



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:46 PM UTC

PDB ID : 5IY8 / pdb_00005iy8
EMDB ID : EMD-8133
Title : Human holo-PIC in the initial transcribing state
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on : 2016-03-24
Resolution : 7.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

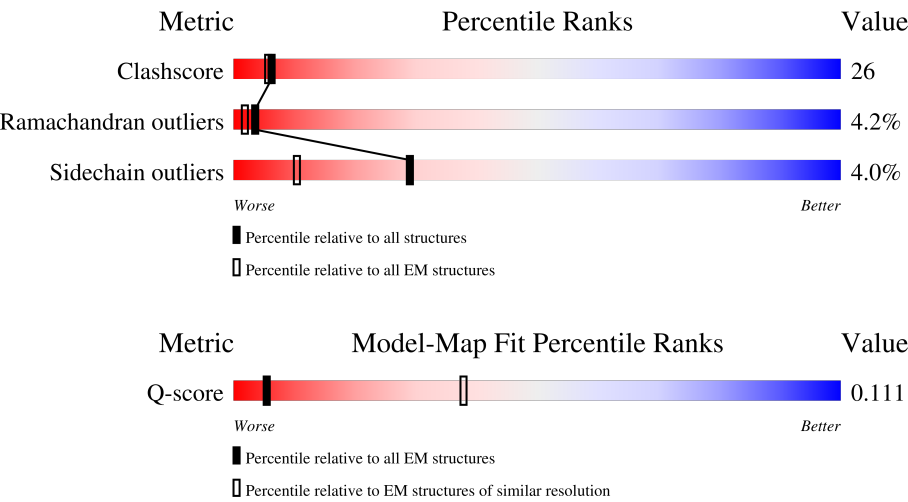
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.90 Å.

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



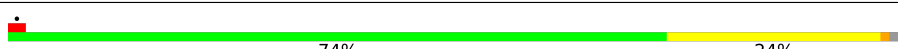
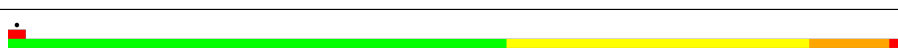
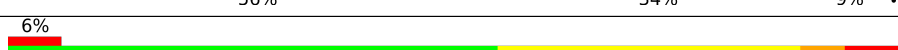
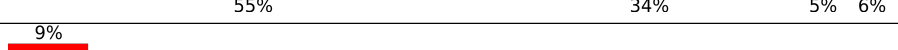
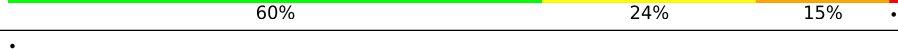
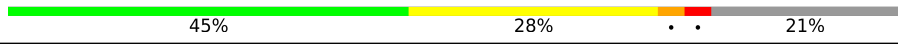
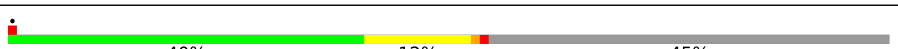
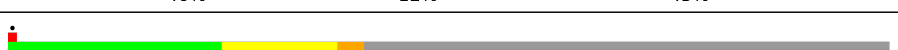
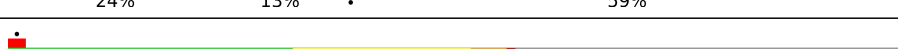
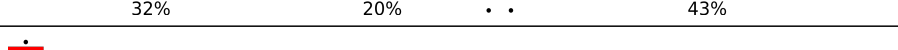
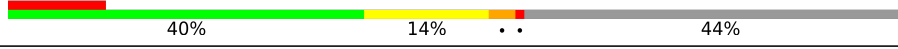
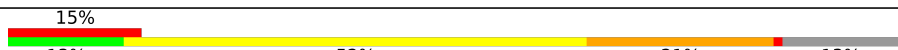
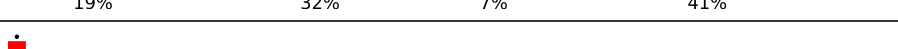
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	366 (7.40 - 8.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

Continued on next page...

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Mol	Chain	Length	Quality of chain
5	E	210	
6	F	127	
7	G	172	
8	H	150	
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	83	
29	Y	83	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 62944 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 A protein 1.

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 TFIIH 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 TFIIH 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 IIH 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 IIH 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 IIH 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 IIH 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	83	Total	C	N	O	P	0	0
			1710	815	307	506	82		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	83	Total	C	N	O	P	0	0
			1681	798	300	501	82		

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	A	2	Total	Mg	0
			2	2	

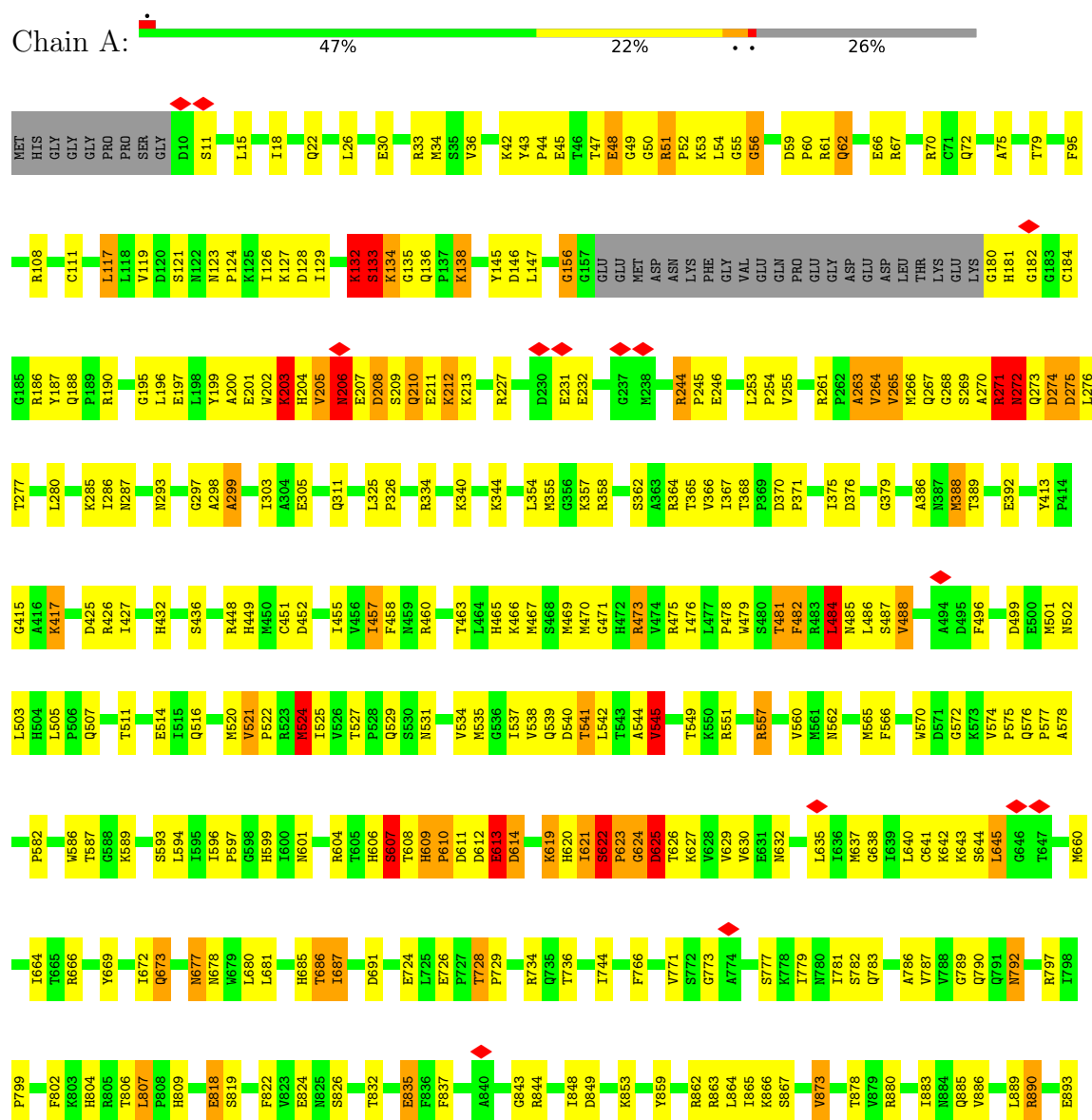
- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Zn	0
			2	2	
31	B	1	Total	Zn	0
			1	1	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	J	1	Total	Zn	0
			1	1	
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.

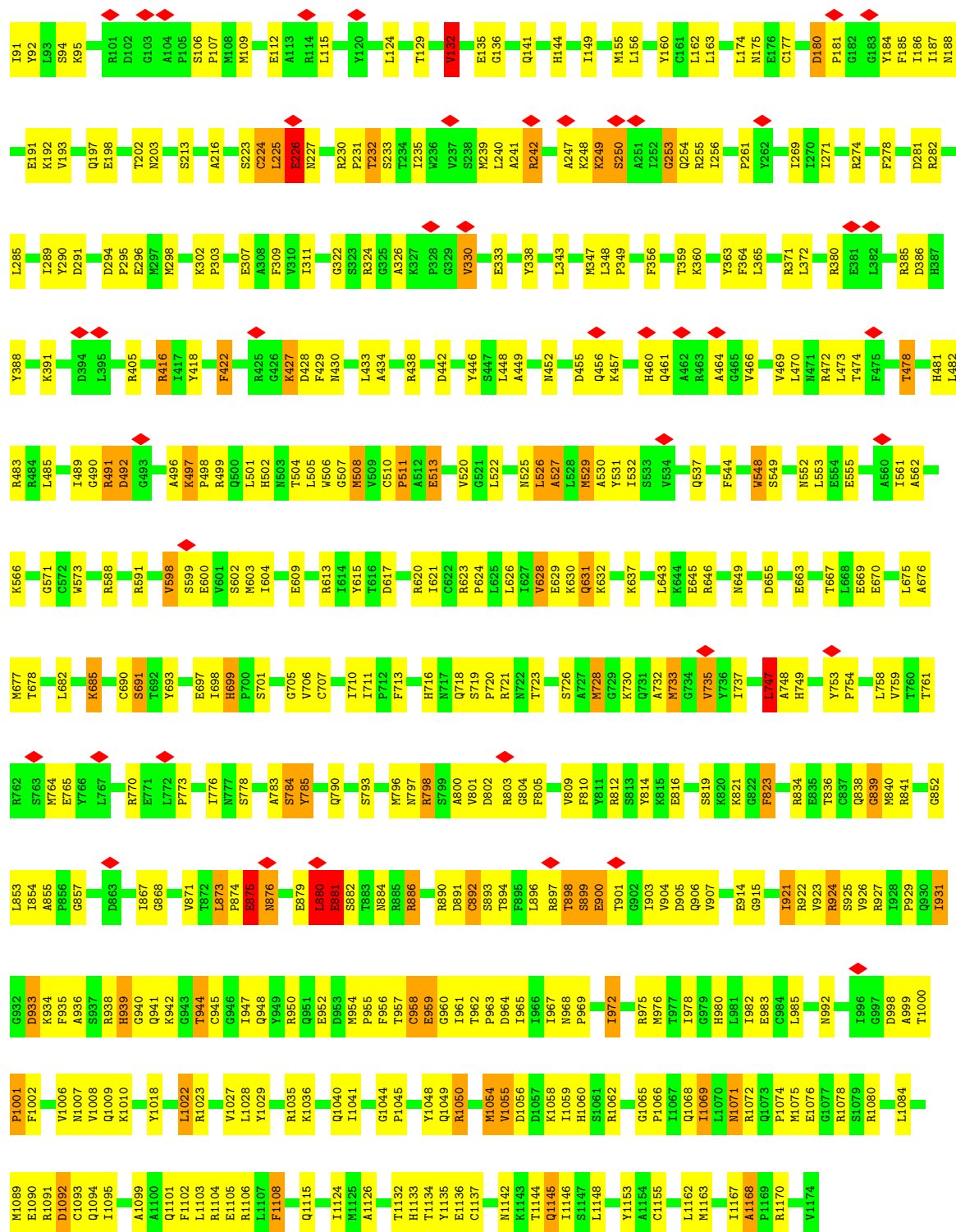
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1





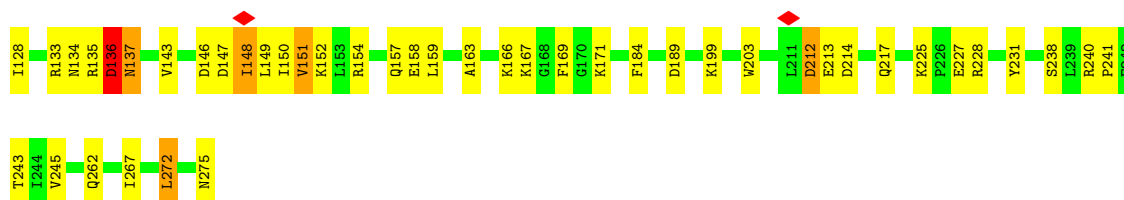
Frequency	Percentage
Often	58%
Sometimes	34%
Rarely	6%



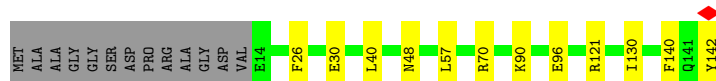
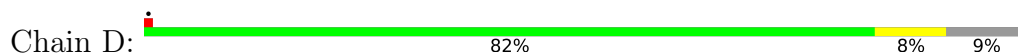


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3





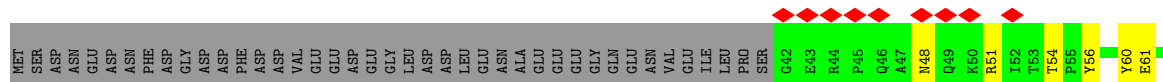
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



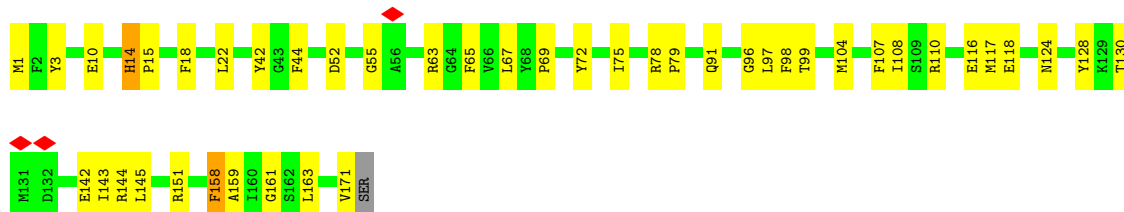
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5



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

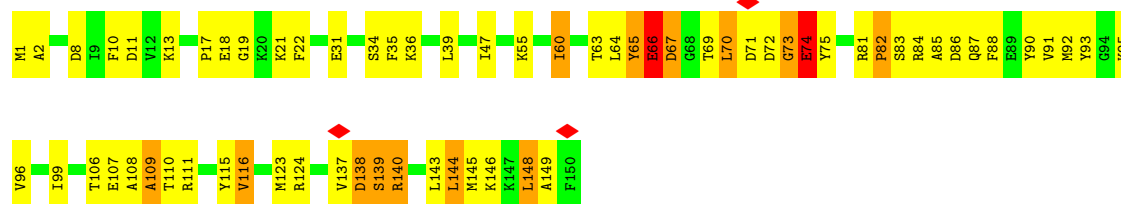


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



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

Chain H: 



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

Chain I: 



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

Chain J: 



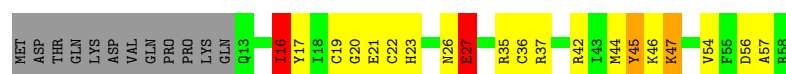
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 



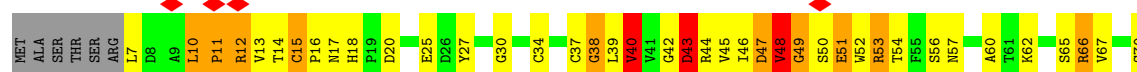
- Molecule 12: DNA-directed RNA polymerase II subunit RPB12

Chain L: 



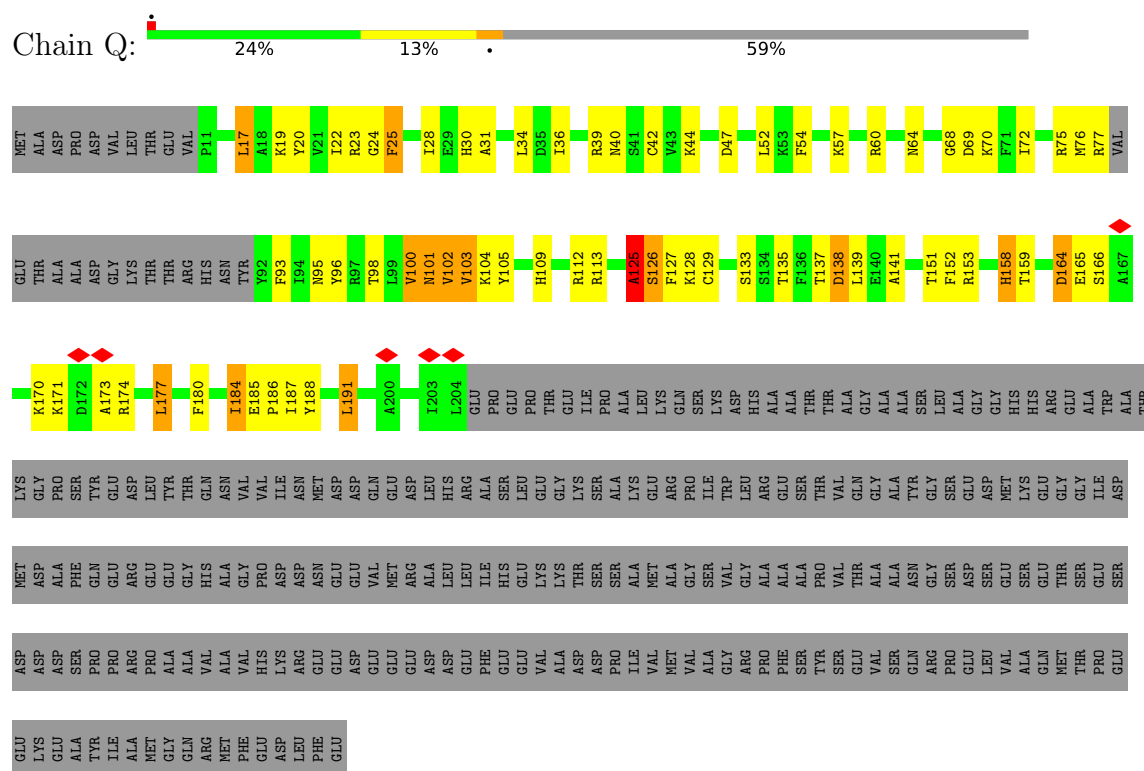
- Molecule 13: Transcription initiation factor IIB

Chain M: 

