SER	N-CA-C	-6.13	94.44	111.00
24	O	183	TYR	CB-CG-CD1	-6.13	117.32	121.00
23	W	77	VAL	CG1-CB-CG2	-6.11	101.12	110.90
29	Y	34	DC	C5'-C4'-C3'	6.04	124.98	114.10
28	X	77	DC	O4'-C1'-C2'	-6.04	101.06	105.90
23	W	673	ASP	CB-CG-OD1	6.02	123.72	118.30
3	C	6	GLN	N-CA-C	6.01	127.22	111.00
28	X	59	DC	O4'-C1'-N1	6.00	112.20	108.00
24	O	218	THR	CA-CB-CG2	-6.00	104.00	112.40
22	V	566	PHE	CB-CG-CD1	5.99	124.99	120.80
22	V	360	ARG	CD-NE-CZ	5.98	131.97	123.60
28	X	72	DC	N1-C1'-C2'	5.97	123.94	112.60
23	W	552	TRP	CD1-NE1-CE2	5.96	114.36	109.00
23	W	156	ARG	CD-NE-CZ	5.95	131.94	123.60
22	V	321	GLU	OE1-CD-OE2	-5.95	116.16	123.30
22	V	663	VAL	CG1-CB-CG2	-5.94	101.39	110.90
22	V	472	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	932	ARG	C-N-CA	-5.92	106.89	121.70
2	B	289	ILE	CG1-CB-CG2	-5.91	98.40	111.40
29	Y	17	DG	P-O3'-C3'	5.91	126.79	119.70
23	W	131	ASP	CB-CG-OD2	5.89	123.60	118.30
29	Y	22	DG	O4'-C1'-C2'	5.88	110.60	105.90
23	W	472	ASP	CB-CG-OD2	5.86	123.57	118.30
29	Y	30	DG	C4-N9-C1'	-5.85	118.89	126.50
22	V	381	TRP	CZ3-CH2-CZ2	-5.85	114.58	121.60
28	X	65	DG	O4'-C1'-N9	5.84	112.09	108.00
22	V	410	TYR	CB-CG-CD2	5.84	124.50	121.00
20	T	234	GLU	CG-CD-OE1	5.83	129.96	118.30
28	X	59	DC	N3-C2-O2	-5.83	117.82	121.90
29	Y	27	DC	O4'-C1'-N1	-5.83	103.92	108.00
23	W	112	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
24	O	171	PHE	CB-CG-CD1	-5.79	116.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	345	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	B	922	ARG	NE-CZ-NH1	-5.77	117.41	120.30
23	W	650	ASP	CB-CG-OD1	5.77	123.49	118.30
24	0	90	TYR	CG-CD2-CE2	-5.75	116.70	121.30
29	Y	20	DA	C3'-C2'-C1'	-5.75	95.61	102.50
23	W	472	ASP	CB-CG-OD1	-5.74	113.14	118.30
24	0	183	TYR	CD1-CE1-CZ	5.73	124.96	119.80
24	0	177	CYS	CA-CB-SG	-5.73	103.69	114.00
23	W	711	ASP	CB-CG-OD1	5.71	123.44	118.30
22	V	655	TYR	CB-CG-CD1	5.70	124.42	121.00
22	V	542	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
23	W	563	ARG	NE-CZ-NH1	5.70	123.15	120.30
24	0	96	PHE	CB-CG-CD1	-5.70	116.81	120.80
23	W	334	ARG	NE-CZ-NH2	-5.69	117.46	120.30
24	0	91	PHE	CG-CD2-CE2	-5.68	114.55	120.80
23	W	641	ARG	CD-NE-CZ	5.68	131.55	123.60
23	W	129	ASP	CB-CG-OD1	5.68	123.41	118.30
22	V	419	ARG	CD-NE-CZ	5.67	131.54	123.60
17	Q	102	VAL	N-CA-C	5.66	126.27	111.00
24	0	80	ARG	CD-NE-CZ	5.65	131.51	123.60
22	V	391	ARG	NE-CZ-NH2	5.65	123.13	120.30
28	X	68	DC	C3'-C2'-C1'	-5.65	95.72	102.50
23	W	708	LEU	CB-CG-CD2	-5.64	101.41	111.00
22	V	284	CYS	CA-CB-SG	-5.64	103.85	114.00
23	W	72	TYR	CB-CG-CD2	-5.63	117.62	121.00
28	X	76	DC	O4'-C1'-N1	-5.63	104.06	108.00
23	W	207	TYR	CA-CB-CG	5.62	124.07	113.40
24	0	226	SER	N-CA-CB	-5.62	102.08	110.50
22	V	430	LEU	CB-CG-CD1	5.61	120.54	111.00
22	V	325	ARG	NE-CZ-NH1	5.61	123.10	120.30
23	W	41	GLU	O-C-N	5.61	131.67	122.70
23	W	684	PHE	CB-CG-CD1	-5.60	116.88	120.80
22	V	571	TYR	CG-CD2-CE2	-5.60	116.82	121.30
22	V	662	LEU	CB-CG-CD2	-5.60	101.48	111.00
22	V	425	ARG	NE-CZ-NH1	5.59	123.10	120.30
23	W	270	VAL	CA-C-O	5.59	131.85	120.10
24	0	201	LEU	CB-CG-CD1	5.58	120.49	111.00
22	V	419	ARG	NH1-CZ-NH2	-5.58	113.26	119.40
23	W	544	TYR	CG-CD2-CE2	-5.58	116.83	121.30
28	X	61	DA	O4'-C4'-C3'	5.58	109.35	106.00
24	0	183	TYR	CG-CD1-CE1	-5.57	116.84	121.30
22	V	328	PHE	C-N-CA	5.57	134.00	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	482	PHE	CB-CG-CD1	-5.57	116.90	120.80
23	W	141	TYR	CG-CD2-CE2	5.57	125.75	121.30
22	V	608	SER	O-C-N	-5.54	113.83	122.70
28	X	58	DT	O4'-C4'-C3'	5.54	109.32	106.00
22	V	640	LEU	CB-CG-CD2	5.52	120.39	111.00
22	V	362	LEU	CB-CG-CD1	-5.51	101.63	111.00
22	V	393	THR	O-C-N	-5.51	113.89	122.70
22	V	289	TYR	CG-CD2-CE2	-5.50	116.90	121.30
23	W	177	LEU	CB-CG-CD1	5.50	120.35	111.00
24	O	65	VAL	CA-CB-CG1	5.50	119.15	110.90
23	W	625	TYR	CZ-CE2-CD2	-5.50	114.85	119.80
18	R	140	LYS	C-N-CD	5.49	139.93	128.40
22	V	634	ARG	CD-NE-CZ	5.48	131.28	123.60
1	A	640	LEU	CB-CG-CD1	-5.48	101.69	111.00
29	Y	23	DT	P-O3'-C3'	5.48	126.27	119.70
23	W	258	ARG	NE-CZ-NH1	5.47	123.04	120.30
28	X	74	DT	O4'-C4'-C3'	-5.47	102.31	104.50
23	W	722	ARG	NE-CZ-NH1	-5.46	117.57	120.30
23	W	631	ARG	NH1-CZ-NH2	-5.45	113.40	119.40
22	V	382	SER	N-CA-CB	-5.43	102.35	110.50
22	V	272	VAL	CA-CB-CG2	-5.43	102.75	110.90
29	Y	17	DG	O4'-C4'-C3'	5.43	109.26	106.00
23	W	205	VAL	CA-CB-CG1	5.43	119.04	110.90
3	C	35	ARG	NE-CZ-NH2	-5.42	117.59	120.30
23	W	690	ARG	CD-NE-CZ	5.42	131.18	123.60
23	W	595	ILE	CB-CA-C	5.41	122.42	111.60
23	W	196	ARG	CD-NE-CZ	5.41	131.17	123.60
23	W	253	ARG	NH1-CZ-NH2	-5.39	113.48	119.40
22	V	571	TYR	CB-CG-CD1	-5.38	117.77	121.00
23	W	224	GLU	OE1-CD-OE2	-5.38	116.84	123.30
23	W	616	ARG	NE-CZ-NH2	5.38	122.99	120.30
22	V	702	ALA	N-CA-CB	-5.38	102.57	110.10
22	V	479	ASP	CB-CG-OD2	5.38	123.14	118.30
5	E	63	ALA	CA-C-N	-5.37	105.38	117.20
23	W	280	ARG	NE-CZ-NH2	5.36	122.98	120.30
26	2	61	PHE	CB-CG-CD2	-5.36	117.05	120.80
28	X	74	DT	O4'-C1'-N1	-5.36	104.25	108.00
5	E	47	LYS	C-N-CD	-5.36	108.81	120.60
23	W	663	CYS	CA-CB-SG	-5.36	104.36	114.00
23	W	162	ASP	CB-CG-OD2	5.35	123.11	118.30
28	X	57	DC	O4'-C4'-C3'	5.34	109.20	106.00
21	U	299	LYS	CD-CE-NZ	5.33	123.97	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	287	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
23	W	33	ASP	CB-CG-OD2	5.33	123.09	118.30
28	X	31	DC	C1'-O4'-C4'	-5.32	104.78	110.10
29	Y	29	DC	N1-C1'-C2'	5.32	122.72	112.60
23	W	286	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
26	2	35	TYR	CB-CA-C	5.32	121.04	110.40
24	0	58	MET	O-C-N	5.32	131.21	122.70
24	0	125	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	B	935	PHE	CB-CG-CD2	-5.30	117.09	120.80
22	V	560	VAL	CA-CB-CG2	5.30	118.86	110.90
5	E	64	HIS	CA-C-N	-5.29	105.56	117.20
1	A	614	ASP	N-CA-C	5.29	125.28	111.00
23	W	686	ARG	NE-CZ-NH2	-5.29	117.66	120.30
23	W	540	THR	O-C-N	-5.28	114.25	122.70
28	X	75	DG	C4'-C3'-C2'	-5.27	98.36	103.10
22	V	666	ASP	CB-CG-OD1	-5.25	113.57	118.30
24	0	90	TYR	CB-CG-CD1	5.25	124.15	121.00
24	0	207	VAL	CA-CB-CG1	5.24	118.76	110.90
23	W	449	GLU	OE1-CD-OE2	-5.24	117.02	123.30
26	2	389	ASP	CB-CG-OD1	-5.24	113.59	118.30
23	W	623	VAL	CG1-CB-CG2	-5.23	102.53	110.90
28	X	59	DC	N1-C2-O2	5.23	122.04	118.90
24	0	213	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
23	W	285	TYR	CB-CG-CD1	-5.22	117.87	121.00
23	W	617	ALA	N-CA-CB	5.20	117.38	110.10
22	V	289	TYR	CB-CG-CD2	-5.20	117.88	121.00
22	V	478	VAL	CA-CB-CG2	-5.20	103.10	110.90
23	W	24	TYR	CB-CG-CD2	-5.18	117.89	121.00
24	0	131	LEU	CB-CG-CD1	5.18	119.81	111.00
24	0	64	VAL	CA-CB-CG1	5.18	118.67	110.90
29	Y	25	DT	P-O5'-C5'	5.17	129.18	120.90
22	V	325	ARG	CD-NE-CZ	5.16	130.83	123.60
24	0	62	TYR	CB-CG-CD1	5.16	124.09	121.00
23	W	461	LEU	CA-CB-CG	5.15	127.15	115.30
22	V	434	GLU	OE1-CD-OE2	5.15	129.48	123.30
23	W	468	PRO	CA-N-CD	-5.15	104.29	111.50
23	W	439	ASP	CB-CG-OD1	5.14	122.93	118.30
2	B	897	ARG	N-CA-C	-5.14	97.12	111.00
22	V	644	LEU	CB-CG-CD2	-5.14	102.26	111.00
23	W	61	ARG	NE-CZ-NH1	5.14	122.87	120.30
23	W	253	ARG	NE-CZ-NH2	5.13	122.87	120.30
23	W	283	ASP	CB-CG-OD2	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	288	LEU	O-C-N	-5.13	114.49	122.70
23	W	94	TYR	CB-CG-CD2	5.12	124.07	121.00
23	W	207	TYR	CB-CG-CD2	-5.12	117.93	121.00
26	2	392	ARG	NE-CZ-NH1	5.12	122.86	120.30
28	X	60	DG	O3'-P-O5'	-5.12	94.27	104.00
1	A	1398	LEU	CB-CG-CD2	-5.12	102.30	111.00
23	W	714	VAL	CA-CB-CG2	5.12	118.58	110.90
22	V	250	ASP	CB-CG-OD1	5.11	122.90	118.30
9	I	84	HIS	N-CA-C	5.11	124.79	111.00
29	Y	35	DG	N1-C6-O6	-5.11	116.84	119.90
22	V	332	ARG	CA-CB-CG	5.10	124.62	113.40
23	W	600	ALA	N-CA-CB	-5.10	102.96	110.10
26	2	457	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	475	ARG	CB-CA-C	5.10	120.60	110.40
23	W	143	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
22	V	398	ASP	CB-CG-OD1	5.08	122.87	118.30
28	X	67	DG	C1'-O4'-C4'	-5.08	105.02	110.10
23	W	636	ARG	CD-NE-CZ	5.07	130.69	123.60
23	W	157	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	A	1192	TRP	CA-CB-CG	5.05	123.30	113.70
24	0	90	TYR	CZ-CE2-CD2	5.05	124.34	119.80
22	V	362	LEU	CB-CG-CD2	5.05	119.58	111.00
22	V	289	TYR	CZ-CE2-CD2	5.04	124.34	119.80
23	W	463	PRO	N-CA-CB	5.04	109.35	103.30
2	B	924	ARG	NE-CZ-NH2	-5.04	117.78	120.30
23	W	676	LEU	CB-CG-CD2	5.04	119.57	111.00
24	0	178	ASP	CB-CG-OD2	-5.04	113.76	118.30
23	W	695	ARG	NE-CZ-NH2	5.04	122.82	120.30
27	3	210	THR	CA-CB-CG2	-5.03	105.35	112.40
1	A	467	MET	CB-CG-SD	5.03	127.50	112.40
22	V	344	ALA	CB-CA-C	5.03	117.65	110.10
25	1	16	MET	CG-SD-CE	5.03	108.24	100.20
23	W	66	GLU	C-N-CA	5.02	134.26	121.70
23	W	87	LEU	CB-CA-C	5.02	119.74	110.20
23	W	346	VAL	CA-CB-CG2	5.02	118.43	110.90
22	V	361	CYS	N-CA-CB	-5.02	101.57	110.60
23	W	599	VAL	CA-CB-CG1	5.02	118.43	110.90
24	0	224	ASP	N-CA-CB	-5.02	101.57	110.60
22	V	546	PHE	CB-CG-CD1	-5.01	117.29	120.80
22	V	607	ILE	CA-CB-CG1	5.01	120.52	111.00
24	0	228	TYR	CB-CG-CD2	-5.01	118.00	121.00
22	V	678	ARG	NE-CZ-NH2	5.01	122.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	312	ASP	N-CA-CB	-5.01	101.59	110.60
23	W	467	TYR	CG-CD1-CE1	-5.01	117.30	121.30
23	W	566	LEU	CB-CG-CD2	-5.00	102.49	111.00
22	V	614	SER	N-CA-C	5.00	124.50	111.00
23	W	450	ARG	NH1-CZ-NH2	-5.00	113.90	119.40

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	0	143	PRO	Mainchain
25	1	17	LYS	Mainchain
26	2	389	ASP	Mainchain,Sidechain
26	2	399	ASP	Sidechain
26	2	403	PHE	Mainchain,Peptide
26	2	406	GLY	Peptide
26	2	409	TYR	Sidechain
26	2	425	ALA	Mainchain
1	A	475	ARG	Sidechain
2	B	234	THR	Peptide
5	E	126	ILE	Peptide
8	H	111	ARG	Peptide
14	N	324	GLU	Peptide
14	N	355	ASP	Peptide
14	N	371	ILE	Peptide
18	R	146	ARG	Peptide
18	R	213	ASP	Sidechain
18	R	214	GLU	Peptide
18	R	215	GLU	Mainchain
18	R	230	GLU	Mainchain
18	R	235	GLU	Sidechain
19	S	148	PRO	Peptide
20	T	123	ASN	Peptide
22	V	247	ASP	Mainchain
22	V	378	PHE	Sidechain
22	V	417	THR	Peptide
22	V	489	TYR	Sidechain
22	V	503	ALA	Peptide
22	V	519	TYR	Sidechain
22	V	530	ARG	Sidechain
22	V	674	THR	Mainchain
23	W	104	PHE	Sidechain