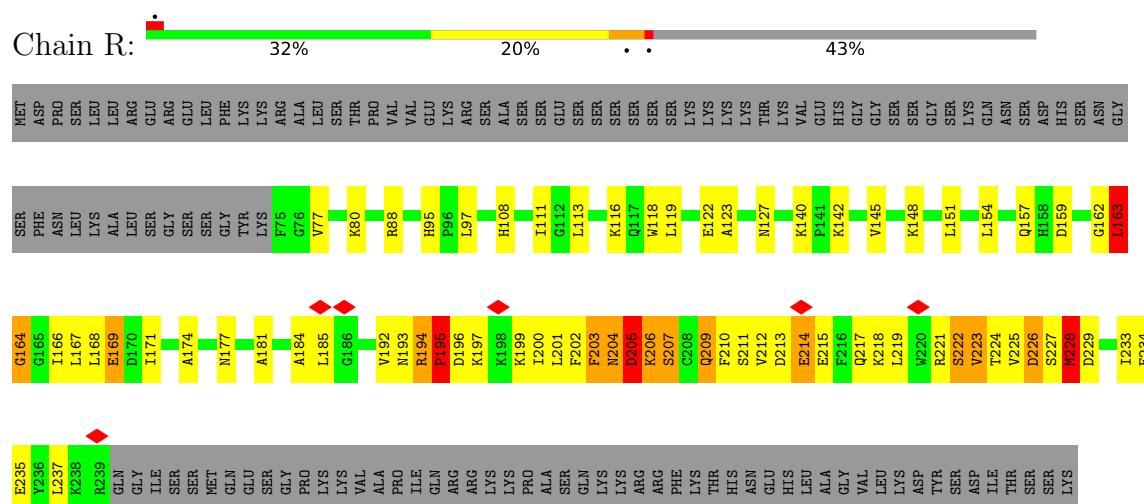




• Molecule 17: General transcription factor IIE subunit 1

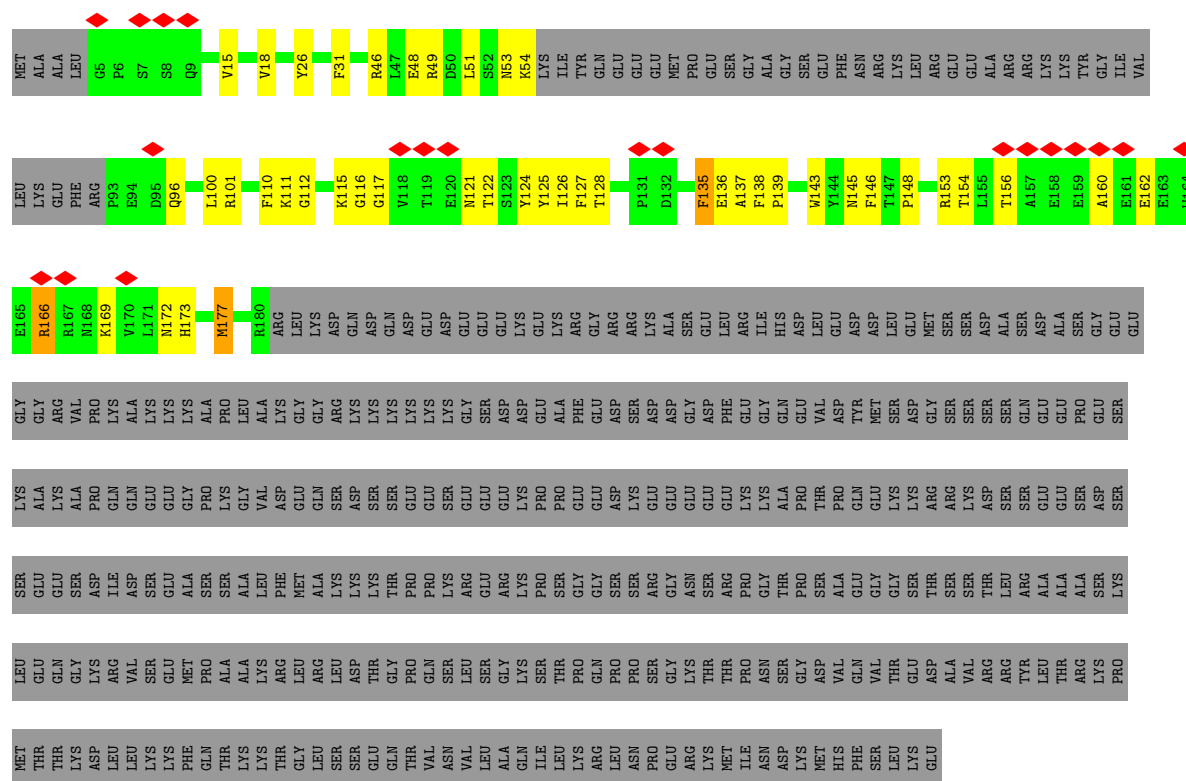


• Molecule 18: Transcription initiation factor IIE subunit beta

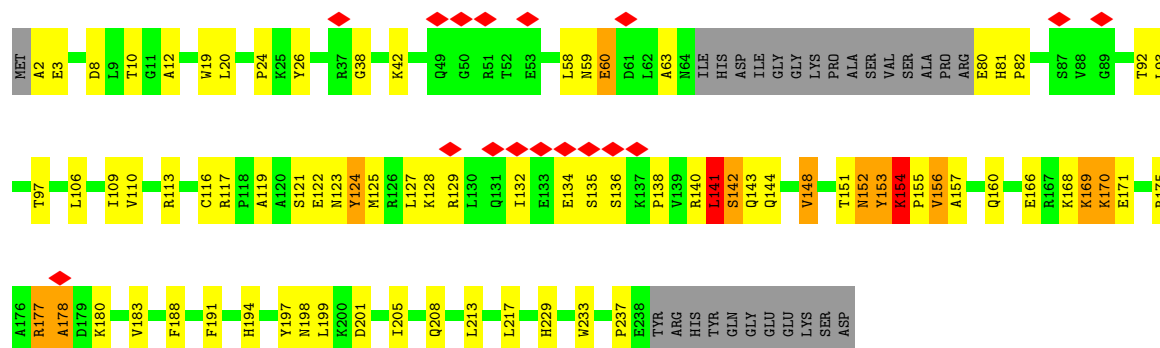


• Molecule 19: General transcription factor IIF subunit 1

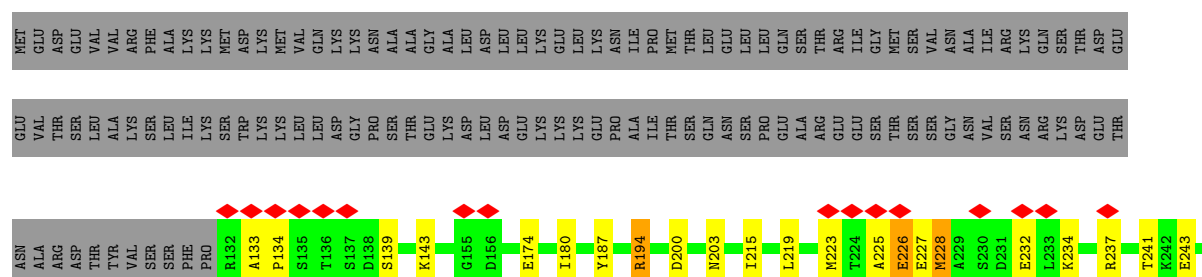




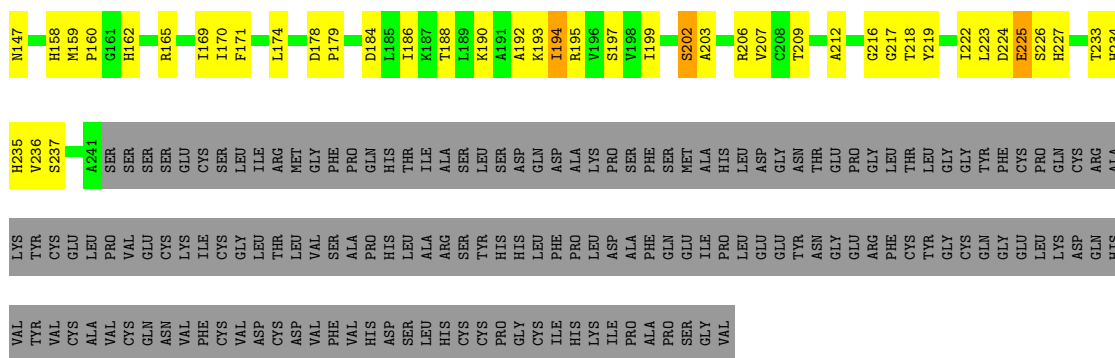
• Molecule 20: General transcription factor IIF subunit 2



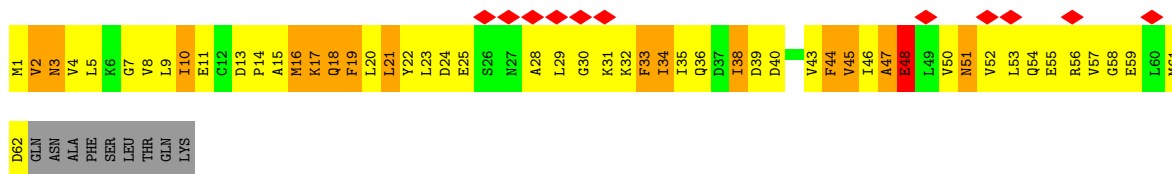
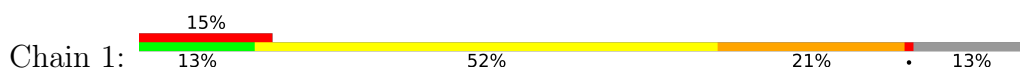
• Molecule 21: Transcription elongation factor A protein 1



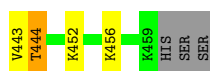
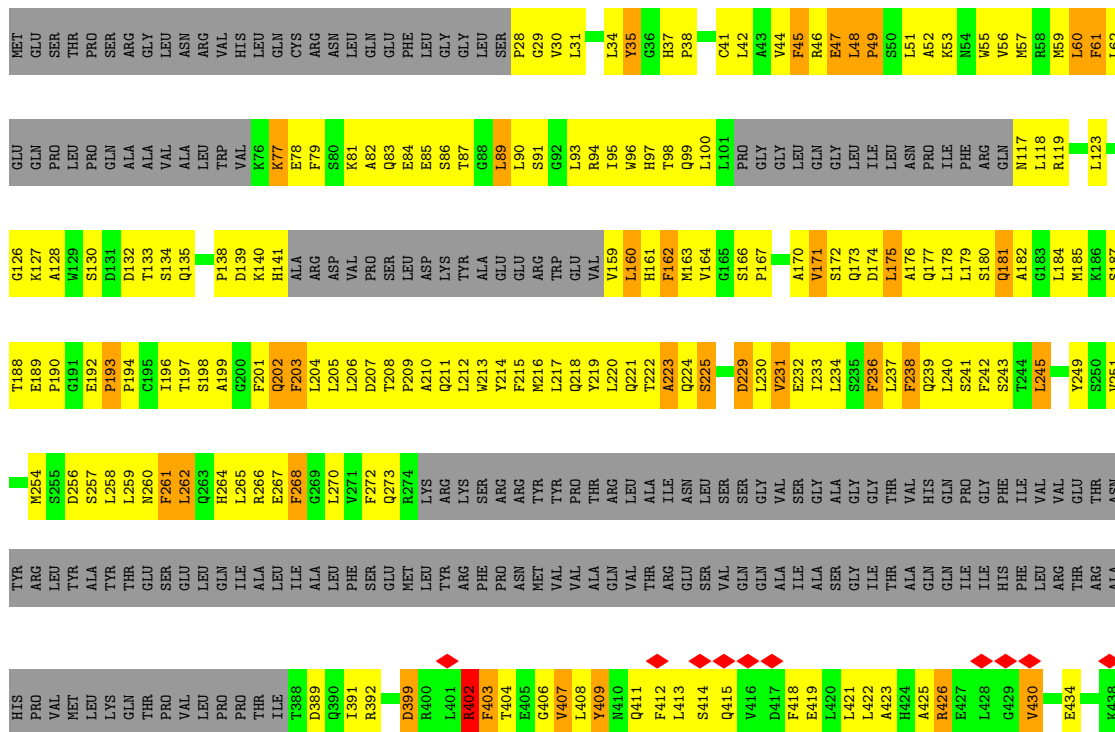




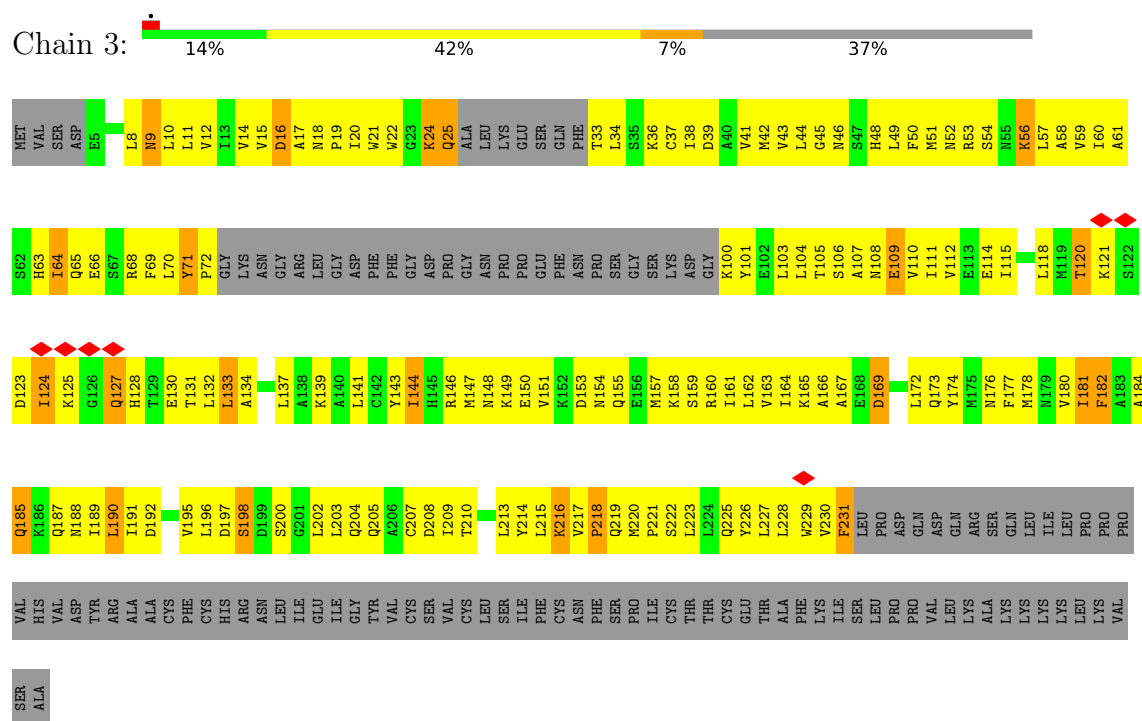
• Molecule 25: General transcription factor IIH subunit 5



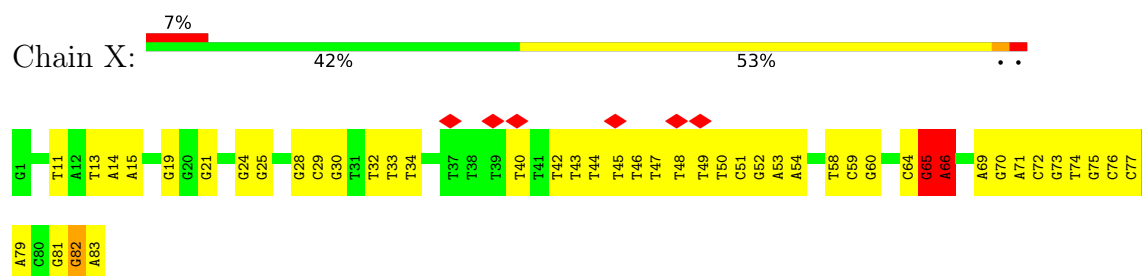
• Molecule 26: General transcription factor IIH subunit 4



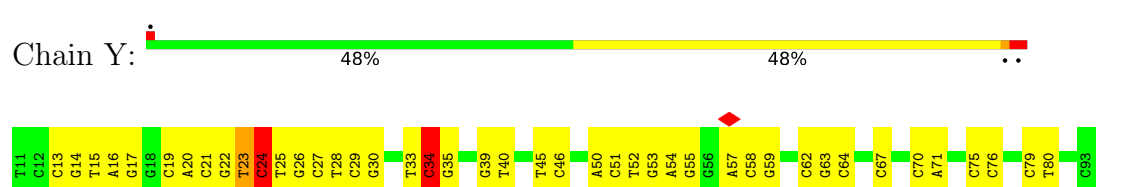
- Molecule 27: General transcription factor IIH subunit 3



- 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	68858	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	0.332	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	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	0.82	13/11727 (0.1%)	1.24	89/15833 (0.6%)
2	B	0.94	10/9503 (0.1%)	1.31	90/12831 (0.7%)
3	C	0.75	0/2259	1.10	14/3073 (0.5%)
4	D	0.30	0/1077	0.81	0/1446
5	E	0.57	0/1753	1.16	10/2368 (0.4%)
6	F	0.83	0/700	1.07	1/946 (0.1%)
7	G	0.39	0/1382	0.93	6/1874 (0.3%)
8	H	0.53	0/1227	1.04	4/1654 (0.2%)
9	I	0.45	0/1038	1.20	10/1407 (0.7%)
10	J	0.84	0/542	1.36	5/730 (0.7%)
11	K	0.65	0/956	1.10	6/1294 (0.5%)
12	L	0.66	0/394	1.14	3/524 (0.6%)
13	M	0.53	0/2429	1.21	24/3281 (0.7%)
14	N	0.34	0/945	1.03	8/1274 (0.6%)
15	O	0.31	0/816	0.83	2/1105 (0.2%)
16	P	0.40	0/1489	0.97	6/2005 (0.3%)
17	Q	0.43	0/1507	0.98	1/2023 (0.0%)
18	R	0.66	3/1380 (0.2%)	1.37	13/1854 (0.7%)
19	S	0.31	0/1167	0.81	0/1576
20	T	0.44	0/1817	1.07	12/2445 (0.5%)
21	U	0.35	0/1358	0.93	3/1820 (0.2%)
22	V	1.90	78/3931 (2.0%)	2.33	243/5298 (4.6%)
23	W	2.05	132/5460 (2.4%)	2.43	361/7390 (4.9%)
24	0	2.09	35/1506 (2.3%)	2.32	75/2038 (3.7%)
25	1	1.29	1/496 (0.2%)	1.82	13/669 (1.9%)
26	2	1.23	0/2243	1.70	40/3024 (1.3%)
27	3	1.28	0/1548	1.56	15/2090 (0.7%)
28	X	0.70	2/1917 (0.1%)	1.12	19/2962 (0.6%)
29	Y	0.64	0/1880	1.09	26/2896 (0.9%)
All	All	1.08	274/64447 (0.4%)	1.47	1099/87730 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
7	G	0	1
14	N	0	2
16	P	0	1
17	Q	0	1
18	R	0	6
19	S	0	1
20	T	0	2
22	V	0	13
23	W	0	19
25	1	0	1
26	2	0	8
28	X	0	4
29	Y	0	4
All	All	0	66