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Mol	Chain	Res	Type	Group
23	W	197	TYR	Sidechain
23	W	206	VAL	Mainchain
23	W	208	SER	Mainchain
23	W	211	TYR	Sidechain
23	W	282	ARG	Sidechain
23	W	286	ARG	Sidechain
23	W	409	THR	Peptide
23	W	616	ARG	Sidechain
23	W	641	ARG	Sidechain
23	W	669	ARG	Sidechain
23	W	674	TYR	Sidechain
23	W	719	TYR	Sidechain
23	W	72	TYR	Sidechain
28	X	59	DC	Sidechain
28	X	66	DA	Sidechain
29	Y	29	DC	Sidechain
29	Y	30	DG	Sidechain
29	Y	35	DG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11617	539	0
2	B	9317	0	9312	408	0
3	C	2213	0	2155	79	0
4	D	1062	0	1042	9	0
5	E	1723	0	1745	100	0
6	F	689	0	715	16	0
7	G	1351	0	1358	31	0
8	H	1205	0	1167	52	0
9	I	1013	0	936	73	0
10	J	533	0	556	48	0
11	K	937	0	959	21	0
12	L	388	0	396	13	0
13	M	2391	0	2411	147	0
14	N	930	0	888	32	0
15	O	806	0	818	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	1462	0	1549	67	0
17	Q	1484	0	1499	145	0
18	R	1357	0	1381	151	0
19	S	1138	0	1103	24	0
20	T	1788	0	1819	113	0
21	U	1343	0	1341	67	0
22	V	3855	0	3871	196	0
23	W	5348	0	5372	145	0
24	O	1479	0	1524	37	0
25	1	491	0	507	238	0
26	2	2196	0	2206	566	0
27	3	1526	0	1561	442	0
28	X	1591	0	865	30	0
29	Y	1561	0	865	59	0
30	A	1	0	0	0	0
30	B	1	0	0	0	0
31	A	2	0	0	0	0
31	B	2	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	Q	1	0	0	0	0
31	U	1	0	0	0	0
All	All	62705	0	61538	3185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (3185) 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)
27:3:59:VAL:HG12	27:3:71:TYR:CD1	1.22	1.73
23:W:421:PHE:CE1	23:W:423:ASP:CB	1.83	1.62
22:V:516:PRO:CG	25:1:15:ALA:HB3	1.20	1.61
1:A:1250:ASP:CB	21:U:227:GLU:HG2	1.26	1.60
27:3:59:VAL:CG1	27:3:71:TYR:HD1	1.12	1.59
17:Q:180:PHE:CZ	18:R:211:SER:HB2	1.39	1.58
22:V:531:ILE:HA	22:V:534:TYR:CE2	1.39	1.58
1:A:926:ASN:HD21	1:A:932:ARG:CG	1.12	1.57
23:W:421:PHE:HE1	23:W:423:ASP:CB	1.12	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:54:ARG:HG3	27:3:182:PHE:CE1	1.42	1.55
22:V:315:VAL:HG13	23:W:500:ASP:CB	1.21	1.55
23:W:421:PHE:CE1	23:W:423:ASP:HB2	1.04	1.53
1:A:271:ARG:CD	13:M:73:PRO:HG2	1.37	1.52
1:A:1250:ASP:HB3	21:U:227:GLU:CG	1.10	1.52
22:V:516:PRO:HG3	25:1:15:ALA:CB	1.11	1.52
1:A:927:GLU:HB3	1:A:931:ARG:CG	1.05	1.52
17:Q:180:PHE:CZ	18:R:211:SER:CB	1.91	1.51
23:W:421:PHE:CD1	23:W:423:ASP:HB2	1.41	1.51
1:A:266:MET:CG	1:A:272:ASN:ND2	1.73	1.49
22:V:315:VAL:CG1	23:W:500:ASP:HB2	1.01	1.48
26:2:117:ASN:ND2	27:3:108:ASN:CB	1.76	1.47
1:A:927:GLU:CB	1:A:931:ARG:HG3	1.44	1.46
26:2:117:ASN:HD21	27:3:108:ASN:CB	1.27	1.45
5:E:51:GLY:O	5:E:52:ARG:CG	1.64	1.45
2:B:90:GLN:NE2	20:T:141:LEU:HD23	1.30	1.43
22:V:321:GLU:HB3	23:W:499:ASN:ND2	1.25	1.42
26:2:30:VAL:CG2	27:3:25:GLN:HB2	1.49	1.41
10:J:62:TYR:C	10:J:64:PRO:HD2	1.36	1.41
1:A:926:ASN:ND2	1:A:932:ARG:CG	1.81	1.40
26:2:117:ASN:CG	27:3:108:ASN:HB2	1.39	1.40
22:V:321:GLU:HB3	23:W:499:ASN:CG	1.38	1.39
3:C:5:ASN:O	3:C:7:PRO:CD	1.69	1.38
13:M:47:ASP:O	13:M:49:GLY:N	1.57	1.38
24:0:54:ARG:CG	27:3:182:PHE:HE1	1.35	1.38
1:A:926:ASN:ND2	1:A:932:ARG:HG3	1.32	1.37
2:B:90:GLN:HE21	20:T:141:LEU:CD2	1.38	1.36
17:Q:180:PHE:HZ	18:R:211:SER:CB	1.27	1.36
26:2:31:LEU:HD21	27:3:33:THR:N	1.36	1.36
2:B:90:GLN:HE22	20:T:141:LEU:CA	1.39	1.34
26:2:28:PRO:N	27:3:25:GLN:CA	1.89	1.33
2:B:80:GLU:CB	2:B:135:GLU:CB	2.06	1.33
26:2:30:VAL:HG23	27:3:25:GLN:CB	1.58	1.33
26:2:117:ASN:OD1	27:3:108:ASN:ND2	1.57	1.33
17:Q:105:TYR:CE1	17:Q:109:HIS:NE2	1.95	1.33
17:Q:105:TYR:CE1	18:R:231:GLU:CD	2.02	1.33
26:2:118:LEU:CD2	27:3:39:ASP:OD1	1.75	1.32
1:A:271:ARG:HD2	13:M:73:PRO:CG	1.57	1.32
1:A:927:GLU:HB3	1:A:931:ARG:CD	1.59	1.32
5:E:52:ARG:HB3	5:E:53:PRO:CD	1.59	1.31
26:2:118:LEU:HD22	27:3:39:ASP:OD1	1.16	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:GLU:CB	1:A:931:ARG:CG	2.00	1.31
1:A:1319:LYS:HG2	1:A:1333:GLU:CD	1.51	1.31
22:V:325:ARG:NH2	23:W:499:ASN:HB3	1.02	1.31
25:1:1:MET:O	26:2:413:LEU:HG	1.28	1.31
13:M:178:LYS:O	20:T:154:LYS:HB3	1.28	1.31
22:V:523:VAL:HG11	25:1:20:LEU:CD2	1.59	1.31
2:B:79:GLU:O	2:B:80:GLU:HG3	1.12	1.30
1:A:1319:LYS:CG	1:A:1333:GLU:CD	2.00	1.29
1:A:266:MET:HG2	1:A:272:ASN:ND2	1.27	1.29
17:Q:180:PHE:CE2	18:R:211:SER:HB2	1.67	1.29
5:E:64:HIS:CD2	5:E:69:THR:H	1.51	1.29
22:V:321:GLU:HB3	23:W:499:ASN:OD1	1.30	1.29
2:B:80:GLU:HB2	2:B:135:GLU:CB	1.59	1.28
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.54	1.28
24:0:97:ASP:O	27:3:208:ASP:HB3	1.12	1.28
24:0:165:ARG:NH1	24:0:192:ALA:O	1.67	1.28
26:2:118:LEU:HD21	27:3:39:ASP:O	1.23	1.28
5:E:47:LYS:HB2	5:E:48:PRO:CD	1.61	1.27
1:A:271:ARG:CD	13:M:73:PRO:CG	2.09	1.27
13:M:11:PRO:O	13:M:12:ARG:HG2	1.20	1.27
22:V:321:GLU:CB	23:W:499:ASN:HD21	1.45	1.27
2:B:80:GLU:OE1	2:B:135:GLU:HB3	1.20	1.26
1:A:1319:LYS:HD3	1:A:1333:GLU:OE2	1.36	1.26
22:V:325:ARG:NH2	23:W:499:ASN:CB	1.97	1.25
1:A:266:MET:CG	1:A:272:ASN:HD22	1.34	1.25
2:B:90:GLN:NE2	20:T:141:LEU:CD2	1.95	1.25
13:M:94:ASP:OD2	13:M:97:GLY:O	1.52	1.25
2:B:91:ILE:CG2	20:T:141:LEU:HD12	1.65	1.25
17:Q:102:VAL:CG1	17:Q:103:VAL:H	1.38	1.25
26:2:28:PRO:N	27:3:25:GLN:HA	0.95	1.25
17:Q:113:ARG:NH2	18:R:218:LYS:HE2	1.52	1.24
1:A:204:HIS:O	1:A:205:VAL:O	1.55	1.24
1:A:199:TYR:OH	13:M:93:PHE:CE2	1.84	1.23
22:V:321:GLU:OE2	23:W:500:ASP:CB	1.85	1.23
1:A:927:GLU:CB	1:A:931:ARG:HD2	1.69	1.23
22:V:674:THR:HG23	26:2:392:ARG:NH2	1.53	1.23
22:V:321:GLU:CB	23:W:499:ASN:OD1	1.88	1.22
17:Q:105:TYR:HE1	18:R:231:GLU:CG	1.51	1.22
23:W:59:TYR:CZ	23:W:62:ALA:CB	2.22	1.22
22:V:531:ILE:CG2	22:V:534:TYR:OH	1.88	1.22
27:3:58:ALA:N	27:3:71:TYR:OH	1.73	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:107:GLU:O	8:H:108:ALA:O	1.58	1.21
9:I:14:ILE:HG13	9:I:16:PHE:CE2	1.77	1.20
18:R:190:LEU:CD1	18:R:205:ASP:OD2	1.90	1.20
3:C:5:ASN:C	3:C:7:PRO:HD3	1.45	1.19
22:V:516:PRO:CG	25:1:15:ALA:CB	1.90	1.19
25:1:59:GLU:OE2	26:2:402:ARG:NH2	1.75	1.19
17:Q:113:ARG:HH22	18:R:218:LYS:CE	1.53	1.19
1:A:927:GLU:HB2	1:A:931:ARG:HD2	1.21	1.19
22:V:531:ILE:HG23	22:V:534:TYR:CZ	1.78	1.19
23:W:209:TYR:OH	23:W:233:PHE:HA	1.39	1.19
5:E:52:ARG:CB	5:E:53:PRO:HD2	1.71	1.18
22:V:531:ILE:CA	22:V:534:TYR:CE2	2.25	1.18
8:H:85:ALA:O	8:H:87:GLN:OE1	1.58	1.18
2:B:80:GLU:HB3	2:B:135:GLU:CG	1.73	1.18
17:Q:29:GLU:CD	18:R:194:ARG:HH21	1.45	1.18
5:E:64:HIS:NE2	5:E:69:THR:OG1	1.74	1.18
23:W:59:TYR:CZ	23:W:62:ALA:HB1	1.77	1.18
27:3:66:GLU:HA	27:3:132:LEU:HD12	1.22	1.17
22:V:325:ARG:HH22	23:W:499:ASN:CB	1.55	1.17
22:V:516:PRO:HB3	25:1:15:ALA:HB1	1.24	1.17
2:B:79:GLU:O	2:B:80:GLU:CG	1.93	1.16
10:J:63:ALA:N	10:J:64:PRO:CD	2.06	1.16
27:3:59:VAL:N	27:3:71:TYR:CE1	2.12	1.16
2:B:133:ILE:HD13	2:B:139:GLN:HB3	1.18	1.16
25:1:28:ALA:HB1	25:1:31:LYS:HD2	1.27	1.16
26:2:117:ASN:ND2	27:3:108:ASN:HB2	0.85	1.16
27:3:59:VAL:CG1	27:3:71:TYR:CD1	1.97	1.16
25:1:2:VAL:CG1	26:2:456:LYS:HG2	1.74	1.16
2:B:90:GLN:NE2	20:T:141:LEU:HA	1.59	1.15
2:B:80:GLU:O	2:B:135:GLU:HG3	1.45	1.15
1:A:133:SER:O	1:A:135:GLY:N	1.77	1.15
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.42	1.15
1:A:927:GLU:CB	1:A:931:ARG:CD	2.19	1.15
1:A:1319:LYS:CD	1:A:1333:GLU:OE2	1.94	1.15
22:V:321:GLU:CB	23:W:499:ASN:ND2	2.05	1.15
5:E:54:ARG:CB	5:E:78:GLU:OE1	1.95	1.15
5:E:64:HIS:CD2	5:E:69:THR:N	2.13	1.15
2:B:861:SER:O	2:B:896:LEU:CD2	1.94	1.14
25:1:2:VAL:HG13	26:2:422:LEU:HD11	1.20	1.14
17:Q:109:HIS:ND1	18:R:224:THR:OG1	1.80	1.14
26:2:28:PRO:HA	27:3:33:THR:HB	1.14	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:GLU:OE1	2:B:135:GLU:O	1.66	1.14
23:W:419:GLU:HB3	23:W:420:PRO:CD	1.76	1.14
25:1:1:MET:CG	26:2:413:LEU:HB3	1.76	1.14
2:B:90:GLN:NE2	20:T:141:LEU:CG	2.10	1.14
23:W:421:PHE:HE1	23:W:423:ASP:HB3	1.12	1.14
17:Q:180:PHE:CE2	18:R:211:SER:CB	2.26	1.13
26:2:211:GLN:HG3	26:2:257:SER:HB3	1.29	1.13
13:M:179:GLU:HA	20:T:154:LYS:HG2	1.25	1.13
2:B:80:GLU:CB	2:B:135:GLU:HB2	1.68	1.12
2:B:91:ILE:HG23	20:T:141:LEU:HD12	1.16	1.12
2:B:90:GLN:HE22	20:T:141:LEU:CB	1.61	1.12
24:0:54:ARG:CG	27:3:182:PHE:CE1	2.17	1.12
3:C:137:ASN:HB2	3:C:145:GLN:HE22	1.13	1.12
5:E:55:ARG:O	5:E:76:PHE:O	1.67	1.12
23:W:59:TYR:CE2	23:W:62:ALA:CB	2.32	1.12
20:T:141:LEU:O	20:T:143:GLN:OE1	1.66	1.11
25:1:9:LEU:HD13	25:1:48:GLU:HA	1.32	1.11
27:3:59:VAL:HG13	27:3:70:LEU:HB2	1.27	1.11
17:Q:102:VAL:HG13	17:Q:103:VAL:N	1.37	1.11
27:3:57:LEU:O	27:3:71:TYR:HE2	1.30	1.11
22:V:315:VAL:CG1	23:W:500:ASP:CB	1.94	1.11
25:1:5:LEU:CD2	26:2:408:LEU:HD13	1.80	1.11
26:2:42:LEU:HD21	26:2:55:TRP:HB2	1.21	1.11
1:A:266:MET:HG3	1:A:272:ASN:ND2	1.51	1.10
1:A:611:ASP:OD2	1:A:627:LYS:HE3	1.51	1.10
1:A:1319:LYS:HG2	1:A:1333:GLU:CG	1.80	1.10
5:E:51:GLY:O	5:E:52:ARG:HG3	0.95	1.10
1:A:1114:ALA:C	1:A:1116:ASN:H	1.43	1.10
23:W:419:GLU:CB	23:W:420:PRO:HD2	1.78	1.10
26:2:160:LEU:HD23	26:2:206:LEU:HD21	1.25	1.10
1:A:326:PRO:HB3	13:M:87:GLY:CA	1.81	1.10
25:1:18:GLN:HB2	25:1:44:PHE:CE2	1.86	1.10
1:A:271:ARG:HG2	13:M:73:PRO:HG3	1.33	1.09
22:V:516:PRO:CG	22:V:706:LYS:HZ3	1.64	1.09
22:V:516:PRO:CB	25:1:15:ALA:HB1	1.81	1.09
22:V:516:PRO:HG2	22:V:706:LYS:HZ3	1.12	1.09
26:2:171:VAL:HG22	26:2:213:TRP:HA	1.27	1.09
9:I:14:ILE:HG13	9:I:16:PHE:CZ	1.86	1.09
21:U:230:SER:O	21:U:231:ASP:HB2	1.50	1.09
22:V:531:ILE:HG23	22:V:534:TYR:OH	0.92	1.09
25:1:2:VAL:HG11	26:2:456:LYS:CG	1.81	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:192:GLU:HG3	26:2:193:PRO:HD2	1.33	1.09
27:3:49:LEU:HB3	27:3:101:TYR:HB3	1.15	1.09
5:E:64:HIS:NE2	5:E:69:THR:N	1.99	1.09
22:V:519:TYR:CE2	25:1:20:LEU:HG	1.87	1.09
1:A:1250:ASP:HB3	21:U:227:GLU:HG3	1.35	1.09
13:M:94:ASP:O	13:M:97:GLY:N	1.84	1.09
25:1:5:LEU:HD11	26:2:408:LEU:HB3	1.17	1.09
17:Q:29:GLU:OE2	18:R:194:ARG:NH2	1.84	1.08
22:V:321:GLU:OE2	23:W:500:ASP:HB3	0.91	1.08
27:3:57:LEU:C	27:3:71:TYR:OH	1.92	1.08
2:B:225:LEU:HD11	2:B:228:SER:CB	1.81	1.08
27:3:137:LEU:HB3	27:3:180:VAL:HG11	1.34	1.08
25:1:13:ASP:CG	25:1:14:PRO:HD2	1.74	1.08
2:B:80:GLU:OE1	2:B:135:GLU:CB	2.01	1.08
25:1:5:LEU:HD21	26:2:408:LEU:CD1	1.82	1.08
26:2:30:VAL:H	27:3:25:GLN:CB	1.67	1.07
26:2:30:VAL:H	27:3:25:GLN:HB3	1.00	1.07
2:B:80:GLU:HB3	2:B:135:GLU:CB	1.81	1.07
26:2:159:VAL:HG13	26:2:161:HIS:H	1.16	1.07
27:3:59:VAL:HB	27:3:71:TYR:CE1	1.89	1.07
2:B:882:SER:O	2:B:887:TYR:CD1	2.06	1.07
10:J:62:TYR:C	10:J:64:PRO:CD	2.22	1.07
22:V:516:PRO:HG2	22:V:706:LYS:NZ	1.70	1.07
25:1:2:VAL:HG11	26:2:456:LYS:HG2	1.09	1.07
5:E:52:ARG:HB3	5:E:53:PRO:HD3	1.30	1.06
24:0:54:ARG:HB2	27:3:209:ILE:HG23	1.35	1.06
13:M:10:LEU:N	13:M:11:PRO:HD2	1.66	1.06
13:M:11:PRO:O	13:M:12:ARG:CG	2.03	1.06
2:B:80:GLU:HB3	2:B:135:GLU:HG3	1.25	1.06
23:W:424:ARG:O	23:W:425:THR:HG23	1.52	1.06
2:B:225:LEU:HD11	2:B:228:SER:HB2	1.38	1.06
24:0:97:ASP:O	27:3:208:ASP:CB	2.02	1.06
5:E:54:ARG:HB2	5:E:78:GLU:OE1	1.51	1.05
17:Q:51:LEU:HD11	18:R:163:LEU:HD11	1.10	1.05
22:V:516:PRO:CG	22:V:706:LYS:NZ	2.18	1.05
17:Q:180:PHE:CZ	18:R:211:SER:HB3	1.84	1.05
27:3:22:TRP:O	27:3:25:GLN:HG3	1.56	1.05
9:I:62:VAL:O	9:I:64:GLU:N	1.89	1.05
17:Q:108:ASP:O	18:R:234:GLU:OE2	1.72	1.05
25:1:1:MET:CB	26:2:413:LEU:HB3	1.87	1.05
22:V:674:THR:HG23	26:2:392:ARG:CZ	1.85	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:57:LEU:O	27:3:71:TYR:CE2	2.10	1.04
13:M:178:LYS:O	20:T:154:LYS:CB	2.04	1.04
17:Q:105:TYR:CE1	18:R:231:GLU:CG	2.34	1.04
17:Q:180:PHE:HZ	18:R:211:SER:CA	1.68	1.04
25:1:5:LEU:HD12	26:2:409:TYR:O	1.56	1.04
1:A:326:PRO:HB3	13:M:87:GLY:HA2	1.38	1.04
1:A:926:ASN:HD22	1:A:932:ARG:HG3	1.22	1.03
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.10	1.03
26:2:234:LEU:HD21	26:2:237:LEU:HD12	1.36	1.03
17:Q:51:LEU:CD1	18:R:163:LEU:HD11	1.87	1.03
22:V:516:PRO:CB	25:1:15:ALA:CB	2.36	1.03
26:2:81:LYS:HE3	26:2:93:LEU:HD21	1.40	1.03
1:A:212:LYS:O	1:A:213:LYS:HB3	1.55	1.02
1:A:326:PRO:CB	13:M:87:GLY:HA2	1.88	1.02
3:C:5:ASN:O	3:C:7:PRO:HD3	0.86	1.02
24:0:54:ARG:CD	27:3:182:PHE:HE1	1.72	1.02
25:1:4:VAL:HG12	26:2:411:GLN:O	1.55	1.02
1:A:927:GLU:CA	1:A:931:ARG:HG3	1.89	1.02
2:B:90:GLN:NE2	20:T:141:LEU:CB	2.22	1.02
5:E:52:ARG:HB3	5:E:53:PRO:HD2	1.26	1.02
16:P:206:GLU:HG3	16:P:236:LYS:NZ	1.75	1.02
24:0:54:ARG:NE	27:3:182:PHE:CE1	2.26	1.02
16:P:206:GLU:HG3	16:P:236:LYS:HZ2	1.20	1.02
2:B:90:GLN:HE22	20:T:141:LEU:HA	0.90	1.02
3:C:212:ASP:O	3:C:214:ASP:N	1.93	1.02
25:1:34:ILE:HG12	25:1:50:VAL:HG11	1.39	1.02
16:P:297:LYS:CB	16:P:298:PRO:CD	2.36	1.01
22:V:528:LYS:HE2	29:Y:25:DT:C5'	1.88	1.01
27:3:196:LEU:HD21	27:3:223:LEU:HD23	1.42	1.01
2:B:1066:PRO:HB3	13:M:46:ILE:HD13	1.38	1.01
29:Y:36:DA:C4	29:Y:37:DG:N7	2.29	1.01
1:A:266:MET:HG2	1:A:272:ASN:HD21	1.24	1.01
2:B:861:SER:O	2:B:896:LEU:HD23	1.57	1.01
22:V:523:VAL:HG11	25:1:20:LEU:HD21	1.02	1.01
26:2:199:ALA:HB3	26:2:202:GLN:HE22	1.22	1.01
27:3:59:VAL:CB	27:3:71:TYR:CE1	2.43	1.01
1:A:265:VAL:O	1:A:272:ASN:ND2	1.91	1.00
1:A:1113:SER:O	1:A:1114:ALA:CB	2.04	1.00
23:W:59:TYR:CE2	23:W:62:ALA:HB3	1.95	1.00
24:0:77:LYS:O	24:0:79:ASN:N	1.93	1.00
2:B:895:PHE:O	2:B:897:ARG:NH1	1.94	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:315:VAL:HG11	23:W:500:ASP:HB2	1.42	1.00
22:V:515:SER:HB3	22:V:539:ASN:HD21	1.27	1.00
1:A:927:GLU:HB3	1:A:931:ARG:HG2	1.42	1.00
5:E:52:ARG:CB	5:E:53:PRO:CD	2.27	1.00
10:J:63:ALA:N	10:J:64:PRO:HD2	1.74	1.00
17:Q:23:ARG:NH2	18:R:209:GLN:H	1.59	1.00
22:V:613:THR:O	22:V:614:SER:HB2	1.59	1.00
27:3:58:ALA:CA	27:3:71:TYR:CZ	2.44	1.00
23:W:419:GLU:HB3	23:W:420:PRO:HD2	1.02	0.99
2:B:92:TYR:HB3	20:T:145:LEU:HB2	1.41	0.99
5:E:47:LYS:CB	5:E:48:PRO:HD2	1.91	0.99
1:A:1113:SER:O	1:A:1114:ALA:HB2	1.56	0.99
1:A:622:SER:O	1:A:624:GLY:N	1.95	0.99
5:E:47:LYS:HB2	5:E:48:PRO:HD2	1.00	0.99
1:A:326:PRO:CA	13:M:87:GLY:HA2	1.92	0.99
26:2:117:ASN:CG	27:3:108:ASN:CB	2.20	0.98
1:A:197:GLU:OE2	13:M:93:PHE:CE2	2.16	0.98
2:B:225:LEU:CD1	2:B:228:SER:HB2	1.92	0.98
23:W:209:TYR:OH	23:W:233:PHE:CA	2.10	0.98
2:B:878:ASP:O	2:B:879:GLU:O	1.81	0.98
27:3:148:ASN:HB2	27:3:157:MET:HE2	1.43	0.98
26:2:196:ILE:HD11	26:2:210:ALA:HB2	1.45	0.98
1:A:271:ARG:CG	13:M:73:PRO:HG3	1.94	0.98
22:V:523:VAL:CG1	25:1:20:LEU:HD21	1.94	0.98
26:2:118:LEU:CD2	27:3:39:ASP:O	2.12	0.98
16:P:206:GLU:CG	16:P:236:LYS:HZ2	1.76	0.97
17:Q:109:HIS:CG	18:R:224:THR:OG1	2.17	0.97
27:3:173:GLN:HA	27:3:176:ASN:HD21	1.28	0.97
23:W:584:TYR:CD1	23:W:594:ALA:HB2	1.99	0.97
5:E:55:ARG:N	5:E:78:GLU:OE2	1.96	0.97
1:A:47:THR:O	1:A:48:GLU:O	1.82	0.97
20:T:153:TYR:CZ	20:T:155:PRO:HB3	2.00	0.97
1:A:265:VAL:O	1:A:272:ASN:OD1	1.82	0.97
26:2:176:ALA:HB1	26:2:178:LEU:HD13	1.47	0.97
26:2:100:LEU:HD11	26:2:119:ARG:HG3	1.46	0.97
27:3:165:LYS:HD2	27:3:195:VAL:HG22	1.44	0.97
2:B:74:ALA:HB2	20:T:201:ASP:HB3	1.46	0.97
8:H:66:GLU:O	8:H:67:ASP:HB2	1.62	0.96
5:E:47:LYS:HE2	5:E:52:ARG:HB2	1.45	0.96
27:3:59:VAL:CB	27:3:71:TYR:CD1	2.47	0.96
17:Q:105:TYR:O	17:Q:109:HIS:CD2	2.19	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:298:ALA:HA	23:W:421:PHE:CE2	2.01	0.96
2:B:91:ILE:HG23	20:T:141:LEU:CD1	1.95	0.96
3:C:212:ASP:C	3:C:214:ASP:H	1.69	0.96
1:A:1319:LYS:CG	1:A:1333:GLU:OE2	2.06	0.96
2:B:133:ILE:HA	2:B:139:GLN:HA	1.48	0.96
3:C:7:PRO:HG2	11:K:97:GLU:OE2	1.65	0.96
1:A:926:ASN:HD21	1:A:932:ARG:HG2	0.82	0.96
1:A:1319:LYS:CD	1:A:1356:ARG:HH12	1.79	0.96
29:Y:36:DA:C6	29:Y:37:DG:C6	2.53	0.95
2:B:861:SER:O	2:B:896:LEU:HD22	1.66	0.95
23:W:59:TYR:CE1	23:W:62:ALA:HB1	2.02	0.95
5:E:54:ARG:HB3	5:E:78:GLU:OE1	1.67	0.95
21:U:251:ALA:O	21:U:253:THR:N	1.97	0.95
27:3:133:LEU:HD23	27:3:177:PHE:CD1	2.01	0.95
1:A:495:ASP:O	1:A:497:ASP:N	1.98	0.95
1:A:1319:LYS:HG2	1:A:1333:GLU:OE2	1.63	0.95
25:1:13:ASP:OD2	25:1:17:LYS:HB3	1.65	0.95
25:1:18:GLN:HB2	25:1:44:PHE:HE2	1.26	0.95
26:2:28:PRO:HA	27:3:33:THR:CB	1.95	0.95
26:2:211:GLN:HA	26:2:261:PHE:CZ	2.02	0.95
27:3:59:VAL:HB	27:3:71:TYR:HE1	1.25	0.95
22:V:321:GLU:CA	23:W:499:ASN:HD21	1.78	0.95
25:1:2:VAL:CG1	26:2:422:LEU:HD11	1.96	0.95
2:B:133:ILE:O	2:B:134:LYS:O	1.83	0.95
5:E:64:HIS:NE2	5:E:69:THR:CA	2.29	0.95
26:2:117:ASN:ND2	27:3:42:MET:HE1	1.82	0.95
26:2:118:LEU:HD11	27:3:43:VAL:CG2	1.95	0.95
22:V:531:ILE:HA	22:V:534:TYR:CD2	2.01	0.94
10:J:63:ALA:N	10:J:64:PRO:HD3	1.79	0.94
22:V:516:PRO:HA	25:1:15:ALA:O	1.65	0.94
25:1:1:MET:HB3	26:2:413:LEU:CG	1.98	0.94
1:A:265:VAL:C	1:A:272:ASN:HD21	1.71	0.94
10:J:64:PRO:C	10:J:66:GLU:H	1.66	0.94
13:M:39:LEU:O	13:M:40:VAL:O	1.84	0.94
21:U:256:THR:OG1	21:U:272:THR:HG22	1.66	0.94
21:U:231:ASP:O	21:U:232:GLU:CG	2.15	0.94
23:W:696:TRP:CD1	23:W:697:ILE:HG12	2.02	0.94
26:2:117:ASN:N	27:3:104:LEU:HD21	1.83	0.94
5:E:64:HIS:CE1	5:E:69:THR:OG1	2.19	0.94
22:V:528:LYS:HE2	29:Y:25:DT:H5'	1.46	0.94
2:B:78:VAL:O	2:B:79:GLU:HB2	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:O	1:A:208:ASP:N	2.00	0.94
18:R:190:LEU:HD11	18:R:205:ASP:OD2	1.65	0.94
26:2:35:TYR:CE1	26:2:62:LEU:HG	2.02	0.94
2:B:76:GLY:O	2:B:77:GLU:HB2	1.67	0.94
22:V:325:ARG:HH21	23:W:499:ASN:HB3	1.20	0.94
25:1:9:LEU:HD22	25:1:51:ASN:HD22	1.33	0.94
22:V:515:SER:CB	22:V:539:ASN:HD21	1.80	0.93
1:A:1310:HIS:HB3	21:U:252:LYS:HD3	1.48	0.93
23:W:209:TYR:HH	23:W:233:PHE:HA	1.32	0.93
2:B:80:GLU:O	2:B:135:GLU:CG	2.16	0.93
16:P:297:LYS:HA	16:P:297:LYS:CE	1.96	0.93
22:V:631:GLY:O	22:V:632:SER:CB	2.14	0.93
27:3:187:GLN:HG3	27:3:189:ILE:HG12	1.51	0.93
5:E:64:HIS:HD2	5:E:68:PRO:HA	1.33	0.93
17:Q:105:TYR:CD1	18:R:231:GLU:OE2	2.21	0.93
8:H:64:LEU:HB3	8:H:84:ARG:HD3	1.48	0.93
8:H:85:ALA:C	8:H:87:GLN:OE1	2.06	0.93
26:2:30:VAL:N	27:3:25:GLN:HB3	1.82	0.93
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.51	0.93
1:A:133:SER:C	1:A:135:GLY:H	1.72	0.93
26:2:177:GLN:HA	26:2:220:LEU:CD2	1.99	0.93
27:3:133:LEU:HD13	27:3:133:LEU:H	1.33	0.93
26:2:118:LEU:HD23	27:3:42:MET:HB2	1.50	0.93
9:I:105:GLU:O	9:I:106:ASP:HB2	1.69	0.92
15:O:3:TYR:O	15:O:5:LEU:N	2.01	0.92
18:R:162:GLY:O	18:R:164:GLY:N	2.01	0.92
3:C:7:PRO:CG	11:K:97:GLU:OE2	2.17	0.92
27:3:11:LEU:HD22	27:3:160:ARG:HG2	1.51	0.92
22:V:523:VAL:CG1	25:1:20:LEU:CD2	2.45	0.92
27:3:190:LEU:HA	27:3:210:THR:HG22	1.50	0.92
2:B:80:GLU:CB	2:B:135:GLU:HB3	1.94	0.92
27:3:165:LYS:HE3	27:3:200:SER:CB	2.00	0.92
17:Q:113:ARG:HH22	18:R:218:LYS:HE3	1.34	0.92
22:V:516:PRO:HB2	22:V:706:LYS:HZ1	1.33	0.92
22:V:531:ILE:HA	22:V:534:TYR:HE2	1.10	0.92
8:H:85:ALA:CA	8:H:87:GLN:OE1	2.18	0.91
21:U:230:SER:O	21:U:231:ASP:CB	2.18	0.91
25:1:8:VAL:HG11	25:1:45:VAL:CG1	1.99	0.91
2:B:80:GLU:CD	2:B:135:GLU:HB3	1.89	0.91
2:B:92:TYR:CG	20:T:145:LEU:HD13	2.03	0.91
20:T:153:TYR:OH	20:T:155:PRO:HB3	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:97:ASP:OD1	27:3:208:ASP:OD1	1.88	0.91
1:A:551:ARG:CD	1:A:625:ASP:OD2	2.17	0.91
16:P:297:LYS:HA	16:P:297:LYS:HE2	1.49	0.91
1:A:926:ASN:ND2	1:A:932:ARG:HG2	1.59	0.91
20:T:177:ARG:C	20:T:179:ASP:H	1.74	0.91
2:B:225:LEU:CD1	2:B:228:SER:CB	2.49	0.91
2:B:721:ARG:HG3	2:B:977:THR:HG22	1.52	0.91
2:B:90:GLN:HE21	20:T:141:LEU:HD23	0.87	0.91
26:2:81:LYS:CE	26:2:93:LEU:HD21	2.00	0.91
27:3:137:LEU:CB	27:3:180:VAL:HG11	2.01	0.91
1:A:1319:LYS:HG2	1:A:1333:GLU:HG2	1.53	0.90
22:V:516:PRO:CB	22:V:706:LYS:HZ1	1.83	0.90
24:0:54:ARG:HG3	27:3:182:PHE:CZ	2.05	0.90
5:E:55:ARG:HG2	5:E:76:PHE:HB3	1.51	0.90
23:W:59:TYR:CE1	23:W:62:ALA:CB	2.53	0.90
26:2:81:LYS:HD2	26:2:89:LEU:HD21	1.52	0.90
25:1:1:MET:HB3	26:2:413:LEU:HB3	1.52	0.90
26:2:159:VAL:HG22	26:2:160:LEU:HD12	1.51	0.90
24:0:98:GLN:OE1	27:3:209:ILE:HA	1.70	0.90
1:A:265:VAL:O	1:A:272:ASN:CG	2.10	0.89
1:A:926:ASN:OD1	1:A:931:ARG:HB3	1.72	0.89
22:V:315:VAL:HG13	23:W:500:ASP:CA	2.03	0.89
3:C:137:ASN:CB	3:C:145:GLN:HE22	1.84	0.89
1:A:1319:LYS:HD3	1:A:1356:ARG:HH12	1.35	0.89
17:Q:105:TYR:CD1	18:R:231:GLU:CD	2.46	0.89
25:1:47:ALA:CB	25:1:50:VAL:HB	2.03	0.89
1:A:1250:ASP:CB	21:U:227:GLU:CG	2.06	0.89
25:1:8:VAL:HG11	25:1:45:VAL:HG13	1.55	0.89
27:3:165:LYS:HG3	27:3:203:LEU:HD12	1.52	0.89
26:2:160:LEU:HB3	26:2:206:LEU:HD11	1.53	0.89
1:A:212:LYS:O	1:A:213:LYS:CB	2.19	0.89
1:A:199:TYR:OH	13:M:93:PHE:HE2	1.26	0.89
1:A:1114:ALA:C	1:A:1116:ASN:N	2.18	0.89
27:3:177:PHE:CE2	27:3:181:ILE:HD11	2.08	0.88
1:A:199:TYR:CZ	13:M:93:PHE:CZ	2.60	0.88
23:W:696:TRP:CD1	23:W:697:ILE:CG1	2.57	0.88
25:1:4:VAL:HG11	26:2:412:PHE:HD2	1.36	0.88
27:3:70:LEU:HD13	27:3:115:ILE:HD11	1.55	0.88
26:2:160:LEU:CA	26:2:206:LEU:HD11	2.04	0.88
2:B:225:LEU:HD11	2:B:228:SER:HB3	1.56	0.88
26:2:117:ASN:CB	27:3:42:MET:CE	2.51	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:HIS:CE1	5:E:69:THR:HG1	1.91	0.88
26:2:243:SER:CB	26:2:258:LEU:HD22	2.04	0.88
17:Q:113:ARG:NH2	18:R:218:LYS:CE	2.23	0.87
26:2:163:MET:SD	26:2:196:ILE:HG21	2.14	0.87
25:1:28:ALA:CB	25:1:31:LYS:HD2	2.04	0.87
26:2:118:LEU:HD11	27:3:43:VAL:HG22	1.56	0.87
27:3:177:PHE:CD2	27:3:181:ILE:HD11	2.08	0.87
10:J:62:TYR:O	10:J:64:PRO:HD2	1.75	0.87
5:E:48:PRO:O	5:E:49:SER:HB2	1.72	0.87
23:W:584:TYR:CE2	23:W:614:TYR:HB2	2.10	0.87
1:A:153:ILE:O	1:A:154:CYS:O	1.93	0.87
16:P:162:VAL:HG23	16:P:164:GLN:NE2	1.88	0.87
26:2:160:LEU:CD2	26:2:206:LEU:HD21	2.04	0.87
26:2:160:LEU:CB	26:2:206:LEU:HD11	2.04	0.87
27:3:59:VAL:CG1	27:3:70:LEU:HB2	2.03	0.87
23:W:37:HIS:CE1	23:W:454:VAL:HG13	2.09	0.87
26:2:45:PHE:HB2	26:2:51:LEU:HD13	1.56	0.87
26:2:117:ASN:OD1	27:3:108:ASN:CB	2.23	0.87
26:2:218:GLN:HB3	26:2:264:HIS:CD2	2.08	0.87
27:3:165:LYS:HE3	27:3:200:SER:HB2	1.56	0.87
1:A:355:MET:SD	2:B:1091:ARG:NH1	2.48	0.87
23:W:430:ASN:HB3	23:W:431:PRO:HD2	1.54	0.87
2:B:91:ILE:CG2	20:T:141:LEU:CD1	2.52	0.87
9:I:85:PRO:O	9:I:86:CYS:C	2.12	0.87
27:3:71:TYR:CD2	27:3:72:PRO:HD2	2.08	0.87
13:M:86:LYS:HA	13:M:86:LYS:CE	2.05	0.87
13:M:182:ALA:HB2	20:T:154:LYS:HG3	1.56	0.87
2:B:80:GLU:CB	2:B:135:GLU:HG3	2.05	0.86
2:B:90:GLN:HE21	20:T:141:LEU:CG	1.80	0.86
26:2:48:LEU:HB3	26:2:49:PRO:HD3	1.57	0.86
26:2:118:LEU:HD22	27:3:39:ASP:CG	1.94	0.86
17:Q:24:GLY:CA	18:R:210:PHE:CE2	2.58	0.86
23:W:421:PHE:CD1	23:W:423:ASP:CB	2.31	0.86
13:M:44:ARG:HE	13:M:46:ILE:CG2	1.88	0.86
15:O:3:TYR:HB3	15:O:98:CYS:SG	2.15	0.86
18:R:162:GLY:C	18:R:164:GLY:H	1.79	0.86
25:1:1:MET:HB3	26:2:413:LEU:CB	2.04	0.86
26:2:138:PRO:HG3	26:2:189:GLU:HG3	1.57	0.86
26:2:224:GLN:HB2	26:2:268:PHE:CZ	2.09	0.86
27:3:14:VAL:HG21	27:3:163:VAL:HG22	1.57	0.86
27:3:64:ILE:HG13	27:3:123:ASP:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:CG	13:M:73:PRO:CG	2.52	0.86
1:A:1319:LYS:HG3	1:A:1333:GLU:CD	1.96	0.86
23:W:59:TYR:CG	23:W:62:ALA:HB2	2.11	0.86
25:1:1:MET:O	26:2:413:LEU:CG	2.21	0.86
26:2:30:VAL:HG23	27:3:25:GLN:HB2	0.86	0.86
2:B:133:ILE:HD13	2:B:139:GLN:CB	2.03	0.86
20:T:177:ARG:NH1	20:T:209:PRO:O	2.07	0.86
26:2:218:GLN:HB3	26:2:264:HIS:HD2	1.38	0.86
26:2:171:VAL:HG22	26:2:213:TRP:CA	2.06	0.86
27:3:58:ALA:C	27:3:71:TYR:CZ	2.49	0.86
17:Q:105:TYR:HE1	18:R:231:GLU:HG3	1.40	0.86
25:1:2:VAL:HG13	26:2:422:LEU:CD1	2.03	0.86
17:Q:105:TYR:CD1	17:Q:109:HIS:NE2	2.32	0.86
27:3:69:PHE:CZ	27:3:139:LYS:HB3	2.10	0.86
26:2:81:LYS:CD	26:2:89:LEU:HD21	2.06	0.85
1:A:271:ARG:NE	13:M:73:PRO:HG2	1.91	0.85
22:V:316:LEU:HB2	22:V:321:GLU:HG3	1.58	0.85
23:W:696:TRP:NE1	23:W:697:ILE:HG12	1.90	0.85
25:1:1:MET:SD	26:2:415:GLN:O	2.34	0.85
26:2:31:LEU:CD2	27:3:33:THR:N	2.32	0.85
27:3:100:LYS:HB3	27:3:103:LEU:HD13	1.58	0.85
1:A:923:ASP:O	1:A:932:ARG:NH1	2.09	0.85
2:B:1066:PRO:CB	13:M:46:ILE:HD13	2.05	0.85
9:I:15:ARG:O	9:I:16:PHE:O	1.93	0.85
21:U:231:ASP:O	21:U:232:GLU:HG2	1.75	0.85
26:2:211:GLN:HG3	26:2:257:SER:CB	2.05	0.85
27:3:160:ARG:HB3	27:3:190:LEU:HD21	1.57	0.85
13:M:107:MET:HG2	29:Y:63:DG:H22	1.41	0.85
22:V:631:GLY:O	22:V:632:SER:HB2	1.76	0.85
26:2:118:LEU:CD2	27:3:42:MET:HB2	2.06	0.85
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.57	0.85
26:2:31:LEU:N	27:3:25:GLN:O	2.08	0.85
26:2:81:LYS:CD	26:2:93:LEU:HD21	2.07	0.85
27:3:59:VAL:HG12	27:3:71:TYR:CG	2.07	0.85
27:3:190:LEU:HA	27:3:210:THR:CG2	2.05	0.85
23:W:59:TYR:CD2	23:W:62:ALA:HB2	2.12	0.85
1:A:324:GLY:HA2	13:M:90:ALA:HB3	1.57	0.85
2:B:751:LEU:HD12	2:B:808:SER:HB3	1.56	0.85
16:P:206:GLU:CG	16:P:236:LYS:NZ	2.36	0.85
26:2:221:GLN:HG2	26:2:268:PHE:CZ	2.11	0.85
5:E:64:HIS:CD2	5:E:70:ASP:H	1.95	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:297:LYS:HB3	16:P:298:PRO:HD2	1.59	0.84
27:3:124:ILE:HD13	27:3:125:LYS:N	1.91	0.84
1:A:930:LEU:O	1:A:931:ARG:O	1.94	0.84
2:B:179:LEU:HD11	2:B:771:GLU:HG2	1.59	0.84
23:W:298:ALA:HA	23:W:421:PHE:CD2	2.12	0.84
26:2:159:VAL:HG22	26:2:160:LEU:H	1.41	0.84
1:A:271:ARG:NE	13:M:73:PRO:CG	2.40	0.84
1:A:477:LEU:HD11	1:A:483:ARG:HD3	1.58	0.84
27:3:49:LEU:HB3	27:3:101:TYR:CB	2.05	0.84
27:3:144:ILE:CD1	27:3:147:MET:HE3	2.07	0.84
8:H:85:ALA:HA	8:H:87:GLN:OE1	1.78	0.84
25:1:2:VAL:CG1	26:2:422:LEU:CD1	2.55	0.84
27:3:49:LEU:CB	27:3:101:TYR:HB3	2.05	0.84
5:E:62:VAL:CG2	5:E:72:MET:HB3	2.07	0.84
26:2:78:GLU:O	26:2:81:LYS:HG2	1.77	0.84
1:A:608:THR:C	1:A:610:PRO:HD2	1.98	0.84
1:A:1313:GLN:HE22	1:A:1318:LYS:HE2	1.41	0.84
17:Q:109:HIS:HA	18:R:234:GLU:OE1	1.76	0.84
26:2:176:ALA:CB	26:2:178:LEU:HD13	2.07	0.84
26:2:177:GLN:HA	26:2:220:LEU:HD21	1.56	0.84
27:3:58:ALA:HA	27:3:71:TYR:CE2	2.12	0.84
26:2:221:GLN:NE2	26:2:230:LEU:HB2	1.93	0.84
17:Q:109:HIS:CG	18:R:224:THR:CB	2.61	0.84
26:2:159:VAL:HG22	26:2:160:LEU:CD1	2.08	0.84
26:2:229:ASP:O	26:2:233:ILE:HG12	1.78	0.84
2:B:91:ILE:HG22	20:T:141:LEU:HD12	1.56	0.83
26:2:118:LEU:CD2	27:3:39:ASP:HA	2.07	0.83
27:3:184:ALA:HA	27:3:187:GLN:HG2	1.57	0.83
1:A:927:GLU:HB3	1:A:931:ARG:HG3	0.84	0.83
26:2:160:LEU:HD23	26:2:206:LEU:CD2	2.07	0.83
17:Q:23:ARG:CZ	18:R:209:GLN:H	1.91	0.83
26:2:118:LEU:HD12	26:2:119:ARG:N	1.92	0.83
1:A:609:HIS:N	1:A:610:PRO:CD	2.41	0.83
22:V:516:PRO:CG	25:1:15:ALA:HB1	1.95	0.83
22:V:516:PRO:HG3	25:1:15:ALA:HB2	1.57	0.83
22:V:531:ILE:HG23	22:V:534:TYR:HH	1.42	0.83
25:1:52:VAL:HG23	25:1:53:LEU:HD12	1.59	0.83
26:2:57:MET:HA	26:2:60:LEU:CD1	2.09	0.83
2:B:80:GLU:HB2	2:B:135:GLU:HB2	0.86	0.83
13:M:94:ASP:O	13:M:97:GLY:CA	2.27	0.83
26:2:167:PRO:O	26:2:171:VAL:HG23	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:94:ASP:HB2	13:M:99:SER:H	1.44	0.83
26:2:30:VAL:CB	27:3:25:GLN:HB2	2.07	0.83
26:2:160:LEU:O	26:2:164:VAL:HG23	1.79	0.83
27:3:196:LEU:HD21	27:3:223:LEU:CD2	2.09	0.83
22:V:703:PHE:HZ	22:V:712:LEU:HD22	1.44	0.83
1:A:326:PRO:HB3	13:M:86:LYS:O	1.78	0.82
18:R:195:PRO:HB2	18:R:199:LYS:CD	2.09	0.82
22:V:315:VAL:HG12	23:W:500:ASP:HB2	1.54	0.82
22:V:612:ASP:C	22:V:614:SER:H	1.83	0.82
25:1:9:LEU:HB2	25:1:51:ASN:HD21	1.43	0.82
26:2:28:PRO:CA	27:3:25:GLN:HA	2.08	0.82
26:2:259:LEU:HD12	26:2:260:ASN:N	1.94	0.82
27:3:57:LEU:HD23	27:3:58:ALA:N	1.91	0.82
13:M:92:SER:O	13:M:93:PHE:O	1.96	0.82
22:V:516:PRO:CD	22:V:706:LYS:HZ3	1.92	0.82
26:2:86:SER:HB3	26:2:140:LYS:HE2	1.60	0.82
1:A:153:ILE:O	1:A:154:CYS:C	2.18	0.82
1:A:271:ARG:HG2	13:M:73:PRO:CG	2.10	0.82
2:B:1117:HIS:HB2	2:B:1127:ILE:HD13	1.61	0.82
25:1:47:ALA:HB2	25:1:50:VAL:HB	1.61	0.82
1:A:999:ARG:HE	8:H:99:ILE:HD12	1.43	0.82
5:E:55:ARG:HG2	5:E:76:PHE:CB	2.10	0.82
27:3:12:VAL:HG21	27:3:161:ILE:HG12	1.61	0.82
22:V:321:GLU:HB2	23:W:499:ASN:OD1	1.78	0.82
22:V:523:VAL:HG21	25:1:20:LEU:HG	1.61	0.82
26:2:100:LEU:HG	26:2:119:ARG:HE	1.45	0.82
26:2:221:GLN:OE1	26:2:224:GLN:HA	1.80	0.82
25:1:52:VAL:CG2	25:1:53:LEU:HD12	2.09	0.82
1:A:1251:ASN:ND2	21:U:227:GLU:HB3	1.95	0.82
1:A:1251:ASN:HA	21:U:234:LYS:HE3	1.61	0.82
26:2:174:ASP:OD1	26:2:179:LEU:HD12	1.80	0.82
1:A:204:HIS:O	1:A:205:VAL:C	2.18	0.81
26:2:174:ASP:O	26:2:220:LEU:HD23	1.79	0.81
3:C:135:ARG:O	3:C:136:ASP:HB3	1.79	0.81
25:1:59:GLU:OE1	26:2:402:ARG:NH1	2.13	0.81
26:2:117:ASN:OD1	27:3:108:ASN:CG	2.18	0.81
17:Q:24:GLY:CA	18:R:210:PHE:HE2	1.92	0.81
15:O:3:TYR:C	15:O:5:LEU:H	1.83	0.81
26:2:175:LEU:HB3	26:2:216:MET:SD	2.20	0.81
27:3:58:ALA:C	27:3:71:TYR:CE1	2.53	0.81
27:3:12:VAL:CG2	27:3:161:ILE:HG12	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:GLN:NE2	1:A:1318:LYS:HB2	1.95	0.81
2:B:133:ILE:HG23	2:B:139:GLN:HG2	1.63	0.81
2:B:223:SER:O	2:B:224:CYS:HB3	1.79	0.81
13:M:179:GLU:CA	20:T:154:LYS:HG2	2.09	0.81
20:T:177:ARG:O	20:T:179:ASP:N	2.14	0.81
22:V:612:ASP:OD2	22:V:635:GLN:OE1	1.98	0.81
1:A:595:ILE:HG21	1:A:675:VAL:HG21	1.62	0.81
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.12	0.81
18:R:195:PRO:HB2	18:R:199:LYS:HD2	1.63	0.81
23:W:59:TYR:CD1	23:W:62:ALA:HB2	2.16	0.81
5:E:64:HIS:NE2	5:E:69:THR:CB	2.42	0.81
25:1:50:VAL:HG12	25:1:54:GLN:HG2	1.62	0.81
1:A:199:TYR:OH	13:M:93:PHE:CZ	2.33	0.80
26:2:37:HIS:HB3	26:2:38:PRO:HD3	1.61	0.80
25:1:34:ILE:HG22	25:1:46:ILE:HD11	1.63	0.80
27:3:216:LYS:H	27:3:216:LYS:HD2	1.43	0.80
26:2:256:ASP:O	26:2:259:LEU:HG	1.82	0.80
1:A:1319:LYS:CD	1:A:1356:ARG:NH1	2.43	0.80
8:H:100:GLU:HG3	8:H:101:GLY:H	1.45	0.80
26:2:30:VAL:HG23	27:3:25:GLN:OE1	1.81	0.80
17:Q:105:TYR:CE1	17:Q:109:HIS:CE1	2.70	0.80
25:1:9:LEU:CD1	25:1:48:GLU:HA	2.09	0.80
1:A:1022:ILE:H	1:A:1034:GLN:HE22	1.29	0.80
2:B:290:TYR:HB3	2:B:562:ALA:HB1	1.62	0.80
26:2:30:VAL:CG2	27:3:25:GLN:OE1	2.29	0.80
26:2:42:LEU:HD12	26:2:59:MET:CE	2.11	0.80
26:2:251:VAL:HG11	26:2:254:MET:HG3	1.62	0.80
27:3:214:TYR:O	27:3:215:LEU:HD23	1.82	0.80
26:2:35:TYR:CD1	26:2:62:LEU:HG	2.16	0.80
27:3:11:LEU:CD2	27:3:160:ARG:HG2	2.12	0.80
27:3:121:LYS:O	27:3:124:ILE:HB	1.81	0.80
1:A:1123:ARG:NH2	1:A:1381:GLU:OE1	2.14	0.80
22:V:674:THR:CG2	26:2:392:ARG:CZ	2.59	0.80
26:2:93:LEU:HA	26:2:96:TRP:CD1	2.17	0.80
2:B:631:GLN:HB3	2:B:685:LYS:HE2	1.64	0.80
17:Q:109:HIS:CB	18:R:224:THR:HB	2.11	0.80
2:B:728:MET:HE2	2:B:942:LYS:HG2	1.64	0.79
25:1:1:MET:HE2	26:2:440:LEU:HD13	1.64	0.79
26:2:224:GLN:HB2	26:2:268:PHE:CE2	2.17	0.79
27:3:165:LYS:HE2	27:3:167:ALA:O	1.81	0.79
29:Y:36:DA:C4	29:Y:37:DG:C5	2.70	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:TRP:CE2	2:B:762:ARG:HG2	2.18	0.79
2:B:1068:GLN:O	2:B:1072:ARG:N	2.15	0.79
1:A:199:TYR:CZ	13:M:93:PHE:CE2	2.70	0.79
5:E:62:VAL:HG23	5:E:72:MET:HB3	1.61	0.79
16:P:162:VAL:O	16:P:163:PRO:C	2.20	0.79
27:3:64:ILE:HG23	27:3:128:HIS:CD2	2.17	0.79
1:A:427:ILE:HG12	13:M:38:GLY:O	1.82	0.79
2:B:882:SER:O	2:B:887:TYR:CE1	2.35	0.79
25:1:1:MET:CB	26:2:413:LEU:CB	2.60	0.79
27:3:14:VAL:CG2	27:3:163:VAL:HG22	2.13	0.79
4:D:54:GLU:OE2	7:G:28:GLN:NE2	2.15	0.79
9:I:85:PRO:O	9:I:86:CYS:O	2.00	0.79
24:0:55:LEU:HD12	27:3:178:MET:HE3	1.61	0.79
25:1:13:ASP:OD2	25:1:17:LYS:CB	2.30	0.79
9:I:14:ILE:HG12	9:I:16:PHE:CG	2.18	0.79
13:M:179:GLU:HG2	20:T:154:LYS:HE3	1.65	0.79
14:N:332:GLU:HG2	15:O:92:LYS:HB3	1.63	0.79
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.13	0.79
17:Q:102:VAL:CG1	17:Q:103:VAL:N	2.12	0.79
26:2:205:LEU:O	26:2:209:PRO:HD2	1.81	0.79
17:Q:70:LYS:NZ	18:R:226:ASP:O	2.16	0.79
17:Q:111:ARG:NH1	17:Q:188:TYR:OH	2.16	0.79
27:3:222:SER:O	27:3:225:GLN:HG2	1.83	0.79
2:B:92:TYR:CD2	20:T:145:LEU:HD13	2.18	0.79
25:1:1:MET:HA	26:2:414:SER:H	1.46	0.79
26:2:52:ALA:O	26:2:56:VAL:HG13	1.81	0.79
9:I:57:LYS:O	9:I:59:THR:HG23	1.83	0.79
2:B:483:ARG:HH11	2:B:526:LEU:HB2	1.48	0.78
17:Q:180:PHE:CE2	18:R:211:SER:HB3	2.09	0.78
27:3:151:VAL:HG12	27:3:155:GLN:O	1.84	0.78
1:A:1319:LYS:HD3	1:A:1356:ARG:NH1	1.97	0.78
17:Q:105:TYR:CE1	18:R:231:GLU:HG3	2.14	0.78
20:T:142:SER:O	20:T:144:GLN:N	2.15	0.78
20:T:145:LEU:O	20:T:147:LYS:N	2.14	0.78
27:3:58:ALA:HA	27:3:71:TYR:CZ	2.18	0.78
1:A:609:HIS:N	1:A:610:PRO:HD2	1.99	0.78
25:1:34:ILE:CG2	25:1:46:ILE:HD11	2.13	0.78
25:1:38:ILE:HA	25:1:44:PHE:HD1	1.48	0.78
26:2:77:LYS:HD3	26:2:78:GLU:N	1.97	0.78
26:2:181:GLN:OE1	26:2:229:ASP:HB2	1.83	0.78
26:2:203:PHE:CD2	26:2:205:LEU:HD23	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLU:OE1	1:A:48:GLU:HG3	1.84	0.78
1:A:45:GLU:OE1	1:A:48:GLU:CG	2.32	0.78
2:B:803:ARG:NH2	2:B:951:GLN:OE1	2.16	0.78
9:I:14:ILE:HG13	9:I:16:PHE:CD2	2.18	0.78
26:2:118:LEU:CD1	27:3:39:ASP:OD1	2.31	0.78
26:2:118:LEU:CG	27:3:39:ASP:OD1	2.32	0.78
26:2:163:MET:HE2	26:2:206:LEU:HD12	1.66	0.78
2:B:714:PRO:HD2	2:B:1001:PRO:HB3	1.64	0.78
17:Q:23:ARG:CZ	18:R:209:GLN:N	2.46	0.78
17:Q:29:GLU:CD	18:R:194:ARG:NH2	2.31	0.78
17:Q:109:HIS:CE1	18:R:224:THR:OG1	2.37	0.78
22:V:523:VAL:CB	25:1:20:LEU:HD23	2.14	0.78
22:V:703:PHE:CZ	22:V:712:LEU:HD22	2.18	0.78
23:W:419:GLU:CB	23:W:420:PRO:CD	2.46	0.78
25:1:1:MET:HB3	26:2:413:LEU:HD23	1.65	0.78
26:2:207:ASP:O	26:2:211:GLN:HG2	1.84	0.78
26:2:234:LEU:O	26:2:234:LEU:HD23	1.83	0.78
21:U:231:ASP:O	21:U:232:GLU:HG3	1.81	0.78
26:2:190:PRO:O	26:2:194:PRO:HD2	1.83	0.78
26:2:211:GLN:CG	26:2:257:SER:HB3	2.13	0.78
5:E:64:HIS:CD2	5:E:70:ASP:N	2.52	0.78
23:W:424:ARG:O	23:W:425:THR:CG2	2.32	0.78
26:2:34:LEU:O	26:2:38:PRO:HD2	1.84	0.78
26:2:196:ILE:CD1	26:2:210:ALA:HB2	2.13	0.78
26:2:53:LYS:O	26:2:56:VAL:HG22	1.84	0.78
26:2:159:VAL:HG13	26:2:161:HIS:N	1.96	0.78
26:2:189:GLU:HB2	26:2:190:PRO:HD3	1.66	0.78
27:3:147:MET:O	27:3:151:VAL:HG23	1.84	0.78
2:B:225:LEU:O	2:B:227:ASN:N	2.15	0.78
17:Q:23:ARG:HH12	18:R:209:GLN:HB2	1.47	0.78
2:B:79:GLU:C	2:B:80:GLU:HG3	2.04	0.77
5:E:61:LEU:HD13	5:E:73:PHE:HD1	1.49	0.77
25:1:13:ASP:OD1	25:1:14:PRO:HD2	1.83	0.77
26:2:221:GLN:HE22	26:2:230:LEU:HB2	1.47	0.77
27:3:59:VAL:HG11	27:3:71:TYR:HD1	1.41	0.77
2:B:133:ILE:CD1	2:B:139:GLN:HB3	2.07	0.77
7:G:111:HIS:NE2	17:Q:124:ARG:O	2.18	0.77
24:0:54:ARG:NE	27:3:182:PHE:HE1	1.73	0.77
25:1:1:MET:HG3	26:2:415:GLN:O	1.85	0.77
25:1:10:ILE:CG2	26:2:407:VAL:HG21	2.15	0.77
26:2:30:VAL:HG23	27:3:25:GLN:CG	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:316:SER:OG	16:P:235:ARG:NH1	2.17	0.77
17:Q:109:HIS:CG	18:R:224:THR:HB	2.19	0.77
27:3:185:GLN:HA	27:3:185:GLN:HE21	1.48	0.77
2:B:735:VAL:HG22	2:B:750:VAL:HG13	1.67	0.77
22:V:516:PRO:CD	25:1:15:ALA:HB3	2.11	0.77
26:2:163:MET:CE	26:2:206:LEU:HD12	2.14	0.77
27:3:185:GLN:NE2	27:3:210:THR:HA	2.00	0.77
1:A:608:THR:CB	1:A:610:PRO:HD2	2.14	0.77
25:1:38:ILE:HG22	25:1:44:PHE:CD1	2.19	0.77
26:2:179:LEU:HB3	26:2:184:LEU:HD11	1.65	0.77
26:2:208:THR:HG23	26:2:209:PRO:HD3	1.66	0.77
26:2:211:GLN:HA	26:2:261:PHE:HZ	1.49	0.77
26:2:42:LEU:HD21	26:2:55:TRP:CB	2.10	0.77
1:A:199:TYR:CZ	13:M:93:PHE:HZ	2.01	0.76
1:A:648:SER:O	1:A:651:SER:OG	2.02	0.76
1:A:1114:ALA:O	1:A:1116:ASN:N	2.13	0.76
18:R:190:LEU:HD12	18:R:205:ASP:OD2	1.86	0.76
26:2:44:VAL:HG13	26:2:45:PHE:CD1	2.20	0.76
27:3:59:VAL:CA	27:3:71:TYR:CE1	2.67	0.76
22:V:674:THR:CG2	26:2:392:ARG:NH2	2.43	0.76
25:1:1:MET:CE	26:2:440:LEU:HD13	2.16	0.76
5:E:40:PHE:CE2	5:E:46:ASP:OD2	2.38	0.76
5:E:51:GLY:C	5:E:52:ARG:HG3	2.01	0.76
24:0:54:ARG:HB2	27:3:209:ILE:CG2	2.14	0.76
1:A:199:TYR:CE1	13:M:93:PHE:CZ	2.73	0.76
1:A:271:ARG:CD	13:M:73:PRO:HG3	2.07	0.76
26:2:117:ASN:HD21	27:3:108:ASN:HB3	1.47	0.76
26:2:208:THR:HG23	26:2:209:PRO:CD	2.16	0.76
27:3:172:LEU:HD13	27:3:172:LEU:O	1.86	0.76
1:A:331:LYS:NZ	29:Y:63:DG:O6	2.19	0.76
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.17	0.76
2:B:896:LEU:HD21	2:B:901:THR:HG21	1.65	0.76
13:M:47:ASP:C	13:M:49:GLY:N	2.39	0.76
27:3:190:LEU:HD23	27:3:190:LEU:H	1.51	0.76
26:2:177:GLN:CD	26:2:220:LEU:HD22	2.06	0.76
16:P:206:GLU:C	16:P:208:ARG:H	1.89	0.76
27:3:14:VAL:CG2	27:3:163:VAL:HA	2.16	0.76
2:B:490:GLY:O	2:B:491:ARG:CB	2.33	0.76
10:J:64:PRO:C	10:J:66:GLU:N	2.34	0.76
17:Q:39:ARG:NH2	18:R:159:ASP:OD2	2.18	0.76
22:V:444:HIS:O	22:V:447:PRO:HD2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:528:LYS:HE2	29:Y:25:DT:H5''	1.65	0.76
27:3:58:ALA:N	27:3:71:TYR:CZ	2.51	0.76
1:A:927:GLU:HG2	1:A:931:ARG:HH11	1.50	0.75
14:N:320:VAL:HG11	16:P:236:LYS:HG2	1.68	0.75
17:Q:108:ASP:C	18:R:234:GLU:OE2	2.25	0.75
22:V:516:PRO:HA	25:1:15:ALA:C	2.04	0.75
22:V:523:VAL:HG11	25:1:20:LEU:HD23	1.64	0.75
22:V:534:TYR:CE1	22:V:535:THR:OG1	2.39	0.75
26:2:86:SER:HB3	26:2:140:LYS:CE	2.16	0.75
26:2:218:GLN:NE2	26:2:265:LEU:HA	2.00	0.75
1:A:131:ALA:O	1:A:133:SER:N	2.18	0.75
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.17	0.75
9:I:14:ILE:CG1	9:I:16:PHE:CD2	2.70	0.75
17:Q:24:GLY:C	18:R:210:PHE:HE2	1.89	0.75
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.21	0.75
25:1:1:MET:HB3	26:2:413:LEU:CD2	2.15	0.75
25:1:38:ILE:H	25:1:38:ILE:HD13	1.50	0.75
26:2:118:LEU:HD22	27:3:39:ASP:HA	1.65	0.75
17:Q:105:TYR:HE1	18:R:231:GLU:CB	2.00	0.75
25:1:1:MET:SD	26:2:413:LEU:HB3	2.25	0.75
1:A:1251:ASN:CG	21:U:227:GLU:HB3	2.07	0.75
17:Q:105:TYR:O	17:Q:109:HIS:HD2	1.69	0.75
25:1:2:VAL:CG1	26:2:456:LYS:CG	2.53	0.75
1:A:326:PRO:HB3	13:M:86:LYS:C	2.07	0.75
1:A:375:ILE:HB	1:A:666:ARG:HD2	1.67	0.75
26:2:127:LYS:N	26:2:178:LEU:HD23	2.01	0.75
26:2:234:LEU:CD2	26:2:237:LEU:HD12	2.14	0.75
2:B:462:ALA:HB2	28:X:40:DT:H5''	1.67	0.75
11:K:39:ASP:OD1	11:K:39:ASP:N	2.18	0.75
23:W:144:ALA:HA	23:W:148:HIS:C	2.06	0.75
25:1:24:ASP:OD2	25:1:57:VAL:HG11	1.85	0.75
26:2:243:SER:HB3	26:2:258:LEU:HD22	1.69	0.75
27:3:8:LEU:HD23	27:3:54:SER:HB3	1.68	0.75