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X	59	DC	O3'-P	-11.13	1.44	1.61
24	0	142	GLU	N-CA	-10.09	1.37	1.45
24	0	158	HIS	CA-C	9.98	1.65	1.52
24	0	99	ASN	CA-CB	9.64	1.63	1.53
23	W	465	ASP	CA-C	9.17	1.64	1.52
22	V	590	MET	CA-C	8.83	1.64	1.52
24	0	122	GLY	N-CA	8.51	1.55	1.45
22	V	376	ALA	CA-C	8.43	1.63	1.52
24	0	142	GLU	CA-C	8.32	1.60	1.52
22	V	255	MET	N-CA	8.31	1.54	1.47
23	W	237	HIS	CE1-NE2	8.28	1.40	1.32
24	0	235	HIS	CE1-NE2	7.91	1.40	1.32
24	0	186	ILE	N-CA	7.86	1.55	1.46
23	W	670	GLY	CA-C	7.76	1.59	1.52
24	0	135	VAL	N-CA	7.67	1.55	1.46
23	W	302	ASP	CA-C	7.65	1.62	1.53
23	W	606	GLU	CA-CB	7.63	1.65	1.53
22	V	289	TYR	N-CA	7.58	1.54	1.46
1	A	521	VAL	CA-CB	7.56	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	168	VAL	CA-CB	7.43	1.58	1.54
18	R	204	ASN	CA-C	7.38	1.61	1.52
22	V	554	ARG	NE-CZ	7.36	1.41	1.33
22	V	391	ARG	CZ-NH2	-7.33	1.24	1.33
24	O	112	LYS	N-CA	7.32	1.56	1.46
24	O	203	ALA	CA-C	7.28	1.61	1.52
23	W	566	LEU	CA-C	7.26	1.61	1.52
23	W	556	GLY	N-CA	7.23	1.52	1.45
23	W	706	LEU	CA-C	7.15	1.62	1.52
23	W	521	GLY	N-CA	7.13	1.55	1.45
22	V	417	THR	CA-C	7.10	1.62	1.52
23	W	272	ARG	CA-CB	7.08	1.64	1.53
24	O	169	ILE	CA-CB	7.08	1.63	1.54
23	W	531	VAL	C-N	7.04	1.39	1.33
22	V	626	ILE	N-CA	7.03	1.55	1.46
23	W	327	GLU	CA-C	7.01	1.61	1.52
1	A	1159	CYS	CA-CB	6.98	1.64	1.53
23	W	546	GLU	C-N	6.97	1.43	1.33
23	W	272	ARG	N-CA	6.88	1.54	1.45
1	A	482	PHE	C-O	-6.86	1.15	1.24
18	R	204	ASN	N-CA	6.84	1.54	1.46
23	W	698	GLN	N-CA	6.77	1.54	1.46
23	W	615	GLY	N-CA	6.76	1.52	1.44
2	B	923	VAL	C-O	-6.74	1.16	1.24
18	R	203	PHE	CA-C	6.72	1.61	1.53
23	W	429	ALA	CA-C	6.69	1.61	1.52
23	W	474	HIS	CD2-NE2	-6.65	1.30	1.37
24	O	188	THR	N-CA	6.64	1.54	1.46
22	V	425	ARG	C-O	-6.63	1.16	1.24
22	V	706	LYS	N-CA	-6.62	1.38	1.46
23	W	683	ARG	CZ-NH2	-6.60	1.24	1.33
22	V	353	ALA	C-N	6.60	1.42	1.33
23	W	674	TYR	N-CA	6.54	1.54	1.45
23	W	115	LEU	N-CA	6.54	1.54	1.46
1	A	481	THR	C-O	-6.48	1.15	1.23
24	O	96	PHE	CA-C	6.48	1.61	1.52
23	W	321	GLY	N-CA	6.48	1.54	1.45
24	O	202	SER	CA-C	6.48	1.62	1.53
22	V	414	GLY	CA-C	6.47	1.59	1.51
22	V	382	SER	N-CA	6.47	1.54	1.46
23	W	291	GLY	CA-C	6.46	1.59	1.52
23	W	522	ASN	CA-C	6.43	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	171	PHE	CA-C	6.42	1.60	1.52
23	W	245	ASP	N-CA	6.40	1.53	1.46
23	W	301	THR	N-CA	6.38	1.54	1.45
22	V	479	ASP	N-CA	-6.36	1.38	1.46
22	V	348	LEU	C-O	-6.34	1.16	1.24
22	V	453	ARG	CZ-NH2	-6.33	1.25	1.33
23	W	494	ILE	C-O	-6.28	1.17	1.24
22	V	712	LEU	CA-C	6.27	1.60	1.52
22	V	252	TYR	CA-CB	6.25	1.62	1.53
22	V	618	PRO	C-O	6.22	1.31	1.23
23	W	693	LEU	CA-CB	6.22	1.61	1.54
23	W	523	LEU	N-CA	6.21	1.53	1.46
23	W	432	ILE	CA-CB	6.21	1.62	1.54
23	W	265	THR	N-CA	6.20	1.54	1.46
23	W	685	ALA	N-CA	6.20	1.53	1.46
23	W	608	ILE	CA-CB	6.14	1.63	1.54
24	0	142	GLU	CA-CB	-6.12	1.46	1.54
23	W	490	LEU	CA-C	6.11	1.59	1.52
23	W	47	GLY	N-CA	6.11	1.54	1.45
23	W	67	VAL	N-CA	6.09	1.53	1.46
23	W	69	LYS	CA-C	6.09	1.60	1.52
22	V	332	ARG	CA-C	6.08	1.60	1.52
24	0	128	ILE	CA-C	6.08	1.60	1.52
23	W	491	CYS	N-CA	6.06	1.53	1.46
22	V	383	THR	CB-OG1	-6.06	1.34	1.43
23	W	18	TYR	CA-CB	6.04	1.62	1.53
24	0	199	ILE	C-N	6.04	1.41	1.33
1	A	502	ASN	CA-C	-6.03	1.45	1.52
23	W	701	LEU	N-CA	6.01	1.54	1.46
23	W	511	ARG	NE-CZ	-6.00	1.26	1.33
23	W	698	GLN	CA-C	5.99	1.60	1.52
22	V	620	ALA	N-CA	5.99	1.54	1.46
22	V	609	LYS	N-CA	5.99	1.54	1.46
2	B	186	ILE	C-O	-5.98	1.17	1.24
23	W	158	TYR	N-CA	5.98	1.53	1.46
23	W	492	PRO	CA-C	5.98	1.59	1.52
24	0	171	PHE	N-CA	-5.97	1.39	1.46
22	V	286	HIS	N-CA	5.97	1.53	1.46
23	W	83	VAL	CA-C	5.96	1.60	1.52
22	V	468	ALA	N-CA	5.96	1.53	1.46
1	A	890	ARG	CA-C	-5.95	1.45	1.52
22	V	638	GLN	N-CA	5.92	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	551	HIS	CA-C	5.92	1.60	1.52
23	W	559	GLU	C-O	-5.92	1.16	1.23
22	V	647	LYS	CA-C	5.90	1.60	1.52
22	V	306	ILE	N-CA	-5.90	1.39	1.46
22	V	269	SER	N-CA	5.89	1.53	1.46
22	V	286	HIS	CB-CG	5.89	1.58	1.50
22	V	633	ARG	CZ-NH1	-5.88	1.24	1.32
22	V	325	ARG	CZ-NH1	-5.87	1.24	1.32
23	W	244	ILE	CA-CB	5.86	1.61	1.54
23	W	242	VAL	N-CA	5.84	1.53	1.46
2	B	939	HIS	CA-C	-5.84	1.45	1.52
23	W	632	ILE	N-CA	5.82	1.53	1.46
23	W	508	PHE	CA-CB	5.79	1.57	1.53
1	A	1159	CYS	N-CA	-5.78	1.39	1.46
23	W	237	HIS	CA-C	5.78	1.60	1.52
23	W	448	PHE	CA-C	5.77	1.60	1.52
22	V	690	ILE	CA-CB	5.77	1.61	1.54
2	B	43	GLN	CA-C	-5.76	1.45	1.52
24	0	207	VAL	CA-CB	5.76	1.61	1.54
22	V	332	ARG	CZ-NH2	-5.76	1.25	1.33
24	0	162	HIS	CA-C	5.76	1.60	1.52
1	A	835	GLU	CA-C	-5.76	1.45	1.52
23	W	666	ARG	NE-CZ	-5.75	1.26	1.33
22	V	657	ALA	CA-C	5.74	1.59	1.52
23	W	648	GLU	C-N	5.74	1.41	1.33
22	V	534	TYR	N-CA	5.73	1.53	1.46
23	W	152	LEU	N-CA	5.72	1.54	1.46
2	B	478	THR	CA-CB	-5.71	1.44	1.53
23	W	705	ASN	C-O	-5.71	1.16	1.24
23	W	106	GLY	CA-C	5.71	1.56	1.51
23	W	703	ASP	CA-C	5.70	1.60	1.53
23	W	343	ARG	CA-C	5.70	1.60	1.52
23	W	42	MET	CA-C	5.69	1.59	1.52
23	W	256	LEU	C-N	-5.68	1.26	1.33
22	V	452	ARG	CZ-NH2	-5.66	1.26	1.33
25	1	47	ALA	CA-C	-5.66	1.48	1.53
23	W	334	ARG	CZ-NH2	-5.65	1.26	1.33
24	0	147	ASN	CA-C	5.65	1.60	1.52
22	V	629	HIS	CE1-NE2	5.65	1.38	1.32
22	V	437	LEU	C-N	5.64	1.41	1.33
22	V	639	ARG	N-CA	5.63	1.53	1.46
23	W	645	GLN	N-CA	5.63	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	461	HIS	CG-CD2	5.61	1.42	1.35
23	W	155	CYS	C-N	5.61	1.43	1.34
23	W	286	ARG	CZ-NH2	-5.60	1.26	1.33
23	W	160	GLU	CA-C	5.59	1.60	1.52
24	O	131	LEU	CA-C	5.58	1.60	1.52
23	W	600	ALA	N-CA	5.56	1.53	1.46
22	V	565	VAL	N-CA	5.56	1.53	1.46
23	W	283	ASP	CA-CB	5.56	1.61	1.53
23	W	291	GLY	C-N	5.56	1.41	1.34
22	V	252	TYR	C-N	5.55	1.41	1.33
22	V	415	HIS	CD2-NE2	5.51	1.44	1.37
22	V	560	VAL	N-CA	-5.51	1.39	1.46
22	V	640	LEU	CA-C	5.51	1.59	1.52
23	W	663	CYS	N-CA	-5.51	1.39	1.46
24	O	190	LYS	N-CA	5.51	1.53	1.46
23	W	552	TRP	C-O	-5.49	1.17	1.24
22	V	474	ASP	N-CA	5.49	1.53	1.46
22	V	392	PHE	C-N	5.49	1.38	1.33
2	B	1048	TYR	CA-C	-5.47	1.46	1.52
24	O	195	ARG	CA-CB	5.47	1.61	1.53
22	V	323	SER	CA-C	5.46	1.59	1.52
23	W	110	SER	CA-CB	5.46	1.63	1.53
23	W	77	VAL	CA-C	5.45	1.57	1.52
2	B	469	VAL	CA-C	-5.43	1.46	1.52
22	V	310	LEU	CA-C	5.43	1.60	1.52
24	O	136	ASP	N-CA	5.43	1.52	1.46
23	W	331	GLY	N-CA	-5.42	1.39	1.45
1	A	673	GLN	C-O	-5.41	1.17	1.24
23	W	405	THR	N-CA	5.40	1.52	1.46
23	W	693	LEU	N-CA	5.38	1.51	1.45
22	V	626	ILE	CB-CG1	5.38	1.64	1.53
23	W	298	ALA	CA-C	5.38	1.59	1.52
22	V	705	THR	CB-OG1	-5.38	1.35	1.43
23	W	85	GLU	CA-C	5.37	1.59	1.52
23	W	185	ARG	CA-CB	5.36	1.61	1.53
23	W	630	SER	CA-C	5.35	1.59	1.52
22	V	692	LYS	CA-C	5.34	1.59	1.52
22	V	296	ASP	CA-C	5.33	1.59	1.52
23	W	48	LYS	N-CA	5.32	1.52	1.46
23	W	592	ARG	CD-NE	5.32	1.53	1.46
23	W	518	ARG	CZ-NH2	-5.31	1.26	1.33
23	W	229	ALA	N-CA	5.31	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X	71	DA	P-O5'	-5.30	1.49	1.60
22	V	332	ARG	NE-CZ	-5.29	1.27	1.33
24	O	217	GLY	N-CA	5.29	1.53	1.45
23	W	510	THR	CA-C	-5.28	1.45	1.52
22	V	636	GLU	N-CA	5.27	1.52	1.46
23	W	72	TYR	CA-C	5.27	1.59	1.52
23	W	154	HIS	CA-CB	5.27	1.62	1.53
1	A	488	VAL	CA-CB	-5.27	1.47	1.54
23	W	548	THR	N-CA	5.27	1.52	1.46
23	W	263	LEU	N-CA	5.26	1.52	1.46
24	O	97	ASP	N-CA	5.26	1.52	1.46
22	V	618	PRO	CA-CB	5.25	1.61	1.53
23	W	412	LYS	N-CA	5.25	1.53	1.46
23	W	713	GLY	CA-C	5.25	1.57	1.52
22	V	699	GLU	CA-C	5.25	1.59	1.52
23	W	501	GLN	CA-C	5.24	1.59	1.52
22	V	420	SER	N-CA	5.23	1.52	1.46
23	W	341	LYS	CA-CB	5.22	1.61	1.53
23	W	96	LYS	N-CA	5.22	1.52	1.46
23	W	675	GLY	N-CA	5.21	1.52	1.45
22	V	386	ASP	N-CA	5.21	1.51	1.46
22	V	561	PHE	C-N	5.21	1.40	1.33
23	W	95	GLU	CA-C	5.21	1.58	1.52
23	W	210	HIS	CE1-NE2	5.21	1.37	1.32
23	W	426	PRO	CA-CB	-5.20	1.47	1.53
23	W	66	GLU	N-CA	5.20	1.53	1.46
22	V	521	GLU	CA-CB	5.19	1.61	1.53
24	O	197	SER	N-CA	-5.19	1.39	1.46
23	W	491	CYS	CA-C	5.19	1.58	1.53
23	W	257	ASP	CA-C	5.19	1.59	1.52
1	A	1160	ARG	CD-NE	-5.18	1.39	1.46
23	W	531	VAL	C-O	-5.18	1.17	1.24
22	V	532	LEU	CA-CB	5.18	1.61	1.53
2	B	924	ARG	CZ-NH1	5.18	1.40	1.32
23	W	75	ARG	CZ-NH2	-5.17	1.26	1.33
22	V	598	HIS	CB-CG	5.17	1.57	1.50
23	W	30	ARG	N-CA	5.17	1.52	1.46
24	O	140	HIS	ND1-CE1	5.17	1.37	1.32
23	W	567	LEU	N-CA	-5.16	1.40	1.45
23	W	148	HIS	CE1-NE2	5.16	1.37	1.32
22	V	410	TYR	N-CA	5.16	1.52	1.46
22	V	398	ASP	N-CA	5.15	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	80	ARG	CA-CB	5.15	1.61	1.53
23	W	310	LEU	CA-CB	5.14	1.60	1.53
22	V	303	ASN	C-N	5.14	1.37	1.33
22	V	316	LEU	CA-CB	5.14	1.61	1.53
23	W	626	VAL	N-CA	5.14	1.52	1.46
23	W	398	THR	CB-OG1	-5.14	1.35	1.43
23	W	482	THR	N-CA	5.13	1.52	1.46
1	A	457	ILE	CA-CB	-5.13	1.48	1.54
23	W	658	ARG	CZ-NH2	-5.13	1.26	1.33
23	W	328	HIS	ND1-CE1	5.12	1.37	1.32
24	0	195	ARG	CZ-NH1	-5.12	1.25	1.32
22	V	693	LEU	CA-C	5.12	1.59	1.53
22	V	623	LEU	C-O	-5.11	1.18	1.24
23	W	168	VAL	N-CA	5.11	1.52	1.46
22	V	333	ALA	CA-C	-5.10	1.45	1.52
22	V	617	LEU	N-CA	5.10	1.51	1.45
2	B	481	HIS	C-O	-5.09	1.18	1.24
23	W	303	ALA	CA-C	5.09	1.59	1.52
23	W	452	GLN	CA-CB	5.08	1.61	1.53
23	W	629	GLN	N-CA	-5.07	1.39	1.46
22	V	408	SER	CA-C	-5.07	1.46	1.52
22	V	367	SER	N-CA	-5.06	1.39	1.46
23	W	679	PHE	CA-CB	5.06	1.62	1.53
24	0	105	GLY	C-N	5.06	1.40	1.33
24	0	61	LEU	N-CA	5.06	1.52	1.46
1	A	835	GLU	C-O	-5.06	1.18	1.24
2	B	785	TYR	CA-C	5.05	1.57	1.53
23	W	418	ILE	N-CA	5.05	1.52	1.46
23	W	122	THR	CA-C	5.05	1.58	1.52
23	W	286	ARG	CZ-NH1	-5.05	1.25	1.32
23	W	699	GLU	N-CA	5.05	1.52	1.46
23	W	20	GLU	C-N	-5.04	1.27	1.33
23	W	322	SER	N-CA	5.04	1.52	1.46
22	V	607	ILE	C-O	-5.03	1.19	1.24
23	W	104	PHE	CG-CD1	5.03	1.49	1.38
23	W	61	ARG	CA-C	5.03	1.59	1.52
23	W	417	ILE	N-CA	5.02	1.51	1.46
23	W	672	THR	N-CA	5.02	1.52	1.46
24	0	225	GLU	N-CA	5.02	1.52	1.46
23	W	434	HIS	ND1-CE1	5.01	1.37	1.32
23	W	201	HIS	CG-ND1	5.01	1.43	1.38
23	W	498	GLY	CA-C	-5.00	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	489	TYR	CA-C	5.00	1.58	1.52
22	V	633	ARG	N-CA	5.00	1.52	1.46
23	W	417	ILE	CA-C	-5.00	1.46	1.52