27:3:11:LEU:HD22	27:3:160:ARG:CG	2.16	0.75
1:A:611:ASP:OD2	1:A:627:LYS:CE	2.34	0.75
22:V:611:GLY:HA2	22:V:615:PHE:HB3	1.68	0.75
26:2:180:SER:O	26:2:184:LEU:HG	1.87	0.75
2:B:80:GLU:CB	2:B:135:GLU:CG	2.48	0.75
26:2:117:ASN:CG	27:3:42:MET:CE	2.55	0.75
1:A:326:PRO:HA	13:M:87:GLY:HA2	1.67	0.74
2:B:490:GLY:O	2:B:491:ARG:HB2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:52:LEU:HB3	17:Q:54:PHE:HD1	1.50	0.74
20:T:177:ARG:C	20:T:179:ASP:N	2.37	0.74
22:V:321:GLU:OE1	23:W:499:ASN:OD1	2.05	0.74
26:2:100:LEU:CD1	26:2:119:ARG:HG3	2.16	0.74
8:H:107:GLU:O	8:H:108:ALA:C	2.26	0.74
27:3:38:ILE:O	27:3:41:VAL:HG12	1.87	0.74
21:U:251:ALA:C	21:U:253:THR:H	1.90	0.74
22:V:523:VAL:HG21	25:1:20:LEU:CD2	2.17	0.74
9:I:14:ILE:CG1	9:I:16:PHE:CE2	2.66	0.74
16:P:206:GLU:CB	16:P:236:LYS:HZ2	2.01	0.74
25:1:1:MET:HB2	26:2:418:PHE:CB	2.18	0.74
26:2:196:ILE:HD11	26:2:210:ALA:CB	2.17	0.74
17:Q:51:LEU:HD11	18:R:163:LEU:CD1	2.05	0.74
23:W:608:ILE:HG23	23:W:614:TYR:CE2	2.22	0.74
27:3:133:LEU:HD23	27:3:177:PHE:HD1	1.50	0.74
13:M:91:ALA:O	13:M:92:SER:CB	2.35	0.74
26:2:53:LYS:HE3	26:2:95:ILE:HD11	1.67	0.74
23:W:430:ASN:HB3	23:W:431:PRO:CD	2.16	0.74
26:2:35:TYR:CD2	26:2:62:LEU:HB3	2.22	0.74
26:2:51:LEU:HD23	26:2:51:LEU:O	1.87	0.74
27:3:57:LEU:C	27:3:71:TYR:CZ	2.60	0.74
1:A:326:PRO:CB	13:M:87:GLY:CA	2.56	0.74
26:2:132:ASP:O	26:2:135:GLN:HG2	1.88	0.74
26:2:160:LEU:HA	26:2:206:LEU:HD11	1.70	0.74
2:B:56:GLN:OE1	20:T:141:LEU:HB2	1.88	0.73
17:Q:23:ARG:NE	18:R:207:SER:O	2.20	0.73
23:W:421:PHE:CE1	23:W:423:ASP:CG	2.60	0.73
1:A:1177:TYR:H	9:I:51:SER:HB3	1.53	0.73
2:B:988:LYS:NZ	2:B:1026:GLU:OE2	2.17	0.73
14:N:341:LYS:HB3	14:N:352:HIS:HB2	1.68	0.73
1:A:117:LEU:N	1:A:232:GLU:OE2	2.19	0.73
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	1.70	0.73
27:3:141:LEU:O	27:3:144:ILE:HG22	1.89	0.73
17:Q:100:VAL:O	17:Q:102:VAL:N	2.20	0.73
22:V:523:VAL:CG1	25:1:20:LEU:HD23	2.19	0.73
25:1:34:ILE:HD13	25:1:54:GLN:OE1	1.88	0.73
26:2:251:VAL:HG11	26:2:254:MET:CG	2.18	0.73
27:3:214:TYR:HE2	27:3:216:LYS:HE2	1.53	0.73
25:1:34:ILE:HG12	25:1:50:VAL:CG1	2.18	0.73
1:A:197:GLU:OE2	13:M:93:PHE:CD2	2.41	0.73
22:V:516:PRO:HG2	22:V:706:LYS:CE	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:667:THR:HA	25:1:62:ASP:OD1	1.89	0.73
1:A:1319:LYS:HD2	1:A:1356:ARG:HH12	1.53	0.73
2:B:914:GLU:OE1	2:B:914:GLU:N	2.21	0.73
3:C:274:ILE:HD12	11:K:84:GLN:HB3	1.69	0.73
8:H:85:ALA:O	8:H:87:GLN:CD	2.26	0.73
25:1:9:LEU:HD22	25:1:51:ASN:ND2	2.04	0.73
26:2:172:SER:HA	26:2:175:LEU:CD2	2.19	0.73
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.71	0.73
18:R:194:ARG:O	18:R:196:ASP:O	2.06	0.73
27:3:226:TYR:HA	27:3:230:VAL:HG23	1.71	0.73
5:E:47:LYS:CE	5:E:52:ARG:HB2	2.18	0.73
8:H:146:LYS:HE2	8:H:147:LYS:HG3	1.71	0.72
17:Q:102:VAL:HG13	17:Q:103:VAL:H	0.60	0.72
22:V:516:PRO:CB	22:V:706:LYS:NZ	2.48	0.72
25:1:1:MET:HG3	26:2:418:PHE:HB2	1.69	0.72
25:1:5:LEU:HD21	26:2:408:LEU:HD13	0.87	0.72
26:2:237:LEU:O	26:2:240:LEU:HD13	1.88	0.72
27:3:111:ILE:HG13	27:3:112:VAL:N	2.02	0.72
23:W:59:TYR:CD2	23:W:62:ALA:CB	2.71	0.72
26:2:41:CYS:O	26:2:44:VAL:HG12	1.88	0.72
26:2:60:LEU:HD11	26:2:95:ILE:HB	1.71	0.72
26:2:218:GLN:HE22	26:2:265:LEU:HA	1.54	0.72
26:2:243:SER:HB2	26:2:258:LEU:HD22	1.71	0.72
22:V:504:LYS:HB3	22:V:654:GLU:O	1.89	0.72
26:2:117:ASN:HB3	27:3:42:MET:CE	2.18	0.72
27:3:12:VAL:HG23	27:3:161:ILE:HG23	1.70	0.72
29:Y:36:DA:C4	29:Y:37:DG:C8	2.78	0.72
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.71	0.72
3:C:40:ALA:HB1	3:C:171:LYS:HB3	1.70	0.72
10:J:64:PRO:O	10:J:66:GLU:N	2.21	0.72
16:P:162:VAL:O	16:P:164:GLN:NE2	2.21	0.72
17:Q:23:ARG:NH1	18:R:209:GLN:HB2	2.03	0.72
21:U:231:ASP:C	21:U:232:GLU:HG2	2.09	0.72
26:2:175:LEU:HD22	26:2:216:MET:SD	2.29	0.72
26:2:198:SER:HG	26:2:238:PHE:HE2	1.37	0.72
26:2:199:ALA:HB3	26:2:202:GLN:NE2	2.02	0.72
3:C:240:ARG:NH1	3:C:242:GLU:OE2	2.23	0.72
20:T:154:LYS:HD2	20:T:154:LYS:H	1.52	0.72
8:H:66:GLU:O	8:H:67:ASP:CB	2.38	0.72
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.69	0.72
16:P:167:ASN:ND2	29:Y:79:DT:O2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:25:GLU:CD	25:1:35:ILE:HG12	2.09	0.72
26:2:42:LEU:HD12	26:2:59:MET:HE3	1.71	0.72
27:3:69:PHE:CE1	27:3:139:LYS:HD2	2.25	0.72
27:3:148:ASN:CB	27:3:157:MET:HE2	2.20	0.72
27:3:222:SER:HB2	27:3:226:TYR:HE2	1.54	0.72
22:V:315:VAL:HG12	23:W:500:ASP:CB	2.17	0.72
23:W:73:CYS:HB2	23:W:209:TYR:CZ	2.24	0.72
26:2:118:LEU:HD22	27:3:39:ASP:CA	2.19	0.72
24:0:76:LEU:O	24:0:77:LYS:O	2.08	0.72
25:1:2:VAL:HG12	26:2:422:LEU:HD13	1.72	0.72
1:A:927:GLU:C	1:A:931:ARG:HG3	2.09	0.72
2:B:874:PRO:O	2:B:877:GLU:OE1	2.08	0.72
26:2:117:ASN:HB2	27:3:104:LEU:HD11	1.71	0.72
27:3:217:VAL:HG13	27:3:226:TYR:CZ	2.25	0.72
26:2:134:SER:O	26:2:138:PRO:HD2	1.89	0.71
27:3:59:VAL:CB	27:3:71:TYR:HE1	1.93	0.71
27:3:66:GLU:CA	27:3:132:LEU:HD12	2.13	0.71
23:W:584:TYR:HD1	23:W:594:ALA:HB2	1.52	0.71
26:2:35:TYR:CG	26:2:62:LEU:HD12	2.25	0.71
26:2:192:GLU:HG3	26:2:193:PRO:CD	2.18	0.71
17:Q:110:MET:SD	18:R:222:SER:HB2	2.30	0.71
17:Q:180:PHE:HZ	18:R:211:SER:HA	1.55	0.71
22:V:519:TYR:HE2	25:1:20:LEU:HG	1.53	0.71
22:V:689:VAL:HB	26:2:391:ILE:HD11	1.69	0.71
26:2:171:VAL:HG12	26:2:216:MET:SD	2.30	0.71
23:W:696:TRP:CD1	23:W:697:ILE:HG13	2.25	0.71
23:W:209:TYR:OH	23:W:234:ASP:N	2.23	0.71
25:1:1:MET:HG2	26:2:413:LEU:HB3	1.71	0.71
25:1:28:ALA:HB3	25:1:31:LYS:HB2	1.71	0.71
27:3:165:LYS:HG3	27:3:203:LEU:CD1	2.20	0.71
1:A:960:ARG:NH2	1:A:961:GLU:OE2	2.24	0.71
3:C:135:ARG:O	3:C:136:ASP:CB	2.38	0.71
22:V:648:LYS:O	22:V:650:MET:N	2.24	0.71
1:A:1319:LYS:CG	1:A:1333:GLU:CG	2.60	0.71
2:B:1085:ARG:NH2	29:Y:53:DG:OP2	2.24	0.71
21:U:229:ALA:HB1	21:U:234:LYS:HB3	1.72	0.71
25:1:18:GLN:CB	25:1:44:PHE:HE2	2.00	0.71
26:2:118:LEU:CD2	27:3:39:ASP:CA	2.68	0.71
3:C:67:ARG:HH12	10:J:2:ILE:HG13	1.55	0.71
5:E:10:LEU:HD21	5:E:55:ARG:HH21	1.55	0.71
22:V:523:VAL:HG21	25:1:20:LEU:CG	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:57:LEU:C	27:3:71:TYR:CE2	2.63	0.71
1:A:1112:VAL:HB	21:U:252:LYS:O	1.90	0.70
26:2:86:SER:CB	26:2:140:LYS:HE2	2.20	0.70
1:A:206:ASN:C	1:A:208:ASP:H	1.94	0.70
4:D:90:LYS:HE2	4:D:130:ILE:HD11	1.72	0.70
5:E:51:GLY:O	5:E:52:ARG:HG2	1.84	0.70
13:M:44:ARG:HE	13:M:46:ILE:HG22	1.53	0.70
23:W:589:GLU:O	23:W:594:ALA:HB1	1.91	0.70
25:1:29:LEU:HD23	25:1:30:GLY:N	2.06	0.70
3:C:137:ASN:HB2	3:C:145:GLN:NE2	1.99	0.70
27:3:177:PHE:CZ	27:3:203:LEU:HD23	2.27	0.70
2:B:777:ASN:O	10:J:47:ARG:NH1	2.24	0.70
2:B:874:PRO:O	2:B:876:ASN:N	2.24	0.70
22:V:516:PRO:CD	22:V:706:LYS:NZ	2.54	0.70
5:E:48:PRO:O	5:E:49:SER:CB	2.39	0.70
9:I:62:VAL:O	9:I:63:ASP:C	2.30	0.70
22:V:515:SER:HB3	22:V:539:ASN:ND2	2.05	0.70
1:A:199:TYR:CE1	13:M:93:PHE:HZ	2.08	0.70
26:2:218:GLN:OE1	26:2:265:LEU:HA	1.92	0.70
27:3:59:VAL:N	27:3:71:TYR:CD1	2.59	0.70
2:B:76:GLY:O	2:B:77:GLU:CB	2.40	0.70
5:E:52:ARG:CB	5:E:53:PRO:HD3	2.11	0.70
22:V:528:LYS:CE	29:Y:25:DT:H5"	2.21	0.70
23:W:209:TYR:HE1	23:W:233:PHE:CD1	2.09	0.70
25:1:2:VAL:HG12	26:2:456:LYS:HE2	1.74	0.70
24:0:54:ARG:NE	27:3:182:PHE:CD1	2.60	0.70
1:A:1192:TRP:HE3	1:A:1192:TRP:H	1.40	0.70
27:3:133:LEU:HD22	27:3:134:ALA:H	1.56	0.70
28:X:65:DG:C2	29:Y:30:DG:C2	2.80	0.70
1:A:79:THR:HG23	13:M:43:ASP:OD1	1.92	0.69
2:B:80:GLU:OE1	2:B:135:GLU:C	2.30	0.69
9:I:14:ILE:HG12	9:I:16:PHE:CD1	2.26	0.69
22:V:519:TYR:CE2	25:1:20:LEU:CG	2.72	0.69
25:1:8:VAL:HG11	25:1:45:VAL:HG12	1.74	0.69
27:3:162:LEU:HA	27:3:192:ASP:OD1	1.92	0.69
2:B:48:ASP:OD1	2:B:159:THR:OG1	2.09	0.69
26:2:163:MET:O	26:2:167:PRO:HD2	1.91	0.69
26:2:189:GLU:HA	26:2:192:GLU:HG2	1.72	0.69
2:B:52:GLN:HE22	20:T:142:SER:HB2	1.55	0.69
2:B:69:ALA:HB2	2:B:423:ILE:HB	1.73	0.69
17:Q:105:TYR:CZ	17:Q:109:HIS:NE2	2.53	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:516:PRO:HB2	22:V:706:LYS:NZ	2.07	0.69
23:W:59:TYR:CE1	23:W:62:ALA:HB2	2.27	0.69
3:C:212:ASP:C	3:C:214:ASP:N	2.38	0.69
22:V:674:THR:OG1	26:2:392:ARG:NE	2.26	0.69
23:W:298:ALA:HA	23:W:421:PHE:HE2	1.55	0.69
26:2:185:MET:SD	26:2:232:GLU:HB2	2.32	0.69
27:3:69:PHE:CZ	27:3:139:LYS:HD2	2.27	0.69
5:E:10:LEU:HD21	5:E:55:ARG:HE	1.56	0.69
9:I:61:GLU:O	9:I:63:ASP:N	2.25	0.69
16:P:206:GLU:O	16:P:208:ARG:N	2.25	0.69
25:1:1:MET:CG	26:2:415:GLN:O	2.41	0.69
2:B:74:ALA:CB	20:T:201:ASP:HB3	2.22	0.69
2:B:295:PRO:HB2	9:I:11:PHE:HD2	1.58	0.69
17:Q:180:PHE:HE2	18:R:211:SER:CB	2.00	0.69
26:2:118:LEU:HD11	27:3:43:VAL:HG23	1.75	0.69
22:V:522:TYR:HE2	25:1:62:ASP:CG	1.96	0.69
26:2:117:ASN:CB	27:3:42:MET:HE3	2.21	0.69
26:2:140:LYS:HD3	26:2:162:PHE:HE1	1.58	0.69
26:2:163:MET:CE	26:2:206:LEU:HB3	2.23	0.69
26:2:199:ALA:CB	26:2:202:GLN:HE22	2.02	0.69
1:A:1250:ASP:CG	21:U:227:GLU:HG2	2.10	0.69
1:A:1313:GLN:HE22	1:A:1318:LYS:CE	2.05	0.69
2:B:313:GLU:OE2	19:S:153:ARG:NH2	2.26	0.69
5:E:10:LEU:CD2	5:E:55:ARG:HE	2.05	0.69
25:1:4:VAL:CG1	26:2:411:GLN:O	2.38	0.69
25:1:53:LEU:HD12	25:1:53:LEU:H	1.57	0.69
26:2:130:SER:O	26:2:133:THR:HG22	1.92	0.69
13:M:39:LEU:O	13:M:40:VAL:C	2.31	0.69
22:V:612:ASP:O	22:V:614:SER:N	2.26	0.69
25:1:1:MET:HG2	26:2:413:LEU:C	2.14	0.69
26:2:81:LYS:HD2	26:2:89:LEU:CD2	2.20	0.69
28:X:65:DG:C2	29:Y:30:DG:N2	2.60	0.69
1:A:1313:GLN:NE2	1:A:1318:LYS:HE2	2.08	0.69
13:M:47:ASP:O	13:M:49:GLY:CA	2.40	0.69
17:Q:102:VAL:HG22	17:Q:103:VAL:HG13	1.75	0.69
26:2:81:LYS:HE3	26:2:93:LEU:CD2	2.20	0.69
1:A:551:ARG:NH1	1:A:625:ASP:OD2	2.26	0.68
24:0:54:ARG:CD	27:3:182:PHE:CE1	2.60	0.68
25:1:55:GLU:OE2	26:2:402:ARG:HG3	1.93	0.68
26:2:48:LEU:CB	26:2:49:PRO:HD3	2.19	0.68
26:2:211:GLN:HA	26:2:261:PHE:CE1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ASN:ND2	1:A:272:ASN:O	2.26	0.68
2:B:323:SER:OG	2:B:335:ARG:NH1	2.27	0.68
27:3:215:LEU:HD12	27:3:230:VAL:CG1	2.23	0.68
1:A:266:MET:HG2	1:A:272:ASN:HD22	1.02	0.68
2:B:78:VAL:O	2:B:79:GLU:CB	2.41	0.68
26:2:118:LEU:HD21	27:3:39:ASP:C	2.12	0.68
1:A:49:GLY:O	1:A:52:PRO:HD2	1.92	0.68
22:V:531:ILE:CG2	22:V:534:TYR:CZ	2.64	0.68
26:2:251:VAL:HG12	26:2:254:MET:H	1.58	0.68
27:3:114:GLU:O	27:3:118:LEU:HD23	1.92	0.68
26:2:176:ALA:HB1	26:2:178:LEU:CD1	2.23	0.68
25:1:1:MET:C	26:2:413:LEU:HG	2.12	0.68
1:A:540:ASP:HB2	2:B:790:GLN:NE2	2.09	0.68
3:C:56:SER:HG	3:C:158:GLU:H	1.40	0.68
13:M:44:ARG:NE	13:M:46:ILE:CG2	2.57	0.68
14:N:324:GLU:HA	16:P:188:ARG:HH12	1.58	0.68
20:T:177:ARG:NH2	20:T:212:TYR:HB2	2.09	0.68
22:V:415:HIS:HA	22:V:421:TRP:CD1	2.29	0.68
22:V:612:ASP:C	22:V:614:SER:N	2.46	0.68
25:1:10:ILE:HG21	26:2:407:VAL:HG21	1.76	0.68
1:A:271:ARG:HD2	13:M:73:PRO:HG2	0.70	0.68
1:A:632:ASN:HA	1:A:992:LYS:HD2	1.74	0.68
5:E:54:ARG:HB2	5:E:78:GLU:CD	2.15	0.68
17:Q:102:VAL:HG13	17:Q:103:VAL:HG22	1.76	0.68
1:A:197:GLU:OE1	1:A:308:LYS:NZ	2.26	0.68
3:C:5:ASN:C	3:C:7:PRO:CD	2.39	0.68
25:1:39:ASP:OD1	25:1:43:VAL:HB	1.94	0.68
1:A:207:GLU:O	1:A:209:SER:N	2.28	0.67
1:A:1180:ASN:HB3	9:I:33:ARG:HH22	1.59	0.67
1:A:1319:LYS:HD2	1:A:1356:ARG:NH1	2.07	0.67
2:B:13:ASP:OD1	2:B:636:LYS:NZ	2.27	0.67
2:B:839:GLY:HA3	2:B:891:ASP:HB3	1.76	0.67
13:M:91:ALA:O	13:M:92:SER:HB2	1.94	0.67
17:Q:52:LEU:HB3	17:Q:54:PHE:CD1	2.28	0.67
18:R:195:PRO:O	18:R:199:LYS:HD2	1.93	0.67
26:2:170:ALA:HB1	26:2:213:TRP:CZ3	2.29	0.67
26:2:211:GLN:HB3	26:2:261:PHE:HE1	1.59	0.67
17:Q:51:LEU:CD1	18:R:163:LEU:CD1	2.70	0.67
26:2:172:SER:O	26:2:175:LEU:HD23	1.95	0.67
27:3:187:GLN:HG3	27:3:189:ILE:CG1	2.24	0.67
1:A:111:CYS:SG	1:A:114:CYS:HB3	2.33	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:TYR:CE2	8:H:70:LEU:HB3	2.30	0.67
1:A:608:THR:OG1	1:A:610:PRO:HD2	1.94	0.67
2:B:591:ARG:NH2	2:B:601:VAL:O	2.27	0.67
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.25	0.67
25:1:19:PHE:O	25:1:23:LEU:HG	1.95	0.67
27:3:130:GLU:HB2	27:3:173:GLN:NE2	2.09	0.67
27:3:159:SER:OG	27:3:189:ILE:HD12	1.94	0.67
1:A:326:PRO:HB3	13:M:87:GLY:N	2.09	0.67
27:3:187:GLN:CG	27:3:189:ILE:HG12	2.24	0.67
26:2:56:VAL:O	26:2:60:LEU:HG	1.94	0.67
26:2:118:LEU:HD13	27:3:39:ASP:OD1	1.93	0.67
27:3:22:TRP:O	27:3:25:GLN:CG	2.40	0.67
27:3:111:ILE:O	27:3:115:ILE:HD13	1.94	0.67
1:A:460:ARG:NH2	1:A:493:ASN:HB2	2.10	0.67
2:B:331:THR:HB	2:B:334:LYS:HB2	1.75	0.67
26:2:56:VAL:HG11	26:2:91:SER:HB2	1.77	0.67
26:2:117:ASN:HB3	27:3:42:MET:HE3	1.75	0.67
1:A:1313:GLN:NE2	1:A:1316:ASN:OD1	2.25	0.67
2:B:90:GLN:NE2	20:T:141:LEU:HG	2.06	0.67
1:A:551:ARG:CZ	1:A:625:ASP:OD2	2.43	0.66
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.76	0.66
15:O:3:TYR:HD1	15:O:98:CYS:HG	1.40	0.66
27:3:217:VAL:HG13	27:3:226:TYR:CE2	2.30	0.66
16:P:203:ARG:HH21	16:P:203:ARG:HG3	1.59	0.66
17:Q:102:VAL:CG1	17:Q:103:VAL:HG22	2.25	0.66
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.76	0.66
22:V:415:HIS:CD2	22:V:416:THR:HG23	2.31	0.66
22:V:516:PRO:HB3	25:1:15:ALA:CB	2.05	0.66
25:1:59:GLU:OE2	26:2:402:ARG:CZ	2.41	0.66
1:A:460:ARG:HH21	1:A:493:ASN:HB2	1.61	0.66
2:B:216:ALA:HB2	2:B:241:ALA:HB2	1.77	0.66
2:B:761:THR:H	2:B:764:MET:HE3	1.60	0.66
9:I:84:HIS:CG	9:I:85:PRO:CD	2.68	0.66
21:U:153:ARG:NH2	21:U:166:GLU:OE2	2.28	0.66
23:W:73:CYS:C	23:W:209:TYR:CE2	2.69	0.66
26:2:160:LEU:HD12	26:2:160:LEU:H	1.60	0.66
28:X:45:DC:H42	29:Y:48:DC:H42	1.41	0.66
1:A:271:ARG:HE	13:M:73:PRO:CD	2.09	0.66
1:A:326:PRO:CB	13:M:86:LYS:O	2.43	0.66
18:R:190:LEU:CD1	18:R:205:ASP:CG	2.64	0.66
26:2:117:ASN:HD21	27:3:108:ASN:CA	2.05	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:218:GLN:CG	26:2:268:PHE:HB3	2.26	0.66
27:3:207:CYS:SG	27:3:214:TYR:HB2	2.34	0.66
29:Y:36:DA:C5	29:Y:37:DG:C5	2.83	0.66
25:1:8:VAL:HG12	25:1:9:LEU:N	2.10	0.66
27:3:18:ASN:CG	27:3:20:ILE:HD13	2.15	0.66
1:A:522:PRO:HA	1:A:666:ARG:HH21	1.59	0.66
13:M:94:ASP:CG	13:M:97:GLY:O	2.34	0.66
17:Q:24:GLY:CA	18:R:210:PHE:CD2	2.79	0.66
27:3:146:ARG:O	27:3:149:LYS:HG2	1.96	0.66
27:3:178:MET:HE2	27:3:202:LEU:CD1	2.25	0.66
8:H:106:THR:O	8:H:108:ALA:N	2.29	0.66
18:R:142:LYS:NZ	18:R:172:GLU:OE2	2.26	0.66
25:1:35:ILE:HG22	25:1:46:ILE:HD12	1.78	0.66
26:2:126:GLY:C	26:2:178:LEU:HD23	2.16	0.66
27:3:45:GLY:O	27:3:49:LEU:HD23	1.96	0.66
5:E:64:HIS:HD2	5:E:68:PRO:CA	2.06	0.66
22:V:631:GLY:O	22:V:632:SER:HB3	1.96	0.66
26:2:171:VAL:HG13	26:2:216:MET:CB	2.26	0.66
2:B:1066:PRO:HB3	13:M:46:ILE:CD1	2.22	0.66
22:V:516:PRO:HD2	22:V:706:LYS:HZ3	1.60	0.66
26:2:270:LEU:HD23	26:2:270:LEU:O	1.96	0.66
27:3:144:ILE:O	27:3:147:MET:HG3	1.96	0.66
1:A:622:SER:C	1:A:624:GLY:H	1.96	0.65
2:B:422:PHE:O	2:B:426:GLY:N	2.29	0.65
17:Q:57:LYS:NZ	28:X:28:DG:OP1	2.29	0.65
20:T:145:LEU:O	20:T:145:LEU:HG	1.96	0.65
2:B:73:HIS:O	2:B:75:SER:N	2.28	0.65
22:V:426:VAL:HG13	22:V:427:MET:H	1.61	0.65
25:1:10:ILE:HG22	26:2:407:VAL:HG21	1.79	0.65
27:3:106:SER:O	27:3:110:VAL:HG23	1.97	0.65
27:3:137:LEU:HB3	27:3:180:VAL:CG1	2.20	0.65
1:A:271:ARG:HE	13:M:73:PRO:CG	2.09	0.65
5:E:47:LYS:CB	5:E:48:PRO:CD	2.42	0.65
9:I:14:ILE:CG1	9:I:16:PHE:CZ	2.74	0.65
20:T:146:ASP:O	20:T:147:LYS:HB3	1.97	0.65
25:1:1:MET:SD	26:2:419:GLU:HB2	2.37	0.65
25:1:34:ILE:CG1	25:1:50:VAL:HG11	2.21	0.65
26:2:270:LEU:HD23	26:2:273:GLN:HE21	1.62	0.65
5:E:64:HIS:CD2	5:E:68:PRO:HA	2.24	0.65
9:I:84:HIS:H	9:I:84:HIS:CD2	2.12	0.65
23:W:421:PHE:HB3	23:W:431:PRO:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:696:TRP:HD1	23:W:697:ILE:HG13	1.61	0.65
26:2:218:GLN:CD	26:2:265:LEU:HA	2.17	0.65
1:A:51:ARG:H	1:A:52:PRO:HD2	1.61	0.65
2:B:490:GLY:O	2:B:491:ARG:CG	2.44	0.65
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.77	0.65
18:R:195:PRO:CB	18:R:199:LYS:HD2	2.26	0.65
18:R:225:VAL:HG12	18:R:227:SER:H	1.61	0.65
26:2:189:GLU:HA	26:2:192:GLU:CG	2.26	0.65
26:2:236:PHE:CZ	26:2:262:LEU:HD22	2.32	0.65
27:3:184:ALA:CA	27:3:187:GLN:HG2	2.25	0.65
26:2:57:MET:HA	26:2:60:LEU:HD11	1.76	0.65
3:C:132:SER:HB3	3:C:147:ASP:HB2	1.78	0.65
13:M:178:LYS:NZ	13:M:279:GLY:O	2.27	0.65
23:W:298:ALA:CA	23:W:421:PHE:CE2	2.80	0.65
2:B:312:GLN:OE1	19:S:153:ARG:NH1	2.29	0.65
22:V:516:PRO:CA	25:1:15:ALA:O	2.44	0.65
29:Y:36:DA:C2	29:Y:37:DG:C4	2.84	0.65
1:A:48:GLU:OE1	1:A:48:GLU:N	2.30	0.65
2:B:873:LEU:HB3	2:B:874:PRO:CD	2.24	0.65
1:A:210:GLN:O	1:A:211:GLU:CB	2.45	0.64
26:2:45:PHE:HB2	26:2:51:LEU:CD1	2.26	0.64
27:3:17:ALA:CB	27:3:63:HIS:HD2	2.10	0.64
27:3:58:ALA:CA	27:3:71:TYR:OH	2.39	0.64
8:H:106:THR:C	8:H:108:ALA:H	2.00	0.64
17:Q:180:PHE:CZ	18:R:211:SER:CA	2.60	0.64
21:U:227:GLU:O	21:U:228:MET:O	2.15	0.64
22:V:366:ASN:HD21	22:V:613:THR:HG22	1.62	0.64
1:A:212:LYS:HB3	1:A:212:LYS:NZ	2.12	0.64
26:2:211:GLN:CB	26:2:261:PHE:HE1	2.11	0.64
26:2:266:ARG:O	26:2:270:LEU:HB2	1.97	0.64
27:3:130:GLU:HB2	27:3:173:GLN:HE22	1.61	0.64
27:3:149:LYS:HG3	27:3:150:GLU:N	2.12	0.64
2:B:133:ILE:C	2:B:134:LYS:O	2.34	0.64
23:W:581:LEU:HD21	23:W:608:ILE:HG21	1.78	0.64
25:1:35:ILE:HG22	25:1:46:ILE:CD1	2.27	0.64
27:3:192:ASP:HB2	27:3:231:PHE:CE1	2.32	0.64
2:B:225:LEU:HD13	2:B:228:SER:HB2	1.77	0.64
17:Q:24:GLY:HA2	18:R:210:PHE:CD2	2.33	0.64
23:W:59:TYR:CZ	23:W:62:ALA:HB2	2.29	0.64
27:3:64:ILE:HB	27:3:123:ASP:OD2	1.98	0.64
2:B:901:THR:OG1	2:B:902:GLY:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:97:LEU:HB3	7:G:108:ILE:HB	1.78	0.64
26:2:202:GLN:HE21	26:2:202:GLN:H	1.44	0.64
27:3:14:VAL:HG22	27:3:163:VAL:HA	1.78	0.64
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.63	0.64
9:I:14:ILE:HG13	9:I:16:PHE:CE1	2.33	0.64
26:2:42:LEU:CD2	26:2:55:TRP:HB2	2.13	0.64
26:2:159:VAL:HG11	26:2:161:HIS:HD2	1.62	0.64
1:A:22:GLN:HE22	1:A:1448:SER:HB2	1.63	0.64
5:E:64:HIS:HD2	5:E:69:THR:N	1.93	0.64
23:W:584:TYR:CZ	23:W:614:TYR:HB2	2.31	0.64
26:2:220:LEU:O	26:2:220:LEU:HD13	1.98	0.64
27:3:144:ILE:HD13	27:3:147:MET:HE3	1.78	0.64
1:A:863:ARG:NH2	1:A:1415:THR:OG1	2.30	0.64
1:A:1027:ASP:OD1	5:E:162:ARG:NH1	2.31	0.64
5:E:64:HIS:NE2	5:E:69:THR:C	2.50	0.64
26:2:181:GLN:HG3	26:2:229:ASP:CG	2.18	0.64
27:3:70:LEU:HD13	27:3:115:ILE:CD1	2.28	0.64
1:A:1298:LEU:O	1:A:1300:GLY:N	2.31	0.64
3:C:84:TYR:CZ	3:C:167:LYS:HE3	2.32	0.64
9:I:14:ILE:CG1	9:I:16:PHE:CG	2.80	0.64
17:Q:109:HIS:HB3	18:R:224:THR:HB	1.78	0.64
25:1:38:ILE:HB	25:1:44:PHE:HE1	1.63	0.64
26:2:160:LEU:HB3	26:2:206:LEU:CD1	2.27	0.64
27:3:178:MET:HE2	27:3:202:LEU:HD12	1.80	0.64
1:A:264:VAL:O	1:A:266:MET:N	2.31	0.63
18:R:190:LEU:HD11	18:R:205:ASP:HB2	1.80	0.63
22:V:517:GLU:HB2	22:V:713:LEU:HD22	1.80	0.63
26:2:117:ASN:ND2	27:3:108:ASN:CA	2.57	0.63
26:2:177:GLN:OE1	26:2:220:LEU:HD22	1.98	0.63
1:A:1196:TYR:OH	1:A:1247:PHE:O	2.11	0.63
2:B:80:GLU:CG	2:B:135:GLU:HB3	2.28	0.63
9:I:84:HIS:CG	9:I:85:PRO:HD3	1.91	0.63
13:M:94:ASP:HB2	13:M:99:SER:N	2.11	0.63
13:M:182:ALA:CB	20:T:154:LYS:HG3	2.29	0.63
1:A:926:ASN:OD1	1:A:931:ARG:HD3	1.98	0.63
2:B:595:ASP:OD1	20:T:129:ARG:NH1	2.30	0.63
13:M:44:ARG:HE	13:M:46:ILE:HG23	1.63	0.63
25:1:13:ASP:OD1	25:1:14:PRO:CD	2.46	0.63
25:1:35:ILE:HA	25:1:46:ILE:HG13	1.80	0.63
27:3:131:THR:O	27:3:133:LEU:HD13	1.97	0.63
2:B:53:MET:SD	20:T:140:ARG:HD2	2.37	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:TYR:HB3	20:T:145:LEU:CB	2.22	0.63
5:E:51:GLY:C	5:E:52:ARG:CG	2.62	0.63
13:M:11:PRO:O	13:M:12:ARG:CB	2.46	0.63
24:0:77:LYS:H	24:0:77:LYS:HD2	1.63	0.63
26:2:44:VAL:HG13	26:2:45:PHE:HD1	1.59	0.63
29:Y:56:DG:H2''	29:Y:57:DA:H5'	1.80	0.63
3:C:78:ILE:HD11	3:C:81:LYS:HE3	1.80	0.63
10:J:62:TYR:HB3	10:J:64:PRO:CD	2.28	0.63
17:Q:29:GLU:OE1	18:R:194:ARG:NH2	2.32	0.63
20:T:177:ARG:HH22	20:T:212:TYR:HB2	1.62	0.63
26:2:35:TYR:CZ	26:2:62:LEU:HG	2.34	0.63
27:3:17:ALA:HB1	27:3:63:HIS:HD2	1.63	0.63
27:3:18:ASN:CG	27:3:64:ILE:HD11	2.19	0.63
27:3:160:ARG:NH2	27:3:190:LEU:HD12	2.13	0.63
16:P:162:VAL:HG23	16:P:164:GLN:HE21	1.62	0.63
26:2:60:LEU:HD11	26:2:95:ILE:CB	2.29	0.63
26:2:140:LYS:HG2	26:2:162:PHE:CE1	2.33	0.63
27:3:64:ILE:CG1	27:3:123:ASP:HB3	2.29	0.63
1:A:1112:VAL:HG12	1:A:1311:LEU:HD21	1.81	0.63
2:B:309:PHE:CE2	9:I:40:ARG:HD2	2.33	0.63
2:B:1120:ASN:HB3	2:B:1145:GLN:HB3	1.81	0.63
25:1:18:GLN:NE2	25:1:44:PHE:HZ	1.97	0.63
26:2:100:LEU:HG	26:2:119:ARG:NE	2.13	0.63
2:B:225:LEU:CD1	2:B:228:SER:HB3	2.23	0.63
11:K:56:VAL:HA	11:K:77:THR:HG22	1.81	0.63
18:R:190:LEU:CD1	18:R:205:ASP:HB2	2.29	0.63
26:2:258:LEU:HG	26:2:262:LEU:CD2	2.28	0.63
27:3:134:ALA:HB2	27:3:176:ASN:OD1	1.99	0.63
27:3:214:TYR:CE2	27:3:216:LYS:HE2	2.32	0.63
1:A:927:GLU:CG	1:A:931:ARG:HH11	2.11	0.63
2:B:225:LEU:C	2:B:227:ASN:H	2.01	0.63
10:J:3:ILE:HD12	10:J:15:GLY:HA2	1.81	0.63
13:M:10:LEU:O	13:M:12:ARG:N	2.32	0.63
26:2:163:MET:HE1	26:2:206:LEU:HB3	1.81	0.63
1:A:927:GLU:H	1:A:931:ARG:CD	2.12	0.62
1:A:1179:PRO:HG2	9:I:33:ARG:HG3	1.79	0.62
14:N:344:ARG:NH2	29:Y:79:DT:OP2	2.30	0.62
26:2:89:LEU:HD23	26:2:89:LEU:O	1.99	0.62
26:2:123:LEU:O	26:2:123:LEU:HD23	1.99	0.62
27:3:24:LYS:HE2	27:3:220:MET:SD	2.38	0.62
27:3:70:LEU:CD1	27:3:115:ILE:HD11	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:HG2	1:A:245:PRO:HD2	1.81	0.62
1:A:339:LEU:HD11	2:B:1161:GLU:HG2	1.81	0.62
1:A:609:HIS:O	1:A:610:PRO:O	2.16	0.62
2:B:958:CYS:SG	2:B:959:GLU:N	2.72	0.62
17:Q:35:ASP:OD1	18:R:161:ARG:NH2	2.33	0.62
17:Q:36:ILE:O	17:Q:41:SER:OG	2.16	0.62
20:T:202:LEU:HD12	20:T:205:ILE:HD11	1.81	0.62
21:U:252:LYS:HA	21:U:252:LYS:CE	2.28	0.62
26:2:173:GLN:HG2	26:2:179:LEU:HG	1.80	0.62
1:A:266:MET:HG3	1:A:272:ASN:CG	2.18	0.62
3:C:5:ASN:O	3:C:7:PRO:CG	2.43	0.62
8:H:23:ASP:O	8:H:25:VAL:N	2.32	0.62
9:I:89:CYS:HB3	9:I:119:CYS:SG	2.39	0.62
13:M:108:SER:HB3	13:M:112:ARG:HH11	1.64	0.62
2:B:133:ILE:HG23	2:B:139:GLN:CG	2.29	0.62
8:H:88:PHE:HD2	8:H:144:LEU:HB3	1.65	0.62
23:W:584:TYR:CG	23:W:594:ALA:HB2	2.34	0.62
25:1:2:VAL:HG12	26:2:422:LEU:CD1	2.27	0.62
25:1:8:VAL:O	26:2:407:VAL:HG12	1.99	0.62
26:2:93:LEU:HA	26:2:96:TRP:HD1	1.64	0.62
26:2:181:GLN:CD	26:2:229:ASP:HB2	2.19	0.62
27:3:59:VAL:HB	27:3:71:TYR:CD1	2.25	0.62
2:B:861:SER:C	2:B:896:LEU:HD23	2.19	0.62
4:D:70:ARG:NH1	7:G:140:ASP:OD1	2.31	0.62
14:N:321:SER:OG	16:P:243:LYS:NZ	2.26	0.62
20:T:236:LYS:NZ	20:T:238:GLU:O	2.33	0.62
22:V:667:THR:HA	25:1:62:ASP:CG	2.19	0.62
25:1:38:ILE:HB	25:1:44:PHE:CE1	2.34	0.62
25:1:50:VAL:HA	25:1:53:LEU:HD13	1.82	0.62
1:A:896:LEU:HD23	1:A:1080:ILE:HD12	1.82	0.62
1:A:927:GLU:CB	1:A:931:ARG:HH11	2.13	0.62
23:W:298:ALA:CA	23:W:421:PHE:HE2	2.12	0.62
26:2:189:GLU:O	26:2:193:PRO:HD2	2.00	0.62
27:3:184:ALA:HA	27:3:187:GLN:CG	2.28	0.62
18:R:144:ASN:ND2	18:R:173:GLU:OE2	2.28	0.62
26:2:28:PRO:CA	27:3:25:GLN:CA	2.73	0.62
26:2:218:GLN:HG2	26:2:268:PHE:HB3	1.82	0.62
27:3:165:LYS:O	27:3:165:LYS:HD3	1.98	0.62
1:A:950:ASN:OD1	1:A:954:ARG:NH1	2.33	0.62
1:A:1375:ARG:NH1	1:A:1379:GLU:OE1	2.32	0.62
6:F:65:VAL:HG13	6:F:104:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:194:ARG:O	18:R:199:LYS:HB2	2.00	0.62
25:1:17:LYS:O	25:1:20:LEU:HB3	2.00	0.62
27:3:9:ASN:O	27:3:56:LYS:HD3	1.99	0.62
1:A:603:ILE:HD11	1:A:988:TRP:CE2	2.35	0.62
25:1:1:MET:HB2	26:2:418:PHE:HB3	1.81	0.62
25:1:1:MET:HG2	26:2:414:SER:N	2.15	0.62
25:1:47:ALA:HB1	25:1:50:VAL:HB	1.81	0.62
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.30	0.61
2:B:952:GLU:OE1	2:B:952:GLU:N	2.25	0.61
1:A:1251:ASN:ND2	21:U:227:GLU:O	2.33	0.61
8:H:105:SER:HB2	8:H:108:ALA:HB2	1.81	0.61
27:3:133:LEU:HD22	27:3:134:ALA:N	2.14	0.61
29:Y:36:DA:C2	29:Y:37:DG:C5	2.88	0.61
1:A:779:ILE:O	1:A:783:GLN:HG3	2.00	0.61
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.82	0.61
2:B:761:THR:H	2:B:764:MET:CE	2.13	0.61
3:C:67:ARG:HH21	3:C:148:ILE:HD11	1.65	0.61
5:E:64:HIS:CE1	5:E:70:ASP:O	2.54	0.61
22:V:316:LEU:HB2	22:V:321:GLU:CG	2.29	0.61
26:2:46:ARG:CD	26:2:85:GLU:HB2	2.30	0.61
1:A:890:ARG:CZ	1:A:1023:VAL:HB	2.30	0.61
2:B:552:ASN:OD1	2:B:553:LEU:N	2.33	0.61
12:L:28:ILE:O	12:L:28:ILE:HG22	2.00	0.61
14:N:333:ASN:OD1	14:N:361:ASN:N	2.26	0.61
23:W:37:HIS:CE1	23:W:454:VAL:CG1	2.82	0.61
23:W:423:ASP:O	23:W:425:THR:N	2.33	0.61
23:W:584:TYR:HB2	23:W:594:ALA:HB2	1.81	0.61
26:2:60:LEU:CD1	26:2:95:ILE:HB	2.31	0.61
27:3:190:LEU:H	27:3:190:LEU:CD2	2.12	0.61
1:A:1313:GLN:HE22	1:A:1318:LYS:CD	2.14	0.61
2:B:924:ARG:NH1	3:C:60:HIS:HB2	2.16	0.61
17:Q:54:PHE:HD2	18:R:194:ARG:HD2	1.65	0.61
22:V:612:ASP:CG	22:V:635:GLN:CD	2.59	0.61
26:2:203:PHE:HD2	26:2:205:LEU:HD23	1.64	0.61
29:Y:36:DA:C6	29:Y:37:DG:O6	2.54	0.61
29:Y:36:DA:C5	29:Y:37:DG:C6	2.88	0.61
26:2:29:GLY:N	27:3:25:GLN:HB3	2.15	0.61
5:E:62:VAL:HG21	5:E:72:MET:HB3	1.82	0.61
5:E:64:HIS:NE2	5:E:70:ASP:N	2.49	0.61
8:H:64:LEU:HB3	8:H:84:ARG:CD	2.28	0.61
9:I:14:ILE:CG1	9:I:16:PHE:CE1	2.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:22:ILE:HD11	14:N:43:LYS:HB2	1.82	0.61
17:Q:54:PHE:CD2	18:R:194:ARG:CD	2.83	0.61
18:R:194:ARG:C	18:R:196:ASP:H	2.02	0.61
26:2:117:ASN:ND2	27:3:42:MET:CE	2.60	0.61
26:2:251:VAL:CG1	26:2:254:MET:HG3	2.30	0.61
27:3:18:ASN:O	27:3:21:TRP:HD1	1.84	0.61
27:3:100:LYS:HG3	27:3:101:TYR:N	2.16	0.61
1:A:1102:MET:HB2	1:A:1389:ASP:OD1	2.00	0.61
2:B:80:GLU:OE1	2:B:135:GLU:CA	2.49	0.61
10:J:63:ALA:O	10:J:65:LEU:N	2.26	0.61
23:W:59:TYR:OH	23:W:63:TYR:CE2	2.52	0.61
23:W:432:ILE:HG12	23:W:434:HIS:CE1	2.36	0.61
25:1:9:LEU:CB	25:1:51:ASN:HD21	2.14	0.61
26:2:236:PHE:CE2	26:2:262:LEU:HD13	2.36	0.61
22:V:368:ALA:O	22:V:371:VAL:HG22	2.00	0.61
22:V:520:ARG:HG3	25:1:23:LEU:HD11	1.83	0.61
27:3:8:LEU:HA	27:3:54:SER:HB3	1.83	0.61
1:A:93:PRO:HB3	1:A:251:THR:HG22	1.82	0.61
7:G:78:ARG:NH1	7:G:79:PRO:O	2.33	0.61
19:S:111:LYS:HE3	19:S:149:LEU:HD21	1.82	0.61
23:W:423:ASP:C	23:W:425:THR:H	2.05	0.61
1:A:267:GLN:H	13:M:49:GLY:HA2	1.66	0.60
2:B:875:GLU:OE1	2:B:875:GLU:HA	2.01	0.60
13:M:182:ALA:HB2	20:T:154:LYS:CG	2.26	0.60
25:1:1:MET:HA	26:2:414:SER:N	2.15	0.60
26:2:56:VAL:HG11	26:2:91:SER:CB	2.31	0.60
2:B:52:GLN:NE2	20:T:142:SER:HB2	2.15	0.60
22:V:612:ASP:CG	22:V:635:GLN:OE1	2.39	0.60
27:3:143:TYR:O	27:3:146:ARG:HG2	2.01	0.60
2:B:133:ILE:O	2:B:133:ILE:HG22	2.00	0.60
2:B:1040:GLN:H	2:B:1040:GLN:CD	2.05	0.60
19:S:115:LYS:NZ	19:S:117:GLY:O	2.32	0.60
22:V:593:LEU:HD11	22:V:615:PHE:CZ	2.36	0.60
26:2:117:ASN:HD22	27:3:42:MET:HE1	1.60	0.60
1:A:927:GLU:O	1:A:931:ARG:HB2	2.00	0.60
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.84	0.60
18:R:190:LEU:HD11	18:R:205:ASP:CB	2.31	0.60
25:1:1:MET:HA	26:2:413:LEU:HA	1.83	0.60
26:2:30:VAL:HG12	26:2:34:LEU:HD23	1.82	0.60
26:2:173:GLN:CD	26:2:179:LEU:HD21	2.21	0.60
16:P:298:PRO:O	16:P:300:ILE:HG12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:51:GLY:O	5:E:52:ARG:CB	2.37	0.60
9:I:61:GLU:C	9:I:63:ASP:H	2.04	0.60
18:R:138:ALA:C	18:R:140:LYS:H	2.05	0.60
27:3:71:TYR:CG	27:3:72:PRO:HD2	2.17	0.60
27:3:222:SER:HB2	27:3:226:TYR:CE2	2.37	0.60
1:A:720:ALA:HB1	9:I:108:MET:HG2	1.84	0.60
1:A:1319:LYS:CG	1:A:1333:GLU:HG2	2.27	0.60
5:E:26:TYR:HD1	5:E:65:ASN:H	1.49	0.60
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.84	0.60
22:V:534:TYR:CD1	22:V:535:THR:N	2.70	0.60
11:K:62:LYS:HE2	11:K:72:ILE:HD11	1.83	0.60
23:W:175:TYR:HD1	23:W:175:TYR:H	1.46	0.60
26:2:83:GLN:OE1	26:2:83:GLN:HA	2.01	0.60
1:A:1250:ASP:OD2	21:U:227:GLU:HB2	2.00	0.60
2:B:90:GLN:NE2	20:T:141:LEU:CA	2.25	0.60
3:C:117:SER:HB3	3:C:130:VAL:HG21	1.83	0.60
5:E:71:GLN:HE21	5:E:99:ILE:HA	1.66	0.60
26:2:159:VAL:HG13	26:2:160:LEU:N	2.17	0.60
27:3:173:GLN:CA	27:3:176:ASN:HD21	2.10	0.60
1:A:425:ASP:HB3	13:M:39:LEU:CD1	2.32	0.60
1:A:621:ILE:HG22	1:A:621:ILE:O	2.02	0.60
2:B:78:VAL:O	2:B:78:VAL:HG12	2.01	0.60
16:P:162:VAL:HG23	16:P:162:VAL:O	2.02	0.60
16:P:206:GLU:C	16:P:208:ARG:N	2.56	0.60
23:W:421:PHE:CB	23:W:431:PRO:HG3	2.32	0.60
17:Q:54:PHE:CD2	18:R:194:ARG:HD2	2.36	0.59
23:W:584:TYR:HB2	23:W:594:ALA:CB	2.32	0.59
26:2:164:VAL:HG13	26:2:209:PRO:HG2	1.83	0.59
25:1:53:LEU:HD12	25:1:53:LEU:N	2.18	0.59
26:2:171:VAL:HG13	26:2:216:MET:HB2	1.83	0.59
27:3:14:VAL:HG23	27:3:163:VAL:HA	1.84	0.59
27:3:196:LEU:CD2	27:3:223:LEU:HD23	2.25	0.59
27:3:213:LEU:HD23	27:3:230:VAL:HG12	1.84	0.59
1:A:153:ILE:O	1:A:153:ILE:HG22	2.03	0.59
1:A:621:ILE:O	1:A:623:PRO:N	2.35	0.59
13:M:44:ARG:NE	13:M:46:ILE:HG22	2.16	0.59
26:2:28:PRO:CA	27:3:25:GLN:C	2.70	0.59
26:2:196:ILE:HA	26:2:202:GLN:OE1	2.02	0.59
26:2:206:LEU:HD22	26:2:206:LEU:N	2.17	0.59
2:B:228:SER:O	2:B:405:ARG:NH1	2.36	0.59
2:B:838:GLN:HB3	2:B:890:ARG:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:612:ASP:OD2	22:V:639:ARG:NH1	2.35	0.59
24:0:55:LEU:HD12	27:3:178:MET:CE	2.31	0.59
28:X:51:DC:H2"	28:X:52:DG:C8	2.37	0.59
1:A:95:PHE:CE2	1:A:218:PRO:HG3	2.37	0.59
2:B:883:THR:O	2:B:884:ASN:C	2.41	0.59
17:Q:117:ASP:OD1	17:Q:174:ARG:NH1	2.35	0.59
25:1:18:GLN:HB2	25:1:44:PHE:CZ	2.37	0.59
27:3:110:VAL:O	27:3:114:GLU:HG2	2.02	0.59
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.83	0.59
2:B:297:MET:SD	2:B:373:LEU:HD22	2.42	0.59
27:3:160:ARG:HB3	27:3:190:LEU:CD2	2.32	0.59
1:A:857:THR:HG21	1:A:1100:THR:HA	1.84	0.59
2:B:490:GLY:O	2:B:491:ARG:HG2	2.02	0.59
18:R:194:ARG:C	18:R:196:ASP:N	2.56	0.59
22:V:703:PHE:CZ	22:V:712:LEU:CD2	2.86	0.59
27:3:215:LEU:CD1	27:3:230:VAL:HG13	2.32	0.59
1:A:478:PRO:HB2	1:A:479:TRP:CE3	2.38	0.59
1:A:1021:VAL:HA	1:A:1034:GLN:NE2	2.18	0.59
18:R:195:PRO:O	18:R:196:ASP:CB	2.50	0.59
26:2:202:GLN:NE2	26:2:202:GLN:H	2.00	0.59
26:2:215:PHE:CD2	26:2:264:HIS:HB2	2.37	0.59
27:3:131:THR:HG23	27:3:133:LEU:CD1	2.32	0.59
1:A:800:PHE:CZ	1:A:815:TYR:HE1	2.21	0.59
2:B:883:THR:O	2:B:885:ARG:N	2.36	0.59
13:M:44:ARG:NE	13:M:46:ILE:HG23	2.17	0.59
25:1:34:ILE:O	25:1:46:ILE:HG13	2.03	0.59
25:1:38:ILE:H	25:1:38:ILE:CD1	2.16	0.59
26:2:203:PHE:CE2	26:2:205:LEU:HD23	2.38	0.59
1:A:1416:ARG:HB3	1:A:1433:GLU:OE1	2.03	0.58
2:B:289:ILE:O	2:B:291:ASP:N	2.35	0.58
5:E:160:LEU:HD21	5:E:167:GLU:HG3	1.84	0.58
17:Q:28:ILE:HG21	18:R:190:LEU:HD13	1.85	0.58
21:U:132:ARG:N	21:U:167:GLU:OE2	2.36	0.58
23:W:37:HIS:ND1	23:W:454:VAL:HG13	2.16	0.58
23:W:209:TYR:CE1	23:W:233:PHE:CD1	2.90	0.58
26:2:44:VAL:HG13	26:2:45:PHE:N	2.17	0.58
26:2:160:LEU:HD12	26:2:160:LEU:N	2.18	0.58
1:A:69:GLY:HA2	1:A:77:ASN:HA	1.85	0.58
1:A:1192:TRP:O	1:A:1196:TYR:N	2.34	0.58
2:B:685:LYS:HA	2:B:688:ALA:HB3	1.86	0.58
22:V:520:ARG:HD3	25:1:19:PHE:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:1:MET:HB3	26:2:413:LEU:HG	1.83	0.58
25:1:2:VAL:HB	26:2:456:LYS:HD3	1.85	0.58
25:1:34:ILE:HG22	25:1:46:ILE:CD1	2.32	0.58
26:2:42:LEU:HD12	26:2:59:MET:HE1	1.84	0.58
26:2:217:LEU:HD23	26:2:233:ILE:CD1	2.32	0.58
27:3:144:ILE:HG12	27:3:147:MET:HE2	1.84	0.58
20:T:141:LEU:C	20:T:141:LEU:HD22	2.23	0.58
21:U:252:LYS:O	21:U:253:THR:CB	2.51	0.58
27:3:169:ASP:CB	27:3:202:LEU:HD23	2.33	0.58
1:A:551:ARG:NE	1:A:625:ASP:OD2	2.36	0.58
1:A:799:PRO:O	1:A:806:THR:HG22	2.03	0.58
1:A:1251:ASN:OD1	21:U:197:ASN:ND2	2.36	0.58
6:F:62:ARG:NH1	6:F:127:ASP:O	2.27	0.58
23:W:73:CYS:CB	23:W:209:TYR:CZ	2.86	0.58
26:2:30:VAL:HG22	27:3:25:GLN:OE1	2.03	0.58
27:3:131:THR:CG2	27:3:133:LEU:HD12	2.33	0.58
27:3:190:LEU:HD23	27:3:190:LEU:N	2.18	0.58
1:A:298:ALA:HB1	1:A:303:ILE:HD11	1.85	0.58
1:A:930:LEU:O	1:A:931:ARG:C	2.42	0.58
25:1:2:VAL:CG1	26:2:456:LYS:CD	2.82	0.58
25:1:13:ASP:CG	25:1:14:PRO:CD	2.61	0.58
26:2:177:GLN:HE22	26:2:220:LEU:HA	1.68	0.58
1:A:35:SER:OG	1:A:37:THR:HG22	2.04	0.58
1:A:643:LYS:HD3	21:U:301:CYS:SG	2.43	0.58
5:E:10:LEU:HD21	5:E:55:ARG:NH2	2.18	0.58
26:2:117:ASN:CG	27:3:108:ASN:ND2	2.50	0.58
1:A:611:ASP:CG	1:A:626:THR:HG1	2.06	0.58
3:C:148:ILE:HG12	10:J:5:VAL:HG22	1.86	0.58
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.85	0.58
23:W:419:GLU:O	23:W:420:PRO:O	2.20	0.58
26:2:35:TYR:CB	26:2:62:LEU:HD12	2.33	0.58
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.85	0.58
1:A:417:LYS:HG2	1:A:449:HIS:CE1	2.39	0.58
1:A:425:ASP:CG	13:M:39:LEU:HD11	2.24	0.58
7:G:31:PHE:HE1	7:G:48:VAL:HB	1.68	0.58
21:U:226:GLU:HG3	21:U:238:LYS:NZ	2.18	0.58
28:X:48:DG:H2"	28:X:49:DA:H5"	1.84	0.58
3:C:137:ASN:CB	3:C:145:GLN:NE2	2.63	0.58
5:E:55:ARG:H	5:E:78:GLU:CD	2.04	0.58
20:T:4:ARG:NE	20:T:102:ASP:OD2	2.35	0.58
22:V:613:THR:O	22:V:614:SER:CB	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:236:PHE:CZ	26:2:258:LEU:HD11	2.39	0.58
29:Y:36:DA:N9	29:Y:37:DG:N7	2.50	0.58
1:A:353:ASN:HD21	2:B:1071:ASN:HD21	1.50	0.58
1:A:375:ILE:HD11	1:A:669:TYR:HB3	1.85	0.58
2:B:1129:ASN:HA	2:B:1135:TYR:HD1	1.69	0.58
9:I:58:ILE:C	9:I:60:HIS:H	2.07	0.58
25:1:8:VAL:HG12	25:1:9:LEU:H	1.69	0.58
27:3:215:LEU:HD12	27:3:230:VAL:HG13	1.85	0.58
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.34	0.57
1:A:1319:LYS:CD	1:A:1333:GLU:CD	2.57	0.57
2:B:471:ASN:OD1	2:B:472:ARG:N	2.37	0.57
13:M:86:LYS:HA	13:M:86:LYS:HE2	1.83	0.57
1:A:522:PRO:CA	1:A:666:ARG:HH21	2.17	0.57
1:A:631:GLU:HG3	1:A:988:TRP:HH2	1.69	0.57
1:A:927:GLU:HG2	1:A:931:ARG:NH1	2.18	0.57
13:M:10:LEU:N	13:M:11:PRO:CD	2.53	0.57
26:2:82:ALA:HA	26:2:89:LEU:HD11	1.85	0.57
26:2:118:LEU:CD2	27:3:39:ASP:C	2.72	0.57
2:B:91:ILE:HG22	20:T:141:LEU:CD1	2.29	0.57
2:B:1016:SER:HB3	2:B:1022:LEU:HB3	1.86	0.57
9:I:14:ILE:CG1	9:I:16:PHE:CD1	2.87	0.57
23:W:209:TYR:OH	23:W:233:PHE:C	2.42	0.57
27:3:16:ASP:O	27:3:21:TRP:NE1	2.27	0.57
1:A:210:GLN:O	1:A:211:GLU:HB2	2.03	0.57
8:H:95:LYS:HB3	8:H:139:SER:HA	1.85	0.57
17:Q:102:VAL:HG13	17:Q:103:VAL:CA	2.32	0.57
22:V:321:GLU:HA	23:W:499:ASN:HD21	1.65	0.57
1:A:480:SER:HB3	2:B:1059:ILE:HD12	1.86	0.57
27:3:46:ASN:CG	27:3:104:LEU:HD22	2.24	0.57
27:3:144:ILE:HG12	27:3:147:MET:CE	2.34	0.57
1:A:948:ILE:HG23	1:A:1007:ILE:HD11	1.85	0.57
2:B:800:ALA:O	2:B:805:PHE:HB3	2.05	0.57
18:R:190:LEU:HD13	18:R:205:ASP:OD2	1.97	0.57
23:W:584:TYR:CB	23:W:594:ALA:HB2	2.33	0.57
26:2:30:VAL:HG23	27:3:25:GLN:CD	2.23	0.57
26:2:117:ASN:CG	27:3:42:MET:HE2	2.24	0.57
27:3:216:LYS:H	27:3:216:LYS:CD	2.13	0.57
10:J:9:THR:OG1	10:J:47:ARG:NH2	2.35	0.57
13:M:10:LEU:C	13:M:12:ARG:H	2.07	0.57
21:U:252:LYS:HA	21:U:252:LYS:HE3	1.86	0.57
24:0:109:THR:HB	24:0:144:SER:H	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:117:ASN:CG	27:3:42:MET:HE1	2.21	0.57
27:3:14:VAL:HG23	27:3:163:VAL:HG13	1.86	0.57
27:3:187:GLN:NE2	27:3:189:ILE:HG13	2.20	0.57
1:A:114:CYS:HB2	1:A:184:CYS:SG	2.44	0.57
1:A:800:PHE:HZ	1:A:815:TYR:HE1	1.53	0.57
1:A:922:PHE:CE2	1:A:932:ARG:NH1	2.73	0.57
2:B:496:ALA:HB3	2:B:498:PRO:HD2	1.87	0.57
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.86	0.57
9:I:62:VAL:HG23	9:I:64:GLU:HG2	1.86	0.57
15:O:3:TYR:CD1	15:O:98:CYS:SG	2.93	0.57
17:Q:24:GLY:HA3	18:R:210:PHE:CD2	2.38	0.57
18:R:144:ASN:OD1	18:R:145:VAL:N	2.36	0.57
25:1:59:GLU:CD	26:2:402:ARG:NH1	2.56	0.57
29:Y:18:DG:C2	29:Y:19:DC:C2	2.93	0.57
1:A:931:ARG:O	1:A:933:THR:N	2.37	0.57
2:B:468:GLN:OE1	2:B:481:HIS:NE2	2.38	0.57
2:B:720:PRO:O	2:B:724:TYR:HD2	1.88	0.57
2:B:755:GLN:HB2	2:B:777:ASN:ND2	2.19	0.57
2:B:1022:LEU:HD12	2:B:1023:ARG:HG3	1.87	0.57
20:T:129:ARG:HA	20:T:132:ILE:HD12	1.87	0.57
24:O:77:LYS:HD2	24:O:77:LYS:N	2.19	0.57
26:2:30:VAL:N	27:3:25:GLN:CB	2.52	0.57
26:2:185:MET:HB2	26:2:229:ASP:OD1	2.04	0.57
26:2:197:THR:HG21	26:2:239:GLN:CD	2.24	0.57
2:B:834:ARG:O	2:B:885:ARG:NH1	2.38	0.57
17:Q:16:ARG:HD2	17:Q:19:LYS:HB2	1.86	0.57
21:U:291:CYS:SG	21:U:293:GLU:HB2	2.45	0.57
22:V:514:MET:SD	22:V:537:ASN:ND2	2.78	0.57
27:3:59:VAL:N	27:3:71:TYR:CZ	2.70	0.57
28:X:14:DA:H2"	28:X:15:DA:C8	2.40	0.57
1:A:129:ILE:O	1:A:132:LYS:HB2	2.05	0.56
2:B:80:GLU:HB3	2:B:135:GLU:HB3	1.71	0.56
2:B:326:ALA:HB2	2:B:338:TYR:CE2	2.40	0.56
2:B:875:GLU:O	2:B:876:ASN:HB2	2.04	0.56
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.86	0.56
3:C:117:SER:OG	3:C:147:ASP:OD2	2.16	0.56
26:2:117:ASN:HB2	27:3:104:LEU:CD1	2.35	0.56
27:3:210:THR:HG22	27:3:210:THR:O	2.04	0.56
27:3:223:LEU:HD11	27:3:227:LEU:HD11	1.87	0.56
29:Y:36:DA:C5	29:Y:37:DG:N7	2.73	0.56
1:A:364:ARG:NH2	1:A:500:GLU:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ASP:O	1:A:615:SER:OG	2.20	0.56
21:U:231:ASP:C	21:U:232:GLU:CG	2.68	0.56
27:3:19:PRO:HG2	27:3:123:ASP:O	2.05	0.56
27:3:195:VAL:HG21	27:3:214:TYR:OH	2.05	0.56
1:A:77:ASN:ND2	13:M:43:ASP:CG	2.59	0.56
1:A:1132:LYS:N	28:X:47:DC:OP1	2.37	0.56
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.39	0.56
17:Q:42:CYS:O	17:Q:95:ASN:ND2	2.38	0.56
20:T:146:ASP:O	20:T:147:LYS:CB	2.53	0.56
22:V:519:TYR:HD2	25:1:20:LEU:HB2	1.71	0.56
25:1:1:MET:CB	26:2:418:PHE:HB2	2.35	0.56
25:1:52:VAL:HG22	25:1:53:LEU:HD12	1.87	0.56
26:2:60:LEU:HD11	26:2:95:ILE:CG2	2.35	0.56
27:3:21:TRP:O	27:3:24:LYS:HB2	2.05	0.56
27:3:178:MET:SD	27:3:181:ILE:HD12	2.46	0.56
2:B:704:LEU:HD22	2:B:708:ALA:CB	2.36	0.56
18:R:99:LEU:HD12	18:R:124:LEU:HD12	1.86	0.56
26:2:47:GLU:HG3	26:2:48:LEU:N	2.20	0.56
26:2:130:SER:HB2	26:2:173:GLN:OE1	2.06	0.56
27:3:42:MET:SD	27:3:111:ILE:HD13	2.46	0.56
27:3:223:LEU:O	27:3:223:LEU:HD13	2.05	0.56
1:A:611:ASP:CG	1:A:626:THR:OG1	2.44	0.56
2:B:882:SER:O	2:B:887:TYR:CG	2.57	0.56
2:B:45:ASP:HB3	2:B:534:VAL:HG11	1.87	0.56
2:B:74:ALA:HB2	20:T:201:ASP:CB	2.29	0.56
3:C:130:VAL:O	3:C:134:ASN:ND2	2.39	0.56
22:V:319:TYR:CE2	22:V:320:GLN:HG3	2.41	0.56
22:V:519:TYR:CD2	25:1:20:LEU:HB2	2.41	0.56
25:1:1:MET:HB2	26:2:418:PHE:HB2	1.88	0.56
26:2:160:LEU:H	26:2:160:LEU:CD1	2.18	0.56
19:S:110:PHE:HD1	19:S:148:PRO:HA	1.70	0.56
27:3:58:ALA:CA	27:3:71:TYR:CE2	2.82	0.56
1:A:464:LEU:HD21	1:A:1100:THR:HG21	1.88	0.56
1:A:631:GLU:HG3	1:A:988:TRP:CH2	2.40	0.56
1:A:939:VAL:HA	1:A:942:VAL:HG22	1.87	0.56
9:I:75:ASP:HB3	9:I:78:LEU:HD12	1.86	0.56
13:M:290:ARG:NH1	28:X:5:DG:OP1	2.39	0.56
19:S:49:ARG:NH1	19:S:96:GLN:O	2.36	0.56
1:A:108:ARG:NH1	1:A:145:TYR:OH	2.36	0.56
1:A:521:VAL:O	1:A:666:ARG:NH2	2.38	0.56
1:A:1085:GLU:OE2	6:F:59:LYS:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:206:GLU:HG3	16:P:236:LYS:HZ3	1.67	0.56
18:R:162:GLY:C	18:R:164:GLY:N	2.46	0.56
25:1:31:LYS:O	25:1:32:LYS:HB2	2.06	0.56
25:1:36:GLN:HB3	25:1:45:VAL:HG12	1.88	0.56
26:2:163:MET:HE2	26:2:206:LEU:CD1	2.35	0.56
26:2:163:MET:HE3	26:2:206:LEU:HD12	1.88	0.56
26:2:206:LEU:HD22	26:2:206:LEU:H	1.71	0.56
1:A:678:ASN:O	1:A:681:LEU:HB3	2.06	0.56
1:A:1223:ASP:OD2	1:A:1224:ARG:NH1	2.38	0.56
3:C:142:TYR:O	3:C:144:GLU:N	2.39	0.56
7:G:93:ASN:OD1	7:G:94:LYS:N	2.38	0.56
21:U:251:ALA:C	21:U:253:THR:N	2.51	0.56
26:2:423:ALA:HA	26:2:426:ARG:HE	1.70	0.56
1:A:1113:SER:O	1:A:1114:ALA:HB3	2.03	0.55
27:3:21:TRP:CD2	27:3:34:LEU:HD23	2.42	0.55
1:A:606:HIS:HB2	1:A:627:LYS:HA	1.87	0.55
1:A:930:LEU:HD21	8:H:107:GLU:OE1	2.06	0.55
1:A:1103:THR:HG23	1:A:1106:THR:H	1.71	0.55
2:B:329:GLY:H	2:B:335:ARG:HH21	1.54	0.55
2:B:747:LEU:HD21	2:B:810:PHE:HE1	1.71	0.55
18:R:190:LEU:HD11	18:R:205:ASP:CG	2.25	0.55
18:R:224:THR:O	18:R:225:VAL:C	2.44	0.55
24:0:54:ARG:C	27:3:209:ILE:HD11	2.25	0.55
26:2:181:GLN:HA	26:2:181:GLN:HE21	1.70	0.55
29:Y:36:DA:N3	29:Y:37:DG:C8	2.75	0.55
1:A:121:SER:HA	1:A:126:ILE:HG21	1.87	0.55
1:A:364:ARG:HE	1:A:500:GLU:CD	2.10	0.55
2:B:92:TYR:HE1	20:T:143:GLN:HE21	1.54	0.55
17:Q:109:HIS:HE1	18:R:231:GLU:CB	2.19	0.55
27:3:44:LEU:HD13	27:3:44:LEU:O	2.06	0.55
1:A:266:MET:CG	1:A:272:ASN:HD21	1.90	0.55
1:A:1319:LYS:HG3	1:A:1333:GLU:OE1	2.07	0.55
2:B:35:ASP:OD2	2:B:646:ARG:NH1	2.37	0.55
15:O:64:THR:HG21	16:P:188:ARG:HD2	1.89	0.55
17:Q:109:HIS:CG	18:R:224:THR:HG1	2.15	0.55
18:R:84:TYR:OH	18:R:88:ARG:NH1	2.38	0.55
22:V:531:ILE:CB	22:V:534:TYR:CE2	2.89	0.55
25:1:1:MET:CG	26:2:418:PHE:HB2	2.35	0.55
1:A:138:LYS:HB2	1:A:1445:HIS:CE1	2.41	0.55
13:M:44:ARG:HG3	13:M:46:ILE:HG23	1.89	0.55
20:T:228:ILE:O	20:T:230:LYS:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:504:LYS:HD2	22:V:654:GLU:O	2.07	0.55
1:A:685:HIS:HB3	2:B:784:SER:OG	2.07	0.55
5:E:55:ARG:N	5:E:78:GLU:CD	2.59	0.55
19:S:172:ASN:OD1	19:S:173:HIS:N	2.38	0.55
25:1:10:ILE:C	25:1:10:ILE:HD13	2.26	0.55
25:1:34:ILE:HG23	25:1:50:VAL:HG11	1.89	0.55
27:3:133:LEU:H	27:3:133:LEU:CD1	2.10	0.55
1:A:279:LYS:HB2	1:A:336:LEU:HD21	1.88	0.55
1:A:428:ASP:OD1	1:A:430:ARG:N	2.37	0.55
1:A:875:TYR:O	6:F:53:THR:HG22	2.06	0.55
5:E:10:LEU:HD21	5:E:55:ARG:NE	2.21	0.55
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.42	0.55
10:J:10:CYS:SG	10:J:11:GLY:N	2.79	0.55
13:M:94:ASP:O	13:M:97:GLY:O	2.25	0.55
17:Q:24:GLY:HA2	18:R:210:PHE:CE2	2.40	0.55
21:U:256:THR:HG1	21:U:272:THR:HG22	1.69	0.55
25:1:52:VAL:HG23	25:1:53:LEU:N	2.21	0.55
26:2:259:LEU:HD12	26:2:259:LEU:C	2.27	0.55
1:A:611:ASP:O	1:A:612:ASP:HB2	2.06	0.55
1:A:1299:GLN:HG2	1:A:1300:GLY:N	2.21	0.55
1:A:1316:ASN:HA	21:U:292:ASN:O	2.07	0.55
2:B:240:LEU:O	2:B:253:GLY:HA2	2.07	0.55
22:V:531:ILE:CA	22:V:534:TYR:HE2	1.90	0.55
5:E:185:ILE:HG13	5:E:189:GLN:OE1	2.07	0.55
7:G:107:PHE:CZ	17:Q:127:PHE:HZ	2.24	0.55
1:A:230:ASP:OD1	1:A:244:ARG:NH1	2.40	0.55
5:E:45:GLY:C	5:E:47:LYS:H	2.11	0.55
10:J:3:ILE:HD13	10:J:18:TRP:CB	2.37	0.55
12:L:19:CYS:SG	12:L:20:GLY:N	2.80	0.55
14:N:323:GLU:HG3	14:N:325:GLY:HA3	1.89	0.55
18:R:93:ASP:O	18:R:140:LYS:NZ	2.35	0.55
26:2:53:LYS:CE	26:2:95:ILE:HD11	2.36	0.55
26:2:208:THR:O	26:2:212:LEU:HG	2.07	0.55
27:3:223:LEU:HD13	27:3:227:LEU:HG	1.88	0.55
2:B:116:ARG:HH12	12:L:42:ARG:HH11	1.53	0.54
2:B:704:LEU:HD22	2:B:708:ALA:HB1	1.89	0.54
22:V:251:PHE:O	22:V:257:LYS:HA	2.06	0.54
22:V:516:PRO:HD2	22:V:706:LYS:NZ	2.22	0.54
26:2:123:LEU:CD2	26:2:178:LEU:HD11	2.37	0.54
26:2:123:LEU:HD21	26:2:178:LEU:CD1	2.38	0.54
26:2:177:GLN:NE2	26:2:220:LEU:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1307:VAL:HG11	1:A:1339:ASP:OD2	2.06	0.54
19:S:47:LEU:HD23	20:T:104:LEU:HD13	1.89	0.54
26:2:159:VAL:HG22	26:2:160:LEU:N	2.16	0.54
22:V:523:VAL:HG21	25:1:20:LEU:HD23	1.88	0.54
26:2:37:HIS:HB3	26:2:38:PRO:CD	2.35	0.54
26:2:211:GLN:HB3	26:2:261:PHE:CE1	2.40	0.54
27:3:64:ILE:HG23	27:3:128:HIS:CG	2.42	0.54
27:3:100:LYS:O	27:3:103:LEU:HB2	2.08	0.54
17:Q:109:HIS:HB3	18:R:224:THR:CB	2.38	0.54
22:V:325:ARG:HH22	23:W:499:ASN:HB3	0.72	0.54
25:1:3:ASN:CB	26:2:412:PHE:O	2.54	0.54
25:1:29:LEU:HD23	25:1:29:LEU:C	2.27	0.54
26:2:117:ASN:CG	27:3:108:ASN:CG	2.65	0.54
29:Y:48:DC:H2"	29:Y:49:DG:C8	2.41	0.54
1:A:549:THR:HG21	1:A:640:LEU:HG	1.90	0.54
1:A:597:PRO:O	1:A:599:HIS:N	2.40	0.54
2:B:133:ILE:O	2:B:134:LYS:C	2.45	0.54
22:V:638:GLN:O	22:V:642:ARG:HG2	2.08	0.54
26:2:199:ALA:HB1	26:2:201:PHE:CD2	2.43	0.54
1:A:924:TYR:OH	1:A:949:GLN:HA	2.08	0.54
5:E:52:ARG:HB2	5:E:53:PRO:HD2	1.80	0.54
16:P:161:ILE:O	16:P:161:ILE:HG23	2.07	0.54
22:V:667:THR:HA	25:1:62:ASP:OD2	2.07	0.54
26:2:28:PRO:CA	27:3:33:THR:HB	2.10	0.54
1:A:133:SER:C	1:A:135:GLY:N	2.40	0.54
2:B:92:TYR:HE2	2:B:146:LYS:NZ	2.06	0.54
3:C:9:VAL:HG11	11:K:105:PHE:HA	1.89	0.54
5:E:54:ARG:HG2	5:E:54:ARG:HH11	1.72	0.54
19:S:126:ILE:O	19:S:137:ALA:HA	2.08	0.54
20:T:141:LEU:O	20:T:143:GLN:N	2.38	0.54
27:3:144:ILE:HD11	27:3:147:MET:HE3	1.90	0.54
1:A:294:GLU:HA	1:A:298:ALA:HB2	1.88	0.54
1:A:1341:VAL:O	1:A:1343:LEU:N	2.38	0.54
26:2:214:TYR:CD2	26:2:261:PHE:CD2	2.95	0.54
27:3:169:ASP:CG	27:3:202:LEU:HD23	2.28	0.54
1:A:1123:ARG:NH1	1:A:1126:GLU:OE1	2.39	0.54
2:B:649:ASN:OD1	2:B:650:ASN:N	2.41	0.54
2:B:991:ALA:HB1	10:J:43:TYR:HB2	1.90	0.54
13:M:290:ARG:HH12	28:X:5:DG:P	2.31	0.54
23:W:428:ILE:HA	23:W:430:ASN:ND2	2.23	0.54
1:A:930:LEU:C	1:A:931:ARG:O	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:TRP:CD2	2:B:762:ARG:HG2	2.43	0.54
2:B:489:ILE:HG13	2:B:490:GLY:H	1.73	0.54
3:C:262:GLN:HG3	11:K:18:LYS:HG2	1.90	0.54
5:E:177:ASP:OD1	5:E:178:PRO:HD2	2.08	0.54
24:0:54:ARG:CB	27:3:209:ILE:HG23	2.25	0.54
26:2:81:LYS:HG3	26:2:82:ALA:N	2.21	0.54
26:2:86:SER:O	26:2:90:LEU:HD13	2.08	0.54
1:A:622:SER:C	1:A:624:GLY:N	2.53	0.53
2:B:739:ASN:HB3	10:J:62:TYR:CZ	2.44	0.53
3:C:7:PRO:HG3	11:K:97:GLU:OE2	2.04	0.53
9:I:14:ILE:HA	9:I:16:PHE:CE1	2.43	0.53
25:1:18:GLN:CD	25:1:44:PHE:HZ	2.11	0.53
25:1:25:GLU:HG2	25:1:32:LYS:HA	1.89	0.53
27:3:106:SER:O	27:3:109:GLU:HG3	2.08	0.53
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.90	0.53
2:B:91:ILE:N	20:T:141:LEU:HG	2.23	0.53
3:C:58:VAL:HG21	10:J:59:LEU:HB3	1.90	0.53
17:Q:14:LEU:HD21	17:Q:102:VAL:HG21	1.90	0.53
17:Q:105:TYR:CE1	18:R:231:GLU:OE1	2.59	0.53
20:T:26:TYR:HE2	20:T:124:TYR:HH	1.54	0.53
22:V:520:ARG:NE	22:V:521:GLU:OE2	2.30	0.53
26:2:62:LEU:HD13	26:2:62:LEU:C	2.28	0.53
26:2:220:LEU:HD13	26:2:220:LEU:C	2.29	0.53
26:2:222:THR:HG23	26:2:222:THR:O	2.07	0.53
1:A:137:PRO:HB2	1:A:1445:HIS:NE2	2.23	0.53
5:E:47:LYS:HB2	5:E:48:PRO:HD3	1.77	0.53
10:J:62:TYR:CA	10:J:64:PRO:HD2	2.30	0.53
13:M:44:ARG:HH11	13:M:46:ILE:HG22	1.72	0.53
25:1:4:VAL:HG11	26:2:412:PHE:CD2	2.29	0.53
1:A:521:VAL:C	1:A:666:ARG:HH21	2.11	0.53
1:A:522:PRO:HA	1:A:666:ARG:NH2	2.24	0.53
1:A:1111:GLY:HA2	21:U:254:GLY:HA2	1.90	0.53
26:2:141:HIS:HA	26:2:162:PHE:CE2	2.43	0.53
26:2:160:LEU:CG	26:2:206:LEU:HD21	2.39	0.53
27:3:191:ILE:N	27:3:210:THR:HG21	2.24	0.53
1:A:460:ARG:NE	1:A:492:TYR:O	2.32	0.53
1:A:603:ILE:HD11	1:A:988:TRP:NE1	2.23	0.53
2:B:853:LEU:HD12	12:L:46:LYS:HE3	1.91	0.53
2:B:1152:PRO:HG2	2:B:1155:CYS:HB2	1.89	0.53
26:2:31:LEU:HG	27:3:25:GLN:O	2.09	0.53
26:2:211:GLN:HE21	26:2:257:SER:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:225:PRO:HG2	13:M:228:VAL:HG23	1.90	0.53
17:Q:105:TYR:HE1	18:R:231:GLU:HB2	1.73	0.53
18:R:140:LYS:HB3	18:R:141:PRO:HD3	1.89	0.53
19:S:103:ASN:HB2	19:S:107:GLY:HA3	1.89	0.53
20:T:12:ALA:HB2	20:T:106:LEU:HD23	1.91	0.53
26:2:118:LEU:HD12	26:2:118:LEU:C	2.28	0.53
27:3:15:VAL:HG23	27:3:15:VAL:O	2.08	0.53
2:B:73:HIS:C	2:B:75:SER:H	2.12	0.53
17:Q:105:TYR:CE1	18:R:231:GLU:HB2	2.43	0.53
18:R:151:LEU:HD13	18:R:154:LEU:HD13	1.89	0.53
26:2:30:VAL:O	26:2:34:LEU:HD23	2.09	0.53
26:2:159:VAL:CG1	26:2:161:HIS:H	2.06	0.53
27:3:21:TRP:CG	27:3:34:LEU:HD23	2.44	0.53
1:A:542:LEU:HD23	1:A:774:ALA:HA	1.91	0.53
5:E:112:PRO:HA	5:E:115:LYS:HE2	1.91	0.53
7:G:94:LYS:HG3	7:G:95:VAL:HG23	1.90	0.53
18:R:78:LEU:HD11	18:R:124:LEU:HD21	1.89	0.53
26:2:138:PRO:O	26:2:139:ASP:HB2	2.08	0.53
26:2:241:SER:O	26:2:245:LEU:HD23	2.09	0.53
27:3:160:ARG:NH2	27:3:192:ASP:HB3	2.23	0.53
27:3:204:GLN:HG2	27:3:214:TYR:CZ	2.44	0.53
1:A:1248:ASN:HD21	1:A:1255:LEU:HA	1.74	0.53
9:I:15:ARG:O	9:I:15:ARG:HG3	2.08	0.53
27:3:105:THR:HG23	27:3:106:SER:N	2.23	0.53
2:B:1029:TYR:HA	2:B:1036:LYS:HA	1.91	0.53
3:C:56:SER:OG	3:C:158:GLU:N	2.27	0.53
27:3:10:LEU:HD21	27:3:143:TYR:CE2	2.44	0.53
1:A:870:SER:HB2	1:A:882:SER:HB3	1.90	0.52
2:B:92:TYR:CB	20:T:145:LEU:HD13	2.38	0.52
17:Q:109:HIS:HE1	18:R:231:GLU:HA	1.73	0.52
22:V:325:ARG:HH21	23:W:499:ASN:CB	1.95	0.52
27:3:44:LEU:HD13	27:3:44:LEU:C	2.30	0.52
28:X:65:DG:N3	29:Y:30:DG:N2	2.57	0.52
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.43	0.52
13:M:47:ASP:O	13:M:48:VAL:C	2.38	0.52
2:B:329:GLY:H	2:B:335:ARG:NH2	2.07	0.52
18:R:190:LEU:HD12	18:R:205:ASP:CG	2.29	0.52
22:V:523:VAL:CG2	25:1:20:LEU:CD2	2.87	0.52
22:V:611:GLY:HA2	22:V:615:PHE:CB	2.37	0.52
29:Y:36:DA:N1	29:Y:37:DG:C6	2.76	0.52
2:B:367:TYR:OH	2:B:371:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:8:VAL:CG1	25:1:45:VAL:HG13	2.35	0.52
26:2:138:PRO:HG3	26:2:189:GLU:CG	2.35	0.52
26:2:192:GLU:CG	26:2:193:PRO:HD2	2.23	0.52
1:A:389:THR:HB	1:A:417:LYS:HD3	1.90	0.52
2:B:157:ARG:N	2:B:161:CYS:SG	2.71	0.52
5:E:29:THR:HG22	5:E:31:ASP:H	1.75	0.52
16:P:203:ARG:HG3	16:P:203:ARG:NH2	2.25	0.52
22:V:531:ILE:O	22:V:534:TYR:CZ	2.62	0.52
27:3:133:LEU:HD13	27:3:133:LEU:N	2.14	0.52
27:3:222:SER:HB3	27:3:225:GLN:HG2	1.92	0.52
2:B:160:TYR:HE1	20:T:144:GLN:HG2	1.74	0.52
2:B:182:GLY:HA2	2:B:184:TYR:CE1	2.45	0.52
2:B:873:LEU:CB	2:B:874:PRO:HD3	2.35	0.52
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.75	0.52
13:M:94:ASP:O	13:M:97:GLY:C	2.48	0.52
14:N:359:ASN:ND2	14:N:364:ASP:OD1	2.43	0.52
22:V:523:VAL:CG2	25:1:20:LEU:HD23	2.39	0.52
22:V:531:ILE:O	22:V:534:TYR:CE2	2.63	0.52
22:V:689:VAL:CB	26:2:391:ILE:HD11	2.39	0.52
25:1:35:ILE:O	25:1:35:ILE:HG13	2.08	0.52
29:Y:36:DA:N3	29:Y:37:DG:C5	2.78	0.52
2:B:45:ASP:OD2	2:B:531:TYR:OH	2.25	0.52
2:B:195:ILE:HD11	2:B:481:HIS:HE2	1.73	0.52
23:W:209:TYR:HH	23:W:234:ASP:H	1.56	0.52
27:3:10:LEU:HD21	27:3:143:TYR:CD2	2.45	0.52
27:3:18:ASN:O	27:3:21:TRP:CD1	2.63	0.52
27:3:70:LEU:HD22	27:3:114:GLU:HB3	1.91	0.52
29:Y:36:DA:C6	29:Y:37:DG:C5	2.97	0.52
1:A:11:SER:O	1:A:13:CYS:N	2.43	0.52
1:A:208:ASP:OD1	1:A:209:SER:N	2.41	0.52
1:A:219:GLU:O	1:A:222:HIS:HB3	2.08	0.52
9:I:105:GLU:O	9:I:106:ASP:CB	2.41	0.52
17:Q:23:ARG:CD	18:R:207:SER:O	2.57	0.52
17:Q:69:ASP:O	17:Q:70:LYS:HB2	2.10	0.52
27:3:172:LEU:HD13	27:3:172:LEU:C	2.29	0.52
1:A:1251:ASN:OD1	21:U:227:GLU:HB3	2.09	0.52
2:B:289:ILE:HD13	2:B:297:MET:SD	2.50	0.52
2:B:952:GLU:HG3	3:C:39:ILE:HG23	1.91	0.52
26:2:193:PRO:HB2	26:2:194:PRO:HD3	1.92	0.52
27:3:10:LEU:HD22	27:3:147:MET:HG2	1.92	0.52
27:3:42:MET:CG	27:3:111:ILE:HD11	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:40:DT:H2''	28:X:41:DT:H5''	1.92	0.52
1:A:602:CYS:HB2	1:A:655:ILE:HD12	1.91	0.52
1:A:800:PHE:HZ	1:A:815:TYR:CE1	2.28	0.52
1:A:1162:GLU:HA	1:A:1304:ILE:HD11	1.92	0.52
2:B:483:ARG:NH1	2:B:526:LEU:HB2	2.20	0.52
2:B:939:HIS:NE2	2:B:980:HIS:HA	2.24	0.52
18:R:194:ARG:O	18:R:196:ASP:N	2.43	0.52
21:U:290:VAL:HG22	21:U:297:ARG:HG2	1.90	0.52
22:V:593:LEU:HD11	22:V:615:PHE:HZ	1.75	0.52
24:O:77:LYS:C	24:O:79:ASN:N	2.56	0.52
26:2:257:SER:O	26:2:261:PHE:HD1	1.93	0.52
27:3:57:LEU:HD23	27:3:58:ALA:C	2.31	0.52
27:3:226:TYR:O	27:3:230:VAL:HB	2.10	0.52
29:Y:30:DG:N3	29:Y:31:DG:C5	2.78	0.52
2:B:733:MET:HE3	2:B:1054:MET:HE3	1.92	0.51
8:H:106:THR:C	8:H:108:ALA:N	2.63	0.51
1:A:47:THR:C	1:A:48:GLU:O	2.46	0.51
1:A:261:ARG:O	1:A:263:ALA:N	2.42	0.51
2:B:92:TYR:CD1	20:T:141:LEU:HD21	2.44	0.51
2:B:151:LYS:N	2:B:441:SER:OG	2.39	0.51
24:O:77:LYS:HG2	24:O:225:GLU:OE2	2.09	0.51
25:1:2:VAL:HG12	26:2:456:LYS:HG2	1.79	0.51
27:3:14:VAL:HG23	27:3:14:VAL:O	2.09	0.51
27:3:64:ILE:HG21	27:3:128:HIS:CB	2.40	0.51
27:3:141:LEU:HG	27:3:187:GLN:HE22	1.75	0.51
23:W:423:ASP:C	23:W:425:THR:N	2.64	0.51
26:2:160:LEU:HB3	26:2:206:LEU:HD21	1.93	0.51
1:A:489:THR:OG1	1:A:494:ALA:O	2.28	0.51
17:Q:108:ASP:OD1	17:Q:111:ARG:NH2	2.19	0.51
23:W:584:TYR:HB2	23:W:591:GLY:HA3	1.92	0.51
1:A:1479:LYS:HD3	6:F:103:PRO:HA	1.93	0.51
2:B:738:THR:HG22	2:B:772:LEU:HD21	1.93	0.51
2:B:866:ILE:HG13	2:B:867:ILE:N	2.25	0.51
14:N:353:LEU:HB2	14:N:370:ALA:HB3	1.91	0.51
27:3:121:LYS:HD3	27:3:121:LYS:N	2.25	0.51
1:A:77:ASN:HD22	13:M:43:ASP:CG	2.14	0.51
1:A:430:ARG:NH2	13:M:26:ASP:OD2	2.40	0.51
1:A:689:ILE:HD13	2:B:985:LEU:HD22	1.93	0.51
18:R:190:LEU:CD1	18:R:205:ASP:CB	2.88	0.51
26:2:179:LEU:CB	26:2:184:LEU:HD11	2.40	0.51
27:3:131:THR:HG23	27:3:133:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:165:LYS:HE3	27:3:200:SER:OG	2.09	0.51
1:A:743:ARG:HD2	21:U:257:GLN:HG2	1.92	0.51
22:V:523:VAL:HB	25:1:20:LEU:HD23	1.93	0.51
25:1:21:LEU:O	25:1:24:ASP:HB3	2.10	0.51
26:2:46:ARG:HD3	26:2:85:GLU:HB2	1.93	0.51
26:2:215:PHE:CE2	26:2:264:HIS:HB2	2.46	0.51
1:A:1172:ASN:OD1	1:A:1173:THR:N	2.43	0.51
2:B:1124:ILE:HD12	2:B:1124:ILE:H	1.76	0.51
3:C:154:ARG:N	3:C:157:GLN:OE1	2.38	0.51
5:E:192:LYS:HE3	5:E:194:ILE:HD11	1.93	0.51
7:G:10:GLU:HB3	7:G:67:LEU:HD11	1.92	0.51
27:3:165:LYS:HD3	27:3:165:LYS:C	2.31	0.51
2:B:1117:HIS:O	2:B:1127:ILE:HG12	2.11	0.51
7:G:151:ARG:HB2	7:G:158:PHE:CE1	2.46	0.51
9:I:57:LYS:C	9:I:59:THR:N	2.63	0.51
18:R:193:ASN:HB3	18:R:197:LYS:HA	1.92	0.51
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.75	0.51
23:W:209:TYR:CZ	23:W:233:PHE:HA	2.40	0.51
26:2:236:PHE:CE2	26:2:262:LEU:CD1	2.94	0.51
26:2:236:PHE:CE1	26:2:261:PHE:CB	2.94	0.51
1:A:476:ILE:HD12	1:A:476:ILE:N	2.25	0.51
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.93	0.51
1:A:980:PRO:HB2	1:A:981:CYS:SG	2.51	0.51
2:B:906:GLN:HG2	12:L:45:TYR:HE1	1.75	0.51
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.93	0.51
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.91	0.51
10:J:62:TYR:CB	10:J:64:PRO:CD	2.88	0.51
16:P:269:ARG:HB3	16:P:335:PHE:HB3	1.92	0.51
26:2:51:LEU:CD2	26:2:55:TRP:CD1	2.94	0.51
26:2:236:PHE:CZ	26:2:262:LEU:CD2	2.94	0.51
27:3:12:VAL:HG12	27:3:58:ALA:HB3	1.92	0.51
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.51	0.50
8:H:10:PHE:CE2	8:H:39:LEU:HD13	2.46	0.50
17:Q:54:PHE:HD2	18:R:194:ARG:CD	2.22	0.50
26:2:57:MET:HA	26:2:60:LEU:CG	2.41	0.50
27:3:165:LYS:HZ1	27:3:200:SER:H	1.59	0.50
29:Y:36:DA:H2"	29:Y:37:DG:H8	1.76	0.50
2:B:116:ARG:NH1	12:L:42:ARG:HH11	2.08	0.50
2:B:499:ARG:HH11	2:B:520:VAL:HG22	1.76	0.50
3:C:267:ILE:HG21	3:C:274:ILE:HD13	1.93	0.50
26:2:231:VAL:O	26:2:234:LEU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:85:PRO:C	9:I:86:CYS:O	2.49	0.50
10:J:28:GLU:HG2	10:J:30:THR:HG22	1.93	0.50
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.46	0.50
17:Q:180:PHE:CZ	18:R:211:SER:HA	2.38	0.50
26:2:199:ALA:HB1	26:2:201:PHE:CE2	2.47	0.50
27:3:100:LYS:HB3	27:3:103:LEU:CD1	2.38	0.50
27:3:187:GLN:O	27:3:188:ASN:HB2	2.12	0.50
1:A:85:PHE:HD1	1:A:257:PRO:HD3	1.76	0.50
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.94	0.50
13:M:52:TRP:CD1	13:M:67:VAL:HG22	2.47	0.50
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.77	0.50
13:M:178:LYS:NZ	29:Y:86:DC:OP1	2.45	0.50
15:O:66:ARG:HB3	15:O:73:THR:HB	1.92	0.50
16:P:297:LYS:HE2	16:P:297:LYS:CA	2.33	0.50
22:V:519:TYR:HE2	25:1:20:LEU:CG	2.19	0.50
26:2:140:LYS:CG	26:2:162:PHE:CE1	2.94	0.50
26:2:214:TYR:CB	26:2:261:PHE:CE2	2.95	0.50
1:A:1313:GLN:CD	1:A:1318:LYS:HB2	2.32	0.50
9:I:84:HIS:ND1	9:I:85:PRO:HD3	2.23	0.50
13:M:17:ASN:OD1	13:M:18:HIS:N	2.44	0.50
21:U:215:ILE:HG23	21:U:219:LEU:HD23	1.92	0.50
21:U:252:LYS:O	21:U:253:THR:HB	2.11	0.50
22:V:516:PRO:HG2	22:V:706:LYS:HE2	1.92	0.50
22:V:520:ARG:CG	25:1:23:LEU:HD11	2.42	0.50
25:1:2:VAL:HG23	25:1:2:VAL:O	2.11	0.50
26:2:35:TYR:CD1	26:2:35:TYR:N	2.79	0.50
1:A:126:ILE:HD13	1:A:129:ILE:HD12	1.93	0.50
1:A:463:THR:HG22	1:A:468:SER:HB3	1.94	0.50
1:A:873:VAL:HB	1:A:1083:PRO:HA	1.94	0.50
1:A:1408:ARG:NH2	1:A:1421:ARG:O	2.45	0.50
2:B:35:ASP:CG	2:B:646:ARG:HH12	2.15	0.50
2:B:160:TYR:CE1	20:T:144:GLN:HG2	2.46	0.50
2:B:351:VAL:HG11	2:B:361:LYS:HA	1.94	0.50
2:B:746:THR:HG22	2:B:812:ARG:NH1	2.27	0.50
13:M:86:LYS:HA	13:M:86:LYS:NZ	2.27	0.50
26:2:57:MET:HA	26:2:60:LEU:HG	1.93	0.50
26:2:93:LEU:CD2	26:2:96:TRP:HE1	2.25	0.50
26:2:223:ALA:O	26:2:224:GLN:HB3	2.12	0.50
27:3:64:ILE:CG2	27:3:128:HIS:HB3	2.42	0.50
1:A:199:TYR:CE1	13:M:93:PHE:CE2	2.98	0.50
2:B:939:HIS:CD2	2:B:980:HIS:HA	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:111:THR:HG21	28:X:58:DT:OP1	2.12	0.50
13:M:178:LYS:C	20:T:154:LYS:CB	2.77	0.50
26:2:30:VAL:CG1	26:2:34:LEU:HD23	2.40	0.50
27:3:60:ILE:HG22	27:3:61:ALA:N	2.26	0.50
27:3:216:LYS:O	27:3:216:LYS:HG2	2.11	0.50
27:3:108:ASN:O	27:3:111:ILE:HG12	2.12	0.50
27:3:202:LEU:HD22	27:3:202:LEU:N	2.27	0.50
2:B:387:HIS:CD2	2:B:504:THR:HG21	2.46	0.50
2:B:714:PRO:O	2:B:717:ASN:HB2	2.11	0.50
8:H:17:PRO:O	8:H:19:GLY:N	2.45	0.50
13:M:57:ASN:ND2	29:Y:54:DA:OP2	2.44	0.50
16:P:311:VAL:HG11	29:Y:81:DA:C2	2.47	0.50
17:Q:58:GLN:OE1	18:R:194:ARG:NH1	2.45	0.50
23:W:73:CYS:O	23:W:209:TYR:CE2	2.65	0.50
23:W:116:CYS:SG	23:W:191:PRO:HD2	2.51	0.50
23:W:430:ASN:CB	23:W:431:PRO:CD	2.86	0.50
24:0:54:ARG:CB	27:3:209:ILE:CG2	2.87	0.50
26:2:77:LYS:CD	26:2:78:GLU:HG3	2.41	0.50
26:2:181:GLN:HE21	26:2:181:GLN:CA	2.23	0.50
26:2:181:GLN:HE22	26:2:220:LEU:HD12	1.76	0.50
27:3:107:ALA:O	27:3:111:ILE:HG23	2.11	0.50
1:A:535:MET:O	1:A:669:TYR:OH	2.25	0.49
1:A:691:ASP:HB3	1:A:766:PHE:HB2	1.94	0.49
2:B:563:ASP:OD1	2:B:610:ARG:NH1	2.45	0.49
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.76	0.49
2:B:1069:ILE:HG12	13:M:48:VAL:CG1	2.42	0.49
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.45	0.49
17:Q:18:ALA:O	17:Q:22:ILE:HG12	2.12	0.49
18:R:93:ASP:HB3	18:R:95:HIS:CE1	2.47	0.49
20:T:139:VAL:HG12	20:T:141:LEU:N	2.27	0.49
20:T:141:LEU:HD23	20:T:143:GLN:NE2	2.27	0.49
23:W:494:ILE:HD11	23:W:680:ALA:HB2	1.93	0.49
25:1:1:MET:HA	26:2:413:LEU:CA	2.42	0.49
26:2:100:LEU:CG	26:2:119:ARG:HE	2.22	0.49
26:2:199:ALA:CB	26:2:201:PHE:CE2	2.95	0.49
27:3:137:LEU:CD1	27:3:177:PHE:CE1	2.95	0.49
28:X:14:DA:N6	29:Y:80:DT:O4	2.43	0.49
28:X:62:DG:N2	29:Y:33:DT:O2	2.45	0.49
1:A:281:ALA:O	1:A:285:LYS:HG3	2.11	0.49
1:A:375:ILE:HG21	1:A:666:ARG:NH1	2.27	0.49
1:A:460:ARG:HB2	1:A:501:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:44:PHE:CD2	7:G:103:PRO:HG2	2.47	0.49
13:M:86:LYS:CE	13:M:86:LYS:CA	2.86	0.49
19:S:125:TYR:CD1	19:S:139:PRO:HA	2.47	0.49
22:V:667:THR:CA	25:1:62:ASP:OD1	2.59	0.49
26:2:208:THR:HG23	26:2:209:PRO:HD2	1.91	0.49
27:3:10:LEU:CD2	27:3:143:TYR:HE2	2.25	0.49
27:3:12:VAL:HG23	27:3:12:VAL:O	2.10	0.49
27:3:12:VAL:HG22	27:3:161:ILE:HA	1.94	0.49
27:3:216:LYS:HD2	27:3:216:LYS:N	2.22	0.49
27:3:217:VAL:CG1	27:3:226:TYR:CE2	2.95	0.49
28:X:47:DC:H42	29:Y:47:DG:H22	1.59	0.49
1:A:817:PRO:HG2	1:A:818:GLU:OE1	2.12	0.49
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.95	0.49
14:N:312:GLU:HB3	14:N:313:PRO:HD3	1.95	0.49
23:W:325:THR:HG22	23:W:329:PHE:CE2	2.47	0.49
25:1:45:VAL:CG2	26:2:409:TYR:CE2	2.95	0.49
26:2:188:THR:HG23	26:2:189:GLU:N	2.27	0.49
26:2:426:ARG:HD2	26:2:444:THR:CG2	2.43	0.49
27:3:215:LEU:HD12	27:3:230:VAL:CG2	2.42	0.49
1:A:1192:TRP:HE1	1:A:1248:ASN:HB3	1.77	0.49
2:B:101:ARG:O	13:M:175:ARG:NH2	2.45	0.49
2:B:628:VAL:HG12	2:B:633:LEU:HD23	1.94	0.49
5:E:54:ARG:HG2	5:E:54:ARG:NH1	2.26	0.49
17:Q:102:VAL:HG13	17:Q:103:VAL:CG2	2.41	0.49
21:U:226:GLU:HG3	21:U:238:LYS:HZ1	1.76	0.49
25:1:1:MET:CE	26:2:415:GLN:C	2.80	0.49
25:1:34:ILE:HG21	25:1:54:GLN:CD	2.32	0.49
26:2:28:PRO:N	27:3:25:GLN:CB	2.71	0.49
26:2:81:LYS:CE	26:2:89:LEU:HD21	2.42	0.49
26:2:89:LEU:HD23	26:2:93:LEU:HG	1.94	0.49
26:2:245:LEU:HD22	26:2:245:LEU:N	2.27	0.49
27:3:10:LEU:CD2	27:3:143:TYR:CE2	2.95	0.49
27:3:53:ARG:HA	27:3:101:TYR:HE1	1.78	0.49
27:3:59:VAL:HG13	27:3:59:VAL:O	2.12	0.49
27:3:220:MET:N	27:3:221:PRO:HD2	2.28	0.49
1:A:85:PHE:CD1	1:A:257:PRO:HD3	2.48	0.49
1:A:138:LYS:HB2	1:A:1445:HIS:HE1	1.76	0.49
1:A:520:MET:HG3	1:A:522:PRO:HD2	1.93	0.49
2:B:509:VAL:HG11	2:B:524:LYS:HB3	1.95	0.49
2:B:905:ASP:OD1	2:B:924:ARG:NH1	2.46	0.49
1:A:606:HIS:O	1:A:608:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:GLU:H	1:A:931:ARG:HD3	1.76	0.49
2:B:191:GLU:OE2	2:B:472:ARG:NH1	2.46	0.49
5:E:62:VAL:CG2	5:E:72:MET:O	2.60	0.49
18:R:213:ASP:HB2	18:R:215:GLU:HA	1.93	0.49
24:0:55:LEU:N	27:3:209:ILE:HD11	2.28	0.49
26:2:35:TYR:CD1	26:2:62:LEU:CD1	2.95	0.49
26:2:42:LEU:HD22	26:2:52:ALA:HA	1.95	0.49
26:2:236:PHE:CZ	26:2:258:LEU:CD1	2.95	0.49
27:3:12:VAL:CG2	27:3:161:ILE:HA	2.42	0.49
27:3:166:ALA:O	27:3:198:SER:HB2	2.13	0.49
27:3:174:TYR:HD1	27:3:202:LEU:HD11	1.78	0.49
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.48	0.49
1:A:924:TYR:CE1	1:A:949:GLN:HG2	2.47	0.49
16:P:311:VAL:HG11	29:Y:81:DA:H2	1.78	0.49
22:V:534:TYR:CD1	22:V:534:TYR:C	2.86	0.49
27:3:100:LYS:HG3	27:3:101:TYR:H	1.74	0.49
27:3:195:VAL:HG23	27:3:214:TYR:CE1	2.48	0.49
27:3:223:LEU:HD13	27:3:223:LEU:C	2.33	0.49
1:A:641:CYS:SG	1:A:643:LYS:N	2.86	0.49
1:A:1213:ARG:NH2	1:A:1215:GLU:OE2	2.46	0.49
2:B:803:ARG:HH12	2:B:951:GLN:HE22	1.59	0.49
20:T:177:ARG:HE	20:T:208:GLN:HB2	1.77	0.49
24:0:54:ARG:CG	27:3:182:PHE:CZ	2.80	0.49
25:1:1:MET:HE3	26:2:415:GLN:N	2.28	0.49
26:2:203:PHE:CE2	26:2:205:LEU:CD2	2.96	0.49
1:A:375:ILE:HG13	1:A:666:ARG:HH11	1.77	0.49
1:A:927:GLU:O	1:A:931:ARG:HG3	2.13	0.49
2:B:309:PHE:HE2	9:I:25:TYR:HE2	1.59	0.49
2:B:474:THR:HG23	2:B:477:SER:H	1.78	0.49
23:W:596:LEU:HG	23:W:597:LEU:N	2.27	0.49
26:2:176:ALA:O	26:2:177:GLN:HB2	2.12	0.49
1:A:924:TYR:CZ	1:A:949:GLN:HA	2.48	0.49
26:2:90:LEU:CD2	26:2:140:LYS:HD3	2.42	0.49
26:2:133:THR:HG23	26:2:134:SER:N	2.28	0.49
26:2:170:ALA:CB	26:2:213:TRP:CZ3	2.95	0.49
27:3:160:ARG:HE	27:3:190:LEU:HG	1.78	0.49
28:X:65:DG:N2	29:Y:30:DG:C2	2.81	0.49
1:A:546:ARG:HB3	1:A:640:LEU:O	2.13	0.48
1:A:1392:TYR:OH	1:A:1394:ASN:HA	2.12	0.48
2:B:68:GLN:OE1	2:B:81:PRO:HB2	2.13	0.48
2:B:513:GLU:HG3	2:B:726:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:37:MET:HG2	8:H:127:GLY:HA3	1.95	0.48
25:1:45:VAL:HG21	26:2:409:TYR:CE2	2.48	0.48
26:2:77:LYS:HD3	26:2:78:GLU:HG3	1.94	0.48
26:2:166:SER:HB3	26:2:167:PRO:CD	2.43	0.48
27:3:177:PHE:CZ	27:3:203:LEU:CD2	2.95	0.48
1:A:484:LEU:N	1:A:484:LEU:HD23	2.28	0.48
2:B:838:GLN:O	2:B:891:ASP:N	2.40	0.48
16:P:242:GLN:HG3	16:P:248:ALA:HB3	1.94	0.48
26:2:159:VAL:N	26:2:162:PHE:HB3	2.28	0.48
26:2:189:GLU:CA	26:2:192:GLU:HG2	2.41	0.48
26:2:198:SER:OG	26:2:238:PHE:HE2	1.96	0.48
27:3:58:ALA:C	27:3:71:TYR:OH	2.51	0.48
2:B:414:GLU:HG2	2:B:436:LYS:HD3	1.95	0.48
9:I:62:VAL:O	9:I:64:GLU:CA	2.61	0.48
20:T:37:ARG:HH22	20:T:62:LEU:HB2	1.78	0.48
23:W:624:PRO:O	23:W:656:ALA:HB1	2.12	0.48
24:0:209:THR:HA	24:0:219:TYR:CD1	2.48	0.48
26:2:35:TYR:CE2	26:2:62:LEU:CB	2.96	0.48
1:A:1427:LEU:HD23	1:A:1456:GLU:HB3	1.94	0.48
2:B:20:ASP:OD1	2:B:21:LEU:N	2.45	0.48
3:C:67:ARG:HH22	10:J:2:ILE:HG13	1.77	0.48
3:C:242:GLU:OE1	3:C:242:GLU:N	2.46	0.48
17:Q:28:ILE:HG21	18:R:205:ASP:OD2	2.13	0.48
17:Q:36:ILE:HD13	17:Q:52:LEU:HD21	1.96	0.48
19:S:118:VAL:HG13	19:S:120:GLU:HG3	1.95	0.48
23:W:37:HIS:NE2	23:W:454:VAL:CG1	2.76	0.48
1:A:621:ILE:O	1:A:623:PRO:HD3	2.14	0.48
3:C:68:LEU:O	3:C:71:ILE:HG12	2.13	0.48
7:G:91:GLN:HG2	17:Q:145:PHE:CE1	2.47	0.48
11:K:61:TYR:HA	11:K:72:ILE:O	2.14	0.48
13:M:79:ASP:OD1	13:M:79:ASP:N	2.46	0.48
20:T:160:GLN:HA	20:T:163:ILE:HD12	1.94	0.48
25:1:34:ILE:HG22	25:1:46:ILE:CG1	2.44	0.48
26:2:211:GLN:HE21	26:2:257:SER:HB3	1.78	0.48
26:2:251:VAL:HG11	26:2:254:MET:SD	2.53	0.48
1:A:45:GLU:OE1	1:A:48:GLU:HG2	2.12	0.48
1:A:1188:GLU:O	1:A:1192:TRP:HZ3	1.97	0.48
1:A:1410:HIS:N	5:E:174:GLN:HE22	2.12	0.48
2:B:1022:LEU:CD1	2:B:1023:ARG:HG3	2.44	0.48
3:C:44:ILE:HD11	3:C:238:SER:HB2	1.94	0.48
7:G:114:PRO:HB2	7:G:116:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:39:CYS:HB3	9:I:42:CYS:SG	2.53	0.48
13:M:297:PRO:HG3	13:M:310:VAL:HG11	1.93	0.48
17:Q:28:ILE:CG2	18:R:205:ASP:OD2	2.62	0.48
21:U:227:GLU:O	21:U:228:MET:C	2.52	0.48
22:V:315:VAL:CG1	23:W:500:ASP:HB3	2.26	0.48
25:1:38:ILE:CG2	25:1:44:PHE:CE1	2.96	0.48
26:2:60:LEU:CD1	26:2:95:ILE:CG2	2.91	0.48
1:A:924:TYR:HH	1:A:949:GLN:HA	1.78	0.48
2:B:100:GLU:O	2:B:103:GLY:N	2.39	0.48
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.95	0.48
5:E:11:TRP:O	5:E:15:LYS:HG2	2.14	0.48
8:H:17:PRO:C	8:H:19:GLY:H	2.17	0.48
8:H:111:ARG:HB3	8:H:127:GLY:O	2.13	0.48
22:V:523:VAL:CB	25:1:20:LEU:CD2	2.85	0.48
26:2:178:LEU:HD12	26:2:178:LEU:N	2.28	0.48
27:3:21:TRP:HA	27:3:24:LYS:CG	2.43	0.48
1:A:809:HIS:CE1	2:B:697:GLU:OE2	2.66	0.48
1:A:1036:ASN:ND2	1:A:1037:ALA:N	2.62	0.48
2:B:841:ARG:HD2	2:B:895:PHE:CZ	2.48	0.48
12:L:27:GLU:HG3	12:L:27:GLU:O	2.13	0.48
13:M:60:ALA:O	13:M:62:LYS:N	2.45	0.48
20:T:194:HIS:HD1	20:T:196:TYR:H	1.62	0.48
21:U:290:VAL:HG13	21:U:297:ARG:HG2	1.96	0.48
23:W:285:TYR:CE1	23:W:403:PHE:CZ	3.01	0.48
26:2:234:LEU:HD23	26:2:234:LEU:C	2.34	0.48
1:A:362:SER:HB3	2:B:1084:LEU:HD12	1.95	0.48
1:A:1155:LYS:HD3	21:U:249:GLN:OE1	2.13	0.48
22:V:504:LYS:CB	22:V:654:GLU:O	2.58	0.48
22:V:531:ILE:C	22:V:534:TYR:CE2	2.85	0.48
23:W:608:ILE:HG23	23:W:614:TYR:CZ	2.48	0.48
25:1:43:VAL:HG12	25:1:44:PHE:N	2.27	0.48
26:2:100:LEU:HD11	26:2:119:ARG:CG	2.31	0.48
27:3:165:LYS:NZ	27:3:200:SER:H	2.12	0.48
28:X:41:DT:H1'	28:X:42:DT:H3'	1.95	0.48
2:B:911:LEU:HD13	2:B:915:GLY:HA2	1.96	0.48
13:M:235:ILE:HD11	13:M:300:PHE:CE1	2.49	0.48
22:V:634:ARG:HG2	22:V:679:PHE:CZ	2.48	0.48
25:1:53:LEU:H	25:1:53:LEU:CD1	2.26	0.48
26:2:35:TYR:CD1	26:2:62:LEU:CG	2.92	0.48
26:2:211:GLN:CA	26:2:261:PHE:CE1	2.95	0.48
27:3:124:ILE:O	27:3:127:GLN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:22:DG:H2'	29:Y:23:DT:C6	2.48	0.48
7:G:98:PHE:CZ	17:Q:152:PHE:HE1	2.31	0.47
13:M:205:SER:OG	16:P:278:GLN:NE2	2.43	0.47
17:Q:23:ARG:NH2	18:R:209:GLN:N	2.43	0.47
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.79	0.47
25:1:18:GLN:OE1	25:1:19:PHE:CD1	2.67	0.47
25:1:59:GLU:CD	26:2:402:ARG:HH12	2.14	0.47
26:2:28:PRO:O	27:3:25:GLN:O	2.32	0.47
26:2:89:LEU:CD2	26:2:93:LEU:HG	2.44	0.47
26:2:171:VAL:CG2	26:2:213:TRP:HA	2.19	0.47
26:2:236:PHE:CD1	26:2:261:PHE:HB3	2.49	0.47
27:3:160:ARG:HB2	27:3:190:LEU:HG	1.96	0.47
1:A:532:ARG:HB3	1:A:649:ALA:HB2	1.96	0.47
1:A:999:ARG:HE	8:H:99:ILE:CD1	2.22	0.47
1:A:1186:VAL:HG12	1:A:1188:GLU:HG2	1.96	0.47
2:B:101:ARG:HB3	13:M:131:PRO:HG2	1.96	0.47
2:B:274:ARG:HE	2:B:308:ALA:HB1	1.80	0.47
4:D:40:LEU:HD13	7:G:75:ILE:HD11	1.95	0.47
17:Q:109:HIS:CB	18:R:224:THR:CB	2.84	0.47
18:R:153:ARG:O	18:R:157:GLN:N	2.46	0.47
22:V:461:HIS:CE1	22:V:462:CYS:HG	2.31	0.47
24:0:165:ARG:HB2	24:0:193:LYS:O	2.14	0.47
25:1:3:ASN:HB2	26:2:412:PHE:O	2.13	0.47
25:1:38:ILE:HG22	25:1:44:PHE:CE1	2.48	0.47
26:2:203:PHE:CD2	26:2:204:LEU:N	2.82	0.47
27:3:216:LYS:O	27:3:218:PRO:HD3	2.14	0.47
5:E:15:LYS:NZ	5:E:33:LEU:O	2.40	0.47
13:M:86:LYS:HE2	13:M:86:LYS:CA	2.43	0.47
19:S:25:LYS:HD3	19:S:141:HIS:CD2	2.49	0.47
20:T:154:LYS:HD2	20:T:154:LYS:N	2.26	0.47
26:2:117:ASN:CB	27:3:42:MET:HE2	2.43	0.47
26:2:218:GLN:HG2	26:2:268:PHE:CB	2.44	0.47
26:2:236:PHE:HE2	26:2:262:LEU:CD1	2.27	0.47
1:A:220:ARG:HD2	1:A:223:GLU:OE1	2.14	0.47
1:A:246:GLU:HG2	1:A:247:TRP:CD1	2.50	0.47
1:A:621:ILE:O	1:A:623:PRO:CD	2.63	0.47
1:A:766:PHE:CE1	1:A:781:ILE:HG12	2.49	0.47
2:B:91:ILE:H	20:T:141:LEU:HG	1.79	0.47
2:B:202:THR:O	2:B:204:THR:N	2.47	0.47
3:C:61:ASP:OD2	12:L:48:ARG:NH1	2.48	0.47
8:H:128:ASP:N	8:H:128:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:10:LEU:C	13:M:12:ARG:N	2.68	0.47
13:M:169:ARG:HH11	13:M:206:VAL:HG21	1.79	0.47
13:M:178:LYS:O	20:T:154:LYS:CG	2.62	0.47
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.96	0.47
20:T:177:ARG:CZ	20:T:212:TYR:HB2	2.44	0.47
22:V:361:CYS:HB3	22:V:405:VAL:HG21	1.96	0.47
25:1:1:MET:HE1	26:2:440:LEU:HD13	1.94	0.47
26:2:93:LEU:CA	26:2:96:TRP:CD1	2.94	0.47
26:2:211:GLN:CB	26:2:261:PHE:CE1	2.95	0.47
27:3:10:LEU:CD1	27:3:56:LYS:HG2	2.44	0.47
27:3:226:TYR:CA	27:3:230:VAL:HG23	2.42	0.47
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.79	0.47
4:D:112:LYS:NZ	4:D:124:ASP:OD2	2.28	0.47
7:G:110:ARG:HA	7:G:113:ILE:HD12	1.97	0.47
8:H:56:PHE:HA	8:H:148:LEU:HA	1.96	0.47
13:M:195:PHE:CZ	13:M:199:LEU:HD11	2.49	0.47
17:Q:25:PHE:CZ	17:Q:110:MET:HE3	2.49	0.47
22:V:321:GLU:OE2	23:W:500:ASP:CA	2.59	0.47
22:V:370:SER:O	22:V:374:TRP:HD1	1.96	0.47
26:2:205:LEU:HD22	26:2:205:LEU:N	2.30	0.47
1:A:90:LEU:O	1:A:291:ARG:NH2	2.47	0.47
1:A:490:THR:HG23	21:U:282:ASP:HB3	1.96	0.47
3:C:171:LYS:HE3	11:K:10:PHE:HB3	1.96	0.47
13:M:44:ARG:NH1	13:M:46:ILE:HG22	2.29	0.47
13:M:235:ILE:HD11	13:M:300:PHE:HE1	1.79	0.47
19:S:174:PHE:O	19:S:178:GLN:HG2	2.14	0.47
22:V:514:MET:HE2	22:V:664:SER:HB3	1.95	0.47
25:1:4:VAL:HG12	26:2:411:GLN:C	2.30	0.47
27:3:10:LEU:HA	27:3:56:LYS:HG2	1.96	0.47
1:A:297:GLY:HA3	17:Q:57:LYS:HG3	1.96	0.47
1:A:351:ARG:HG3	2:B:1088:GLU:OE2	2.15	0.47
1:A:777:SER:OG	1:A:779:ILE:HG22	2.15	0.47
1:A:1128:ILE:HD11	1:A:1401:LEU:HD21	1.97	0.47
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.39	0.47
2:B:26:CYS:SG	2:B:27:TRP:N	2.87	0.47
2:B:754:PRO:HB2	2:B:773:PRO:CG	2.45	0.47
3:C:143:VAL:HG23	3:C:144:GLU:H	1.80	0.47
5:E:55:ARG:HG2	5:E:76:PHE:HB2	1.94	0.47
15:O:64:THR:OG1	15:O:75:VAL:HB	2.15	0.47
16:P:297:LYS:C	16:P:299:ARG:H	2.17	0.47
21:U:292:ASN:O	21:U:294:CYS:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:50:VAL:CG1	25:1:54:GLN:HG2	2.41	0.47
26:2:46:ARG:CD	26:2:85:GLU:CB	2.93	0.47
26:2:201:PHE:CD1	26:2:202:GLN:N	2.83	0.47
29:Y:36:DA:C1'	29:Y:37:DG:C8	2.97	0.47
1:A:220:ARG:O	1:A:221:VAL:C	2.52	0.47
1:A:1408:ARG:HD2	1:A:1422:GLN:HE22	1.80	0.47
2:B:613:ARG:HD3	2:B:615:TYR:CE2	2.50	0.47
2:B:628:VAL:HG22	2:B:694:THR:C	2.35	0.47
3:C:67:ARG:NH1	10:J:2:ILE:HG13	2.28	0.47
8:H:66:GLU:O	8:H:66:GLU:HG2	2.13	0.47
17:Q:105:TYR:CE1	18:R:231:GLU:CB	2.86	0.47
20:T:142:SER:C	20:T:144:GLN:H	2.12	0.47
23:W:73:CYS:HB3	23:W:209:TYR:CG	2.49	0.47
23:W:143:ARG:HG2	23:W:143:ARG:HH11	1.80	0.47
23:W:657:MET:O	23:W:660:ALA:HB3	2.15	0.47
25:1:9:LEU:N	25:1:9:LEU:HD12	2.30	0.47
25:1:38:ILE:CB	25:1:44:PHE:CE1	2.98	0.47
27:3:70:LEU:HD22	27:3:114:GLU:CB	2.44	0.47
27:3:131:THR:HG23	27:3:133:LEU:HD13	1.95	0.47
27:3:137:LEU:HD11	27:3:177:PHE:CE1	2.50	0.47
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.74	0.47
1:A:1013:VAL:HG11	1:A:1046:ARG:HG2	1.97	0.47
2:B:119:THR:HG23	2:B:187:ILE:HA	1.97	0.47
2:B:1062:ARG:HH11	2:B:1082:GLY:HA2	1.80	0.47
5:E:21:CYS:SG	5:E:62:VAL:HG11	2.55	0.47
15:O:66:ARG:N	15:O:73:THR:O	2.48	0.47
17:Q:110:MET:SD	18:R:222:SER:CB	3.02	0.47
21:U:226:GLU:CG	21:U:238:LYS:NZ	2.78	0.47
22:V:689:VAL:CG2	26:2:391:ILE:CD1	2.93	0.47
25:1:22:TYR:O	25:1:25:GLU:HB3	2.15	0.47
26:2:51:LEU:HD21	26:2:55:TRP:CD1	2.50	0.47
26:2:84:GLU:OE1	26:2:84:GLU:HA	2.15	0.47
26:2:85:GLU:O	26:2:89:LEU:HB2	2.15	0.47
27:3:64:ILE:HG21	27:3:128:HIS:HB3	1.97	0.47
27:3:177:PHE:O	27:3:181:ILE:HG13	2.15	0.47
1:A:1250:ASP:HB3	21:U:227:GLU:HG2	0.47	0.47
1:A:1274:GLU:O	1:A:1276:VAL:N	2.48	0.47
1:A:1408:ARG:HD2	1:A:1422:GLN:NE2	2.30	0.47
2:B:873:LEU:CB	2:B:874:PRO:CD	2.90	0.47
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.96	0.47
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:593:LEU:HD21	22:V:615:PHE:HZ	1.78	0.47
25:1:38:ILE:O	25:1:38:ILE:HG12	2.15	0.47
25:1:53:LEU:O	25:1:57:VAL:HG12	2.15	0.47
26:2:96:TRP:CH2	26:2:97:HIS:CE1	3.03	0.47
26:2:221:GLN:CD	26:2:230:LEU:HB2	2.34	0.47
27:3:56:LYS:HD3	27:3:56:LYS:N	2.30	0.47
28:X:45:DC:H2'	28:X:46:DG:C8	2.49	0.47
29:Y:30:DG:C4	29:Y:31:DG:C5	3.02	0.47
29:Y:31:DG:H2''	29:Y:32:DC:C6	2.50	0.47
1:A:199:TYR:CZ	13:M:93:PHE:HE2	2.23	0.46
8:H:7:GLU:OE2	8:H:57:ARG:NH2	2.48	0.46
9:I:93:GLU:O	9:I:115:THR:HG22	2.15	0.46
23:W:73:CYS:HB2	23:W:209:TYR:CE1	2.50	0.46
26:2:240:LEU:HD12	26:2:240:LEU:N	2.30	0.46
27:3:12:VAL:CG2	27:3:161:ILE:HG23	2.43	0.46
1:A:561:MET:HG2	11:K:58:PHE:CD1	2.50	0.46
1:A:592:PHE:CZ	1:A:595:ILE:HD11	2.50	0.46
2:B:195:ILE:HG21	2:B:486:ASN:HB2	1.97	0.46
2:B:1115:GLN:OE1	2:B:1115:GLN:N	2.47	0.46
5:E:55:ARG:HB3	5:E:76:PHE:O	2.16	0.46
20:T:94:THR:HG22	20:T:109:ILE:HA	1.97	0.46
22:V:366:ASN:ND2	22:V:613:THR:HG22	2.30	0.46
23:W:73:CYS:CB	23:W:209:TYR:CE1	2.99	0.46
23:W:73:CYS:HB3	23:W:209:TYR:CD1	2.51	0.46
28:X:39:DT:H2'	28:X:40:DT:C6	2.49	0.46
1:A:111:CYS:SG	1:A:114:CYS:CB	3.02	0.46
1:A:1036:ASN:C	1:A:1036:ASN:HD22	2.18	0.46
2:B:91:ILE:HG22	20:T:141:LEU:CG	2.45	0.46
2:B:187:ILE:HD11	2:B:448:LEU:HD23	1.98	0.46
2:B:854:ILE:O	2:B:907:VAL:HG21	2.15	0.46
2:B:936:ALA:HB2	2:B:942:LYS:HA	1.97	0.46
2:B:992:ASN:O	10:J:46:ARG:NH2	2.48	0.46
3:C:149:LEU:HD21	3:C:152:LYS:HE3	1.97	0.46
15:O:50:GLN:O	15:O:53:ARG:NH1	2.47	0.46
17:Q:172:ASP:O	17:Q:176:LEU:N	2.39	0.46
19:S:125:TYR:HD1	19:S:139:PRO:HA	1.81	0.46
26:2:30:VAL:HB	27:3:25:GLN:O	2.16	0.46
27:3:196:LEU:HB3	27:3:220:MET:SD	2.56	0.46
1:A:117:LEU:HD23	1:A:119:VAL:H	1.80	0.46
1:A:495:ASP:HB3	2:B:792:ASP:OD2	2.16	0.46
1:A:1181:PRO:C	1:A:1183:SER:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ASP:N	2:B:212:ASP:OD1	2.46	0.46
13:M:12:ARG:NH1	13:M:23:LEU:O	2.48	0.46
18:R:78:LEU:HB2	18:R:119:LEU:HD22	1.98	0.46
22:V:321:GLU:CG	23:W:499:ASN:ND2	2.76	0.46
23:W:175:TYR:CD1	23:W:175:TYR:N	2.76	0.46
25:1:40:ASP:HB2	25:1:43:VAL:H	1.81	0.46
26:2:30:VAL:HB	27:3:24:LYS:O	2.15	0.46
1:A:1251:ASN:HD21	21:U:227:GLU:HB3	1.77	0.46
2:B:80:GLU:O	2:B:135:GLU:HG2	2.10	0.46
2:B:651:TYR:HA	2:B:655:ASP:OD2	2.16	0.46
2:B:1069:ILE:HA	2:B:1072:ARG:HE	1.80	0.46
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.81	0.46
17:Q:109:HIS:HE1	18:R:231:GLU:CA	2.28	0.46
17:Q:113:ARG:HH21	18:R:218:LYS:HE2	1.68	0.46
18:R:195:PRO:HB2	18:R:199:LYS:CB	2.46	0.46
23:W:581:LEU:C	23:W:581:LEU:HD13	2.36	0.46
6:F:56:TYR:HD1	6:F:124:ILE:HB	1.80	0.46
13:M:289:TYR:HA	13:M:292:ILE:HG12	1.96	0.46
18:R:149:LYS:HD2	18:R:175:LEU:H	1.81	0.46
18:R:195:PRO:HB2	18:R:199:LYS:HD3	1.94	0.46
20:T:179:ASP:O	20:T:181:GLN:N	2.48	0.46
25:1:2:VAL:HG11	26:2:456:LYS:CB	2.44	0.46
26:2:96:TRP:CZ2	26:2:97:HIS:NE2	2.83	0.46
26:2:217:LEU:CD2	26:2:233:ILE:HD11	2.45	0.46
27:3:10:LEU:N	27:3:56:LYS:HE3	2.31	0.46
27:3:10:LEU:HB2	27:3:56:LYS:HE3	1.97	0.46
1:A:406:VAL:HG21	1:A:440:LEU:HD11	1.97	0.46
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.55	0.46
2:B:751:LEU:HD12	2:B:751:LEU:HA	1.81	0.46
3:C:138:ASP:OD1	3:C:139:PRO:HD2	2.16	0.46
5:E:62:VAL:HG22	5:E:72:MET:O	2.15	0.46
9:I:15:ARG:NH1	9:I:46:GLN:OE1	2.48	0.46
13:M:22:ILE:HG23	13:M:35:PRO:HG2	1.96	0.46
17:Q:35:ASP:CG	18:R:161:ARG:HH22	2.18	0.46
21:U:280:SER:HB2	21:U:284:PRO:HA	1.98	0.46
22:V:444:HIS:O	22:V:447:PRO:CD	2.61	0.46
24:0:77:LYS:HA	24:0:77:LYS:HE3	1.97	0.46
25:1:2:VAL:HG12	26:2:456:LYS:CE	2.44	0.46
25:1:10:ILE:HG12	25:1:43:VAL:CG1	2.45	0.46
26:2:81:LYS:CG	26:2:82:ALA:N	2.79	0.46
1:A:27:SER:O	1:A:31:LEU:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:HIS:N	1:A:181:HIS:CD2	2.82	0.46
1:A:890:ARG:NH2	1:A:1023:VAL:HB	2.30	0.46
2:B:739:ASN:HB3	10:J:62:TYR:OH	2.16	0.46
5:E:172:ARG:HD2	5:E:210:GLN:HB3	1.98	0.46
8:H:65:TYR:CD2	8:H:70:LEU:HD23	2.50	0.46
1:A:608:THR:OG1	1:A:610:PRO:CD	2.64	0.46
1:A:1195:VAL:HG12	21:U:192:ARG:HD3	1.98	0.46
2:B:1125:MET:HG3	2:B:1163:MET:HE1	1.98	0.46
3:C:5:ASN:O	3:C:7:PRO:N	2.42	0.46
3:C:262:GLN:O	3:C:266:GLU:HG2	2.16	0.46
5:E:14:ARG:NH1	5:E:58:LEU:O	2.49	0.46
13:M:99:SER:HG	28:X:34:DA:H61	1.64	0.46
14:N:11:PRO:HA	14:N:14:TYR:HD2	1.81	0.46
15:O:3:TYR:C	15:O:5:LEU:N	2.51	0.46
22:V:321:GLU:CA	23:W:499:ASN:ND2	2.58	0.46
23:W:37:HIS:CG	23:W:454:VAL:HG13	2.50	0.46