All (1099) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	42	GLY	N-CA-C	19.39	138.18	111.03
9	I	84	HIS	C-N-CD	-14.74	64.58	125.00
18	R	194	ARG	C-N-CD	-14.31	66.32	125.00
9	I	61	GLU	N-CA-C	-14.25	90.87	110.68
28	X	59	DC	P-O3'-C3'	13.86	141.00	120.20
24	0	77	LYS	C-N-CD	-12.76	72.67	125.00
28	X	65	DG	C4'-C3'-O3'	12.38	128.57	110.00
2	B	80	GLU	CA-C-N	-12.29	107.72	120.38
2	B	80	GLU	C-N-CA	-12.29	107.72	120.38
27	3	71	TYR	C-N-CD	-12.15	75.17	125.00
1	A	521	VAL	CB-CA-C	-11.94	102.36	113.70
22	V	520	ARG	O-C-N	11.77	135.65	122.11
23	W	26	ARG	NE-CZ-NH2	11.56	129.60	119.20
22	V	520	ARG	CA-C-N	-11.54	100.84	120.58
22	V	520	ARG	C-N-CA	-11.54	100.84	120.58
2	B	880	LEU	N-CA-C	11.54	126.66	112.58
1	A	370	ASP	CA-C-N	11.18	133.82	119.84
1	A	370	ASP	C-N-CA	11.18	133.82	119.84
22	V	550	PHE	CA-CB-CG	11.07	124.87	113.80
26	2	236	PHE	CA-CB-CG	-11.03	102.77	113.80
22	V	358	ARG	NE-CZ-NH2	11.02	129.12	119.20
23	W	335	ARG	NE-CZ-NH1	-10.96	110.53	121.50
18	R	205	ASP	N-CA-C	10.84	122.17	108.19
18	R	204	ASN	N-CA-C	10.71	122.84	108.38
29	Y	29	DC	O5'-C5'-C4'	10.64	126.76	110.80
22	V	270	PHE	CA-CB-CG	10.63	124.43	113.80
11	K	62	LYS	CA-C-N	-10.60	115.39	122.60
11	K	62	LYS	C-N-CA	-10.60	115.39	122.60
23	W	167	GLU	CA-C-N	10.46	128.70	120.33
23	W	167	GLU	C-N-CA	10.46	128.70	120.33
1	A	271	ARG	N-CA-C	-10.39	92.00	108.63
13	M	51	GLU	N-CA-C	10.34	122.14	111.07
18	R	195	PRO	N-CA-C	-10.33	91.18	112.47
18	R	214	GLU	N-CA-C	-10.23	99.94	111.71
13	M	94	ASP	N-CA-C	-10.05	89.39	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	91	ALA	N-CA-C	-9.92	89.67	110.80
23	W	287	ARG	NE-CZ-NH2	9.86	128.08	119.20
2	B	882	SER	N-CA-C	-9.78	89.97	110.80
23	W	117	ILE	N-CA-C	9.75	119.69	110.53
23	W	26	ARG	NH1-CZ-NH2	-9.75	106.63	119.30
22	V	586	GLN	OE1-CD-NE2	-9.74	112.86	122.60
22	V	638	GLN	OE1-CD-NE2	-9.60	113.00	122.60
25	1	44	PHE	CA-CB-CG	-9.59	104.21	113.80
23	W	645	GLN	OE1-CD-NE2	-9.50	113.10	122.60
22	V	388	GLN	OE1-CD-NE2	-9.49	113.11	122.60
5	E	63	ALA	N-CA-C	9.47	125.37	107.75
22	V	634	ARG	NE-CZ-NH2	9.45	127.71	119.20
20	T	60	GLU	N-CA-C	-9.45	100.33	112.23
22	V	377	GLN	OE1-CD-NE2	-9.42	113.18	122.60
23	W	147	GLN	OE1-CD-NE2	-9.42	113.18	122.60
22	V	621	ASN	CA-CB-CG	9.34	121.94	112.60
28	X	65	DG	P-O3'-C3'	9.29	134.14	120.20
2	B	719	SER	CA-C-N	-9.29	110.18	119.56
2	B	719	SER	C-N-CA	-9.29	110.18	119.56
2	B	699	HIS	CA-C-N	9.27	129.34	119.05
2	B	699	HIS	C-N-CA	9.27	129.34	119.05
5	E	64	HIS	N-CA-C	9.17	130.34	110.80
2	B	62	ALA	CA-C-N	-9.13	110.98	120.38
2	B	62	ALA	C-N-CA	-9.13	110.98	120.38
27	3	231	PHE	CA-CB-CG	-9.10	104.70	113.80
23	W	335	ARG	NE-CZ-NH2	9.07	127.36	119.20
3	C	6	GLN	C-N-CD	-9.01	88.07	125.00
2	B	224	CYS	N-CA-C	8.99	123.55	110.42
22	V	668	GLN	OE1-CD-NE2	-8.98	113.62	122.60
22	V	334	ARG	CD-NE-CZ	8.97	136.96	124.40
26	2	61	PHE	CB-CA-C	-8.95	97.08	110.95
23	W	530	VAL	N-CA-CB	8.93	120.75	110.65
23	W	270	VAL	CA-C-O	8.89	131.89	120.78
2	B	294	ASP	CA-C-N	8.87	129.03	119.28
2	B	294	ASP	C-N-CA	8.87	129.03	119.28
5	E	47	LYS	CA-C-N	-8.80	108.83	119.84
5	E	47	LYS	C-N-CA	-8.80	108.83	119.84
23	W	112	ARG	CA-C-N	8.80	132.07	120.28
23	W	112	ARG	C-N-CA	8.80	132.07	120.28
12	L	27	GLU	CA-C-N	-8.78	111.04	122.37
12	L	27	GLU	C-N-CA	-8.78	111.04	122.37
22	V	665	GLN	OE1-CD-NE2	-8.77	113.83	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	34	ILE	CA-C-N	-8.73	111.77	123.12
25	1	34	ILE	C-N-CA	-8.73	111.77	123.12
18	R	194	ARG	CA-C-N	8.71	130.72	119.84
18	R	194	ARG	C-N-CA	8.71	130.72	119.84
23	W	76	THR	CA-CB-OG1	8.69	122.63	109.60
8	H	74	GLU	N-CA-C	-8.68	92.32	110.80
23	W	332	PHE	CA-CB-CG	8.67	122.47	113.80
26	2	268	PHE	CA-CB-CG	-8.67	105.13	113.80
29	Y	14	DG	O4'-C1'-N9	8.66	121.39	108.40
25	1	47	ALA	CB-CA-C	-8.57	106.68	116.54
22	V	484	ILE	N-CA-C	8.45	119.08	111.81
23	W	469	LYS	CA-C-N	8.45	131.37	120.56
23	W	469	LYS	C-N-CA	8.45	131.37	120.56
23	W	263	LEU	N-CA-CB	-8.41	97.76	110.12
28	X	66	DA	P-O5'-C5'	8.40	132.59	120.00
23	W	193	PHE	CA-CB-CG	8.37	122.17	113.80
23	W	343	ARG	NE-CZ-NH2	8.36	126.72	119.20
14	N	326	GLN	N-CA-C	8.31	124.84	113.37
9	I	84	HIS	CA-C-N	8.28	130.19	119.84
9	I	84	HIS	C-N-CA	8.28	130.19	119.84
23	W	157	PHE	CA-CB-CG	8.27	122.07	113.80
23	W	77	VAL	N-CA-CB	-8.26	105.30	110.50
1	A	524	MET	CA-C-N	-8.24	114.76	123.08
1	A	524	MET	C-N-CA	-8.24	114.76	123.08
1	A	545	VAL	N-CA-C	8.24	119.02	110.62
23	W	521	GLY	CA-C-N	8.16	131.04	120.44
23	W	521	GLY	C-N-CA	8.16	131.04	120.44
22	V	392	PHE	CA-CB-CG	8.14	121.94	113.80
1	A	677	ASN	N-CA-C	8.09	120.10	111.28
26	2	47	GLU	N-CA-C	8.08	120.00	111.03
23	W	106	GLY	CA-C-O	-8.05	114.56	121.57
22	V	433	GLN	N-CA-C	8.04	121.66	112.57
23	W	148	HIS	CE1-NE2-CD2	-8.02	100.98	109.00
1	A	673	GLN	N-CA-C	8.00	120.08	111.36
22	V	333	ALA	N-CA-C	8.00	121.99	111.75
2	B	1044	GLY	CA-C-N	-7.99	112.48	120.31
2	B	1044	GLY	C-N-CA	-7.99	112.48	120.31
23	W	395	SER	CA-C-O	-7.97	110.61	118.34
3	C	137	ASN	N-CA-C	-7.97	93.83	110.80
29	Y	28	DT	O3'-P-O5'	7.97	115.95	104.00
23	W	667	ALA	N-CA-C	7.94	119.57	111.07
2	B	492	ASP	N-CA-C	7.94	122.46	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	700	HIS	CB-CG-CD2	-7.89	120.94	131.20
22	V	394	SER	N-CA-C	7.86	121.97	112.38
23	W	345	ARG	N-CA-C	7.84	122.19	112.47
1	A	1314	THR	N-CA-C	-7.84	104.88	114.75
23	W	16	TYR	N-CA-C	7.83	118.32	108.45
23	W	696	TRP	N-CA-C	7.80	120.82	110.53
1	A	1308	TYR	N-CA-C	7.79	119.99	108.14
26	2	160	LEU	N-CA-C	-7.79	102.78	111.28
9	I	58	ILE	N-CA-C	-7.77	93.18	109.34
2	B	748	ALA	N-CA-C	7.75	121.16	108.99
13	M	87	GLY	CA-C-N	-7.74	108.37	122.38
13	M	87	GLY	C-N-CA	-7.74	108.37	122.38
22	V	415	HIS	CG-CD2-NE2	-7.72	99.48	107.20
23	W	724	MET	CA-C-N	7.71	130.61	120.28
23	W	724	MET	C-N-CA	7.71	130.61	120.28
18	R	203	PHE	N-CA-C	7.69	118.84	108.23
1	A	565	MET	N-CA-C	7.69	119.66	111.28
10	J	46	ARG	N-CA-C	7.69	119.44	111.14
22	V	710	GLN	CA-C-N	7.67	130.41	120.44
22	V	710	GLN	C-N-CA	7.67	130.41	120.44
23	W	499	ASN	OD1-CG-ND2	-7.67	114.93	122.60
26	2	162	PHE	CA-CB-CG	-7.66	106.14	113.80
10	J	45	CYS	N-CA-C	-7.65	102.94	111.82
27	3	182	PHE	CA-CB-CG	-7.64	106.16	113.80
23	W	497	ARG	CD-NE-CZ	7.64	135.09	124.40
22	V	422	GLU	CA-C-O	7.63	128.88	119.11
24	0	237	SER	CA-C-N	7.62	128.23	120.38
24	0	237	SER	C-N-CA	7.62	128.23	120.38
22	V	640	LEU	O-C-N	7.59	130.20	122.08
28	X	78	DT	N1-C1'-C2'	7.59	124.88	113.50
13	M	89	GLY	N-CA-C	-7.58	95.21	113.18
1	A	777	SER	N-CA-C	7.57	118.23	108.24
23	W	304	HIS	CB-CG-CD2	-7.56	121.37	131.20
1	A	1057	GLU	N-CA-C	7.55	119.29	111.14
23	W	295	ALA	N-CA-C	7.54	119.28	111.14
23	W	700	HIS	ND1-CG-CD2	7.53	113.63	106.10
23	W	509	GLU	N-CA-C	7.52	122.12	112.34
23	W	165	GLY	CA-C-N	7.51	130.95	120.29
23	W	165	GLY	C-N-CA	7.51	130.95	120.29
23	W	41	GLU	O-C-N	7.50	131.74	123.27
22	V	355	CYS	CA-C-N	7.48	130.62	120.44
22	V	355	CYS	C-N-CA	7.48	130.62	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1425	GLY	CA-C-N	7.48	127.35	119.05
1	A	1425	GLY	C-N-CA	7.48	127.35	119.05
26	2	35	TYR	CA-CB-CG	-7.47	100.45	113.90
27	3	127	GLN	N-CA-C	-7.47	103.22	111.36
29	Y	30	DG	O5'-C5'-C4'	7.46	121.99	110.80
23	W	250	ASN	OD1-CG-ND2	-7.45	115.16	122.60
24	0	206	ARG	NH1-CZ-NH2	-7.44	109.63	119.30
22	V	669	GLU	CA-C-N	7.43	131.60	120.31
22	V	669	GLU	C-N-CA	7.43	131.60	120.31
2	B	473	LEU	N-CA-C	7.43	119.38	111.28
23	W	329	PHE	CA-CB-CG	7.43	121.23	113.80
13	M	130	LEU	CA-C-N	7.42	127.38	120.03
13	M	130	LEU	C-N-CA	7.42	127.38	120.03
24	0	98	GLN	OE1-CD-NE2	-7.42	115.18	122.60
24	0	123	ASN	CA-C-N	7.41	127.43	119.28
24	0	123	ASN	C-N-CA	7.41	127.43	119.28
26	2	245	LEU	N-CA-C	-7.38	101.33	110.41
23	W	302	ASP	CA-C-O	7.37	126.82	119.08
1	A	611	ASP	N-CA-C	7.37	120.54	108.08
13	M	49	GLY	N-CA-C	7.36	123.41	113.99
27	3	16	ASP	CA-C-N	7.33	132.97	120.72
27	3	16	ASP	C-N-CA	7.33	132.97	120.72
22	V	614	SER	N-CA-C	7.32	126.39	110.80
11	K	3	ALA	CA-C-N	7.32	124.93	119.66
11	K	3	ALA	C-N-CA	7.32	124.93	119.66
23	W	487	ARG	N-CA-C	7.32	120.12	111.71
1	A	1371	ILE	N-CA-C	7.30	118.09	110.72
29	Y	29	DC	C5'-C4'-C3'	7.29	125.84	114.90
24	0	195	ARG	NE-CZ-NH1	7.28	128.78	121.50
24	0	92	VAL	O-C-N	7.26	129.03	121.91
23	W	654	PHE	CA-C-N	7.26	130.00	120.28
23	W	654	PHE	C-N-CA	7.26	130.00	120.28
23	W	683	ARG	NE-CZ-NH2	7.25	125.73	119.20
29	Y	21	DC	C6-N1-C1'	7.25	130.58	119.70
18	R	162	GLY	N-CA-C	7.21	130.26	113.18
22	V	580	ILE	CA-C-O	7.19	127.98	120.36
23	W	690	ARG	NE-CZ-NH2	7.17	125.65	119.20
9	I	84	HIS	N-CA-C	7.17	125.66	109.81
22	V	486	PRO	CA-C-N	7.17	132.67	121.99
22	V	486	PRO	C-N-CA	7.17	132.67	121.99
23	W	288	LEU	O-C-N	-7.15	114.59	122.03
23	W	419	GLU	C-N-CD	-7.15	95.69	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	267	THR	CA-C-O	-7.14	111.90	120.32
23	W	24	TYR	N-CA-C	7.14	121.22	112.23
2	B	785	TYR	CB-CA-C	-7.13	108.36	116.63
23	W	323	ILE	CA-C-N	7.11	129.81	120.28
23	W	323	ILE	C-N-CA	7.11	129.81	120.28
2	B	58	ILE	N-CA-C	7.10	117.90	110.72
2	B	798	ARG	N-CA-C	7.09	119.01	111.28
22	V	598	HIS	CB-CG-CD2	-7.09	121.99	131.20
26	2	193	PRO	N-CA-C	7.08	119.34	110.70
2	B	1055	VAL	N-CA-C	7.07	117.83	110.62
26	2	89	LEU	N-CA-C	-7.07	103.65	111.36
2	B	180	ASP	CA-C-N	7.06	128.67	119.84
2	B	180	ASP	C-N-CA	7.06	128.67	119.84
23	W	653	THR	CA-C-N	7.04	129.72	120.28
23	W	653	THR	C-N-CA	7.04	129.72	120.28
29	Y	21	DC	C2-N1-C1'	-7.04	109.14	119.70
22	V	393	THR	O-C-N	-7.03	113.89	122.68
23	W	232	VAL	CA-CB-CG1	7.03	122.35	110.40
1	A	539	GLN	CB-CA-C	-7.03	108.48	116.63
23	W	715	GLN	OE1-CD-NE2	-7.02	115.58	122.60
28	X	82	DG	C4'-C3'-O3'	-6.99	99.51	110.00
23	W	186	ARG	NE-CZ-NH1	6.99	128.49	121.50
26	2	225	SER	N-CA-C	-6.98	103.60	111.14
1	A	539	GLN	N-CA-C	6.97	119.86	108.08
13	M	86	LYS	N-CA-C	6.97	119.30	110.24
23	W	340	VAL	CA-C-N	6.97	129.61	120.28
23	W	340	VAL	C-N-CA	6.97	129.61	120.28
24	0	147	ASN	OD1-CG-ND2	-6.96	115.64	122.60
22	V	558	ILE	N-CA-CB	-6.93	101.40	111.52
22	V	715	LYS	N-CA-C	6.92	118.82	111.28
20	T	154	LYS	N-CA-C	6.91	125.08	109.81
13	M	15	CYS	CA-C-N	6.91	126.15	118.97
13	M	15	CYS	C-N-CA	6.91	126.15	118.97
23	W	98	GLU	CA-C-N	6.90	130.22	122.15
23	W	98	GLU	C-N-CA	6.90	130.22	122.15
25	1	45	VAL	CA-C-N	-6.89	113.48	122.51
25	1	45	VAL	C-N-CA	-6.89	113.48	122.51
22	V	274	GLN	O-C-N	-6.89	116.64	123.46
28	X	83	DA	O4'-C1'-N9	6.89	118.73	108.40
2	B	132	VAL	N-CA-C	6.88	116.53	106.55
23	W	328	HIS	CB-CG-CD2	-6.86	122.28	131.20
23	W	659	HIS	CA-CB-CG	6.85	120.65	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	193	PRO	CA-N-CD	-6.84	102.43	112.00
1	A	244	ARG	CA-C-N	6.83	127.11	119.32
1	A	244	ARG	C-N-CA	6.83	127.11	119.32
23	W	97	GLN	OE1-CD-NE2	-6.82	115.78	122.60
23	W	462	SER	CA-C-N	6.82	126.51	119.82
23	W	462	SER	C-N-CA	6.82	126.51	119.82
1	A	843	GLY	N-CA-C	6.81	120.91	112.73
23	W	343	ARG	NE-CZ-NH1	-6.80	114.70	121.50
23	W	595	ILE	CB-CA-C	6.80	122.45	111.29
22	V	348	LEU	CA-C-O	-6.80	113.34	120.55
23	W	703	ASP	N-CA-C	6.80	120.92	111.74
23	W	66	GLU	CA-C-N	6.80	134.20	121.97
23	W	66	GLU	C-N-CA	6.80	134.20	121.97
23	W	497	ARG	NE-CZ-NH1	6.79	128.29	121.50
23	W	562	GLN	OE1-CD-NE2	-6.79	115.81	122.60
24	0	145	LEU	N-CA-C	6.79	118.68	111.28
5	E	13	ILE	N-CA-C	6.79	117.57	110.72
23	W	263	LEU	O-C-N	-6.78	114.93	122.12
23	W	270	VAL	CA-C-N	6.78	130.61	120.17
23	W	270	VAL	C-N-CA	6.78	130.61	120.17
22	V	641	GLY	N-CA-C	6.77	120.86	112.73
23	W	34	ALA	CA-C-N	6.77	132.44	122.82
23	W	34	ALA	C-N-CA	6.77	132.44	122.82
23	W	467	TYR	CA-C-N	6.76	126.72	119.28
23	W	467	TYR	C-N-CA	6.76	126.72	119.28
1	A	417	LYS	N-CA-C	6.75	119.63	111.40
2	B	162	LEU	N-CA-C	6.74	120.38	111.75
9	I	85	PRO	N-CA-C	6.74	126.36	112.47
22	V	317	ARG	CA-C-O	-6.73	113.08	120.69
2	B	924	ARG	NE-CZ-NH1	-6.73	114.77	121.50
23	W	131	ASP	CA-C-N	6.73	127.45	119.98
23	W	131	ASP	C-N-CA	6.73	127.45	119.98
22	V	608	SER	O-C-N	-6.71	113.88	122.20
22	V	711	GLN	OE1-CD-NE2	-6.70	115.90	122.60
23	W	723	GLN	OE1-CD-NE2	-6.70	115.90	122.60
22	V	331	GLY	CA-C-N	6.70	129.25	120.28
22	V	331	GLY	C-N-CA	6.70	129.25	120.28
22	V	629	HIS	CB-CG-CD2	-6.69	122.50	131.20
23	W	473	PHE	CA-CB-CG	-6.69	107.11	113.80
23	W	591	GLY	CA-C-O	-6.69	113.77	121.47
24	0	64	VAL	O-C-N	-6.69	116.04	123.26
24	0	92	VAL	CA-C-O	-6.69	114.08	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	0	236	VAL	CA-CB-CG1	6.68	121.77	110.40
21	U	232	GLU	N-CA-C	6.68	121.01	112.86
1	A	1307	VAL	N-CA-C	6.68	123.23	109.34
23	W	629	GLN	CA-C-O	-6.67	113.68	120.96
23	W	613	HIS	CA-C-N	6.66	129.21	120.28
23	W	613	HIS	C-N-CA	6.66	129.21	120.28
23	W	540	THR	O-C-N	-6.64	114.10	122.27
2	B	938	ARG	N-CA-C	6.61	121.06	113.19
22	V	418	LYS	CA-C-O	-6.61	114.09	120.90
13	M	43	ASP	N-CA-C	-6.61	94.61	107.62
22	V	598	HIS	CB-CG-ND1	6.61	132.61	122.70
22	V	701	LEU	O-C-N	-6.61	115.50	123.10
22	V	553	ARG	NE-CZ-NH2	6.60	125.14	119.20
1	A	521	VAL	N-CA-CB	6.60	114.94	110.52
22	V	714	GLN	OE1-CD-NE2	-6.59	116.01	122.60
23	W	152	LEU	O-C-N	-6.59	113.74	121.32
18	R	169	GLU	N-CA-C	6.58	118.46	111.28
23	W	80	ILE	N-CA-CB	6.58	119.49	110.54
25	1	19	PHE	CA-CB-CG	6.57	120.37	113.80
1	A	566	PHE	N-CA-C	6.57	120.55	112.54
26	2	272	PHE	CA-CB-CG	-6.56	107.24	113.80
22	V	358	ARG	NH1-CZ-NH2	-6.55	110.78	119.30
1	A	133	SER	N-CA-C	6.55	124.75	110.80
1	A	844	ARG	N-CA-C	6.55	118.42	111.28
3	C	199	LYS	CA-C-N	6.55	126.24	119.56
3	C	199	LYS	C-N-CA	6.55	126.24	119.56
22	V	624	ILE	N-CA-CB	-6.54	103.14	111.64
23	W	187	GLN	OE1-CD-NE2	-6.54	116.06	122.60
23	W	314	VAL	N-CA-CB	6.54	118.20	110.55
22	V	388	GLN	CG-CD-NE2	6.52	126.18	116.40
24	0	59	ARG	NE-CZ-NH2	6.52	125.07	119.20
2	B	186	ILE	CA-C-N	-6.51	114.61	123.14
2	B	186	ILE	C-N-CA	-6.51	114.61	123.14
1	A	1121	VAL	CB-CA-C	-6.50	107.52	113.70
26	2	242	PHE	CA-CB-CG	-6.50	107.30	113.80
22	V	366	ASN	CA-CB-CG	6.50	119.10	112.60
16	P	292	ILE	N-CA-C	6.49	117.18	107.51
22	V	328	PHE	CA-C-N	6.49	134.13	121.41
22	V	328	PHE	C-N-CA	6.49	134.13	121.41
23	W	120	GLU	CA-C-N	6.48	128.86	120.56
23	W	120	GLU	C-N-CA	6.48	128.86	120.56
22	V	409	THR	CA-C-N	6.48	131.06	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	409	THR	C-N-CA	6.48	131.06	120.63
22	V	434	GLU	N-CA-C	6.47	118.42	111.36
1	A	476	ILE	N-CA-C	6.47	117.39	109.30
23	W	161	PHE	CA-CB-CG	6.47	120.27	113.80
24	O	58	MET	O-C-N	6.46	131.15	123.27
14	N	356	GLY	N-CA-C	6.45	128.47	113.18
1	A	1481	LYS	N-CA-C	6.44	118.30	111.28
23	W	33	ASP	N-CA-C	6.44	119.12	111.71
23	W	166	ARG	CD-NE-CZ	6.44	133.42	124.40
23	W	698	GLN	OE1-CD-NE2	-6.44	116.16	122.60
23	W	138	THR	CA-C-O	-6.44	113.72	120.55
22	V	467	THR	N-CA-C	6.43	118.64	108.79
23	W	491	CYS	CA-C-N	6.43	126.81	119.92
23	W	491	CYS	C-N-CA	6.43	126.81	119.92
22	V	709	GLN	CA-C-N	6.43	128.90	120.28
22	V	709	GLN	C-N-CA	6.43	128.90	120.28
23	W	88	ARG	CA-C-N	6.42	129.41	120.29
23	W	88	ARG	C-N-CA	6.42	129.41	120.29
23	W	406	LEU	CA-C-O	-6.41	114.27	121.00
23	W	299	ARG	NE-CZ-NH1	6.41	127.91	121.50
22	V	281	GLN	O-C-N	6.40	128.75	122.09
22	V	454	VAL	CA-C-N	6.40	129.38	120.29
22	V	454	VAL	C-N-CA	6.40	129.38	120.29
27	3	218	PRO	N-CA-C	-6.40	99.08	111.69
23	W	210	HIS	ND1-CG-CD2	6.40	112.50	106.10
26	2	238	PHE	CA-CB-CG	-6.40	107.40	113.80
29	Y	23	DT	N1-C1'-C2'	6.40	123.10	113.50
23	W	196	ARG	CA-C-N	6.39	128.84	120.28
23	W	196	ARG	C-N-CA	6.39	128.84	120.28
22	V	643	VAL	CA-CB-CG1	6.38	121.25	110.40
22	V	373	GLN	OE1-CD-NE2	-6.37	116.23	122.60
10	J	63	ALA	O-C-N	6.37	126.15	120.48
9	I	104	ALA	CA-C-N	-6.37	109.38	121.54
9	I	104	ALA	C-N-CA	-6.37	109.38	121.54
23	W	416	ILE	CA-C-N	6.36	131.84	123.06
23	W	416	ILE	C-N-CA	6.36	131.84	123.06
23	W	552	TRP	N-CA-C	-6.36	104.27	111.14