25:1:22:TYR:HD1	25:1:23:LEU:HD23	1.80	0.46
26:2:35:TYR:CD2	26:2:62:LEU:CB	2.95	0.46
27:3:8:LEU:HD23	27:3:54:SER:CB	2.42	0.46
1:A:19:LYS:HD3	2:B:1174:VAL:HG23	1.98	0.46
1:A:691:ASP:OD1	1:A:765:ASN:N	2.48	0.46
1:A:809:HIS:HE1	2:B:697:GLU:OE2	1.98	0.46
1:A:1450:PRO:O	1:A:1452:LYS:HG3	2.15	0.46
3:C:45:ILE:HG22	3:C:73:LEU:HD12	1.98	0.46
3:C:49:TRP:O	3:C:163:ALA:HA	2.16	0.46
6:F:56:TYR:CD1	6:F:124:ILE:HB	2.50	0.46
9:I:98:GLN:NE2	9:I:108:MET:SD	2.89	0.46
20:T:139:VAL:C	20:T:141:LEU:H	2.18	0.46
25:1:38:ILE:CG2	25:1:44:PHE:CD1	2.94	0.46
25:1:57:VAL:HG13	25:1:58:GLY:N	2.31	0.46
26:2:187:SER:OG	26:2:190:PRO:HD2	2.16	0.46
26:2:214:TYR:CE1	26:2:233:ILE:HG23	2.51	0.46
27:3:64:ILE:CG2	27:3:128:HIS:CB	2.94	0.46
1:A:693:ILE:HG21	2:B:1023:ARG:NE	2.31	0.45
3:C:44:ILE:HD11	3:C:238:SER:CB	2.46	0.45
5:E:25:GLY:O	5:E:65:ASN:HA	2.16	0.45
7:G:152:VAL:HG22	7:G:157:ILE:HG13	1.98	0.45
8:H:23:ASP:OD1	8:H:23:ASP:N	2.49	0.45
18:R:138:ALA:O	18:R:140:LYS:N	2.49	0.45
25:1:38:ILE:HA	25:1:44:PHE:CD1	2.37	0.45
26:2:118:LEU:HD21	27:3:39:ASP:OD1	1.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:69:PHE:HE1	27:3:139:LYS:HD2	1.77	0.45
1:A:632:ASN:CA	1:A:992:LYS:HD2	2.43	0.45
2:B:163:LEU:HD12	2:B:163:LEU:N	2.31	0.45
2:B:201:ALA:HB3	2:B:206:TYR:OH	2.16	0.45
2:B:952:GLU:HG3	3:C:39:ILE:CG2	2.46	0.45
2:B:961:ILE:H	2:B:961:ILE:HG13	1.55	0.45
8:H:24:ARG:O	8:H:45:ILE:N	2.49	0.45
8:H:100:GLU:HG3	8:H:101:GLY:N	2.25	0.45
10:J:44:CYS:O	10:J:47:ARG:HG3	2.15	0.45
23:W:623:VAL:HG23	23:W:681:ASP:HB2	1.98	0.45
26:2:221:GLN:HG2	26:2:268:PHE:HZ	1.75	0.45
27:3:15:VAL:HG12	27:3:164:ILE:HD12	1.97	0.45
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.98	0.45
2:B:403:LEU:O	2:B:407:MET:HG2	2.17	0.45
2:B:487:SER:HA	2:B:488:PRO:HD3	1.67	0.45
5:E:62:VAL:HG23	5:E:72:MET:CB	2.40	0.45
6:F:109:TYR:CD1	6:F:115:TYR:HB3	2.51	0.45
16:P:239:ARG:HD2	16:P:239:ARG:HA	1.57	0.45
26:2:203:PHE:CG	26:2:204:LEU:N	2.84	0.45
27:3:190:LEU:HA	27:3:210:THR:HG21	1.91	0.45
28:X:32:DG:H2''	28:X:33:DA:O5'	2.16	0.45
28:X:67:DG:C2	28:X:68:DC:C2	3.04	0.45
1:A:262:PRO:HD3	1:A:342:ARG:HH12	1.81	0.45
1:A:533:PRO:CG	1:A:654:HIS:HB2	2.46	0.45
1:A:595:ILE:C	1:A:595:ILE:HD12	2.37	0.45
5:E:40:PHE:HE2	5:E:46:ASP:OD2	1.93	0.45
5:E:64:HIS:CD2	5:E:67:ASP:O	2.69	0.45
14:N:354:LYS:HA	14:N:369:LYS:HA	1.99	0.45
16:P:206:GLU:HB3	16:P:236:LYS:HZ2	1.81	0.45
20:T:191:PHE:HA	20:T:197:TYR:HE2	1.81	0.45
23:W:299:ARG:HG3	23:W:300:GLU:HG2	1.97	0.45
26:2:90:LEU:HD21	26:2:140:LYS:HD3	1.98	0.45
26:2:117:ASN:HB2	27:3:104:LEU:CG	2.46	0.45
27:3:64:ILE:CG2	27:3:128:HIS:CG	2.99	0.45
29:Y:56:DG:C2'	29:Y:57:DA:H5'	2.46	0.45
1:A:37:THR:O	1:A:39:GLY:N	2.50	0.45
1:A:261:ARG:HB3	1:A:276:LEU:HD22	1.98	0.45
1:A:686:THR:OG1	1:A:687:ILE:N	2.49	0.45
3:C:71:ILE:HG13	3:C:71:ILE:O	2.16	0.45
8:H:65:TYR:HE2	8:H:70:LEU:HB3	1.79	0.45
9:I:54:TYR:OH	9:I:56:ASN:ND2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:LYS:HB3	12:L:23:HIS:HE1	1.82	0.45
18:R:77:VAL:HA	18:R:80:LYS:HE3	1.98	0.45
25:1:54:GLN:O	25:1:57:VAL:HG12	2.16	0.45
26:2:30:VAL:N	27:3:25:GLN:O	2.50	0.45
26:2:51:LEU:HD23	26:2:51:LEU:C	2.37	0.45
27:3:42:MET:CG	27:3:111:ILE:CD1	2.95	0.45
1:A:1112:VAL:HB	21:U:253:THR:HB	1.99	0.45
2:B:285:LEU:O	2:B:289:ILE:HG22	2.16	0.45
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.99	0.45
10:J:63:ALA:H	10:J:64:PRO:HD3	1.75	0.45
17:Q:109:HIS:CE1	18:R:231:GLU:HG3	2.52	0.45
18:R:138:ALA:C	18:R:140:LYS:N	2.70	0.45
20:T:26:TYR:HE2	20:T:124:TYR:OH	2.00	0.45
26:2:30:VAL:CG1	26:2:34:LEU:CD2	2.94	0.45
27:3:42:MET:HE1	27:3:108:ASN:HB2	1.98	0.45
27:3:160:ARG:HE	27:3:160:ARG:HB2	1.58	0.45
29:Y:71:DA:H2'	29:Y:71:DA:OP2	2.15	0.45
1:A:780:ASN:ND2	2:B:976:MET:SD	2.89	0.45
2:B:529:MET:HE2	2:B:623:ARG:HB2	1.98	0.45
2:B:698:ILE:O	2:B:699:HIS:HB2	2.17	0.45
2:B:1101:GLN:OE1	6:F:64:ARG:NH1	2.50	0.45
3:C:149:LEU:HD23	10:J:2:ILE:HD13	1.98	0.45
7:G:97:LEU:HD23	7:G:108:ILE:HD12	1.97	0.45
19:S:165:GLU:HA	19:S:168:ASN:HB2	1.97	0.45
27:3:219:GLN:OE1	27:3:219:GLN:HA	2.17	0.45
28:X:13:DT:H2''	28:X:14:DA:H8	1.81	0.45
1:A:275:ASP:HA	1:A:278:HIS:HB2	1.99	0.45
1:A:1192:TRP:HA	1:A:1195:VAL:HB	1.98	0.45
1:A:1319:LYS:H	1:A:1356:ARG:HH22	1.64	0.45
2:B:758:LEU:O	2:B:996:ILE:HG23	2.16	0.45
2:B:968:ASN:CG	2:B:969:PRO:HD2	2.37	0.45
3:C:147:ASP:OD2	3:C:148:ILE:HG22	2.17	0.45
14:N:315:ASN:HA	16:P:239:ARG:HH12	1.82	0.45
18:R:157:GLN:HG2	18:R:160:GLN:HB3	1.99	0.45
20:T:8:ASP:HB3	20:T:105:SER:HA	1.99	0.45
27:3:121:LYS:HD3	27:3:121:LYS:H	1.80	0.45
27:3:148:ASN:ND2	27:3:157:MET:HG3	2.32	0.45
1:A:267:GLN:H	13:M:49:GLY:CA	2.29	0.45
1:A:546:ARG:HG3	1:A:547:LYS:H	1.81	0.45
1:A:581:LYS:NZ	8:H:86:ASP:O	2.49	0.45
1:A:625:ASP:O	1:A:638:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:GLY:O	1:A:1470:CYS:HB2	2.17	0.45
2:B:243:GLY:N	2:B:252:ILE:HG21	2.32	0.45
3:C:260:GLN:O	3:C:260:GLN:HG3	2.17	0.45
5:E:172:ARG:CD	5:E:210:GLN:HB3	2.47	0.45
8:H:113:SER:OG	8:H:126:GLN:HG2	2.17	0.45
23:W:37:HIS:NE2	23:W:454:VAL:HG11	2.32	0.45
1:A:157:GLY:N	1:A:181:HIS:NE2	2.64	0.45
1:A:608:THR:HB	1:A:610:PRO:HD2	1.97	0.45
1:A:1250:ASP:CA	21:U:227:GLU:HG3	2.47	0.45
2:B:380:ARG:HE	2:B:609:GLU:CD	2.19	0.45
17:Q:71:PHE:CE1	17:Q:106:LYS:HE3	2.52	0.45
26:2:117:ASN:HB3	27:3:42:MET:HE2	1.99	0.45
26:2:164:VAL:HG13	26:2:209:PRO:CG	2.45	0.45
1:A:611:ASP:OD2	1:A:627:LYS:HG3	2.17	0.44
2:B:62:ALA:N	2:B:63:PRO:HD3	2.32	0.44
2:B:298:MET:O	2:B:301:VAL:HG12	2.15	0.44
2:B:514:THR:HG21	2:B:521:GLY:HA2	1.99	0.44
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.98	0.44
9:I:119:CYS:HB3	9:I:121:HIS:H	1.82	0.44
13:M:92:SER:O	13:M:93:PHE:C	2.56	0.44
17:Q:24:GLY:O	18:R:210:PHE:HE2	1.99	0.44
18:R:157:GLN:OE1	18:R:162:GLY:HA2	2.17	0.44
24:0:106:ILE:HD11	24:0:127:HIS:HB3	1.99	0.44
26:2:35:TYR:HB2	26:2:62:LEU:HD12	1.98	0.44
1:A:138:LYS:NZ	1:A:1441:GLU:OE2	2.45	0.44
1:A:389:THR:HB	1:A:417:LYS:CD	2.48	0.44
1:A:797:ARG:NH2	1:A:820:ARG:HB2	2.33	0.44
2:B:235:ILE:HD11	2:B:347:MET:HG3	1.99	0.44
2:B:1116:VAL:HG11	2:B:1125:MET:SD	2.57	0.44
9:I:14:ILE:HA	9:I:16:PHE:CD1	2.52	0.44
13:M:91:ALA:O	13:M:92:SER:OG	2.36	0.44
13:M:246:PRO:HB2	16:P:306:VAL:HG21	1.99	0.44
14:N:324:GLU:HA	16:P:188:ARG:NH1	2.29	0.44
16:P:171:THR:HG22	16:P:220:VAL:HG22	1.98	0.44
16:P:298:PRO:HB2	16:P:320:GLU:HB3	1.99	0.44
22:V:517:GLU:CB	22:V:713:LEU:HD22	2.46	0.44
22:V:647:LYS:O	22:V:648:LYS:O	2.35	0.44
22:V:666:ASP:CB	25:1:17:LYS:HZ3	2.29	0.44
26:2:203:PHE:CD2	26:2:205:LEU:CD2	2.95	0.44
26:2:217:LEU:CD2	26:2:233:ILE:CD1	2.95	0.44
27:3:71:TYR:CG	27:3:71:TYR:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:144:ILE:O	27:3:144:ILE:HD13	2.17	0.44
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.44
2:B:132:VAL:HG12	2:B:134:LYS:HG3	1.99	0.44
2:B:549:SER:OG	2:B:577:HIS:NE2	2.44	0.44
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.99	0.44
9:I:61:GLU:HG3	9:I:103:ARG:CZ	2.48	0.44
10:J:21:TYR:CG	10:J:49:LEU:HD21	2.52	0.44
16:P:180:LEU:HA	16:P:183:ILE:HD12	1.99	0.44
21:U:225:ALA:HB3	21:U:228:MET:HA	1.99	0.44
27:3:24:LYS:HE2	27:3:196:LEU:HB3	1.98	0.44
27:3:228:LEU:O	27:3:228:LEU:HD23	2.18	0.44
29:Y:30:DG:H1'	29:Y:31:DG:C8	2.52	0.44
1:A:107:LEU:HD23	1:A:191:ILE:HD13	1.99	0.44
1:A:1050:CYS:HB3	1:A:1053:ARG:HG2	1.98	0.44
2:B:711:ILE:HA	2:B:712:PRO:HD3	1.95	0.44
16:P:165:LEU:HD23	16:P:168:ILE:HD11	1.99	0.44
17:Q:102:VAL:HG11	17:Q:103:VAL:HG22	1.99	0.44
20:T:177:ARG:NH1	20:T:212:TYR:HB2	2.33	0.44
24:0:54:ARG:HA	27:3:209:ILE:HD13	1.06	0.44
26:2:130:SER:HB2	26:2:179:LEU:HD23	1.98	0.44
26:2:189:GLU:HB2	26:2:190:PRO:CD	2.43	0.44
28:X:38:DT:H4'	28:X:39:DT:H4'	1.98	0.44
29:Y:36:DA:N3	29:Y:37:DG:C4	2.86	0.44
1:A:206:ASN:C	1:A:208:ASP:N	2.61	0.44
2:B:87:LYS:NZ	2:B:89:GLU:OE2	2.51	0.44
2:B:302:LYS:HE2	9:I:23:MET:SD	2.57	0.44
2:B:453:TRP:CG	2:B:463:ARG:HB2	2.53	0.44
2:B:646:ARG:HA	2:B:649:ASN:HB3	1.98	0.44
2:B:803:ARG:HH21	3:C:177:ASN:HD22	1.66	0.44
2:B:898:THR:OG1	2:B:899:SER:N	2.49	0.44
2:B:1066:PRO:HA	13:M:46:ILE:HG21	1.99	0.44
5:E:61:LEU:HD11	5:E:71:GLN:HG3	2.00	0.44
9:I:15:ARG:C	9:I:16:PHE:O	2.53	0.44
15:O:84:VAL:HG23	15:O:85:THR:HG23	1.99	0.44
18:R:223:VAL:O	18:R:223:VAL:HG23	2.17	0.44
22:V:370:SER:O	22:V:374:TRP:CD1	2.71	0.44
23:W:37:HIS:CD2	23:W:454:VAL:CG1	3.00	0.44
25:1:11:GLU:HG2	26:2:404:THR:OG1	2.17	0.44
25:1:18:GLN:HG3	25:1:19:PHE:H	1.82	0.44
26:2:123:LEU:CD2	26:2:178:LEU:CD1	2.95	0.44
27:3:60:ILE:HG23	27:3:68:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:349:TRP:HB3	14:N:351:PHE:CE1	2.52	0.44
19:S:45:ALA:HA	19:S:102:VAL:HA	2.00	0.44
25:1:3:ASN:HB3	26:2:412:PHE:O	2.18	0.44
25:1:4:VAL:HG22	25:1:5:LEU:N	2.32	0.44
26:2:159:VAL:HG12	26:2:161:HIS:HB2	1.99	0.44
27:3:65:GLN:O	27:3:132:LEU:HD11	2.18	0.44
1:A:262:PRO:O	1:A:263:ALA:HB3	2.18	0.44
1:A:425:ASP:HB3	13:M:39:LEU:HD11	2.00	0.44
1:A:640:LEU:HD13	1:A:645:LEU:HD13	2.00	0.44
2:B:295:PRO:HB2	9:I:11:PHE:CD2	2.46	0.44
2:B:714:PRO:CD	2:B:1001:PRO:HB3	2.41	0.44
2:B:1028:LEU:HA	2:B:1028:LEU:HD12	1.51	0.44
8:H:130:ASN:O	8:H:134:GLY:N	2.50	0.44
11:K:29:ASN:ND2	11:K:78:THR:O	2.50	0.44
17:Q:128:LYS:N	17:Q:163:GLU:O	2.51	0.44
25:1:1:MET:SD	26:2:419:GLU:N	2.90	0.44
26:2:204:LEU:HD23	26:2:254:MET:HE2	1.99	0.44
26:2:218:GLN:HE22	26:2:265:LEU:CA	2.28	0.44
27:3:34:LEU:O	27:3:34:LEU:HD13	2.17	0.44
27:3:160:ARG:CB	27:3:190:LEU:CD2	2.95	0.44
1:A:19:LYS:HD2	2:B:1173:SER:H	1.81	0.44
1:A:51:ARG:NH2	2:B:878:ASP:OD1	2.51	0.44
1:A:203:LYS:HA	1:A:203:LYS:CE	2.46	0.44
1:A:728:THR:HG23	1:A:736:THR:HG23	1.99	0.44
2:B:116:ARG:O	2:B:117:ASN:HB2	2.18	0.44
2:B:872:THR:HG23	2:B:888:THR:O	2.18	0.44
3:C:1:MET:HA	3:C:2:PRO:HD3	1.83	0.44
3:C:149:LEU:HD23	10:J:2:ILE:CD1	2.47	0.44
7:G:98:PHE:CZ	17:Q:145:PHE:HB2	2.53	0.44
8:H:65:TYR:HD2	8:H:70:LEU:HD23	1.82	0.44
10:J:21:TYR:HB2	10:J:38:LEU:CD1	2.48	0.44
17:Q:19:LYS:HA	17:Q:22:ILE:HG12	1.98	0.44
22:V:282:LYS:HE3	22:V:482:PHE:CD1	2.53	0.44
23:W:419:GLU:HB2	23:W:432:ILE:HG22	1.98	0.44
26:2:61:PHE:CE1	26:2:99:GLN:NE2	2.85	0.44
26:2:206:LEU:CD2	26:2:206:LEU:H	2.31	0.44
26:2:214:TYR:HB3	26:2:261:PHE:CE2	2.53	0.44
26:2:258:LEU:HG	26:2:262:LEU:HD21	1.99	0.44
1:A:350:VAL:HG11	1:A:1431:SER:HA	1.99	0.44
1:A:610:PRO:O	1:A:612:ASP:N	2.50	0.44
1:A:929:ALA:C	1:A:931:ARG:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:646:ARG:O	2:B:646:ARG:HG2	2.16	0.44
4:D:26:PHE:HE2	7:G:78:ARG:HG2	1.82	0.44
9:I:35:LEU:HB3	9:I:48:ALA:HB3	1.99	0.44
24:0:165:ARG:HD3	24:0:194:ILE:HG12	2.00	0.44
25:1:34:ILE:CG2	25:1:50:VAL:HG11	2.48	0.44
26:2:28:PRO:N	27:3:25:GLN:C	2.65	0.44
26:2:60:LEU:CD1	26:2:95:ILE:CB	2.95	0.44
26:2:117:ASN:ND2	27:3:104:LEU:O	2.51	0.44
27:3:124:ILE:O	27:3:124:ILE:HG23	2.18	0.44
1:A:368:THR:OG1	1:A:483:ARG:NH1	2.51	0.43
1:A:689:ILE:O	1:A:692:SER:OG	2.29	0.43
1:A:1249:ASP:HB2	21:U:196:SER:HB2	2.00	0.43
1:A:1484:MET:H	1:A:1484:MET:HG2	1.54	0.43
2:B:319:ASN:OD1	2:B:332:LYS:HG3	2.18	0.43
2:B:1107:LEU:HD23	2:B:1107:LEU:HA	1.80	0.43
3:C:10:ARG:NH2	3:C:24:GLU:OE2	2.36	0.43
4:D:71:PHE:HE1	7:G:142:GLU:HG2	1.83	0.43
10:J:62:TYR:CB	10:J:64:PRO:HD2	2.46	0.43
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.99	0.43
17:Q:23:ARG:NH1	18:R:209:GLN:CB	2.79	0.43
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.83	0.43
20:T:177:ARG:NE	20:T:208:GLN:HB2	2.33	0.43
22:V:405:VAL:HG12	22:V:406:ALA:H	1.82	0.43
22:V:531:ILE:CG1	22:V:534:TYR:HE2	2.31	0.43
24:0:60:HIS:CE1	24:0:159:MET:SD	3.11	0.43
26:2:140:LYS:HD3	26:2:162:PHE:CE1	2.47	0.43
29:Y:80:DT:H2"	29:Y:81:DA:C8	2.52	0.43
1:A:1301:ILE:HG21	1:A:1345:ARG:CZ	2.48	0.43
2:B:81:PRO:O	2:B:82:PRO:C	2.55	0.43
2:B:193:VAL:N	2:B:468:GLN:O	2.41	0.43
2:B:453:TRP:HB2	2:B:463:ARG:HB2	2.00	0.43
13:M:10:LEU:HD12	13:M:10:LEU:HA	1.81	0.43
16:P:163:PRO:HA	16:P:262:CYS:HB3	2.01	0.43
20:T:98:GLU:HA	20:T:104:LEU:HD23	2.00	0.43
22:V:415:HIS:HD2	22:V:416:THR:HG23	1.82	0.43
22:V:446:ILE:HD12	22:V:451:PHE:HB3	1.99	0.43
26:2:56:VAL:HG23	26:2:57:MET:N	2.31	0.43
26:2:117:ASN:ND2	27:3:108:ASN:N	2.65	0.43
26:2:166:SER:HB3	26:2:167:PRO:HD3	2.01	0.43
26:2:243:SER:HB3	26:2:258:LEU:CD2	2.45	0.43
29:Y:46:DC:H2"	29:Y:47:DG:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:VAL:HG21	1:A:322:LEU:HD21	1.99	0.43
1:A:378:VAL:O	1:A:475:ARG:N	2.51	0.43
1:A:416:ALA:HA	1:A:448:ARG:HA	1.99	0.43
1:A:546:ARG:HG3	1:A:547:LYS:N	2.34	0.43
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.17	0.43
2:B:249:LYS:O	2:B:249:LYS:HG2	2.19	0.43
3:C:52:ILE:HG21	3:C:55:ASN:HB2	2.01	0.43
7:G:158:PHE:CE1	17:Q:139:LEU:HB2	2.53	0.43
23:W:209:TYR:HH	23:W:233:PHE:CA	2.10	0.43
27:3:165:LYS:HZ1	27:3:200:SER:N	2.15	0.43
27:3:178:MET:O	27:3:182:PHE:HD2	2.01	0.43
27:3:178:MET:HA	27:3:181:ILE:HD12	2.00	0.43
1:A:527:THR:HG22	1:A:532:ARG:O	2.17	0.43
1:A:608:THR:OG1	1:A:610:PRO:HG2	2.18	0.43
2:B:22:TRP:O	2:B:24:GLU:N	2.51	0.43
2:B:1069:ILE:HG12	13:M:48:VAL:HG11	2.01	0.43
10:J:66:GLU:HB3	12:L:23:HIS:CE1	2.54	0.43
14:N:332:GLU:CD	15:O:92:LYS:HD3	2.38	0.43
17:Q:23:ARG:CZ	18:R:209:GLN:HB2	2.48	0.43
18:R:194:ARG:HD3	18:R:194:ARG:HA	1.44	0.43
19:S:31:PHE:N	20:T:92:THR:O	2.40	0.43
22:V:514:MET:SD	22:V:537:ASN:CG	2.97	0.43
26:2:35:TYR:CD1	26:2:62:LEU:HD12	2.53	0.43
26:2:223:ALA:H	26:2:268:PHE:HE1	1.64	0.43
27:3:59:VAL:CA	27:3:71:TYR:CD1	2.99	0.43
2:B:906:GLN:HG2	12:L:45:TYR:CE1	2.51	0.43
3:C:155:LYS:HB3	10:J:65:LEU:HD22	1.99	0.43
5:E:73:PHE:HD2	5:E:90:TYR:OH	2.02	0.43
6:F:121:ASP:N	6:F:121:ASP:OD1	2.51	0.43
8:H:75:TYR:HD1	8:H:75:TYR:H	1.65	0.43
17:Q:100:VAL:C	17:Q:102:VAL:N	2.72	0.43
21:U:247:GLU:HA	21:U:250:MET:HG2	2.00	0.43
22:V:612:ASP:OD2	22:V:635:GLN:CD	2.56	0.43
26:2:28:PRO:C	27:3:25:GLN:O	2.57	0.43
26:2:117:ASN:CA	27:3:104:LEU:HD21	2.47	0.43
27:3:121:LYS:H	27:3:121:LYS:CD	2.32	0.43
1:A:936:GLU:HB2	1:A:939:VAL:HG23	2.00	0.43
2:B:880:LEU:HD13	2:B:880:LEU:HA	1.79	0.43
8:H:34:SER:HB2	8:H:36:LYS:NZ	2.33	0.43
14:N:22:ILE:HG13	14:N:43:LYS:HD2	2.00	0.43
15:O:64:THR:CG2	16:P:188:ARG:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:109:HIS:CE1	18:R:231:GLU:HB2	2.54	0.43
20:T:159:HIS:O	20:T:162:ASN:HB3	2.18	0.43
23:W:416:ILE:HA	23:W:434:HIS:O	2.19	0.43
26:2:94:ARG:HD2	26:2:95:ILE:CD1	2.47	0.43
26:2:214:TYR:OH	26:2:265:LEU:HD13	2.18	0.43
26:2:224:GLN:N	26:2:268:PHE:HZ	2.16	0.43
26:2:236:PHE:HZ	26:2:258:LEU:HD11	1.83	0.43
1:A:865:ILE:HD12	1:A:866:LYS:N	2.34	0.43
1:A:1158:LEU:HD21	1:A:1308:TYR:CE2	2.54	0.43
1:A:1168:LYS:HD3	1:A:1306:LYS:HG2	2.01	0.43
14:N:46:TRP:HZ2	15:O:11:LEU:HD12	1.83	0.43
16:P:237:TYR:O	16:P:240:VAL:HG22	2.19	0.43
19:S:16:VAL:O	20:T:39:GLU:HA	2.19	0.43
23:W:263:LEU:C	23:W:263:LEU:HD23	2.39	0.43
25:1:22:TYR:CD1	25:1:22:TYR:C	2.92	0.43
26:2:127:LYS:CA	26:2:178:LEU:HD23	2.48	0.43
26:2:159:VAL:HG22	26:2:160:LEU:HD13	1.95	0.43
26:2:203:PHE:HD2	26:2:205:LEU:H	1.65	0.43
26:2:409:TYR:CD2	26:2:443:VAL:HG22	2.54	0.43
29:Y:36:DA:N9	29:Y:37:DG:C8	2.87	0.43
1:A:371:PRO:HD2	2:B:788:TYR:CZ	2.54	0.43
1:A:376:ASP:CB	1:A:522:PRO:HD3	2.45	0.43
1:A:477:LEU:HB2	1:A:478:PRO:HD2	2.00	0.43
1:A:609:HIS:N	1:A:610:PRO:HD3	2.30	0.43
1:A:1412:MET:SD	1:A:1422:GLN:NE2	2.92	0.43
11:K:111:ASP:O	11:K:113:GLN:N	2.52	0.43
13:M:106:THR:HA	29:Y:63:DG:H21	1.84	0.43
22:V:519:TYR:HA	22:V:522:TYR:HB3	2.01	0.43
23:W:28:LEU:HD13	23:W:28:LEU:C	2.38	0.43
26:2:117:ASN:HD21	27:3:108:ASN:N	2.16	0.43
26:2:215:PHE:CE2	26:2:264:HIS:ND1	2.86	0.43
26:2:270:LEU:HA	26:2:273:GLN:HG3	2.00	0.43
29:Y:18:DG:N2	29:Y:19:DC:C2	2.87	0.43
1:A:220:ARG:O	1:A:223:GLU:N	2.52	0.43
1:A:485:ASN:OD1	1:A:486:LEU:N	2.52	0.43
1:A:486:LEU:HD12	1:A:496:PHE:CE2	2.53	0.43
1:A:522:PRO:HG3	1:A:666:ARG:HE	1.84	0.43
1:A:561:MET:SD	11:K:51:LEU:HD21	2.59	0.43
1:A:927:GLU:N	1:A:931:ARG:CD	2.80	0.43
1:A:1282:ASP:OD1	1:A:1283:VAL:HG23	2.19	0.43
2:B:42:GLN:HG2	2:B:526:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HD13	2:B:51:ILE:HA	1.89	0.43
2:B:1022:LEU:HD11	2:B:1023:ARG:NH1	2.34	0.43
10:J:44:CYS:SG	10:J:45:CYS:N	2.92	0.43
16:P:206:GLU:OE1	16:P:236:LYS:NZ	2.52	0.43
17:Q:109:HIS:HE1	18:R:231:GLU:HB2	1.83	0.43
17:Q:151:THR:HB	17:Q:152:PHE:H	1.74	0.43
22:V:524:ALA:HB2	25:1:23:LEU:HD13	2.01	0.43
23:W:584:TYR:CB	23:W:591:GLY:HA3	2.49	0.43
25:1:13:ASP:OD2	25:1:17:LYS:HB2	2.15	0.43
25:1:25:GLU:OE2	25:1:35:ILE:HG12	2.18	0.43
25:1:50:VAL:HG12	25:1:50:VAL:O	2.18	0.43
26:2:35:TYR:CG	26:2:62:LEU:CD1	2.99	0.43
27:3:178:MET:CE	27:3:202:LEU:CD1	2.95	0.43
29:Y:64:DC:N4	29:Y:65:DG:O6	2.51	0.43
1:A:910:LYS:HB3	1:A:963:ARG:HH12	1.84	0.43
1:A:1177:TYR:N	9:I:51:SER:HB3	2.27	0.43
2:B:728:MET:SD	2:B:940:GLY:HA2	2.59	0.43
2:B:1119:CYS:HB3	2:B:1122:CYS:O	2.18	0.43
6:F:64:ARG:HH22	7:G:61:PRO:HB3	1.82	0.43
9:I:57:LYS:HB3	9:I:59:THR:CG2	2.49	0.43
9:I:62:VAL:O	9:I:64:GLU:CB	2.66	0.43
10:J:62:TYR:HB2	10:J:64:PRO:HG2	2.00	0.43
16:P:190:ALA:HB2	16:P:202:MET:HG2	2.01	0.43
20:T:165:TYR:O	20:T:169:LYS:HG2	2.18	0.43
22:V:615:PHE:CD1	22:V:615:PHE:C	2.91	0.43
25:1:8:VAL:CG1	25:1:9:LEU:N	2.80	0.43
26:2:34:LEU:N	26:2:34:LEU:HD22	2.33	0.43
26:2:118:LEU:HD23	27:3:42:MET:CB	2.35	0.43
1:A:365:THR:HG22	1:A:482:PHE:CE2	2.54	0.42
1:A:483:ARG:NH2	2:B:788:TYR:CE2	2.87	0.42
1:A:1029:LEU:H	5:E:162:ARG:NH1	2.17	0.42
1:A:1130:ILE:HD12	1:A:1411:LEU:HD13	2.01	0.42
2:B:80:GLU:C	2:B:135:GLU:HG3	2.29	0.42
2:B:92:TYR:HD1	20:T:141:LEU:HD21	1.82	0.42
2:B:229:SER:HA	2:B:405:ARG:HH22	1.84	0.42
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.02	0.42
2:B:1005:ALA:O	2:B:1007:ASN:N	2.52	0.42
10:J:62:TYR:HB3	10:J:64:PRO:HD3	2.00	0.42
13:M:32:MET:O	13:M:40:VAL:HA	2.19	0.42
14:N:28:ILE:HD13	15:O:35:GLN:HG2	2.01	0.42
14:N:46:TRP:CZ2	15:O:11:LEU:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:141:LEU:CD2	20:T:141:LEU:C	2.88	0.42
22:V:315:VAL:CG1	23:W:500:ASP:CG	2.80	0.42
22:V:519:TYR:HB3	25:1:16:MET:HG3	2.00	0.42
26:2:236:PHE:CE1	26:2:239:GLN:NE2	2.87	0.42
27:3:184:ALA:O	27:3:187:GLN:HG2	2.19	0.42
29:Y:89:DC:H2''	29:Y:90:DC:C5	2.54	0.42
1:A:613:GLU:HG2	21:U:262:THR:HB	2.01	0.42
1:A:620:HIS:O	1:A:621:ILE:HB	2.19	0.42
1:A:1319:LYS:HD2	1:A:1319:LYS:HA	1.36	0.42
2:B:1162:LEU:HD23	2:B:1162:LEU:HA	1.68	0.42
5:E:11:TRP:CZ2	5:E:36:THR:HA	2.54	0.42
14:N:32:ASP:HB3	14:N:34:VAL:HG23	2.00	0.42
20:T:121:SER:OG	20:T:122:GLU:N	2.52	0.42
20:T:159:HIS:ND1	20:T:160:GLN:N	2.65	0.42
22:V:514:MET:HB3	25:1:16:MET:SD	2.59	0.42
26:2:118:LEU:HD22	27:3:39:ASP:CB	2.49	0.42
26:2:138:PRO:HD3	26:2:189:GLU:CD	2.40	0.42
27:3:141:LEU:HA	27:3:144:ILE:HG22	2.01	0.42
1:A:1050:CYS:SG	1:A:1051:SER:N	2.92	0.42
2:B:17:ILE:HG23	2:B:18:THR:HG23	2.01	0.42
2:B:127:ASP:OD2	2:B:144:HIS:NE2	2.47	0.42
2:B:819:SER:H	2:B:827:GLU:HB2	1.84	0.42
2:B:953:ASP:O	2:B:1031:GLY:HA3	2.19	0.42
8:H:81:ARG:C	8:H:83:SER:H	2.22	0.42
9:I:84:HIS:HB2	9:I:85:PRO:HD3	0.86	0.42
13:M:35:PRO:HB2	13:M:36:GLU:OE1	2.19	0.42
22:V:615:PHE:O	22:V:615:PHE:CG	2.70	0.42
25:1:4:VAL:CG1	26:2:412:PHE:HD2	2.20	0.42
26:2:57:MET:CA	26:2:60:LEU:HG	2.49	0.42
26:2:171:VAL:CG1	26:2:216:MET:SD	3.06	0.42
27:3:124:ILE:HD13	27:3:124:ILE:C	2.38	0.42
27:3:133:LEU:CD2	27:3:134:ALA:N	2.82	0.42
1:A:197:GLU:HG3	1:A:199:TYR:HE1	1.84	0.42
1:A:265:VAL:HG23	1:A:266:MET:H	1.85	0.42
1:A:359:VAL:HA	2:B:1111:SER:HB3	2.00	0.42
1:A:1036:ASN:ND2	1:A:1036:ASN:C	2.73	0.42
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.54	0.42
1:A:1473:LEU:HB3	7:G:59:ILE:HD12	2.01	0.42
2:B:90:GLN:HE21	20:T:141:LEU:HG	1.72	0.42
2:B:92:TYR:HE1	20:T:143:GLN:NE2	2.15	0.42
2:B:757:PRO:HA	2:B:1047:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:TYR:CE1	3:C:167:LYS:HE3	2.55	0.42
9:I:16:PHE:HB3	9:I:22:ASN:O	2.19	0.42
14:N:314:LEU:HD12	16:P:242:GLN:NE2	2.34	0.42
17:Q:30:HIS:CE1	17:Q:62:VAL:HG22	2.54	0.42
26:2:133:THR:CG2	26:2:134:SER:N	2.83	0.42
27:3:137:LEU:HD12	27:3:177:PHE:CE1	2.54	0.42
27:3:160:ARG:CZ	27:3:190:LEU:CD1	2.97	0.42
1:A:689:ILE:HG13	1:A:690:GLY:N	2.34	0.42
1:A:1413:ALA:O	1:A:1418:GLY:HA3	2.19	0.42
2:B:184:TYR:HE2	2:B:191:GLU:HG2	1.84	0.42
13:M:252:SER:OG	29:Y:85:DG:OP1	2.30	0.42
16:P:298:PRO:O	16:P:299:ARG:C	2.57	0.42
22:V:689:VAL:CG2	26:2:391:ILE:HD13	2.50	0.42
23:W:73:CYS:CB	23:W:209:TYR:CE2	3.02	0.42
23:W:73:CYS:HB3	23:W:209:TYR:CD2	2.54	0.42
26:2:159:VAL:HG11	26:2:161:HIS:CD2	2.49	0.42
26:2:188:THR:CG2	26:2:189:GLU:N	2.83	0.42
27:3:69:PHE:CZ	27:3:139:LYS:CB	2.95	0.42
27:3:144:ILE:HG13	27:3:159:SER:OG	2.20	0.42
28:X:1:DG:H2"	28:X:2:DA:C8	2.55	0.42
1:A:81:CYS:HA	1:A:82:PRO:HD2	1.89	0.42
1:A:927:GLU:CA	1:A:931:ARG:CG	2.72	0.42
1:A:1410:HIS:HB2	5:E:174:GLN:NE2	2.34	0.42
2:B:422:PHE:CZ	2:B:429:PHE:HB2	2.55	0.42
2:B:871:VAL:HG13	2:B:890:ARG:HB2	2.01	0.42
3:C:27:ASP:OD1	3:C:28:LEU:N	2.53	0.42
4:D:103:LEU:HD13	4:D:114:LEU:HD13	2.02	0.42
5:E:64:HIS:ND1	5:E:70:ASP:O	2.52	0.42
8:H:65:TYR:CD2	8:H:70:LEU:HB3	2.54	0.42
10:J:6:ARG:H	10:J:14:VAL:H	1.65	0.42
13:M:39:LEU:C	13:M:40:VAL:O	2.56	0.42
13:M:108:SER:HB3	13:M:112:ARG:NH1	2.32	0.42
14:N:333:ASN:HB3	14:N:359:ASN:O	2.20	0.42
17:Q:35:ASP:HA	17:Q:38:ILE:HD12	2.01	0.42
18:R:177:ASN:HD22	18:R:177:ASN:C	2.19	0.42
20:T:138:PRO:HG2	20:T:140:ARG:NH2	2.35	0.42
21:U:257:GLN:NE2	21:U:257:GLN:HA	2.34	0.42
27:3:9:ASN:OD1	27:3:158:LYS:HB3	2.19	0.42
27:3:42:MET:SD	27:3:111:ILE:CD1	3.07	0.42
1:A:1176:TYR:HE1	9:I:52:CYS:HB2	1.85	0.42
2:B:251:ALA:O	2:B:254:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:PRO:HD2	2:B:271:ILE:HD12	2.02	0.42
2:B:1114:TYR:HE2	2:B:1156:LYS:HD3	1.84	0.42
3:C:146:ASP:O	3:C:148:ILE:N	2.49	0.42
7:G:91:GLN:HG2	17:Q:145:PHE:CZ	2.55	0.42
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.34	0.42
12:L:35:ARG:NH1	12:L:42:ARG:HE	2.17	0.42
15:O:3:TYR:CB	15:O:98:CYS:SG	2.97	0.42
16:P:325:PHE:HA	16:P:328:ILE:HG22	2.01	0.42
22:V:321:GLU:CB	23:W:499:ASN:CG	2.32	0.42
27:3:71:TYR:HD2	27:3:72:PRO:HD2	1.72	0.42
27:3:100:LYS:HB2	27:3:100:LYS:HE2	1.89	0.42
27:3:100:LYS:CB	27:3:103:LEU:HD13	2.41	0.42
27:3:128:HIS:NE2	27:3:130:GLU:CG	2.82	0.42
27:3:197:ASP:O	27:3:198:SER:HB3	2.20	0.42
28:X:16:DA:H2"	28:X:17:DA:C8	2.55	0.42
1:A:364:ARG:NE	1:A:500:GLU:CD	2.73	0.42
1:A:425:ASP:CB	13:M:39:LEU:HD11	2.49	0.42
1:A:1178:ASP:HB3	1:A:1260:ARG:HH22	1.85	0.42
1:A:1473:LEU:HD23	6:F:104:ILE:HD12	2.02	0.42
2:B:132:VAL:CG1	2:B:134:LYS:HG3	2.50	0.42
2:B:707:CYS:SG	2:B:730:LYS:NZ	2.92	0.42
4:D:126:GLU:O	4:D:130:ILE:N	2.43	0.42
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.55	0.42
25:1:18:GLN:CB	25:1:44:PHE:CE2	2.76	0.42
26:2:47:GLU:HG3	26:2:48:LEU:H	1.83	0.42
26:2:140:LYS:CD	26:2:162:PHE:HE1	2.29	0.42
27:3:14:VAL:CG2	27:3:163:VAL:HG13	2.48	0.42
1:A:271:ARG:HD2	13:M:73:PRO:CB	2.38	0.42
1:A:1432:PHE:HD1	1:A:1433:GLU:HB2	1.84	0.42
2:B:475:PHE:CE2	2:B:479:LEU:HD22	2.55	0.42
2:B:527:ALA:HA	2:B:705:GLY:HA2	2.02	0.42
2:B:874:PRO:C	2:B:876:ASN:H	2.17	0.42
9:I:28:GLU:HG3	9:I:29:ASP:N	2.34	0.42
11:K:5:PRO:HD2	11:K:8:GLU:OE1	2.19	0.42
13:M:37:CYS:SG	13:M:38:GLY:N	2.88	0.42
16:P:206:GLU:HB3	16:P:207:PRO:HD3	1.74	0.42
21:U:278:THR:HG22	21:U:285:MET:SD	2.60	0.42
22:V:315:VAL:HG13	23:W:500:ASP:HB2	0.42	0.42
23:W:421:PHE:HD1	23:W:423:ASP:CB	2.13	0.42
26:2:77:LYS:HD3	26:2:78:GLU:CG	2.50	0.42
27:3:11:LEU:CD1	27:3:48:HIS:NE2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:18:ASN:ND2	27:3:64:ILE:HD11	2.35	0.42
1:A:743:ARG:HD2	21:U:257:GLN:CG	2.50	0.42
1:A:1098:PRO:HA	1:A:1101:GLN:OE1	2.20	0.42
2:B:196:ALA:HB3	2:B:485:LEU:HA	2.02	0.42
2:B:225:LEU:C	2:B:227:ASN:N	2.67	0.42
2:B:232:THR:OG1	2:B:233:SER:N	2.46	0.42
15:O:79:VAL:HG21	15:O:93:VAL:HG12	2.01	0.42
16:P:162:VAL:CG2	16:P:164:GLN:NE2	2.72	0.42
23:W:25:MET:SD	23:W:58:ALA:HB2	2.59	0.42
26:2:28:PRO:HA	27:3:25:GLN:C	2.40	0.42
26:2:159:VAL:CG2	26:2:160:LEU:N	2.81	0.42
26:2:236:PHE:CE1	26:2:261:PHE:HB3	2.54	0.42
27:3:111:ILE:HG13	27:3:112:VAL:H	1.84	0.42
27:3:202:LEU:N	27:3:202:LEU:CD2	2.82	0.42
2:B:38:GLY:H	2:B:41:ARG:HG2	1.85	0.41
2:B:380:ARG:NE	2:B:609:GLU:OE1	2.48	0.41
2:B:711:ILE:HG21	2:B:711:ILE:HD13	1.76	0.41
17:Q:24:GLY:O	18:R:210:PHE:CE2	2.73	0.41
23:W:15:ASP:HA	23:W:100:GLU:OE2	2.20	0.41
23:W:419:GLU:HB3	23:W:420:PRO:HD3	1.84	0.41
26:2:171:VAL:HG13	26:2:216:MET:HB3	1.98	0.41
27:3:105:THR:CG2	27:3:106:SER:N	2.82	0.41
27:3:147:MET:CE	27:3:157:MET:SD	3.07	0.41
1:A:16:ARG:NE	2:B:1172:MET:SD	2.92	0.41
1:A:366:VAL:O	1:A:481:THR:HB	2.21	0.41
1:A:546:ARG:NH2	1:A:550:LYS:HD2	2.35	0.41
1:A:608:THR:CA	1:A:610:PRO:HD2	2.49	0.41
1:A:1313:GLN:HE22	1:A:1318:LYS:HD2	1.82	0.41
2:B:422:PHE:CD1	2:B:422:PHE:C	2.92	0.41
2:B:715:ASP:OD1	2:B:715:ASP:N	2.46	0.41
3:C:1:MET:HB3	3:C:3:TYR:CE2	2.56	0.41
8:H:96:VAL:HB	8:H:137:VAL:O	2.20	0.41
14:N:318:ASP:OD1	16:P:239:ARG:NH2	2.53	0.41
18:R:195:PRO:O	18:R:196:ASP:HB2	2.19	0.41
22:V:534:TYR:HE1	22:V:535:THR:OG1	1.98	0.41
25:1:1:MET:N	26:2:418:PHE:CB	2.83	0.41
26:2:117:ASN:CB	27:3:42:MET:HE1	2.48	0.41
26:2:176:ALA:HB3	26:2:178:LEU:HD13	1.97	0.41
27:3:64:ILE:CB	27:3:123:ASP:HB3	2.50	0.41
27:3:217:VAL:HG12	27:3:218:PRO:O	2.20	0.41
1:A:24:GLY:O	2:B:1166:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:HG22	1:A:155:GLU:OE2	2.20	0.41
1:A:693:ILE:HG21	2:B:1023:ARG:HE	1.85	0.41
3:C:259:LEU:HD22	11:K:42:LEU:HD11	2.00	0.41
10:J:35:LEU:HD22	10:J:40:LEU:HD22	2.02	0.41
17:Q:154:CYS:SG	17:Q:155:THR:N	2.94	0.41
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.55	0.41
20:T:174:LYS:HG2	28:X:20:DG:H4'	2.02	0.41
22:V:423:ALA:HA	22:V:427:MET:SD	2.60	0.41
26:2:221:GLN:O	26:2:268:PHE:CE1	2.74	0.41
26:2:223:ALA:C	26:2:225:SER:H	2.24	0.41
27:3:14:VAL:HG22	27:3:162:LEU:O	2.21	0.41
27:3:109:GLU:HG3	27:3:110:VAL:N	2.35	0.41
1:A:592:PHE:CZ	1:A:640:LEU:HD11	2.55	0.41
1:A:595:ILE:HD12	1:A:596:ILE:N	2.36	0.41
1:A:692:SER:O	1:A:828:LEU:HD22	2.20	0.41
1:A:908:THR:C	1:A:910:LYS:H	2.23	0.41
1:A:1043:ILE:HG22	1:A:1046:ARG:HH22	1.86	0.41
2:B:65:ILE:O	2:B:85:LEU:HD12	2.20	0.41
2:B:414:GLU:HA	2:B:417:ILE:HG22	2.01	0.41
2:B:728:MET:HE2	2:B:942:LYS:CG	2.43	0.41
2:B:771:GLU:OE2	10:J:58:LYS:HE3	2.20	0.41
2:B:1073:GLN:HG2	2:B:1112:ASP:HB2	2.03	0.41
5:E:64:HIS:CE1	5:E:69:THR:C	2.94	0.41
6:F:68:THR:HG21	7:G:59:ILE:HG21	2.02	0.41
9:I:58:ILE:C	9:I:60:HIS:N	2.73	0.41
9:I:68:ILE:HG23	9:I:122:ARG:HD2	2.00	0.41
16:P:171:THR:HG23	16:P:256:GLN:HG3	2.02	0.41
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.20	0.41
18:R:151:LEU:HB3	18:R:154:LEU:HB3	2.02	0.41
26:2:93:LEU:HD23	26:2:96:TRP:HE1	1.85	0.41
27:3:41:VAL:HG13	27:3:42:MET:N	2.35	0.41
1:A:320:ASN:HB2	1:A:338:SER:HB3	2.03	0.41
1:A:366:VAL:HB	1:A:481:THR:HG22	2.01	0.41
1:A:542:LEU:O	1:A:545:VAL:HG12	2.20	0.41
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.55	0.41
1:A:602:CYS:HB2	1:A:655:ILE:CD1	2.51	0.41
2:B:501:LEU:CD1	2:B:505:LEU:HD22	2.50	0.41
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.55	0.41
3:C:70:LEU:HD23	3:C:70:LEU:HA	1.84	0.41
25:1:1:MET:HG2	26:2:413:LEU:CB	2.47	0.41
29:Y:80:DT:H6	29:Y:80:DT:H2'	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:PRO:O	1:A:479:TRP:HB2	2.20	0.41
1:A:566:PHE:HB3	1:A:674:THR:HG22	2.01	0.41
1:A:576:GLN:HB2	8:H:73:GLY:O	2.20	0.41
2:B:274:ARG:HA	2:B:278:PHE:O	2.20	0.41
2:B:280:SER:HB2	2:B:283:ASP:OD2	2.21	0.41
2:B:962:THR:HA	2:B:963:PRO:HD3	1.80	0.41
5:E:61:LEU:HD12	5:E:72:MET:O	2.21	0.41
9:I:101:SER:OG	9:I:104:ALA:HB2	2.21	0.41
13:M:36:GLU:OE1	13:M:36:GLU:N	2.54	0.41
16:P:283:TYR:CD2	16:P:285:PRO:HD3	2.55	0.41
16:P:295:MET:HG3	16:P:297:LYS:H	1.85	0.41
22:V:518:PHE:CD1	22:V:713:LEU:HD13	2.55	0.41
22:V:612:ASP:OD1	22:V:635:GLN:CG	2.69	0.41
25:1:43:VAL:CG1	25:1:44:PHE:N	2.83	0.41
25:1:52:VAL:CG2	25:1:53:LEU:N	2.83	0.41
26:2:175:LEU:CD2	26:2:216:MET:SD	3.07	0.41
26:2:202:GLN:HE21	26:2:202:GLN:N	2.15	0.41
29:Y:77:DT:C6	29:Y:78:DT:H72	2.56	0.41
1:A:153:ILE:HD13	1:A:153:ILE:N	2.36	0.41
1:A:608:THR:OG1	1:A:610:PRO:CG	2.68	0.41
1:A:823:VAL:HG13	1:A:835:GLU:HB3	2.02	0.41
1:A:1179:PRO:HA	1:A:1209:PRO:HA	2.03	0.41
1:A:1250:ASP:CB	21:U:227:GLU:HG3	2.14	0.41
1:A:1251:ASN:OD1	21:U:227:GLU:O	2.37	0.41
2:B:41:ARG:HD2	2:B:41:ARG:HA	1.68	0.41
2:B:237:VAL:HG12	2:B:372:LEU:HD22	2.03	0.41
2:B:810:PHE:N	2:B:925:SER:O	2.43	0.41
2:B:1043:ILE:HG21	2:B:1043:ILE:HD13	1.74	0.41
3:C:4:ALA:HB2	11:K:93:ASP:OD1	2.21	0.41
9:I:11:PHE:CD1	9:I:55:VAL:HG22	2.56	0.41
13:M:45:VAL:HG13	13:M:48:VAL:HG22	2.03	0.41
17:Q:54:PHE:CD2	18:R:194:ARG:HG3	2.56	0.41
26:2:31:LEU:HG	27:3:25:GLN:C	2.41	0.41
1:A:271:ARG:NE	13:M:73:PRO:CD	2.76	0.41
1:A:537:ILE:HD13	1:A:537:ILE:HA	1.82	0.41
2:B:282:ARG:HH11	9:I:21:ASN:HD21	1.67	0.41
2:B:299:GLU:OE2	2:B:302:LYS:HE3	2.21	0.41
2:B:631:GLN:HE21	2:B:685:LYS:HD2	1.85	0.41
3:C:116:THR:HG21	3:C:146:ASP:HB2	2.03	0.41
14:N:12:LYS:O	14:N:15:ARG:HB2	2.21	0.41
16:P:206:GLU:OE2	16:P:206:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:161:TYR:O	20:T:164:GLU:HB3	2.21	0.41
21:U:165:GLU:OE1	21:U:165:GLU:N	2.53	0.41
22:V:390:CYS:SG	22:V:399:LYS:HE3	2.61	0.41
26:2:123:LEU:HD23	26:2:123:LEU:C	2.41	0.41
26:2:206:LEU:CD2	26:2:206:LEU:N	2.84	0.41
26:2:224:GLN:CB	26:2:268:PHE:CZ	2.94	0.41
27:3:9:ASN:C	27:3:56:LYS:HE3	2.41	0.41
27:3:125:LYS:C	27:3:127:GLN:H	2.24	0.41
1:A:271:ARG:HB3	1:A:272:ASN:H	1.52	0.41
1:A:505:LEU:HA	1:A:506:PRO:HD2	1.83	0.41
1:A:544:ALA:HB2	1:A:680:LEU:HD22	2.03	0.41
1:A:598:GLY:HA2	1:A:633:GLY:HA3	2.02	0.41
1:A:924:TYR:OH	1:A:952:LEU:HB2	2.21	0.41
1:A:954:ARG:HA	1:A:954:ARG:HD3	1.80	0.41
1:A:1024:ASN:OD1	1:A:1025:GLY:N	2.54	0.41
2:B:73:HIS:C	2:B:75:SER:N	2.71	0.41
2:B:128:ILE:HG21	2:B:431:LEU:HD21	2.03	0.41
2:B:451:GLY:HA2	2:B:467:SER:HB3	2.02	0.41
2:B:626:LEU:HG	2:B:698:ILE:HG22	2.03	0.41
2:B:849:ASP:OD1	2:B:850:ASP:N	2.53	0.41
2:B:877:GLU:OE1	2:B:877:GLU:N	2.54	0.41
5:E:11:TRP:HZ2	5:E:36:THR:HA	1.86	0.41
5:E:171:PRO:HB2	5:E:207:ARG:HD2	2.02	0.41
7:G:31:PHE:CE1	7:G:48:VAL:HB	2.52	0.41
8:H:78:THR:HG21	11:K:78:THR:CG2	2.51	0.41
9:I:61:GLU:C	9:I:63:ASP:N	2.67	0.41
10:J:8:PHE:H	10:J:48:MET:HE3	1.86	0.41
16:P:157:GLU:CD	16:P:333:LYS:HD3	2.40	0.41
16:P:229:GLN:HA	16:P:232:LEU:HB3	2.03	0.41
18:R:133:ILE:HG13	18:R:136:LYS:HG3	2.02	0.41
18:R:167:LEU:HD22	18:R:200:ILE:HB	2.02	0.41
18:R:195:PRO:CB	18:R:199:LYS:CD	2.86	0.41
22:V:518:PHE:HB2	25:1:16:MET:SD	2.61	0.41
22:V:519:TYR:CE2	22:V:523:VAL:HG21	2.55	0.41
22:V:531:ILE:HG23	22:V:534:TYR:CE2	2.45	0.41
25:1:14:PRO:HG2	25:1:17:LYS:HB2	2.02	0.41
25:1:52:VAL:O	25:1:56:ARG:HG2	2.21	0.41
26:2:28:PRO:CA	27:3:33:THR:CB	2.84	0.41
26:2:86:SER:HB2	26:2:140:LYS:HE2	2.03	0.41
26:2:170:ALA:C	26:2:213:TRP:CZ3	2.94	0.41
26:2:211:GLN:CD	26:2:261:PHE:CE1	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:236:PHE:HZ	26:2:258:LEU:CD1	2.34	0.41
27:3:141:LEU:C	27:3:144:ILE:HG22	2.41	0.41
27:3:187:GLN:CG	27:3:189:ILE:CG1	2.94	0.41
28:X:44:DT:H2''	28:X:45:DC:C4'	2.51	0.41
1:A:1161:LEU:HD11	1:A:1346:VAL:HG22	2.02	0.41
2:B:971:ALA:O	2:B:975:ARG:HD2	2.21	0.41
9:I:62:VAL:O	9:I:64:GLU:HB3	2.21	0.41
9:I:84:HIS:CD2	9:I:84:HIS:N	2.83	0.41
20:T:155:PRO:O	20:T:156:VAL:HG22	2.21	0.41
20:T:179:ASP:OD1	20:T:183:VAL:HG23	2.21	0.41
26:2:181:GLN:HA	26:2:181:GLN:NE2	2.34	0.41
26:2:236:PHE:CD1	26:2:239:GLN:CD	2.95	0.41
27:3:69:PHE:HZ	27:3:139:LYS:HD2	1.80	0.41
1:A:67:ARG:HH21	13:M:45:VAL:HB	1.85	0.40
1:A:517:GLU:OE1	6:F:62:ARG:NE	2.43	0.40
1:A:1231:ILE:O	1:A:1235:ILE:HG12	2.21	0.40
2:B:613:ARG:HD3	2:B:615:TYR:HE2	1.86	0.40
2:B:617:ASP:O	2:B:620:ARG:NH2	2.50	0.40
2:B:927:ARG:NH2	2:B:1057:ASP:OD1	2.54	0.40
3:C:42:VAL:CB	3:C:178:PRO:HG3	2.44	0.40
5:E:116:GLN:O	5:E:119:VAL:HB	2.21	0.40
9:I:66:THR:C	9:I:68:ILE:H	2.24	0.40
9:I:96:PHE:HB3	9:I:112:TYR:CD1	2.55	0.40
20:T:139:VAL:HG12	20:T:141:LEU:H	1.86	0.40
22:V:297:PHE:CG	22:V:298:ARG:N	2.89	0.40
25:1:18:GLN:CD	25:1:44:PHE:CZ	2.92	0.40
26:2:174:ASP:OD2	26:2:213:TRP:CZ3	2.74	0.40
26:2:251:VAL:CG1	26:2:254:MET:CG	2.95	0.40
27:3:159:SER:HG	27:3:189:ILE:HD12	1.86	0.40
27:3:222:SER:HB3	27:3:225:GLN:CG	2.51	0.40
1:A:297:GLY:HA3	17:Q:57:LYS:CG	2.50	0.40
1:A:818:GLU:HG2	1:A:819:SER:N	2.36	0.40
1:A:974:ASP:HB2	1:A:1317:LYS:NZ	2.36	0.40
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.51	0.40
1:A:1176:TYR:HB2	1:A:1211:LEU:HD23	2.03	0.40
2:B:1040:GLN:CD	2:B:1040:GLN:N	2.71	0.40
5:E:197:SER:HB3	5:E:201:GLY:H	1.85	0.40
8:H:15:ILE:HG13	8:H:52:LEU:HD23	2.04	0.40
12:L:18:ILE:HD11	12:L:47:LYS:HG3	2.02	0.40
13:M:200:LYS:HB3	13:M:200:LYS:HE2	1.75	0.40
16:P:268:ILE:O	16:P:337:LYS:HE3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:136:PHE:HD1	17:Q:140:GLU:OE1	2.03	0.40
19:S:177:MET:HE3	19:S:177:MET:HB3	1.85	0.40
20:T:168:LYS:C	20:T:170:LYS:H	2.24	0.40
20:T:177:ARG:HH22	20:T:212:TYR:CB	2.29	0.40
21:U:247:GLU:OE1	21:U:250:MET:HG3	2.22	0.40
22:V:353:ALA:O	22:V:357:VAL:HG23	2.21	0.40
22:V:520:ARG:HB2	25:1:19:PHE:HB2	2.02	0.40
22:V:593:LEU:HD11	22:V:615:PHE:CE1	2.56	0.40
25:1:13:ASP:CB	25:1:14:PRO:HD2	2.49	0.40
26:2:34:LEU:CD2	26:2:34:LEU:N	2.84	0.40
26:2:93:LEU:HA	26:2:93:LEU:HD23	1.77	0.40
26:2:93:LEU:O	26:2:96:TRP:CD1	2.74	0.40
26:2:236:PHE:HZ	26:2:262:LEU:CD2	2.35	0.40
27:3:60:ILE:CG2	27:3:61:ALA:N	2.84	0.40
27:3:114:GLU:OE1	27:3:114:GLU:HA	2.21	0.40
27:3:146:ARG:HG3	27:3:147:MET:N	2.35	0.40
27:3:191:ILE:H	27:3:210:THR:HG21	1.85	0.40
27:3:222:SER:HB3	27:3:225:GLN:OE1	2.21	0.40
1:A:212:LYS:HB3	1:A:212:LYS:HZ3	1.85	0.40
1:A:275:ASP:OD1	1:A:276:LEU:N	2.55	0.40
1:A:713:VAL:HG21	1:A:745:LEU:HD11	2.04	0.40
1:A:927:GLU:HG3	1:A:929:ALA:H	1.86	0.40
2:B:957:THR:HG21	2:B:1026:GLU:OE1	2.22	0.40
2:B:1152:PRO:HG2	2:B:1155:CYS:CB	2.51	0.40
10:J:2:ILE:HD12	10:J:3:ILE:N	2.36	0.40
17:Q:182:GLU:O	17:Q:186:PRO:HD3	2.22	0.40
25:1:39:ASP:OD2	26:2:434:GLU:OE2	2.39	0.40
26:2:30:VAL:CB	27:3:25:GLN:CB	2.91	0.40
26:2:93:LEU:CA	26:2:96:TRP:HD1	2.31	0.40
26:2:399:ASP:OD1	26:2:402:ARG:NH1	2.55	0.40
27:3:228:LEU:HD23	27:3:228:LEU:C	2.41	0.40
1:A:286:ILE:HD11	1:A:310:LEU:HA	2.04	0.40
2:B:51:ILE:HD12	2:B:51:ILE:HG23	1.64	0.40
2:B:698:ILE:HD13	2:B:698:ILE:HG21	1.71	0.40
5:E:64:HIS:C	5:E:65:ASN:O	2.60	0.40
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.56	0.40
18:R:149:LYS:HD3	18:R:175:LEU:HB2	2.03	0.40
20:T:142:SER:C	20:T:144:GLN:N	2.73	0.40
22:V:516:PRO:CA	25:1:15:ALA:C	2.83	0.40
23:W:233:PHE:HB2	23:W:456:ILE:HG22	2.02	0.40
23:W:299:ARG:O	23:W:300:GLU:CD	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:10:ILE:HG23	25:1:10:ILE:O	2.21	0.40
25:1:38:ILE:CB	25:1:44:PHE:CD1	3.04	0.40
26:2:89:LEU:HD23	26:2:89:LEU:C	2.42	0.40
1:A:118:LEU:HD12	1:A:148:CYS:HB3	2.02	0.40
1:A:136:GLN:HG3	1:A:139:LYS:H	1.85	0.40
1:A:823:VAL:HA	1:A:835:GLU:HG2	2.03	0.40
1:A:1471:PHE:HZ	6:F:61:GLU:HA	1.87	0.40
2:B:181:PRO:HD3	2:B:475:PHE:HE1	1.86	0.40
2:B:191:GLU:OE1	2:B:472:ARG:HD2	2.21	0.40
16:P:206:GLU:CB	16:P:236:LYS:NZ	2.76	0.40
16:P:206:GLU:CD	16:P:236:LYS:NZ	2.75	0.40
17:Q:149:THR:HG23	17:Q:151:THR:H	1.86	0.40
18:R:224:THR:O	18:R:224:THR:HG23	2.20	0.40
20:T:37:ARG:NH2	20:T:62:LEU:HB2	2.36	0.40
23:W:535:ILE:HG12	23:W:617:ALA:HB3	2.04	0.40
26:2:94:ARG:HD2	26:2:95:ILE:HD13	2.02	0.40
26:2:195:CYS:SG	26:2:196:ILE:N	2.95	0.40
27:3:42:MET:HG2	27:3:111:ILE:CD1	2.52	0.40
27:3:222:SER:O	27:3:226:TYR:CD2	2.75	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1450/1970 (74%)	1262 (87%)	123 (8%)	65 (4%)	2	22
2	B	1163/1174 (99%)	1011 (87%)	106 (9%)	46 (4%)	3	23
3	C	273/275 (99%)	242 (89%)	21 (8%)	10 (4%)	3	24
4	D	127/142 (89%)	118 (93%)	9 (7%)	0	100	100
5	E	208/210 (99%)	188 (90%)	13 (6%)	7 (3%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	84/127 (66%)	78 (93%)	6 (7%)	0	100	100
7	G	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
8	H	148/150 (99%)	119 (80%)	19 (13%)	10 (7%)	1	15
9	I	123/125 (98%)	92 (75%)	18 (15%)	13 (11%)	0	8
10	J	65/67 (97%)	51 (78%)	8 (12%)	6 (9%)	1	11
11	K	115/117 (98%)	110 (96%)	2 (2%)	3 (3%)	5	31
12	L	44/58 (76%)	33 (75%)	9 (20%)	2 (4%)	2	22
13	M	308/316 (98%)	263 (85%)	25 (8%)	20 (6%)	1	16
14	N	109/376 (29%)	100 (92%)	7 (6%)	2 (2%)	8	40
15	O	97/109 (89%)	92 (95%)	4 (4%)	1 (1%)	15	55
16	P	183/339 (54%)	169 (92%)	9 (5%)	5 (3%)	5	31
17	Q	176/439 (40%)	154 (88%)	14 (8%)	8 (4%)	2	22
18	R	163/291 (56%)	132 (81%)	21 (13%)	10 (6%)	1	17
19	S	134/517 (26%)	123 (92%)	8 (6%)	3 (2%)	6	35
20	T	218/249 (88%)	185 (85%)	20 (9%)	13 (6%)	1	17
21	U	168/301 (56%)	149 (89%)	10 (6%)	9 (5%)	2	19
22	V	473/782 (60%)	400 (85%)	44 (9%)	29 (6%)	1	17
23	W	661/760 (87%)	570 (86%)	68 (10%)	23 (4%)	3	25
24	0	186/395 (47%)	168 (90%)	13 (7%)	5 (3%)	5	31
25	1	60/71 (84%)	53 (88%)	5 (8%)	2 (3%)	4	26
26	2	264/462 (57%)	246 (93%)	14 (5%)	4 (2%)	10	46
27	3	187/308 (61%)	176 (94%)	9 (5%)	2 (1%)	14	52
All	All	7356/10302 (71%)	6448 (88%)	610 (8%)	298 (4%)	5	23

All (298) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ALA
1	A	48	GLU
1	A	132	LYS
1	A	134	LYS
1	A	154	CYS
1	A	205	VAL
1	A	208	ASP

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Mol	Chain	Res	Type
1	A	211	GLU
1	A	261	ARG
1	A	262	PRO
1	A	264	VAL
1	A	265	VAL
1	A	295	GLN
1	A	344	LYS
1	A	496	PHE
1	A	598	GLY
1	A	605	THR
1	A	607	SER
1	A	610	PRO
1	A	622	SER
1	A	623	PRO
1	A	911	PRO
1	A	931	ARG
1	A	932	ARG
1	A	1114	ALA
1	A	1117	VAL
1	A	1200	PRO
1	A	1299	GLN
1	A	1342	SER
2	B	61	ASP
2	B	63	PRO
2	B	74	ALA
2	B	77	GLU
2	B	78	VAL
2	B	79	GLU
2	B	81	PRO
2	B	134	LYS
2	B	141	GLN
2	B	203	ASN
2	B	226	GLU
2	B	231	PRO
2	B	249	LYS
2	B	491	ARG
2	B	876	ASN
2	B	879	GLU
2	B	898	THR
2	B	901	THR
2	B	1136	GLU
2	B	1166	SER

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Mol	Chain	Res	Type
3	C	6	GLN
3	C	7	PRO
3	C	136	ASP
3	C	139	PRO
3	C	143	VAL
3	C	213	GLU
5	E	47	LYS
5	E	49	SER
5	E	53	PRO
5	E	64	HIS
5	E	65	ASN
8	H	18	GLU
8	H	65	TYR
8	H	67	ASP
8	H	86	ASP
8	H	107	GLU
8	H	108	ALA
9	I	15	ARG
9	I	16	PHE
9	I	62	VAL
9	I	63	ASP
9	I	85	PRO
9	I	86	CYS
9	I	99	SER
9	I	106	ASP
9	I	118	HIS
10	J	64	PRO
11	K	112	LYS
13	M	11	PRO
13	M	12	ARG
13	M	40	VAL
13	M	42	GLY
13	M	43	ASP
13	M	48	VAL
13	M	92	SER
13	M	93	PHE
13	M	94	ASP
14	N	355	ASP
15	O	4	GLN
16	P	207	PRO
17	Q	25	PHE
17	Q	102	VAL