2	B	713	PHE	CB-CA-C	-6.35	104.74	110.71
24	O	224	ASP	N-CA-CB	-6.35	101.53	111.56
23	W	662	GLN	OE1-CD-NE2	-6.34	116.26	122.60
7	G	124	ASN	CA-C-N	-6.34	113.85	120.38
7	G	124	ASN	C-N-CA	-6.34	113.85	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	86	LEU	N-CA-C	6.33	119.22	108.90
13	M	72	ASN	CA-C-N	6.33	126.03	119.64
13	M	72	ASN	C-N-CA	6.33	126.03	119.64
20	T	109	ILE	N-CA-C	6.32	117.02	108.17
23	W	113	LYS	CA-C-O	-6.32	113.85	120.55
6	F	64	ARG	N-CA-C	6.32	117.83	111.07
23	W	83	VAL	CA-C-N	6.31	128.51	120.56
23	W	83	VAL	C-N-CA	6.31	128.51	120.56
22	V	396	ALA	CA-C-N	6.31	132.87	121.89
22	V	396	ALA	C-N-CA	6.31	132.87	121.89
23	W	416	ILE	O-C-N	-6.30	115.76	122.95
23	W	511	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	A	611	ASP	CB-CA-C	-6.29	109.33	116.63
23	W	447	VAL	O-C-N	6.29	127.97	121.87
24	O	111	SER	CA-C-N	6.29	132.93	123.05
24	O	111	SER	C-N-CA	6.29	132.93	123.05
22	V	480	LEU	CA-C-N	6.29	128.71	120.28
22	V	480	LEU	C-N-CA	6.29	128.71	120.28
23	W	257	ASP	CA-CB-CG	-6.29	106.31	112.60
28	X	65	DG	O4'-C1'-C2'	-6.28	96.98	106.40
23	W	258	ARG	CA-C-O	-6.28	113.76	120.42
22	V	391	ARG	NE-CZ-NH1	-6.28	115.22	121.50
23	W	70	LEU	CA-C-O	-6.28	113.64	120.36
2	B	982	ILE	N-CA-C	6.28	117.02	110.62
22	V	689	VAL	O-C-N	-6.27	116.60	123.18
22	V	341	PRO	CB-CA-C	-6.27	103.36	111.39
20	T	134	GLU	N-CA-C	6.27	118.11	111.28
23	W	238	ASN	OD1-CG-ND2	-6.27	116.33	122.60
22	V	449	LYS	N-CA-C	6.26	118.11	111.28
9	I	120	GLY	N-CA-C	-6.26	105.26	114.90
1	A	1376	LYS	N-CA-C	6.26	117.90	111.14
24	O	105	GLY	CA-C-O	-6.26	116.12	121.57
17	Q	103	VAL	N-CA-C	6.26	117.19	111.81
23	W	63	TYR	CA-C-N	6.25	126.16	119.28
23	W	63	TYR	C-N-CA	6.25	126.16	119.28
23	W	299	ARG	N-CA-C	-6.25	104.86	113.18
1	A	596	ILE	CA-C-N	6.25	126.46	119.90
1	A	596	ILE	C-N-CA	6.25	126.46	119.90
27	3	181	ILE	CB-CA-C	-6.25	103.98	111.97
23	W	125	ARG	CD-NE-CZ	6.24	133.13	124.40
3	C	71	ILE	CB-CA-C	-6.22	104.90	111.00
23	W	286	ARG	NE-CZ-NH2	6.22	124.80	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	545	GLN	N-CA-C	6.21	118.05	111.28
24	O	206	ARG	NE-CZ-NH1	6.21	127.71	121.50
23	W	242	VAL	CA-C-O	-6.20	114.28	120.85
23	W	662	GLN	CG-CD-NE2	6.20	125.69	116.40
29	Y	15	DT	O4'-C1'-N1	6.19	117.69	108.40
23	W	332	PHE	O-C-N	-6.19	115.56	122.12
22	V	337	VAL	CA-C-N	6.19	131.59	122.99
22	V	337	VAL	C-N-CA	6.19	131.59	122.99
23	W	50	VAL	CA-CB-CG1	6.19	120.92	110.40
23	W	461	LEU	CA-C-N	6.19	128.75	120.58
23	W	461	LEU	C-N-CA	6.19	128.75	120.58
26	2	229	ASP	CA-CB-CG	-6.18	106.42	112.60
1	A	1071	GLU	N-CA-C	6.17	118.09	111.36
23	W	272	ARG	NH1-CZ-NH2	-6.17	111.28	119.30
2	B	63	PRO	CA-C-N	-6.17	113.42	119.90
2	B	63	PRO	C-N-CA	-6.17	113.42	119.90
22	V	251	PHE	CA-C-N	6.17	130.32	121.50
22	V	251	PHE	C-N-CA	6.17	130.32	121.50
22	V	474	ASP	CA-C-N	6.17	133.32	121.54
22	V	474	ASP	C-N-CA	6.17	133.32	121.54
29	Y	19	DC	P-O5'-C5'	6.17	129.25	120.00
5	E	45	GLY	O-C-N	6.16	127.50	122.51
23	W	592	ARG	NH1-CZ-NH2	-6.15	111.30	119.30
23	W	345	ARG	CD-NE-CZ	6.15	133.01	124.40
2	B	507	GLY	N-CA-C	-6.14	107.29	115.40
22	V	341	PRO	N-CA-CB	6.14	108.48	103.32
28	X	81	DG	C4-N9-C1'	-6.14	117.79	127.00
22	V	524	ALA	N-CA-C	6.13	117.96	111.28
23	W	463	PRO	N-CA-CB	6.13	109.34	103.52
1	A	867	SER	N-CA-C	6.13	117.83	111.03
22	V	529	LYS	O-C-N	-6.13	115.22	122.20
2	B	598	VAL	N-CA-C	6.12	116.31	110.74
14	N	310	GLU	N-CA-C	-6.12	104.43	113.61
23	W	301	THR	CA-C-N	6.12	130.44	120.23
23	W	301	THR	C-N-CA	6.12	130.44	120.23
24	O	184	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	744	ILE	N-CA-C	6.11	116.85	110.62
22	V	337	VAL	CA-C-O	-6.11	115.58	121.63
24	O	140	HIS	CB-CG-CD2	-6.11	123.26	131.20
21	U	283	GLU	CA-C-N	6.11	126.12	119.89
21	U	283	GLU	C-N-CA	6.11	126.12	119.89
22	V	330	ASN	CA-C-O	-6.11	113.46	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	944	THR	CA-C-N	6.10	131.18	121.66
2	B	944	THR	C-N-CA	6.10	131.18	121.66
22	V	713	LEU	CA-C-O	-6.10	114.37	120.90
16	P	153	THR	CA-C-N	6.10	127.46	119.84
16	P	153	THR	C-N-CA	6.10	127.46	119.84
22	V	367	SER	CA-C-N	6.09	128.94	120.29
22	V	367	SER	C-N-CA	6.09	128.94	120.29
23	W	312	ASP	N-CA-C	6.09	117.72	111.14
24	O	62	TYR	CA-C-O	6.09	126.88	120.54
22	V	651	VAL	CA-C-O	-6.08	113.17	120.78
29	Y	24	DC	C2-N1-C1'	-6.08	110.58	119.70
23	W	183	LEU	CA-C-N	6.08	126.69	120.00
23	W	183	LEU	C-N-CA	6.08	126.69	120.00
22	V	286	HIS	CE1-NE2-CD2	-6.07	102.93	109.00
24	O	123	ASN	OD1-CG-ND2	-6.07	116.53	122.60
11	K	82	SER	CA-C-N	6.06	125.94	119.28
11	K	82	SER	C-N-CA	6.06	125.94	119.28
22	V	709	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	A	527	THR	CA-C-N	6.05	126.84	120.12
1	A	527	THR	C-N-CA	6.05	126.84	120.12
8	H	60	ILE	N-CA-C	6.05	116.83	108.12
22	V	379	LYS	N-CA-C	6.04	119.48	111.75
23	W	210	HIS	CB-CG-CD2	-6.04	123.35	131.20
2	B	446	TYR	N-CA-C	6.04	117.53	111.07
23	W	314	VAL	N-CA-C	6.04	116.22	110.42
23	W	30	ARG	CD-NE-CZ	6.04	132.85	124.40
23	W	585	GLN	O-C-N	6.03	130.07	122.23
26	2	79	PHE	CA-CB-CG	-6.03	107.77	113.80
2	B	706	VAL	N-CA-C	-6.03	105.94	111.67
22	V	404	SER	CB-CA-C	6.02	122.41	110.42
28	X	65	DG	O4'-C1'-N9	6.01	117.42	108.40
24	O	235	HIS	CB-CG-CD2	-6.01	123.39	131.20
23	W	122	THR	CA-C-N	6.00	127.35	119.84
23	W	122	THR	C-N-CA	6.00	127.35	119.84
22	V	278	GLU	CA-C-O	-6.00	112.69	120.25
3	C	35	ARG	CG-CD-NE	-6.00	98.80	112.00
22	V	603	ASN	CA-CB-CG	6.00	118.60	112.60
22	V	607	ILE	CA-CB-CG1	5.99	120.59	110.40
23	W	164	HIS	CB-CG-CD2	-5.99	123.42	131.20
26	2	171	VAL	CB-CA-C	-5.98	104.31	111.97
23	W	161	PHE	O-C-N	-5.98	115.87	122.09
10	J	59	LEU	N-CA-C	5.98	117.80	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	459	GLN	CA-C-N	5.98	132.96	121.54
22	V	459	GLN	C-N-CA	5.98	132.96	121.54
23	W	590	ASN	N-CA-C	5.98	119.82	110.32
22	V	561	PHE	O-C-N	-5.97	116.52	123.27
26	2	203	PHE	CA-CB-CG	-5.97	107.83	113.80
23	W	621	PHE	CA-CB-CG	-5.97	107.83	113.80
24	0	130	SER	N-CA-C	5.96	117.86	111.36
22	V	410	TYR	CA-C-N	5.95	129.57	120.82
22	V	410	TYR	C-N-CA	5.95	129.57	120.82
22	V	307	ASN	CA-CB-CG	5.95	118.55	112.60
23	W	148	HIS	CG-CD2-NE2	5.95	113.15	107.20
24	0	74	GLN	OE1-CD-NE2	-5.94	116.66	122.60
18	R	163	LEU	N-CA-C	5.93	123.43	110.80
23	W	569	ILE	N-CA-CB	-5.93	105.31	112.07
23	W	470	ILE	CB-CG1-CD1	-5.93	101.34	113.80
22	V	403	CYS	N-CA-CB	-5.92	102.05	110.46
1	A	1307	VAL	CA-C-N	-5.92	111.08	122.09
1	A	1307	VAL	C-N-CA	-5.92	111.08	122.09
29	Y	19	DC	O5'-C5'-C4'	5.92	119.67	110.80
2	B	959	GLU	N-CA-C	-5.91	105.17	112.38
23	W	442	LEU	CA-C-N	5.91	128.68	120.29
23	W	442	LEU	C-N-CA	5.91	128.68	120.29
1	A	609	HIS	O-C-N	5.91	126.16	120.55
23	W	416	ILE	CA-C-O	5.90	127.38	120.71
23	W	592	ARG	NE-CZ-NH1	5.90	127.40	121.50
24	0	158	HIS	CB-CG-CD2	-5.90	123.53	131.20
29	Y	28	DT	C2-N1-C1'	-5.90	110.51	119.35
23	W	20	GLU	CA-C-O	-5.89	114.30	120.55
2	B	144	HIS	N-CA-C	5.89	119.42	109.76
2	B	1058	LYS	N-CA-C	5.89	120.20	112.89
18	R	169	GLU	CB-CA-C	-5.89	101.01	110.79
22	V	369	VAL	CA-CB-CG1	5.89	120.41	110.40
23	W	480	THR	CA-CB-OG1	5.88	118.43	109.60
3	C	49	TRP	CA-CB-CG	5.88	124.78	113.60
23	W	207	TYR	CA-C-O	-5.88	115.12	121.36
22	V	527	THR	CA-C-O	-5.87	115.29	121.99
7	G	96	GLY	N-CA-C	5.87	118.78	110.74
29	Y	27	DC	C6-N1-C1'	5.87	128.51	119.70
29	Y	28	DT	C6-N1-C1'	5.87	128.16	119.35
23	W	152	LEU	CA-C-N	5.87	125.80	119.76
23	W	152	LEU	C-N-CA	5.87	125.80	119.76
23	W	280	ARG	CA-C-O	-5.86	114.21	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	716	VAL	N-CA-CB	5.86	119.37	110.58
24	0	190	LYS	N-CA-C	-5.86	104.97	111.36
24	0	203	ALA	N-CA-C	5.86	119.03	108.48
28	X	81	DG	C8-N9-C1'	5.86	135.79	127.00
22	V	674	THR	CA-C-N	5.86	128.06	120.44
22	V	674	THR	C-N-CA	5.86	128.06	120.44
23	W	606	GLU	O-C-N	-5.86	115.37	122.22
23	W	685	ALA	N-CA-C	5.86	118.42	111.33
23	W	650	ASP	CA-C-O	-5.85	114.67	120.70
23	W	37	HIS	N-CA-C	5.85	117.74	108.79
23	W	92	ASN	OD1-CG-ND2	-5.84	116.75	122.60
26	2	175	LEU	N-CA-CB	5.84	119.22	110.22
23	W	548	THR	CA-C-O	-5.83	114.70	120.82
27	3	153	ASP	N-CA-C	-5.83	104.92	111.28
1	A	368	THR	CA-C-N	-5.83	113.96	120.14
1	A	368	THR	C-N-CA	-5.83	113.96	120.14
23	W	289	VAL	N-CA-C	5.83	116.57	110.62
14	N	325	GLY	N-CA-C	5.83	126.99	113.18
23	W	623	VAL	N-CA-C	-5.82	103.62	108.63
23	W	722	ARG	CD-NE-CZ	5.82	132.55	124.40
22	V	633	ARG	NE-CZ-NH2	-5.82	113.96	119.20
22	V	335	SER	N-CA-C	5.82	117.91	109.07
25	1	34	ILE	N-CA-C	5.82	116.00	110.42
27	3	64	ILE	CB-CA-C	-5.81	104.53	111.97
22	V	281	GLN	N-CA-C	5.81	118.08	111.11
1	A	502	ASN	N-CA-CB	-5.80	101.35	110.69
22	V	461	HIS	CB-CG-CD2	-5.80	123.66	131.20
1	A	123	ASN	CA-C-N	5.80	125.93	119.32
1	A	123	ASN	C-N-CA	5.80	125.93	119.32
7	G	14	HIS	CA-C-N	5.80	125.93	119.32
7	G	14	HIS	C-N-CA	5.80	125.93	119.32
22	V	416	THR	CB-CA-C	-5.80	99.56	109.65
23	W	312	ASP	N-CA-CB	-5.79	101.67	110.07
2	B	1103	LEU	N-CA-C	5.79	117.26	111.07
23	W	683	ARG	CD-NE-CZ	5.79	132.50	124.40
23	W	586	GLU	N-CA-C	5.78	117.26	111.07
22	V	276	MET	CA-C-O	-5.78	114.79	121.26
23	W	206	VAL	CA-CB-CG1	5.78	120.23	110.40
2	B	945	CYS	CA-CB-SG	5.78	127.69	114.40
2	B	956	PHE	N-CA-C	5.78	117.75	109.14
3	C	159	LEU	N-CA-C	5.78	117.80	107.80
1	A	728	THR	CA-C-N	5.78	126.11	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	728	THR	C-N-CA	5.78	126.11	119.93
13	M	34	CYS	CA-C-N	5.78	127.06	119.84
13	M	34	CYS	C-N-CA	5.78	127.06	119.84
22	V	594	GLN	O-C-N	-5.77	115.86	122.09
2	B	785	TYR	N-CA-C	5.77	117.83	108.08
22	V	332	ARG	NE-CZ-NH1	5.77	127.27	121.50
24	O	92	VAL	CB-CA-C	-5.77	104.58	111.97
2	B	941	GLN	CA-CB-CG	-5.77	102.56	114.10
23	W	213	LEU	N-CA-C	5.76	118.34	111.71
24	O	56	GLY	CA-C-N	5.76	131.67	122.10
24	O	56	GLY	C-N-CA	5.76	131.67	122.10
23	W	702	THR	N-CA-C	5.76	119.93	113.01
22	V	435	TRP	CE2-CD2-CE3	-5.76	113.04	118.80
22	V	679	PHE	CA-CB-CG	5.76	119.56	113.80
23	W	218	ALA	N-CA-C	5.76	117.56	111.28
5	E	92	GLN	N-CA-C	-5.76	105.00	111.28
23	W	154	HIS	CB-CG-ND1	5.76	131.34	122.70
2	B	1093	CYS	N-CA-C	5.75	117.55	111.28
23	W	112	ARG	NE-CZ-NH1	5.75	127.25	121.50
8	H	74	GLU	CA-C-N	5.75	132.51	121.54
8	H	74	GLU	C-N-CA	5.75	132.51	121.54
23	W	672	THR	N-CA-C	5.75	119.92	113.02
22	V	656	ASN	CA-CB-CG	5.74	118.34	112.60
23	W	447	VAL	CA-C-O	-5.74	114.98	120.95
22	V	338	ILE	CA-C-O	-5.74	114.28	120.36
25	1	48	GLU	N-CA-C	-5.74	98.58	110.80
22	V	485	GLY	CA-C-N	5.73	126.06	119.92
22	V	485	GLY	C-N-CA	5.73	126.06	119.92
24	O	160	PRO	CA-C-N	5.73	132.64	121.41
24	O	160	PRO	C-N-CA	5.73	132.64	121.41
14	N	21	VAL	N-CA-C	5.73	115.92	110.42
22	V	636	GLU	N-CA-C	-5.73	105.04	111.28
23	W	92	ASN	CB-CG-ND2	5.73	124.99	116.40
26	2	444	THR	CA-CB-OG1	5.73	118.19	109.60
22	V	479	ASP	N-CA-C	5.72	118.46	111.82
22	V	532	LEU	N-CA-C	5.72	118.46	111.82
29	Y	27	DC	C2-N1-C1'	-5.72	111.11	119.70
23	W	593	GLY	CA-C-N	5.72	132.83	122.02
23	W	593	GLY	C-N-CA	5.72	132.83	122.02
23	W	272	ARG	NE-CZ-NH1	5.72	127.22	121.50
26	2	403	PHE	CA-C-N	5.72	132.73	122.09
26	2	403	PHE	C-N-CA	5.72	132.73	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	216	SER	N-CA-C	5.72	117.20	110.97
28	X	66	DA	O4'-C1'-N9	5.72	116.98	108.40
1	A	388	MET	N-CA-C	5.72	118.56	109.24
23	W	239	ILE	N-CA-C	5.71	116.44	110.62
22	V	354	ALA	N-CA-C	5.71	117.50	111.28
22	V	488	LEU	N-CA-C	5.71	117.58	111.36
22	V	393	THR	N-CA-C	5.71	115.55	108.19
22	V	497	GLN	OE1-CD-NE2	-5.70	116.90	122.60
22	V	520	ARG	NE-CZ-NH2	5.70	124.33	119.20
23	W	434	HIS	CB-CG-CD2	-5.70	123.79	131.20
23	W	175	TYR	O-C-N	5.70	129.73	123.01
22	V	579	TYR	N-CA-C	5.70	118.50	109.50
24	O	178	ASP	O-C-N	-5.70	116.23	121.30
22	V	412	MET	O-C-N	-5.69	115.16	122.21
1	A	645	LEU	N-CA-C	5.68	120.22	113.28
22	V	506	GLN	OE1-CD-NE2	-5.68	116.92	122.60
22	V	702	ALA	N-CA-CB	-5.68	102.52	110.25
22	V	307	ASN	N-CA-CB	-5.68	102.17	111.66
23	W	270	VAL	O-C-N	-5.68	115.47	122.57
23	W	415	THR	CA-C-O	5.68	127.53	120.54
23	W	109	LEU	CA-C-N	5.68	133.44	121.91
23	W	109	LEU	C-N-CA	5.68	133.44	121.91
22	V	551	HIS	CA-CB-CG	-5.68	108.12	113.80
1	A	1396	ARG	CA-C-N	5.68	128.16	120.44
1	A	1396	ARG	C-N-CA	5.68	128.16	120.44
23	W	44	SER	CA-C-O	5.68	126.36	119.49
22	V	665	GLN	CG-CD-NE2	5.67	124.91	116.40
22	V	526	LYS	CA-C-N	5.66	131.71	121.06
22	V	526	LYS	C-N-CA	5.66	131.71	121.06
22	V	567	ALA	CA-C-N	5.66	128.19	120.54
22	V	567	ALA	C-N-CA	5.66	128.19	120.54
23	W	215	PRO	CA-C-N	5.66	127.86	120.28
23	W	215	PRO	C-N-CA	5.66	127.86	120.28
23	W	339	TYR	CA-C-N	5.66	128.45	120.42
23	W	339	TYR	C-N-CA	5.66	128.45	120.42
23	W	177	LEU	N-CA-C	5.65	117.12	111.07
22	V	527	THR	N-CA-C	5.65	117.36	110.41
23	W	16	TYR	CA-C-N	5.65	129.92	122.51
23	W	16	TYR	C-N-CA	5.65	129.92	122.51
23	W	669	ARG	NE-CZ-NH1	5.65	127.15	121.50
2	B	972	ILE	CA-C-N	5.65	125.11	119.24
2	B	972	ILE	C-N-CA	5.65	125.11	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	104	PHE	CA-CB-CG	5.64	119.44	113.80
23	W	216	LYS	CA-C-O	-5.64	114.57	120.55
29	Y	15	DT	O3'-P-O5'	5.64	112.46	104.00
22	V	295	TYR	N-CA-C	5.64	117.97	110.53
22	V	477	ILE	CA-CB-CG1	5.64	119.98	110.40
23	W	421	PHE	CA-C-N	-5.63	114.14	122.35
23	W	421	PHE	C-N-CA	-5.63	114.14	122.35
23	W	193	PHE	N-CA-C	5.62	117.41	111.28
27	3	120	THR	CA-C-N	5.62	127.82	120.28
27	3	120	THR	C-N-CA	5.62	127.82	120.28
23	W	414	PHE	CA-CB-CG	5.62	119.42	113.80
23	W	306	ALA	CA-C-O	-5.62	114.60	120.55
23	W	651	PHE	CA-CB-CG	5.62	119.42	113.80
22	V	703	PHE	N-CA-CB	-5.61	103.48	111.84
23	W	697	ILE	N-CA-C	5.61	121.02	109.34
24	0	113	ARG	N-CA-C	5.61	117.94	109.41
23	W	103	PRO	CB-CA-C	5.61	120.82	111.56
23	W	154	HIS	CA-CB-CG	-5.61	108.19	113.80
22	V	429	TRP	CA-C-N	5.61	133.29	122.53
22	V	429	TRP	C-N-CA	5.61	133.29	122.53
29	Y	24	DC	O4'-C1'-N1	5.61	116.81	108.40
22	V	375	LYS	CA-C-N	5.60	127.79	120.28
22	V	375	LYS	C-N-CA	5.60	127.79	120.28
22	V	444	HIS	CA-C-N	5.60	128.56	120.38
22	V	444	HIS	C-N-CA	5.60	128.56	120.38
1	A	206	ASN	N-CA-C	5.60	122.72	110.80
26	2	262	LEU	CB-CA-C	-5.59	102.10	110.88
23	W	305	LEU	CA-C-N	5.59	127.77	120.28
23	W	305	LEU	C-N-CA	5.59	127.77	120.28
16	P	186	ARG	N-CA-C	5.58	117.17	111.14
29	Y	20	DA	N9-C1'-C2'	5.58	121.87	113.50
1	A	848	ILE	CB-CA-C	-5.58	104.53	112.22
26	2	61	PHE	N-CA-CB	5.58	118.06	109.98
2	B	1054	MET	CB-CG-SD	5.57	129.42	112.70
22	V	439	ILE	CB-CG1-CD1	5.57	125.50	113.80
23	W	207	TYR	CA-CB-CG	5.57	123.93	113.90
23	W	220	LEU	O-C-N	-5.57	115.80	122.15
1	A	1371	ILE	CB-CA-C	-5.57	104.54	112.22
22	V	405	VAL	CB-CA-C	5.57	120.42	111.29
23	W	265	THR	CA-C-N	5.57	129.51	120.60
23	W	265	THR	C-N-CA	5.57	129.51	120.60
23	W	590	ASN	CA-C-N	5.56	129.06	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	590	ASN	C-N-CA	5.56	129.06	121.83
24	O	99	ASN	N-CA-C	5.56	119.91	110.02
23	W	703	ASP	CA-C-N	5.56	132.15	121.54
23	W	703	ASP	C-N-CA	5.56	132.15	121.54
24	O	98	GLN	CA-C-O	5.55	126.31	120.42
22	V	355	CYS	O-C-N	-5.55	116.24	122.12
22	V	677	GLN	N-CA-C	5.55	117.00	111.07
2	B	925	SER	CA-C-N	-5.54	115.73	123.10
2	B	925	SER	C-N-CA	-5.54	115.73	123.10
2	B	51	ILE	N-CA-C	5.54	116.31	110.72
24	O	194	ILE	CA-C-O	5.54	127.16	120.74
2	B	497	LYS	CA-C-N	-5.53	111.36	120.88
2	B	497	LYS	C-N-CA	-5.53	111.36	120.88
22	V	567	ALA	O-C-N	5.53	128.46	122.15
3	C	66	HIS	N-CA-C	5.53	116.99	111.07
23	W	197	TYR	CA-C-O	5.53	126.41	120.55
23	W	685	ALA	CA-C-O	5.53	126.60	120.63
26	2	182	ALA	N-CA-C	-5.53	102.83	110.35
23	W	68	THR	CA-C-O	-5.52	115.79	121.87
23	W	170	LEU	O-C-N	-5.52	116.02	120.38
23	W	468	PRO	CA-N-CD	-5.52	104.27	112.00
24	O	123	ASN	O-C-N	-5.51	114.83	121.12
1	A	622	SER	C-N-CD	-5.51	102.41	125.00
24	O	79	ASN	CA-C-N	-5.51	112.90	120.28
24	O	79	ASN	C-N-CA	-5.51	112.90	120.28
22	V	572	ALA	N-CA-C	5.50	117.28	111.28
24	O	227	HIS	CA-CB-CG	5.50	119.30	113.80
22	V	457	ILE	N-CA-CB	-5.50	102.16	111.23
22	V	675	LYS	N-CA-C	5.50	116.95	111.07
24	O	75	ASP	N-CA-C	5.49	117.27	111.28
2	B	923	VAL	O-C-N	-5.49	117.42	123.18
23	W	53	LEU	CA-C-O	-5.49	114.74	120.55
22	V	268	VAL	CA-C-N	5.48	129.03	120.75
22	V	268	VAL	C-N-CA	5.48	129.03	120.75
23	W	606	GLU	CA-C-O	5.48	126.30	120.10
1	A	466	LYS	N-CA-C	5.48	118.77	111.75
23	W	251	LEU	CB-CA-C	5.48	119.40	109.37
23	W	726	GLN	OE1-CD-NE2	-5.48	117.12	122.60
2	B	637	LYS	N-CA-C	5.48	118.01	111.71
3	C	68	LEU	N-CA-C	5.47	117.33	111.36
23	W	439	ASP	CA-C-O	5.47	127.17	120.60
13	M	87	GLY	N-CA-C	5.47	126.14	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	601	ARG	NE-CZ-NH2	-5.47	114.28	119.20
26	2	45	PHE	CA-CB-CG	-5.46	108.33	113.80
26	2	267	GLU	CA-C-N	-5.46	115.74	122.84
26	2	267	GLU	C-N-CA	-5.46	115.74	122.84
16	P	293	TYR	N-CA-C	5.46	117.63	108.73
28	X	79	DA	C2'-C3'-O3'	5.46	119.69	111.50
23	W	57	MET	CA-C-N	5.46	129.33	120.60
23	W	57	MET	C-N-CA	5.46	129.33	120.60
1	A	1385	VAL	N-CA-C	5.45	116.18	110.62
22	V	514	MET	CB-CA-C	5.45	118.86	110.14
22	V	542	ARG	NE-CZ-NH2	5.45	124.10	119.20
23	W	489	CYS	CA-C-N	5.45	130.45	122.39
23	W	489	CYS	C-N-CA	5.45	130.45	122.39
24	0	236	VAL	CB-CA-C	-5.45	104.78	112.14
20	T	170	LYS	CA-C-N	5.44	131.94	121.54
20	T	170	LYS	C-N-CA	5.44	131.94	121.54
22	V	360	ARG	CD-NE-CZ	5.44	132.02	124.40
22	V	637	ALA	N-CA-C	5.44	118.13	111.82
23	W	334	ARG	N-CA-CB	-5.44	102.12	110.01
23	W	454	VAL	CA-C-N	5.44	131.03	122.33
23	W	454	VAL	C-N-CA	5.44	131.03	122.33
24	0	226	SER	N-CA-CB	-5.43	102.13	110.12
23	W	76	THR	N-CA-C	5.43	117.33	109.07
25	1	51	ASN	CA-CB-CG	-5.43	107.17	112.60
29	Y	34	DC	O5'-C5'-C4'	5.43	118.94	110.80
24	0	186	ILE	N-CA-C	5.43	116.16	110.62
2	B	1155	CYS	N-CA-C	5.42	117.27	111.36
23	W	463	PRO	CA-C-N	5.42	131.90	121.54
23	W	463	PRO	C-N-CA	5.42	131.90	121.54
22	V	662	LEU	N-CA-CB	-5.42	101.59	110.43
1	A	502	ASN	N-CA-C	5.41	118.30	109.59
23	W	148	HIS	ND1-CE1-NE2	5.40	113.80	108.40
1	A	138	LYS	N-CA-C	5.40	116.84	111.07
2	B	924	ARG	NH1-CZ-NH2	5.40	126.31	119.30
26	2	35	TYR	CB-CA-C	5.39	121.03	110.67
23	W	455	ILE	N-CA-C	5.39	115.66	108.27
14	N	319	ASP	N-CA-C	5.39	119.69	113.38
23	W	156	ARG	CD-NE-CZ	5.38	131.94	124.40
26	2	98	THR	CA-C-N	5.38	128.03	120.28
26	2	98	THR	C-N-CA	5.38	128.03	120.28
23	W	560	ASN	CA-CB-CG	-5.38	107.22	112.60
23	W	487	ARG	NH1-CZ-NH2	-5.38	112.31	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	75	ARG	NE-CZ-NH1	5.37	126.87	121.50
23	W	197	TYR	O-C-N	-5.37	116.42	122.12
23	W	645	GLN	CA-C-N	5.37	131.64	121.97
23	W	645	GLN	C-N-CA	5.37	131.64	121.97
28	X	81	DG	C2'-C3'-O3'	5.37	119.56	111.50
2	B	63	PRO	N-CA-C	5.37	117.25	110.70
22	V	677	GLN	OE1-CD-NE2	-5.37	117.23	122.60
20	T	152	ASN	N-CA-C	5.36	119.10	112.24
22	V	253	GLU	CA-C-N	5.36	131.78	121.54
22	V	253	GLU	C-N-CA	5.36	131.78	121.54
23	W	313	GLU	N-CA-C	5.36	116.81	111.07
23	W	141	TYR	N-CA-C	5.36	117.12	111.28
24	0	134	ALA	CA-C-O	5.36	126.10	120.42
25	1	33	PHE	CA-CB-CG	-5.36	108.44	113.80
22	V	339	VAL	CA-C-O	5.36	126.02	120.39
24	0	178	ASP	CA-C-N	5.36	124.87	119.19
24	0	178	ASP	C-N-CA	5.36	124.87	119.19
1	A	458	PHE	N-CA-CB	-5.35	102.07	110.69
20	T	205	ILE	N-CA-C	5.35	117.78	111.09
22	V	317	ARG	O-C-N	5.35	127.42	121.43
22	V	576	ASN	N-CA-CB	-5.35	103.87	111.84
22	V	564	ASN	CA-C-N	5.34	127.78	120.46
22	V	564	ASN	C-N-CA	5.34	127.78	120.46
24	0	142	GLU	O-C-N	5.34	125.72	121.55
18	R	223	VAL	CA-CB-CG2	5.34	119.48	110.40
2	B	115	LEU	N-CA-C	5.34	117.18	111.36
23	W	282	ARG	CA-C-N	5.34	127.43	120.28
23	W	282	ARG	C-N-CA	5.34	127.43	120.28
23	W	686	ARG	CA-C-N	5.34	127.00	120.22
23	W	686	ARG	C-N-CA	5.34	127.00	120.22
22	V	381	TRP	CZ3-CH2-CZ2	-5.34	114.56	121.50
22	V	555	ASN	N-CA-C	5.33	118.79	111.54
23	W	455	ILE	CA-C-O	-5.33	114.93	120.64
1	A	503	LEU	CA-CB-CG	5.33	134.96	116.30
2	B	1168	ALA	CA-C-N	5.33	125.09	119.76
2	B	1168	ALA	C-N-CA	5.33	125.09	119.76
22	V	703	PHE	N-CA-C	5.33	118.79	111.54
22	V	286	HIS	CG-CD2-NE2	5.33	112.53	107.20
24	0	170	ILE	CA-CB-CG1	5.32	119.45	110.40
23	W	37	HIS	CA-C-N	5.32	127.84	120.92
23	W	37	HIS	C-N-CA	5.32	127.84	120.92
28	X	79	DA	C1'-O4'-C4'	-5.32	101.72	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	576	ASN	CA-C-O	5.32	127.71	121.54
2	B	80	GLU	N-CA-C	5.31	121.55	109.81
28	X	66	DA	N9-C1'-C2'	5.31	121.47	113.50
2	B	296	GLU	N-CA-C	5.31	116.75	111.07
2	B	723	THR	CB-CA-C	-5.31	101.83	110.85
23	W	202	ALA	N-CA-C	5.31	118.20	109.76
22	V	552	GLU	N-CA-C	5.30	117.81	111.71
23	W	118	HIS	CB-CG-CD2	-5.30	124.30	131.20
23	W	169	PRO	N-CA-CB	5.30	109.11	103.39
29	Y	22	DG	C2'-C3'-O3'	5.30	119.45	111.50
22	V	433	GLN	OE1-CD-NE2	-5.30	117.30	122.60
22	V	361	CYS	N-CA-CB	-5.29	101.62	110.83
23	W	562	GLN	CB-CG-CD	5.29	121.60	112.60
24	O	131	LEU	O-C-N	-5.29	115.76	122.27
23	W	102	LEU	CA-C-N	5.29	126.45	119.84
23	W	102	LEU	C-N-CA	5.29	126.45	119.84
22	V	332	ARG	NH1-CZ-NH2	-5.29	112.43	119.30
23	W	450	ARG	N-CA-C	5.29	122.06	110.80
23	W	600	ALA	CA-C-N	5.28	127.89	120.28
23	W	600	ALA	C-N-CA	5.28	127.89	120.28
23	W	669	ARG	NH1-CZ-NH2	-5.28	112.43	119.30
29	Y	24	DC	C6-N1-C1'	5.28	127.62	119.70
2	B	508	MET	N-CA-C	5.28	119.70	112.68
22	V	699	GLU	N-CA-C	5.28	116.83	108.96
23	W	621	PHE	O-C-N	5.28	129.35	122.38
22	V	469	THR	CA-C-N	5.28	131.62	121.54
22	V	469	THR	C-N-CA	5.28	131.62	121.54
22	V	575	LEU	CA-C-N	5.28	129.62	122.07
22	V	575	LEU	C-N-CA	5.28	129.62	122.07
22	V	332	ARG	CA-CB-CG	5.28	124.65	114.10
23	W	494	ILE	O-C-N	-5.28	117.19	123.05
2	B	1001	PRO	CA-C-N	-5.27	115.36	122.95
2	B	1001	PRO	C-N-CA	-5.27	115.36	122.95
22	V	435	TRP	CA-C-O	-5.27	114.87	121.46
26	2	60	LEU	CB-CA-C	-5.27	102.60	110.88
2	B	156	LEU	N-CA-C	5.27	118.08	110.28
22	V	366	ASN	N-CA-C	5.27	119.42	112.89
23	W	253	ARG	N-CA-C	5.27	117.02	111.28
29	Y	21	DC	C1'-O4'-C4'	-5.27	101.80	109.70
24	O	73	ASP	CA-CB-CG	5.27	117.87	112.60
23	W	435	PHE	CA-C-N	5.26	128.32	120.95
23	W	435	PHE	C-N-CA	5.26	128.32	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	135	SER	N-CA-C	5.26	117.10	111.36
23	W	149	ASP	O-C-N	-5.26	116.54	122.12
24	0	90	TYR	CA-C-N	5.26	127.33	120.28
24	0	90	TYR	C-N-CA	5.26	127.33	120.28
22	V	282	LYS	CG-CD-CE	5.26	123.40	111.30
2	B	529	MET	CB-CG-SD	5.26	128.47	112.70
22	V	634	ARG	NE-CZ-NH1	-5.26	116.24	121.50
23	W	24	TYR	CA-C-N	5.25	127.27	120.44
23	W	24	TYR	C-N-CA	5.25	127.27	120.44
22	V	399	LYS	CA-C-N	5.25	124.86	119.56
22	V	399	LYS	C-N-CA	5.25	124.86	119.56
23	W	454	VAL	N-CA-CB	-5.25	105.83	112.60
1	A	432	HIS	CA-C-N	5.25	125.56	119.47
1	A	432	HIS	C-N-CA	5.25	125.56	119.47
3	C	212	ASP	N-CA-C	-5.25	106.56	113.17
24	0	59	ARG	NH1-CZ-NH2	-5.25	112.48	119.30
22	V	297	PHE	N-CA-C	5.25	117.05	109.07
23	W	457	THR	N-CA-CB	-5.25	103.43	111.56
22	V	315	VAL	CA-C-O	-5.25	114.88	120.39
22	V	341	PRO	N-CA-C	5.24	119.44	111.11
23	W	534	GLY	O-C-N	-5.24	118.90	122.62
28	X	79	DA	P-O3'-C3'	5.24	128.06	120.20
29	Y	27	DC	O5'-C5'-C4'	5.24	118.66	110.80
24	0	237	SER	N-CA-C	5.24	116.01	109.57
22	V	562	ALA	CA-C-N	5.23	131.53	121.54
22	V	562	ALA	C-N-CA	5.23	131.53	121.54
23	W	284	GLU	N-CA-CB	5.23	117.59	110.01
23	W	87	LEU	CB-CA-C	5.23	119.74	110.85
23	W	205	VAL	CA-C-N	5.23	130.33	123.11
23	W	205	VAL	C-N-CA	5.23	130.33	123.11
2	B	753	TYR	CA-C-N	-5.23	115.19	120.31
2	B	753	TYR	C-N-CA	-5.23	115.19	120.31
23	W	516	VAL	N-CA-C	5.23	115.95	110.62
24	0	135	VAL	N-CA-C	5.23	115.95	110.62
27	3	50	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	807	LEU	CA-C-N	-5.23	114.32	120.12
1	A	807	LEU	C-N-CA	-5.23	114.32	120.12
23	W	46	THR	CA-CB-OG1	5.22	117.44	109.60
23	W	711	ASP	CA-CB-CG	-5.22	107.38	112.60
2	B	256	ILE	N-CA-C	5.22	115.98	108.93
28	X	66	DA	P-O3'-C3'	5.22	128.03	120.20
24	0	99	ASN	OD1-CG-ND2	-5.22	117.38	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	LEU	N-CA-C	5.21	117.74	109.50
1	A	1035	GLU	N-CA-C	5.21	116.65	111.07
23	W	319	VAL	CA-C-N	5.21	126.35	119.84
23	W	319	VAL	C-N-CA	5.21	126.35	119.84
13	M	126	ASP	N-CA-C	5.21	117.86	111.82
22	V	272	VAL	O-C-N	5.21	126.92	121.87
25	1	3	ASN	CA-C-N	-5.21	115.21	122.71
25	1	3	ASN	C-N-CA	-5.21	115.21	122.71
22	V	341	PRO	CA-C-N	5.20	129.88	122.08
22	V	341	PRO	C-N-CA	5.20	129.88	122.08
23	W	50	VAL	O-C-N	5.20	127.19	121.83
24	0	179	PRO	CA-C-O	-5.20	111.69	119.34
22	V	285	ILE	CA-CB-CG2	5.20	119.34	110.50
1	A	1311	LEU	N-CA-C	5.20	118.57	109.48
13	M	42	GLY	CA-C-O	5.20	125.86	120.98
23	W	199	ILE	O-C-N	-5.20	116.83	121.87
23	W	399	LEU	CA-C-O	-5.19	115.35	120.70
26	2	402	ARG	N-CA-C	5.19	117.56	110.24
1	A	593	SER	N-CA-C	5.19	118.72	112.38
22	V	525	ILE	CA-C-O	-5.19	114.58	120.65
7	G	159	ALA	N-CA-C	5.19	117.57	109.52
22	V	252	TYR	O-C-N	-5.19	116.97	123.04
22	V	678	ARG	CA-C-O	-5.19	115.05	120.55
23	W	128	LYS	CA-C-N	5.19	128.08	120.71
23	W	128	LYS	C-N-CA	5.19	128.08	120.71
2	B	1050	ARG	N-CA-C	-5.19	101.25	109.76
1	A	609	HIS	CA-C-N	5.18	126.32	119.84
1	A	609	HIS	C-N-CA	5.18	126.32	119.84
3	C	71	ILE	N-CA-C	5.18	113.84	109.02
22	V	283	ARG	NE-CZ-NH2	-5.18	114.54	119.20
22	V	708	GLU	O-C-N	5.18	127.61	122.12
26	2	261	PHE	CB-CA-C	-5.18	102.75	110.88
22	V	344	ALA	N-CA-CB	-5.18	101.30	111.60
1	A	1405	MET	N-CA-C	5.18	116.92	111.28
22	V	545	GLN	CA-C-N	5.18	127.22	120.28
22	V	545	GLN	C-N-CA	5.18	127.22	120.28
22	V	564	ASN	CB-CA-C	5.18	118.60	109.80
23	W	64	PRO	CA-N-CD	-5.17	104.76	112.00
23	W	152	LEU	N-CA-C	5.17	121.23	109.81
23	W	96	LYS	N-CA-C	5.17	121.81	110.80
23	W	707	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	473	ARG	CG-CD-NE	-5.17	100.64	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	VAL	N-CA-C	5.16	115.93	110.72
22	V	251	PHE	N-CA-C	5.16	116.91	109.07
23	W	153	PRO	CB-CA-C	5.16	118.12	111.46
22	V	305	ASP	CA-C-N	5.16	131.25	121.97
22	V	305	ASP	C-N-CA	5.16	131.25	121.97
22	V	357	VAL	N-CA-CB	5.16	117.55	110.54
27	3	169	ASP	CA-CB-CG	-5.15	107.45	112.60
22	V	680	LEU	N-CA-C	5.15	116.90	111.28
29	Y	14	DG	C4-N9-C1'	-5.15	119.27	127.00
5	E	70	ASP	CB-CA-C	-5.15	110.23	117.23
2	B	728	MET	N-CA-C	5.14	117.78	111.82
22	V	397	LYS	CA-CB-CG	5.14	124.39	114.10
23	W	641	ARG	CD-NE-CZ	5.14	131.60	124.40
24	0	212	ALA	CA-C-N	5.14	127.43	120.44
24	0	212	ALA	C-N-CA	5.14	127.43	120.44
23	W	98	GLU	O-C-N	-5.14	115.75	122.59
14	N	362	GLY	CA-C-N	-5.14	113.89	122.21
14	N	362	GLY	C-N-CA	-5.14	113.89	122.21
23	W	693	LEU	CB-CA-C	5.14	116.94	109.08
5	E	62	VAL	O-C-N	5.13	128.61	123.07
23	W	511	ARG	CA-C-N	5.13	131.36	122.32
23	W	511	ARG	C-N-CA	5.13	131.36	122.32
23	W	564	ASN	OD1-CG-ND2	-5.13	117.47	122.60
23	W	154	HIS	CG-CD2-NE2	5.13	112.33	107.20
1	A	545	VAL	CB-CA-C	-5.13	105.22	112.14
22	V	366	ASN	OD1-CG-ND2	5.13	127.73	122.60
23	W	69	LYS	CG-CD-CE	5.13	123.09	111.30
3	C	240	ARG	CA-C-N	5.12	124.57	119.24
3	C	240	ARG	C-N-CA	5.12	124.57	119.24
23	W	71	ILE	N-CA-C	5.12	115.86	108.48
24	0	65	VAL	CA-CB-CG1	5.12	119.11	110.40
22	V	628	SER	CA-C-N	5.12	131.32	121.54
22	V	628	SER	C-N-CA	5.12	131.32	121.54
23	W	538	PHE	O-C-N	5.12	129.10	123.16
22	V	574	ARG	O-C-N	-5.12	116.31	122.15
23	W	143	ARG	CA-CB-CG	-5.12	103.86	114.10
2	B	896	LEU	N-CA-C	5.12	117.59	109.96
26	2	128	ALA	CA-C-N	-5.12	115.54	123.17
26	2	128	ALA	C-N-CA	-5.12	115.54	123.17
23	W	672	THR	CA-C-N	5.12	130.76	122.53
23	W	672	THR	C-N-CA	5.12	130.76	122.53
1	A	541	THR	CA-C-N	-5.11	113.43	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	THR	C-N-CA	-5.11	113.43	120.28
20	T	136	SER	N-CA-C	5.11	119.61	113.17
10	J	48	MET	N-CA-C	-5.11	105.40	110.97
16	P	325	PHE	N-CA-C	5.11	116.93	111.36
23	W	660	ALA	CA-C-N	5.11	127.64	120.28
23	W	660	ALA	C-N-CA	5.11	127.64	120.28
1	A	773	GLY	N-CA-C	-5.11	107.77	115.32
24	O	80	ARG	CD-NE-CZ	5.11	131.55	124.40
2	B	982	ILE	CB-CA-C	-5.10	105.25	112.14
22	V	452	ARG	CA-CB-CG	5.10	124.30	114.10
23	W	519	ASN	CA-CB-CG	5.10	117.70	112.60
27	3	9	ASN	CA-CB-CG	-5.10	107.50	112.60
29	Y	21	DC	C4'-C3'-O3'	-5.10	102.35	110.00
22	V	577	LYS	CA-C-O	-5.10	115.45	120.19
23	W	175	TYR	CA-C-O	-5.10	115.24	121.05
2	B	747	LEU	CA-CB-CG	-5.09	98.47	116.30
22	V	639	ARG	NE-CZ-NH2	5.09	123.78	119.20
23	W	158	TYR	CA-C-N	5.09	127.61	120.28
23	W	158	TYR	C-N-CA	5.09	127.61	120.28
24	O	234	HIS	CA-CB-CG	5.09	118.89	113.80
2	B	735	VAL	CB-CA-C	-5.09	105.12	111.08
2	B	933	ASP	N-CA-C	-5.09	101.41	109.96
13	M	179	GLU	N-CA-C	5.09	116.91	111.36
23	W	23	SER	CB-CA-C	-5.09	102.89	110.88
26	2	48	LEU	N-CA-C	5.09	121.06	109.81
24	O	233	THR	CA-CB-OG1	5.08	117.22	109.60
23	W	483	MET	N-CA-CB	-5.08	102.70	110.42
12	L	47	LYS	N-CA-C	5.08	117.08	110.43
23	W	720	PHE	CA-CB-CG	5.08	118.88	113.80
22	V	419	ARG	CD-NE-CZ	5.08	131.50	124.40
23	W	87	LEU	CA-C-N	5.07	127.08	120.28
23	W	87	LEU	C-N-CA	5.07	127.08	120.28
2	B	1134	THR	CB-CA-C	-5.07	108.06	114.40
20	T	142	SER	CA-C-N	-5.07	111.85	121.54
20	T	142	SER	C-N-CA	-5.07	111.85	121.54
22	V	466	LEU	N-CA-CB	-5.07	102.03	110.80
2	B	603	MET	N-CA-C	5.07	116.67	108.26
22	V	363	VAL	CA-C-N	-5.07	116.01	123.00
22	V	363	VAL	C-N-CA	-5.07	116.01	123.00
23	W	205	VAL	CA-CB-CG1	5.07	119.01	110.40
23	W	31	THR	CA-CB-CG2	5.06	119.11	110.50
2	B	735	VAL	N-CA-C	5.06	116.03	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	43	PRO	CA-C-N	5.06	128.69	120.60
23	W	43	PRO	C-N-CA	5.06	128.69	120.60
23	W	570	GLU	CA-C-N	5.06	129.79	122.36
23	W	570	GLU	C-N-CA	5.06	129.79	122.36
13	M	140	ASN	N-CA-C	5.05	116.47	111.07
22	V	580	ILE	O-C-N	-5.05	117.75	123.20
23	W	718	LYS	CA-C-N	5.05	127.04	120.28
23	W	718	LYS	C-N-CA	5.05	127.04	120.28
2	B	643	LEU	N-CA-C	5.05	116.78	111.28
23	W	459	GLY	O-C-N	5.05	129.26	122.70
23	W	629	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	951	GLU	N-CA-C	5.04	116.85	111.36
1	A	133	SER	CA-C-N	-5.04	111.92	121.54
1	A	133	SER	C-N-CA	-5.04	111.92	121.54
1	A	686	THR	N-CA-C	5.04	114.98	107.88
1	A	1308	TYR	CA-C-N	5.03	128.38	121.33
1	A	1308	TYR	C-N-CA	5.03	128.38	121.33
23	W	195	ALA	O-C-N	5.03	127.25	122.07
23	W	434	HIS	CA-C-N	5.03	131.62	123.37
23	W	434	HIS	C-N-CA	5.03	131.62	123.37
23	W	553	TYR	CB-CA-C	5.03	118.83	110.78
24	0	124	PRO	CA-C-N	5.03	127.02	120.28
24	0	124	PRO	C-N-CA	5.03	127.02	120.28
26	2	249	TYR	CA-C-N	-5.03	114.60	122.05
26	2	249	TYR	C-N-CA	-5.03	114.60	122.05
22	V	465	GLY	CA-C-O	-5.03	116.01	120.94
23	W	260	GLN	CA-C-N	5.03	125.56	119.98
23	W	260	GLN	C-N-CA	5.03	125.56	119.98
23	W	468	PRO	N-CA-CB	5.03	108.82	103.39
28	X	76	DC	C2'-C3'-O3'	-5.03	103.95	111.50
22	V	316	LEU	CB-CA-C	-5.03	101.54	111.60
23	W	172	ALA	CA-C-N	5.02	131.26	121.41
23	W	172	ALA	C-N-CA	5.02	131.26	121.41
15	O	29	THR	CA-C-N	5.02	125.05	119.32
15	O	29	THR	C-N-CA	5.02	125.05	119.32
23	W	414	PHE	CA-C-O	-5.02	115.75	121.68
1	A	898	GLY	N-CA-C	5.02	120.23	114.16
22	V	560	VAL	O-C-N	-5.02	117.23	123.10
23	W	699	GLU	CB-CA-C	5.02	118.33	109.80
2	B	163	LEU	N-CA-C	5.01	118.50	112.38
22	V	581	TYR	CA-C-O	-5.01	115.94	121.31
23	W	189	TRP	NE1-CE2-CD2	-5.01	100.88	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	687	GLY	CA-C-N	5.01	127.41	120.29
23	W	687	GLY	C-N-CA	5.01	127.41	120.29
24	0	207	VAL	CA-C-N	5.01	127.41	120.29
24	0	207	VAL	C-N-CA	5.01	127.41	120.29
22	V	543	ALA	N-CA-C	5.01	116.74	111.28
22	V	634	ARG	N-CA-C	5.01	117.64	111.82
5	E	145	VAL	N-CA-C	5.01	112.82	107.76
22	V	487	LYS	CA-C-N	5.01	127.40	120.29
22	V	487	LYS	C-N-CA	5.01	127.40	120.29
23	W	321	GLY	O-C-N	-5.01	116.19	122.70
2	B	915	GLY	N-CA-C	-5.00	108.33	115.64
22	V	287	LEU	N-CA-CB	-5.00	101.82	110.32
24	0	106	ILE	CA-C-N	5.00	130.64	122.69
24	0	106	ILE	C-N-CA	5.00	130.64	122.69