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Mol	Chain	Res	Type
17	Q	118	GLU
18	R	140	LYS
18	R	195	PRO
18	R	196	ASP
18	R	215	GLU
20	T	124	TYR
20	T	143	GLN
20	T	145	LEU
20	T	146	ASP
21	U	228	MET
21	U	231	ASP
21	U	253	THR
21	U	277	GLN
21	U	293	GLU
22	V	385	ASP
22	V	427	MET
22	V	461	HIS
22	V	491	ALA
22	V	499	ASN
22	V	613	THR
22	V	614	SER
22	V	616	ASP
22	V	632	SER
22	V	648	LYS
22	V	649	GLY
23	W	67	VAL
23	W	420	PRO
23	W	424	ARG
23	W	430	ASN
23	W	504	ILE
23	W	573	ASP
23	W	595	ILE
23	W	630	SER
24	0	77	LYS
24	0	78	PRO
25	1	48	GLU
26	2	49	PRO
27	3	120	THR
1	A	77	ASN
1	A	195	GLY
1	A	207	GLU
1	A	213	LYS

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Mol	Chain	Res	Type
1	A	299	ALA
1	A	452	ASP
1	A	531	ASN
1	A	611	ASP
1	A	929	ALA
1	A	1115	LYS
1	A	1275	VAL
1	A	1315	ASP
2	B	23	GLN
2	B	224	CYS
2	B	428	ASP
2	B	518	HIS
2	B	527	ALA
2	B	549	SER
2	B	561	ILE
2	B	875	GLU
2	B	897	ARG
5	E	48	PRO
8	H	149	ALA
9	I	92	LYS
10	J	2	ILE
16	P	208	ARG
16	P	297	LYS
16	P	299	ARG
17	Q	70	LYS
17	Q	101	ASN
17	Q	125	ALA
18	R	147	ASP
18	R	163	LEU
20	T	147	LYS
20	T	156	VAL
20	T	171	GLU
20	T	180	LYS
20	T	229	HIS
21	U	252	LYS
22	V	254	GLN
22	V	404	SER
22	V	460	ALA
22	V	615	PHE
23	W	124	LEU
23	W	408	SER
23	W	646	ILE

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Mol	Chain	Res	Type
26	2	223	ALA
26	2	231	VAL
1	A	184	CYS
1	A	374	SER
1	A	599	HIS
1	A	894	ASP
1	A	1102	MET
1	A	1103	THR
1	A	1265	ASP
1	A	1435	THR
2	B	513	GLU
2	B	685	LYS
2	B	884	ASN
8	H	24	ARG
10	J	6	ARG
10	J	65	LEU
11	K	69	HIS
11	K	80	ASP
13	M	10	LEU
13	M	56	SER
13	M	61	THR
13	M	86	LYS
13	M	87	GLY
13	M	95	GLU
13	M	306	PHE
17	Q	158	HIS
18	R	149	LYS
18	R	174	ALA
19	S	154	THR
20	T	142	SER
20	T	155	PRO
21	U	279	ARG
21	U	294	CYS
22	V	343	GLY
23	W	147	GLN
23	W	155	CYS
23	W	509	GLU
27	3	198	SER
1	A	300	ALA
1	A	615	SER
2	B	80	GLU
2	B	118	LEU

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Mol	Chain	Res	Type
2	B	839	GLY
2	B	873	LEU
2	B	1006	VAL
12	L	16	ILE
13	M	44	ARG
13	M	89	GLY
13	M	101	TYR
14	N	312	GLU
16	P	163	PRO
17	Q	126	SER
18	R	156	ASP
19	S	151	ARG
20	T	141	LEU
20	T	178	ALA
21	U	233	LEU
22	V	310	LEU
22	V	475	ASP
22	V	502	ILE
22	V	629	HIS
1	A	51	ARG
1	A	65	ILE
1	A	204	HIS
1	A	271	ARG
1	A	485	ASN
1	A	817	PRO
1	A	935	GLN
1	A	1274	GLU
2	B	75	SER
2	B	290	TYR
2	B	460	HIS
2	B	493	GLY
2	B	521	GLY
2	B	1025	ASN
2	B	1129	ASN
3	C	147	ASP
9	I	12	VAL
10	J	30	THR
19	S	160	ALA
22	V	470	LEU
22	V	650	MET
23	W	152	LEU
23	W	551	SER