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	1086	MET	Peptide
2	B	416	ARG	Sidechain
2	B	525	ASN	Peptide
7	G	151	ARG	Sidechain
14	N	355	ASP	Peptide
14	N	371	ILE	Peptide
16	P	158	SER	Peptide
17	Q	125	ALA	Peptide
18	R	215	GLU	Mainchain
18	R	221	ARG	Mainchain
18	R	222	SER	Peptide
18	R	228	MET	Peptide
18	R	229	ASP	Sidechain
18	R	235	GLU	Sidechain
19	S	148	PRO	Peptide
20	T	123	ASN	Peptide

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Mol	Chain	Res	Type	Group
20	T	177	ARG	Peptide
22	V	247	ASP	Mainchain
22	V	251	PHE	Sidechain
22	V	319	TYR	Sidechain
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	534	TYR	Sidechain
22	V	674	THR	Mainchain
22	V	679	PHE	Sidechain
22	V	703	PHE	Sidechain
23	W	104	PHE	Sidechain
23	W	175	TYR	Sidechain
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	293	ARG	Sidechain
23	W	409	THR	Peptide
23	W	423	ASP	Peptide
23	W	553	TYR	Sidechain
23	W	614	TYR	Sidechain
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	60	DG	Sidechain
28	X	65	DG	Sidechain
28	X	66	DA	Sidechain
28	X	72	DC	Sidechain
29	Y	23	DT	Sidechain
29	Y	24	DC	Sidechain
29	Y	33	DT	Sidechain
29	Y	34	DC	Sidechain