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Mol	Chain	Res	Type
24	0	79	ASN
26	2	430	VAL
1	A	612	ASP
1	A	650	GLY
1	A	726	GLU
1	A	729	PRO
3	C	74	ILE
8	H	21	LYS
8	H	139	SER
9	I	67	GLN
18	R	139	PHE
22	V	436	GLY
22	V	582	GLY
23	W	36	GLY
23	W	111	SER
23	W	345	ARG
23	W	697	ILE
1	A	687	ILE
22	V	311	LYS
22	V	651	VAL
2	B	253	GLY
3	C	218	ALA
9	I	68	ILE
12	L	20	GLY
22	V	457	ILE
23	W	495	ILE
24	0	216	GLY
1	A	621	ILE
13	M	38	GLY
22	V	405	VAL
23	W	174	ILE
25	1	2	VAL
2	B	136	GLY
3	C	151	VAL
5	E	52	ARG
10	J	5	VAL
22	V	426	VAL
23	W	45	GLY
24	0	56	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1279/1748 (73%)	1230 (96%)	49 (4%)	33	57
2	B	1020/1028 (99%)	994 (98%)	26 (2%)	47	68
3	C	252/252 (100%)	247 (98%)	5 (2%)	55	74
4	D	119/126 (94%)	119 (100%)	0	100	100
5	E	192/192 (100%)	184 (96%)	8 (4%)	30	54
6	F	74/111 (67%)	73 (99%)	1 (1%)	67	80
7	G	152/153 (99%)	150 (99%)	2 (1%)	69	81
8	H	131/131 (100%)	127 (97%)	4 (3%)	40	62
9	I	112/112 (100%)	105 (94%)	7 (6%)	18	43
10	J	56/56 (100%)	54 (96%)	2 (4%)	35	59
11	K	106/106 (100%)	101 (95%)	5 (5%)	26	51
12	L	43/55 (78%)	42 (98%)	1 (2%)	50	70
13	M	263/268 (98%)	255 (97%)	8 (3%)	41	63
14	N	105/324 (32%)	104 (99%)	1 (1%)	76	86
15	O	90/98 (92%)	89 (99%)	1 (1%)	73	84
16	P	159/293 (54%)	156 (98%)	3 (2%)	57	75
17	Q	164/373 (44%)	158 (96%)	6 (4%)	34	58
18	R	150/261 (58%)	143 (95%)	7 (5%)	26	51
19	S	121/448 (27%)	118 (98%)	3 (2%)	47	68
20	T	196/218 (90%)	188 (96%)	8 (4%)	30	55
21	U	148/266 (56%)	139 (94%)	9 (6%)	18	44
22	V	422/688 (61%)	404 (96%)	18 (4%)	29	53
23	W	577/664 (87%)	541 (94%)	36 (6%)	18	43
24	0	171/352 (49%)	163 (95%)	8 (5%)	26	51
25	1	56/64 (88%)	52 (93%)	4 (7%)	14	39
26	2	238/399 (60%)	229 (96%)	9 (4%)	33	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	3	171/272 (63%)	158 (92%)	13 (8%)	13	37
All	All	6567/9058 (72%)	6323 (96%)	244 (4%)	37	58

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	87	HIS
1	A	117	LEU
1	A	132	LYS
1	A	181	HIS
1	A	203	LYS
1	A	212	LYS
1	A	220	ARG
1	A	231	GLU
1	A	261	ARG
1	A	264	VAL
1	A	271	ARG
1	A	277	THR
1	A	343	LEU
1	A	449	HIS
1	A	463	THR
1	A	475	ARG
1	A	477	LEU
1	A	500	GLU
1	A	508	SER
1	A	546	ARG
1	A	587	THR
1	A	595	ILE
1	A	611	ASP
1	A	619	LYS
1	A	620	HIS
1	A	625	ASP
1	A	839	HIS
1	A	849	ASP
1	A	908	THR
1	A	954	ARG
1	A	981	CYS
1	A	1036	ASN
1	A	1050	CYS
1	A	1066	ASP
1	A	1075	LYS

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Mol	Chain	Res	Type
1	A	1115	LYS
1	A	1139	LEU
1	A	1192	TRP
1	A	1203	ASP
1	A	1282	ASP
1	A	1298	LEU
1	A	1309	MET
1	A	1319	LYS
1	A	1337	GLU
1	A	1339	ASP
1	A	1375	ARG
1	A	1420	ASN
1	A	1484	MET
2	B	73	HIS
2	B	79	GLU
2	B	129	THR
2	B	146	LYS
2	B	161	CYS
2	B	168	ASP
2	B	225	LEU
2	B	226	GLU
2	B	287	HIS
2	B	302	LYS
2	B	414	GLU
2	B	422	PHE
2	B	483	ARG
2	B	548	TRP
2	B	591	ARG
2	B	666	ASP
2	B	711	ILE
2	B	737	ILE
2	B	785	TYR
2	B	793	SER
2	B	853	LEU
2	B	880	LEU
2	B	897	ARG
2	B	957	THR
2	B	1054	MET
2	B	1069	ILE
3	C	5	ASN
3	C	63	PHE
3	C	114	HIS

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Mol	Chain	Res	Type
3	C	195	THR
3	C	273	THR
5	E	46	ASP
5	E	47	LYS
5	E	50	GLU
5	E	55	ARG
5	E	62	VAL
5	E	64	HIS
5	E	127	LEU
5	E	172	ARG
6	F	121	ASP
7	G	22	LEU
7	G	128	TYR
8	H	38	ASP
8	H	70	LEU
8	H	84	ARG
8	H	107	GLU
9	I	14	ILE
9	I	15	ARG
9	I	60	HIS
9	I	61	GLU
9	I	62	VAL
9	I	66	THR
9	I	103	ARG
10	J	36	ASP
10	J	47	ARG
11	K	39	ASP
11	K	48	SER
11	K	63	VAL
11	K	111	ASP
11	K	112	LYS
12	L	19	CYS
13	M	10	LEU
13	M	14	THR
13	M	31	ASP
13	M	47	ASP
13	M	86	LYS
13	M	129	ASN
13	M	133	ASN
13	M	151	LEU
14	N	20	ASP
15	O	3	TYR

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Mol	Chain	Res	Type
16	P	203	ARG
16	P	239	ARG
16	P	297	LYS
17	Q	16	ARG
17	Q	102	VAL
17	Q	135	THR
17	Q	139	LEU
17	Q	177	LEU
17	Q	202	GLU
18	R	108	HIS
18	R	163	LEU
18	R	177	ASN
18	R	194	ARG
18	R	205	ASP
18	R	206	LYS
18	R	209	GLN
19	S	35	ASP
19	S	166	ARG
19	S	177	MET
20	T	141	LEU
20	T	153	TYR
20	T	154	LYS
20	T	156	VAL
20	T	177	ARG
20	T	185	ASP
20	T	201	ASP
20	T	204	ASP
21	U	205	ASN
21	U	226	GLU
21	U	227	GLU
21	U	233	LEU
21	U	252	LYS
21	U	257	GLN
21	U	276	VAL
21	U	292	ASN
21	U	301	CYS
22	V	246	MET
22	V	332	ARG
22	V	362	LEU
22	V	366	ASN
22	V	427	MET
22	V	429	TRP

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Mol	Chain	Res	Type
22	V	458	VAL
22	V	471	VAL
22	V	479	ASP
22	V	482	PHE
22	V	492	ASN
22	V	517	GLU
22	V	530	ARG
22	V	566	PHE
22	V	568	LEU
22	V	581	TYR
22	V	590	MET
22	V	612	ASP
23	W	37	HIS
23	W	64	PRO
23	W	95	GLU
23	W	101	LYS
23	W	112	ARG
23	W	122	THR
23	W	123	PRO
23	W	166	ARG
23	W	175	TYR
23	W	196	ARG
23	W	207	TYR
23	W	263	LEU
23	W	283	ASP
23	W	285	TYR
23	W	288	LEU
23	W	299	ARG
23	W	309	VAL
23	W	333	LEU
23	W	345	ARG
23	W	346	VAL
23	W	425	THR
23	W	461	LEU
23	W	489	CYS
23	W	523	LEU
23	W	533	ASP
23	W	543	GLN
23	W	544	TYR
23	W	554	GLU
23	W	584	TYR
23	W	596	LEU

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Mol	Chain	Res	Type
23	W	610	PHE
23	W	620	MET
23	W	647	ARG
23	W	654	PHE
23	W	669	ARG
23	W	676	LEU
24	0	77	LYS
24	0	103	GLN
24	0	125	ARG
24	0	137	MET
24	0	174	LEU
24	0	202	SER
24	0	218	THR
24	0	222	ILE
25	1	10	ILE
25	1	16	MET
25	1	18	GLN
25	1	38	ILE
26	2	61	PHE
26	2	77	LYS
26	2	181	GLN
26	2	202	GLN
26	2	402	ARG
26	2	407	VAL
26	2	426	ARG
26	2	430	VAL
26	2	452	LYS
27	3	37	CYS
27	3	56	LYS
27	3	66	GLU
27	3	109	GLU
27	3	121	LYS
27	3	124	ILE
27	3	133	LEU
27	3	144	ILE
27	3	147	MET
27	3	157	MET
27	3	185	GLN
27	3	190	LEU
27	3	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	272	ASN
1	A	353	ASN
1	A	539	GLN
1	A	1034	GLN
1	A	1036	ASN
1	A	1313	GLN
1	A	1316	ASN
1	A	1445	HIS
2	B	90	GLN
2	B	175	ASN
2	B	1021	HIS
3	C	6	GLN
3	C	145	GLN
3	C	260	GLN
5	E	22	HIS
5	E	148	HIS
7	G	24	ASN
9	I	84	HIS
10	J	61	ASN
11	K	29	ASN
12	L	23	HIS
13	M	129	ASN
19	S	141	HIS
22	V	281	GLN
22	V	286	HIS
22	V	366	ASN
22	V	415	HIS
22	V	539	ASN
22	V	677	GLN
23	W	187	GLN
23	W	430	ASN
23	W	590	ASN
24	0	60	HIS
24	0	103	GLN
25	1	51	ASN
26	2	117	ASN
26	2	161	HIS
26	2	181	GLN
26	2	202	GLN
26	2	221	GLN
26	2	239	GLN
26	2	263	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
26	2	273	GLN
27	3	52	ASN
27	3	63	HIS
27	3	148	ASN
27	3	155	GLN
27	3	185	GLN
27	3	187	GLN
27	3	225	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

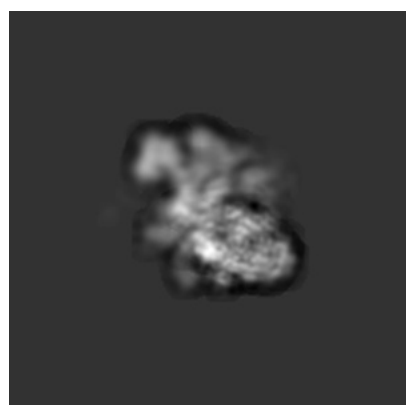
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8132. These allow visual inspection of the internal detail of the map and identification of artifacts.

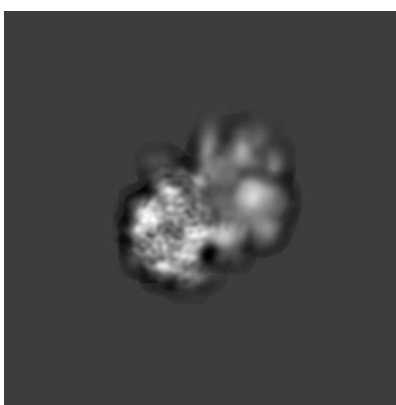
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

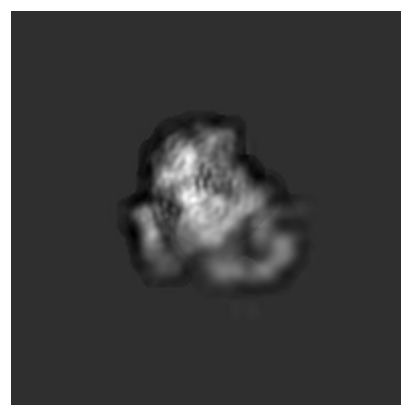
#### 6.1.1 Primary map



X



Y

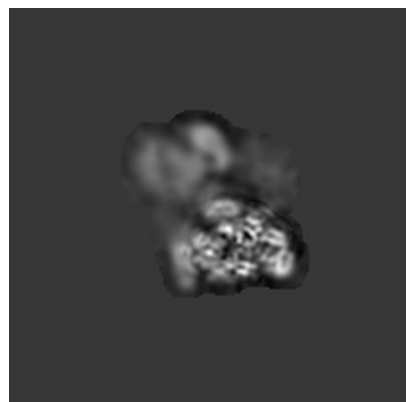


Z

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

### 6.2 Central slices [i](#)

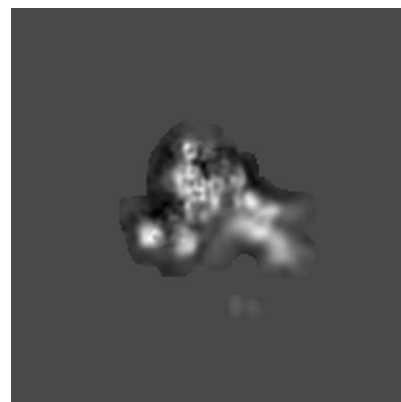
#### 6.2.1 Primary map



X Index: 96



Y Index: 96

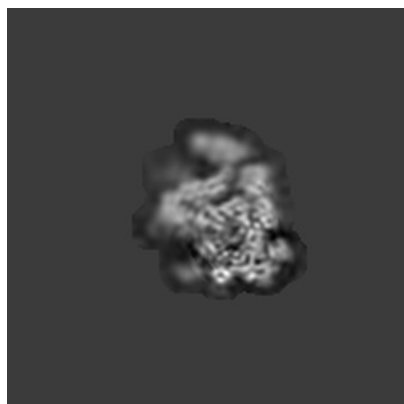


Z Index: 96

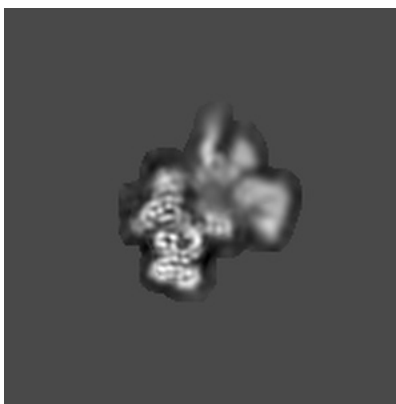
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

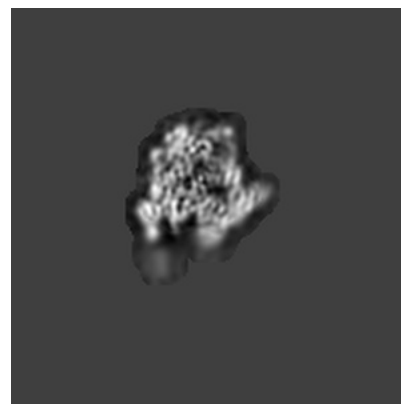
### 6.3.1 Primary map



X Index: 84



Y Index: 93

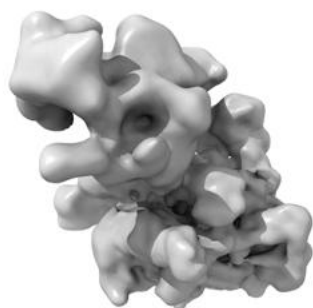


Z Index: 76

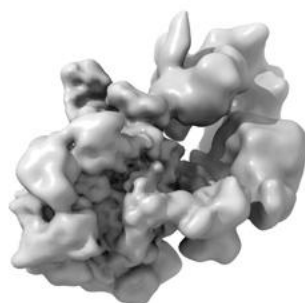
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

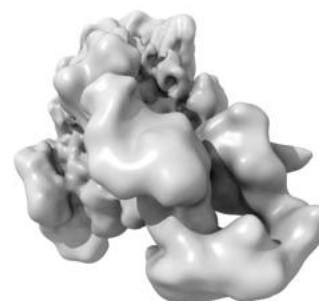
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

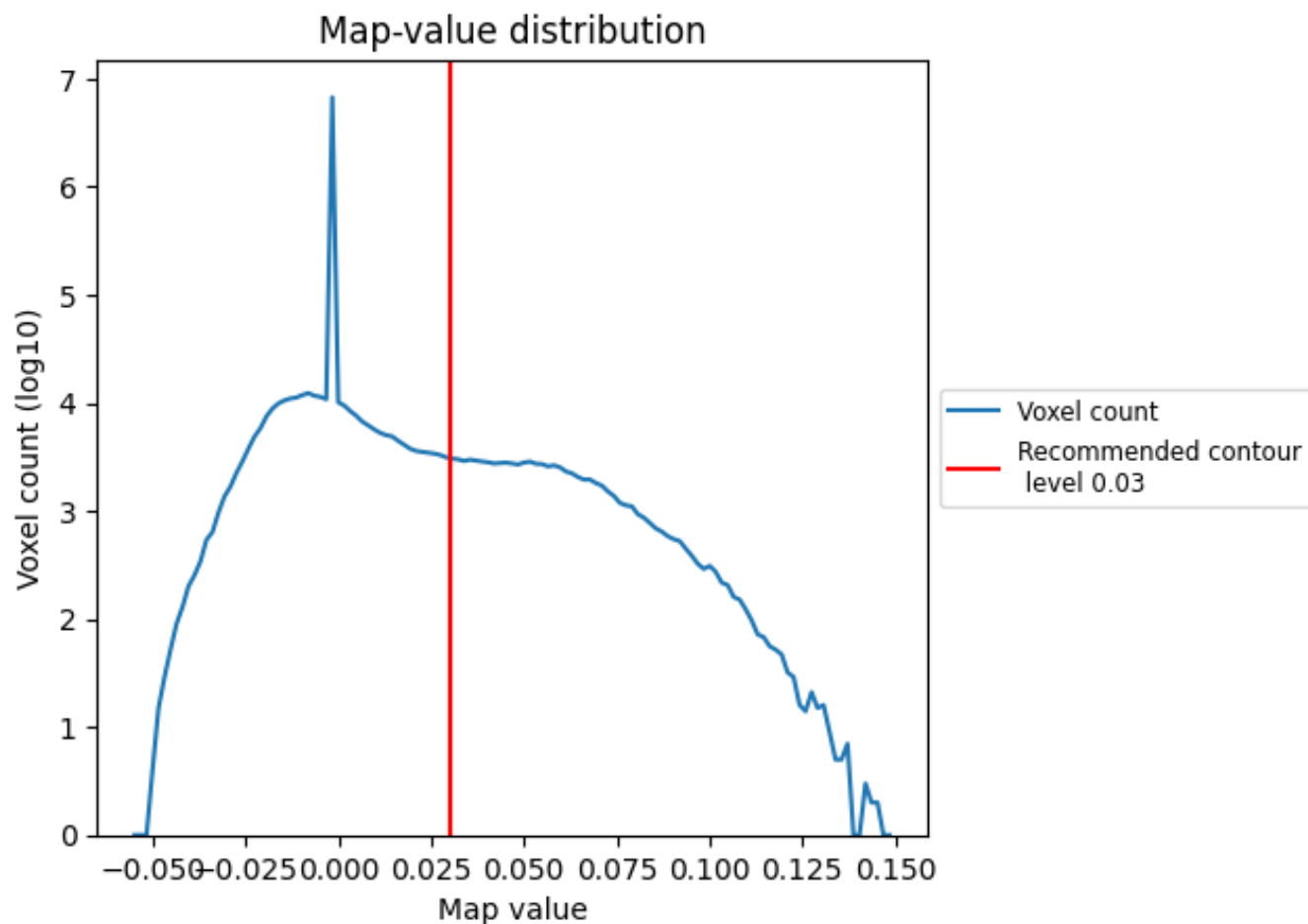
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

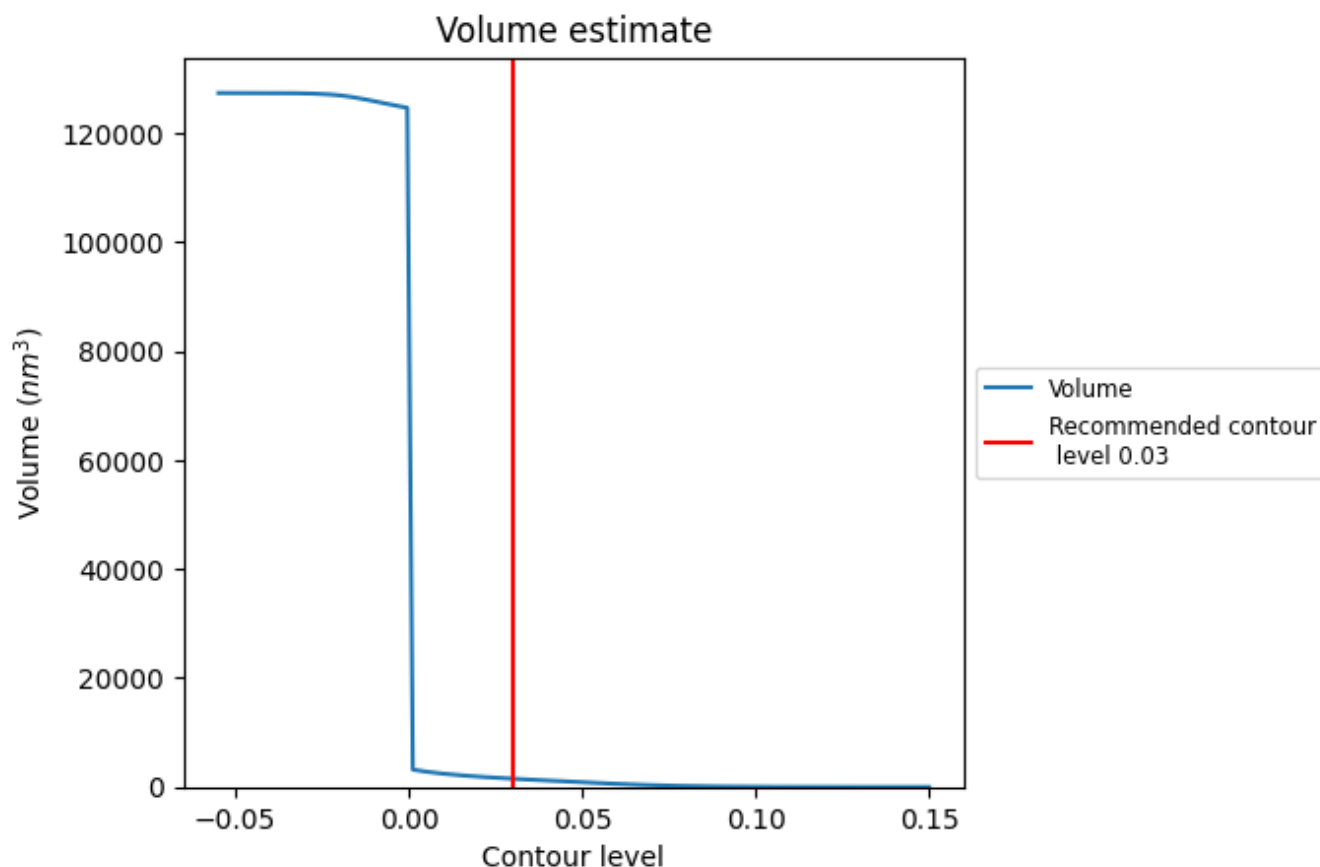
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

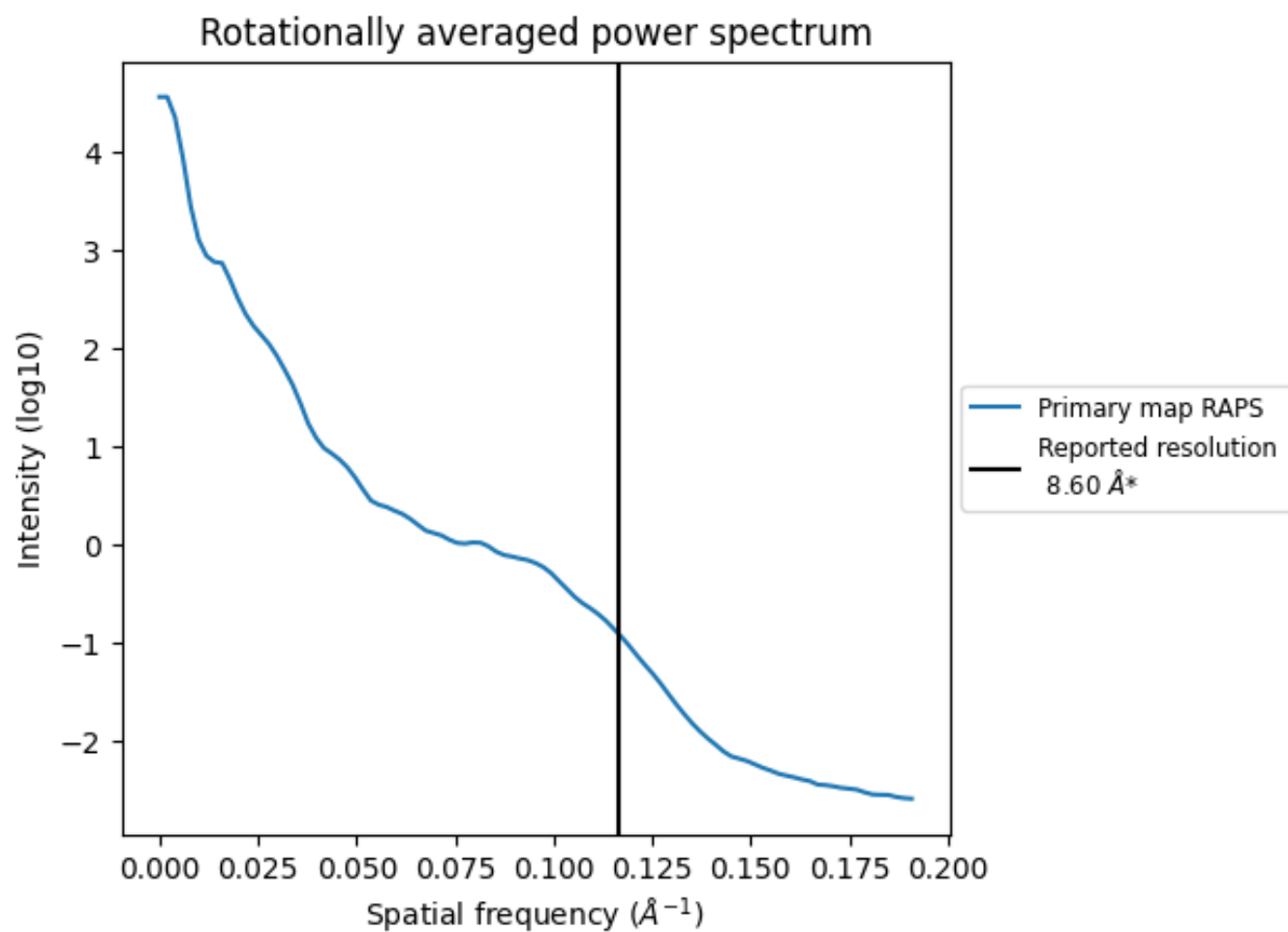
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1510  $\text{nm}^3$ ; this corresponds to an approximate mass of 1364 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



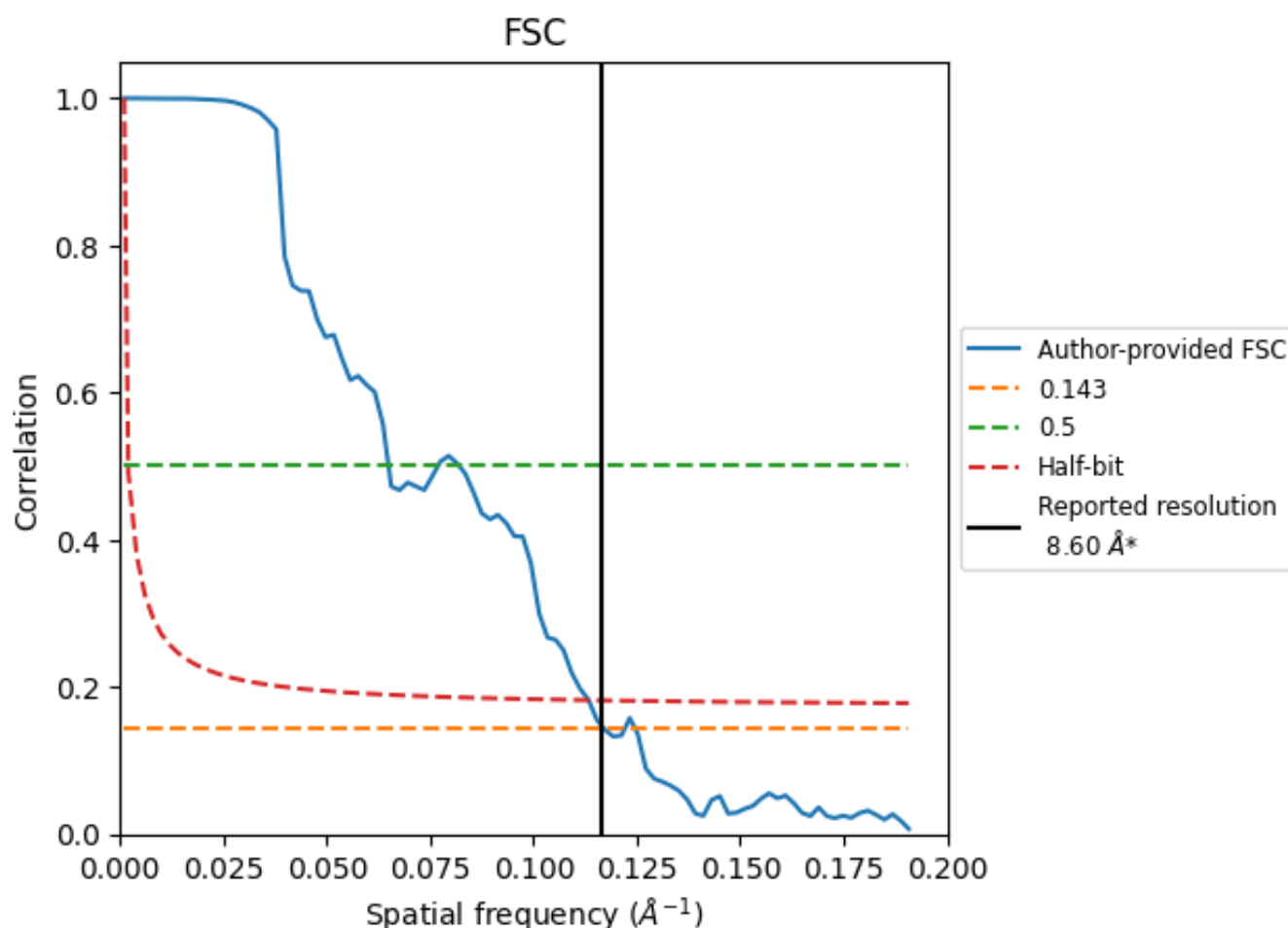
\*Reported resolution corresponds to spatial frequency of 0.116 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.116  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

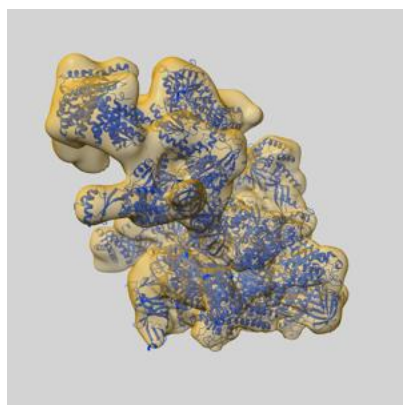
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.60	-	-
Author-provided FSC curve	8.55	15.38	8.82
Unmasked-calculated*	-	-	-

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

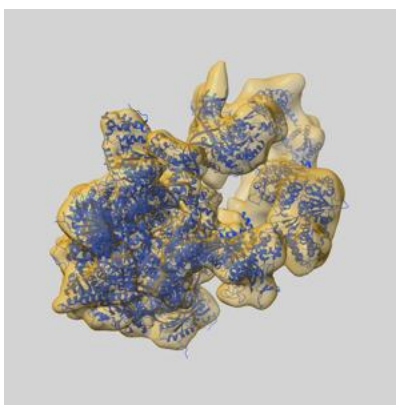
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8132 and PDB model 5IY7. Per-residue inclusion information can be found in section 3 on page 9.

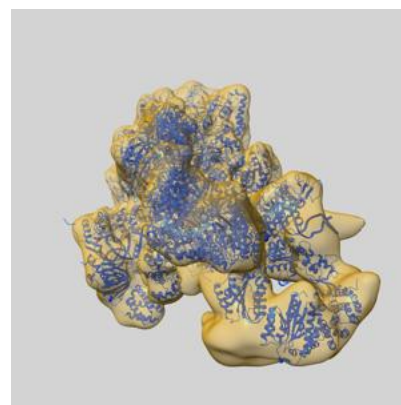
### 9.1 Map-model overlay [i](#)



X



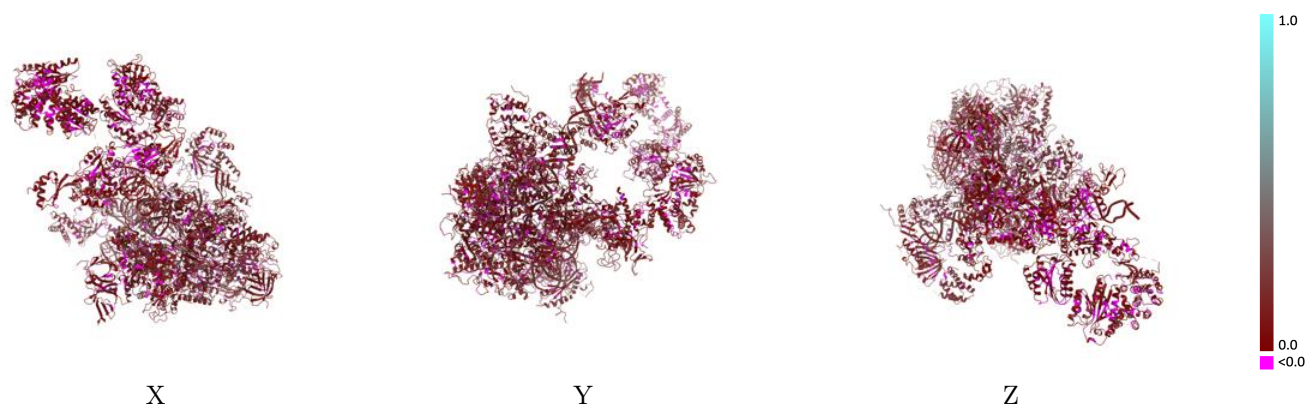
Y



Z

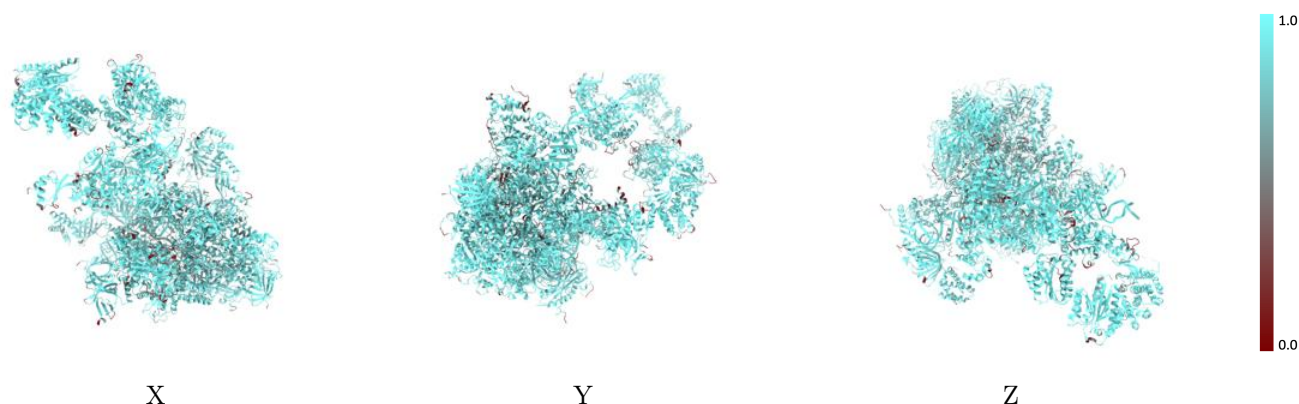
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



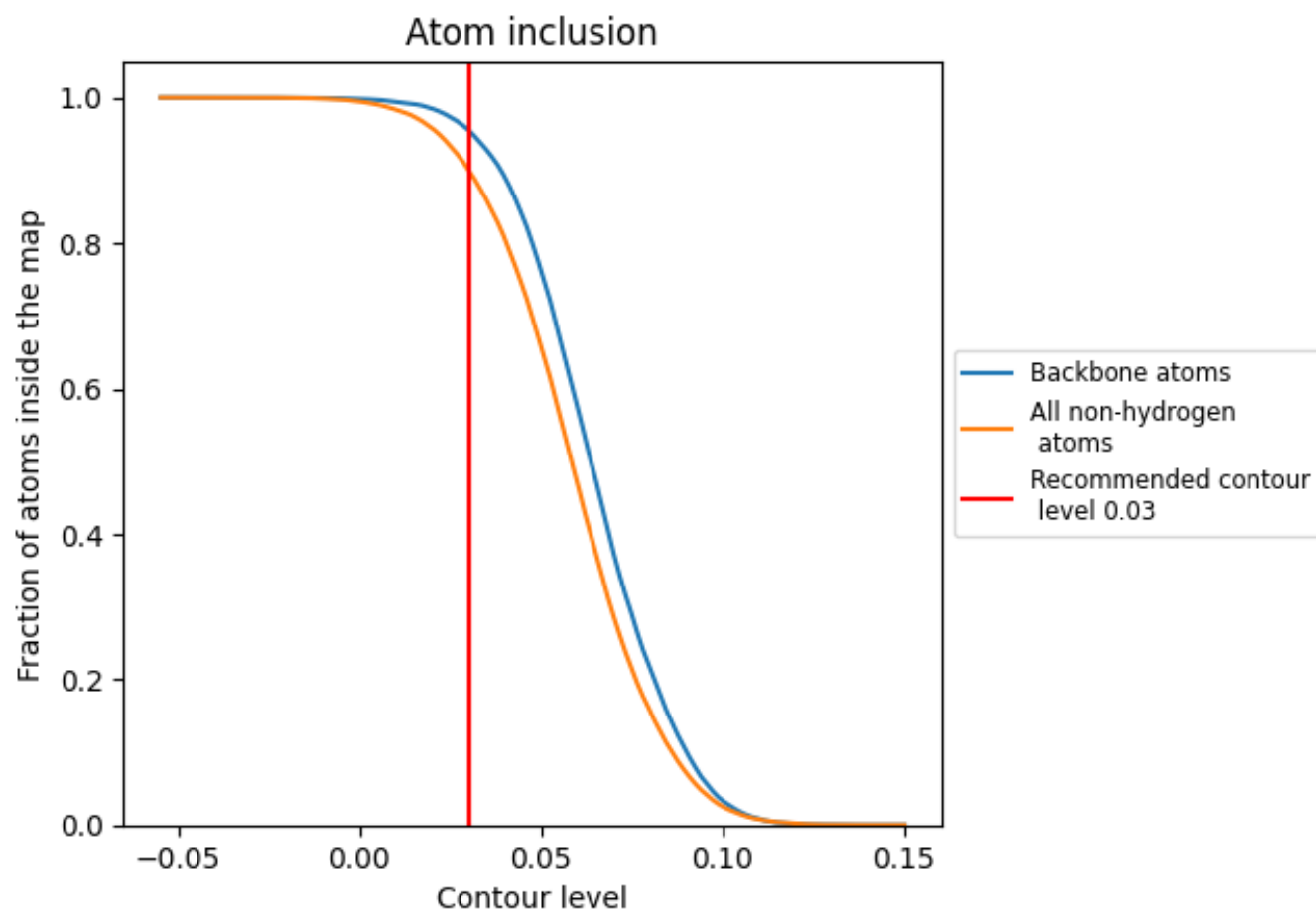
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9005	 0.1050
0	 0.9277	 0.0520
1	 0.8258	 0.0650
2	 0.9350	 0.0720
3	 0.9523	 0.0610
A	 0.8902	 0.1260
B	 0.8753	 0.1170
C	 0.9326	 0.1170
D	 0.8987	 0.1120
E	 0.9245	 0.1250
F	 0.8039	 0.1300
G	 0.9369	 0.1050
H	 0.9380	 0.1170
I	 0.8731	 0.0950
J	 0.9654	 0.1190
K	 0.9419	 0.1420
L	 0.9462	 0.1240
M	 0.8858	 0.1170
N	 0.9039	 0.0930
O	 0.9594	 0.0820
P	 0.9664	 0.1140
Q	 0.9342	 0.1030
R	 0.8854	 0.1030
S	 0.8972	 0.0720
T	 0.8796	 0.1030
U	 0.6407	 0.0780
V	 0.9219	 0.0640
W	 0.9131	 0.0670
X	 0.9428	 0.1560
Y	 0.9161	 0.1590