5.2 Too-close contacts

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	11607	557	0
2	B	9317	0	9308	381	0
3	C	2213	0	2153	87	0
4	D	1062	0	1042	10	0
5	E	1723	0	1745	75	0
6	F	689	0	715	20	0
7	G	1351	0	1358	25	0
8	H	1205	0	1168	57	0
9	I	1013	0	930	70	0
10	J	533	0	553	35	0
11	K	937	0	959	22	0
12	L	388	0	393	38	0
13	M	2391	0	2410	138	0
14	N	930	0	888	25	0
15	O	806	0	818	17	0
16	P	1462	0	1549	56	0
17	Q	1484	0	1494	153	0
18	R	1357	0	1380	190	0
19	S	1138	0	1103	38	0
20	T	1788	0	1819	90	0
21	U	1343	0	1337	62	0
22	V	3855	0	3871	154	0
23	W	5348	0	5372	124	0
24	0	1479	0	1524	41	0
25	1	491	0	507	230	0
26	2	2196	0	2206	582	0
27	3	1526	0	1561	482	0
28	X	1710	0	941	50	0
29	Y	1681	0	932	52	0
30	A	2	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Q	1	0	0	0	0
31	U	1	0	0	0	0
All	All	62944	0	61643	3194	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 (3194) 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	1.24	1.67
22:V:516:PRO:CG	25:1:15:ALA:HB3	1.19	1.60
22:V:315:VAL:HG13	23:W:500:ASP:CB	1.21	1.55
24:0:54:ARG:HG3	27:3:182:PHE:CE1	1.42	1.54
27:3:59:VAL:CG1	27:3:71:TYR:HD1	1.16	1.53
22:V:321:GLU:CG	23:W:499:ASN:HB3	1.39	1.53
26:2:31:LEU:HD11	27:3:33:THR:CB	1.39	1.53
22:V:516:PRO:HG3	25:1:15:ALA:CB	1.10	1.51
22:V:315:VAL:CG1	23:W:500:ASP:HB2	1.01	1.49
26:2:31:LEU:HD11	27:3:33:THR:CG2	1.42	1.48
18:R:195:PRO:HG2	18:R:199:LYS:CB	1.01	1.48
18:R:195:PRO:CG	18:R:199:LYS:CB	1.86	1.47
16:P:206:GLU:CG	16:P:236:LYS:NZ	1.77	1.47
17:Q:23:ARG:NH2	18:R:206:LYS:CA	1.75	1.46
26:2:117:ASN:ND2	27:3:108:ASN:CB	1.76	1.46
5:E:64:HIS:CD2	5:E:69:THR:H	1.30	1.46
26:2:117:ASN:HD21	27:3:108:ASN:CB	1.27	1.46
1:A:1158:LEU:HD11	1:A:1308:TYR:CD2	1.50	1.45
17:Q:23:ARG:NH2	18:R:206:LYS:CB	1.76	1.44
26:2:117:ASN:CG	27:3:108:ASN:HB2	1.39	1.44
29:Y:24:DC:H2"	29:Y:25:DT:C7	1.49	1.42
26:2:28:PRO:N	27:3:25:GLN:HA	1.31	1.42
1:A:926:ASN:CB	1:A:931:ARG:NH1	1.86	1.39
16:P:206:GLU:CG	16:P:236:LYS:HZ3	1.33	1.38
17:Q:113:ARG:NH2	18:R:218:LYS:HE3	1.34	1.38
22:V:325:ARG:NH2	23:W:499:ASN:HB2	1.05	1.37
26:2:29:GLY:N	27:3:25:GLN:HG3	1.38	1.37
26:2:31:LEU:HD21	27:3:33:THR:N	1.34	1.37
17:Q:20:TYR:CE2	18:R:210:PHE:CB	1.93	1.37
24:0:54:ARG:CG	27:3:182:PHE:HE1	1.35	1.37
1:A:926:ASN:HB3	1:A:931:ARG:NH1	1.04	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:523:VAL:HG11	25:1:20:LEU:CD2	1.50	1.37
17:Q:112:ARG:CD	18:R:237:LEU:HD11	1.54	1.36
9:I:103:ARG:O	9:I:105:GLU:N	1.59	1.36
22:V:321:GLU:OE1	23:W:499:ASN:N	1.57	1.35
26:2:117:ASN:OD1	27:3:108:ASN:ND2	1.57	1.35
1:A:201:GLU:HA	1:A:212:LYS:O	1.24	1.34
5:E:64:HIS:CD2	5:E:69:THR:N	1.95	1.34
22:V:516:PRO:CG	22:V:706:LYS:HZ3	1.40	1.34
22:V:321:GLU:CD	23:W:499:ASN:HB3	1.49	1.34
22:V:366:ASN:HD21	22:V:613:THR:CG2	1.41	1.33
26:2:118:LEU:CD2	27:3:39:ASP:OD1	1.75	1.33
26:2:30:VAL:HG23	27:3:25:GLN:CB	1.57	1.33
17:Q:23:ARG:NH2	18:R:206:LYS:HB3	1.35	1.32
1:A:1110:ALA:CB	21:U:256:THR:HG21	1.59	1.32
18:R:195:PRO:CG	18:R:199:LYS:HB3	1.50	1.32
22:V:615:PHE:O	22:V:617:LEU:N	1.60	1.31
26:2:118:LEU:HD22	27:3:39:ASP:OD1	1.16	1.31
17:Q:113:ARG:NH2	18:R:218:LYS:CE	1.93	1.31
25:1:1:MET:O	26:2:413:LEU:HG	1.28	1.30
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.47	1.30
16:P:298:PRO:O	16:P:300:ILE:HG12	1.14	1.30
1:A:133:SER:OG	1:A:136:GLN:HB2	1.23	1.30
1:A:263:ALA:O	1:A:264:VAL:CG1	1.80	1.29
17:Q:112:ARG:NE	18:R:237:LEU:HD11	1.45	1.29
24:0:165:ARG:NH1	24:0:192:ALA:O	1.66	1.29
26:2:118:LEU:HD21	27:3:39:ASP:O	1.23	1.29
8:H:85:ALA:O	8:H:87:GLN:N	1.63	1.28
16:P:206:GLU:HG3	16:P:236:LYS:NZ	1.35	1.28
1:A:263:ALA:CB	1:A:272:ASN:O	1.82	1.28
1:A:199:TYR:OH	13:M:93:PHE:CE2	1.79	1.28
17:Q:23:ARG:HH22	18:R:206:LYS:CB	1.34	1.27
26:2:28:PRO:N	27:3:25:GLN:CA	1.97	1.27
12:L:17:TYR:CE1	12:L:46:LYS:HG3	1.70	1.27
22:V:325:ARG:NH2	23:W:499:ASN:CB	1.97	1.26
1:A:1158:LEU:HD21	1:A:1308:TYR:CE2	1.70	1.26
5:E:64:HIS:CE1	5:E:69:THR:O	1.87	1.26
24:0:97:ASP:O	27:3:208:ASP:HB2	1.10	1.26
1:A:263:ALA:HB1	1:A:272:ASN:O	1.13	1.25
1:A:926:ASN:HB3	1:A:931:ARG:CZ	1.66	1.25
26:2:30:VAL:CG2	27:3:25:GLN:HB3	1.66	1.25
1:A:932:ARG:HD2	1:A:943:LEU:CD2	1.66	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:187:ILE:HD13	18:R:210:PHE:O	1.37	1.24
1:A:425:ASP:OD2	13:M:39:LEU:HD11	1.22	1.24
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.32	1.24
22:V:674:THR:HG23	26:2:392:ARG:NH2	1.53	1.24
8:H:74:GLU:O	8:H:75:TYR:CD1	1.90	1.23
18:R:195:PRO:CG	18:R:199:LYS:HB2	1.54	1.23
3:C:5:ASN:O	3:C:7:PRO:HD3	1.33	1.23
23:W:59:TYR:CZ	23:W:62:ALA:CB	2.21	1.23
17:Q:20:TYR:CE2	18:R:210:PHE:HB3	1.08	1.22
1:A:608:THR:C	1:A:610:PRO:HD2	1.64	1.22
1:A:932:ARG:CD	1:A:943:LEU:HD21	1.68	1.22
13:M:94:ASP:OD2	13:M:97:GLY:O	1.55	1.22
27:3:58:ALA:N	27:3:71:TYR:OH	1.73	1.21
17:Q:23:ARG:NH2	18:R:206:LYS:C	1.77	1.21
26:2:31:LEU:CD1	27:3:33:THR:HB	1.69	1.21
23:W:209:TYR:OH	23:W:233:PHE:HA	1.38	1.21
3:C:6:GLN:HB2	11:K:104:ARG:NH1	1.57	1.20
27:3:59:VAL:CG1	27:3:71:TYR:CD1	1.98	1.20
22:V:516:PRO:CG	25:1:15:ALA:CB	1.90	1.20
25:1:59:GLU:OE2	26:2:402:ARG:NH2	1.75	1.20
13:M:47:ASP:O	13:M:49:GLY:N	1.73	1.19
27:3:66:GLU:HA	27:3:132:LEU:HD12	1.22	1.19
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.19	1.19
17:Q:23:ARG:HH22	18:R:206:LYS:CA	1.45	1.19
2:B:92:TYR:HA	20:T:141:LEU:HD11	1.18	1.18
22:V:366:ASN:ND2	22:V:613:THR:CG2	2.05	1.18
1:A:132:LYS:O	1:A:133:SER:HB2	1.43	1.18
22:V:516:PRO:HB3	25:1:15:ALA:HB1	1.24	1.18
1:A:622:SER:O	1:A:624:GLY:N	1.77	1.18
5:E:46:ASP:O	5:E:48:PRO:HD3	1.42	1.18
26:2:31:LEU:CD1	27:3:33:THR:CG2	2.21	1.18
23:W:59:TYR:CZ	23:W:62:ALA:HB1	1.77	1.17
16:P:298:PRO:O	16:P:300:ILE:CG1	1.93	1.17
18:R:151:LEU:CD1	18:R:163:LEU:HD21	1.75	1.17
22:V:428:GLU:O	22:V:433:GLN:HA	1.42	1.17
17:Q:105:TYR:CE1	18:R:234:GLU:CD	2.22	1.17
17:Q:180:PHE:CZ	18:R:213:ASP:CA	2.26	1.17
17:Q:180:PHE:CZ	18:R:213:ASP:HA	1.79	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
25:1:2:VAL:CG1	26:2:456:LYS:HG2	1.74	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:PRO:O	13:M:12:ARG:CG	1.92	1.16
22:V:325:ARG:HH22	23:W:499:ASN:CB	1.56	1.16
3:C:6:GLN:CB	11:K:104:ARG:HH12	1.58	1.16
21:U:256:THR:OG1	21:U:272:THR:HG21	1.45	1.15
1:A:199:TYR:OH	13:M:93:PHE:CZ	1.96	1.15
13:M:11:PRO:O	13:M:12:ARG:HG2	1.01	1.15
1:A:425:ASP:OD2	13:M:39:LEU:CD1	1.94	1.15
18:R:164:GLY:CA	18:R:203:PHE:CZ	2.30	1.15
26:2:30:VAL:HB	27:3:25:GLN:O	1.46	1.15
22:V:321:GLU:CD	23:W:499:ASN:CB	2.19	1.15
25:1:13:ASP:CG	25:1:14:PRO:HD2	1.72	1.15
27:3:57:LEU:O	27:3:71:TYR:HE2	1.27	1.14
23:W:419:GLU:HB3	23:W:420:PRO:CD	1.76	1.14
25:1:2:VAL:HG13	26:2:422:LEU:HD11	1.20	1.14
24:0:54:ARG:CG	27:3:182:PHE:CE1	2.17	1.13
28:X:15:DA:N6	29:Y:79:DC:H42	1.45	1.13
21:U:227:GLU:O	21:U:228:MET:HE2	1.45	1.13
25:1:1:MET:CG	26:2:413:LEU:HB3	1.76	1.13
27:3:59:VAL:HG13	27:3:70:LEU:HB2	1.27	1.13
1:A:263:ALA:O	1:A:264:VAL:HG13	0.95	1.13
16:P:206:GLU:HG2	16:P:236:LYS:NZ	1.52	1.13
2:B:225:LEU:C	2:B:227:ASN:H	1.52	1.13
18:R:164:GLY:HA2	18:R:203:PHE:CZ	1.83	1.13
3:C:212:ASP:O	3:C:214:ASP:N	1.82	1.13
22:V:321:GLU:OE1	23:W:499:ASN:CA	1.96	1.12
22:V:321:GLU:OE1	23:W:499:ASN:CB	1.97	1.12
22:V:516:PRO:HG2	22:V:706:LYS:HZ3	0.96	1.12
26:2:160:LEU:HD23	26:2:206:LEU:HD21	1.25	1.12
22:V:321:GLU:HG2	23:W:499:ASN:HB3	1.28	1.12
1:A:1113:SER:HB3	1:A:1309:MET:SD	1.88	1.12
1:A:1158:LEU:HD21	1:A:1308:TYR:HE2	0.97	1.12
23:W:59:TYR:CE2	23:W:62:ALA:CB	2.32	1.12
27:3:33:THR:HG23	27:3:36:LYS:H	1.13	1.12
27:3:57:LEU:C	27:3:71:TYR:OH	1.93	1.12
2:B:90:GLN:NE2	20:T:141:LEU:HA	1.63	1.11
21:U:257:GLN:NE2	21:U:270:ASN:OD1	1.83	1.11
26:2:42:LEU:HD21	26:2:55:TRP:HB2	1.20	1.11
27:3:59:VAL:N	27:3:71:TYR:CE1	2.17	1.11
27:3:208:ASP:OD1	27:3:209:ILE:N	1.82	1.11
26:2:171:VAL:HG22	26:2:213:TRP:HA	1.27	1.11
1:A:927:GLU:O	1:A:931:ARG:NH2	1.83	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:211:GLN:HG3	26:2:257:SER:HB3	1.29	1.11
3:C:133:ARG:HA	3:C:136:ASP:OD2	1.51	1.11
12:L:17:TYR:HE1	12:L:46:LYS:CG	1.63	1.11
16:P:206:GLU:HB3	16:P:207:PRO:HD3	1.33	1.11
25:1:9:LEU:HD13	25:1:48:GLU:HA	1.32	1.11
25:1:5:LEU:CD2	26:2:408:LEU:HD13	1.80	1.10
25:1:5:LEU:HD11	26:2:408:LEU:HB3	1.17	1.10
26:2:163:MET:HE2	26:2:206:LEU:HD12	1.30	1.10
16:P:206:GLU:HB3	16:P:207:PRO:CD	1.81	1.10
29:Y:24:DC:C2'	29:Y:25:DT:H71	1.80	1.10
1:A:1110:ALA:HB2	21:U:256:THR:HG21	1.23	1.10
26:2:28:PRO:N	27:3:25:GLN:C	2.10	1.09
26:2:31:LEU:CD1	27:3:33:THR:CB	2.27	1.09
1:A:1290:SER:HB3	2:B:250:SER:HB3	1.32	1.09
25:1:2:VAL:HG11	26:2:456:LYS:CG	1.81	1.09
22:V:516:PRO:CB	25:1:15:ALA:HB1	1.81	1.09
25:1:18:GLN:HB2	25:1:44:PHE:CE2	1.86	1.09
2:B:91:ILE:HG23	20:T:141:LEU:HD12	1.33	1.09
27:3:49:LEU:HB3	27:3:101:TYR:HB3	1.14	1.09
22:V:315:VAL:CG1	23:W:500:ASP:CB	1.94	1.09
1:A:930:LEU:HB3	1:A:934:LEU:HB2	1.35	1.08
26:2:192:GLU:HG3	26:2:193:PRO:HD2	1.34	1.08
21:U:256:THR:CB	21:U:272:THR:CG2	2.31	1.08
16:P:206:GLU:CB	16:P:207:PRO:CD	2.32	1.08
25:1:5:LEU:HD21	26:2:408:LEU:CD1	1.82	1.08
27:3:59:VAL:HB	27:3:71:TYR:CE1	1.88	1.08
27:3:205:GLN:O	27:3:208:ASP:OD1	1.70	1.08
9:I:104:ALA:O	9:I:106:ASP:N	1.86	1.08
27:3:137:LEU:HB3	27:3:180:VAL:HG11	1.34	1.08
29:Y:24:DC:C2'	29:Y:25:DT:C7	2.31	1.08
23:W:419:GLU:CB	23:W:420:PRO:HD2	1.79	1.08
1:A:1158:LEU:CD1	1:A:1308:TYR:HD2	1.66	1.07
2:B:880:LEU:O	2:B:881:GLU:HB2	1.27	1.07
22:V:516:PRO:HG2	22:V:706:LYS:NZ	1.70	1.07
26:2:159:VAL:HG13	26:2:161:HIS:H	1.16	1.07
1:A:930:LEU:HD22	1:A:934:LEU:HD13	1.07	1.07
1:A:1158:LEU:CD1	1:A:1308:TYR:CD2	2.37	1.07
12:L:17:TYR:HE1	12:L:46:LYS:HG3	0.94	1.07
21:U:256:THR:O	21:U:272:THR:HG22	1.54	1.07
17:Q:112:ARG:NE	18:R:237:LEU:CD1	2.15	1.06
18:R:225:VAL:HG12	18:R:227:SER:HB2	1.10	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:206:GLU:HG2	16:P:236:LYS:HZ3	1.02	1.06
25:1:2:VAL:HG11	26:2:456:LYS:HG2	1.09	1.06
1:A:132:LYS:O	1:A:133:SER:CB	2.04	1.06
22:V:523:VAL:HG11	25:1:20:LEU:HD21	1.11	1.06
24:0:54:ARG:HB2	27:3:209:ILE:HG23	1.36	1.05
27:3:57:LEU:O	27:3:71:TYR:CE2	2.10	1.05
26:2:31:LEU:HD11	27:3:33:THR:HG22	1.37	1.05
24:0:97:ASP:O	27:3:208:ASP:CB	2.02	1.05
25:1:5:LEU:HD12	26:2:409:TYR:O	1.56	1.05
22:V:321:GLU:CG	23:W:499:ASN:CB	2.35	1.05
22:V:674:THR:HG23	26:2:392:ARG:CZ	1.85	1.05
16:P:297:LYS:CB	16:P:298:PRO:CD	2.35	1.04
1:A:1110:ALA:HB1	21:U:256:THR:HG21	1.38	1.04
18:R:195:PRO:HG2	18:R:199:LYS:CA	1.85	1.04
21:U:256:THR:HB	21:U:272:THR:CG2	1.87	1.04
25:1:1:MET:CB	26:2:413:LEU:HB3	1.87	1.04
2:B:92:TYR:CA	20:T:141:LEU:HD11	1.80	1.04
17:Q:180:PHE:CE1	18:R:212:VAL:O	2.10	1.04
18:R:164:GLY:HA3	18:R:203:PHE:HZ	1.23	1.04
21:U:227:GLU:O	21:U:228:MET:HB3	1.50	1.04
1:A:1112:VAL:O	21:U:252:LYS:HB3	1.57	1.04
17:Q:180:PHE:CZ	18:R:212:VAL:O	2.10	1.04
26:2:31:LEU:HD11	27:3:33:THR:HB	1.15	1.04
21:U:256:THR:OG1	21:U:272:THR:CG2	2.06	1.04
22:V:426:VAL:O	22:V:427:MET:O	1.76	1.04
22:V:612:ASP:OD2	22:V:635:GLN:OE1	1.72	1.03
5:E:64:HIS:NE2	5:E:69:THR:N	2.05	1.03
17:Q:112:ARG:HD3	18:R:237:LEU:HD11	1.35	1.03
18:R:154:LEU:HD23	18:R:163:LEU:HD23	1.37	1.03
22:V:516:PRO:CB	25:1:15:ALA:CB	2.36	1.03
25:1:34:ILE:HG12	25:1:50:VAL:HG11	1.39	1.03
26:2:117:ASN:CG	27:3:108:ASN:CB	2.20	1.03
5:E:64:HIS:CE1	5:E:69:THR:C	2.37	1.03
22:V:516:PRO:CG	22:V:706:LYS:NZ	2.18	1.03
24:0:54:ARG:NE	27:3:182:PHE:CE1	2.26	1.03
26:2:81:LYS:HE3	26:2:93:LEU:HD21	1.40	1.03
1:A:47:THR:HG23	1:A:53:LYS:HG2	1.05	1.02
22:V:523:VAL:HG11	25:1:20:LEU:HD23	1.37	1.02
22:V:366:ASN:HD21	22:V:613:THR:HG22	1.19	1.02
1:A:206:ASN:O	1:A:207:GLU:HB2	1.59	1.02
24:0:54:ARG:CD	27:3:182:PHE:HE1	1.71	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:4:VAL:HG12	26:2:411:GLN:O	1.55	1.02
27:3:59:VAL:HB	27:3:71:TYR:HE1	1.24	1.02
26:2:234:LEU:HD21	26:2:237:LEU:HD12	1.36	1.02
23:W:59:TYR:CE2	23:W:62:ALA:HB3	1.94	1.01
23:W:419:GLU:HB3	23:W:420:PRO:HD2	1.04	1.01
27:3:196:LEU:HD21	27:3:223:LEU:HD23	1.42	1.01
2:B:90:GLN:HE21	20:T:141:LEU:HA	0.85	1.01
1:A:609:HIS:N	1:A:610:PRO:CD	2.24	1.01
1:A:1110:ALA:CB	21:U:256:THR:CG2	2.39	1.00
26:2:28:PRO:CD	27:3:25:GLN:HA	1.90	1.00
1:A:1290:SER:CB	2:B:250:SER:HB3	1.89	1.00
22:V:515:SER:HB3	22:V:539:ASN:HD21	1.26	1.00
26:2:199:ALA:HB3	26:2:202:GLN:HE22	1.22	1.00
3:C:134:ASN:N	3:C:136:ASP:OD1	1.93	1.00
23:W:209:TYR:OH	23:W:233:PHE:CA	2.09	1.00
24:0:77:LYS:O	24:0:79:ASN:N	1.93	1.00
27:3:58:ALA:CA	27:3:71:TYR:CZ	2.43	1.00
1:A:535:MET:O	1:A:669:TYR:OH	1.80	0.99
27:3:148:ASN:HB2	27:3:157:MET:HE2	1.42	0.99
28:X:15:DA:H61	29:Y:79:DC:H42	1.01	0.99
9:I:85:PRO:O	9:I:86:CYS:C	2.04	0.99
27:3:59:VAL:CB	27:3:71:TYR:CE1	2.44	0.99
16:P:206:GLU:HB2	16:P:207:PRO:HD2	1.45	0.99
17:Q:184:ILE:HD13	18:R:218:LYS:HZ1	1.23	0.99
29:Y:24:DC:C2	29:Y:25:DT:C4	2.51	0.99
2:B:92:TYR:HD1	20:T:141:LEU:HD21	1.28	0.99
1:A:427:ILE:HG12	13:M:38:GLY:O	1.63	0.98
10:J:63:ALA:HB3	10:J:64:PRO:HD3	1.41	0.98
22:V:315:VAL:HG11	23:W:500:ASP:HB2	1.42	0.98
17:Q:105:TYR:CD1	18:R:234:GLU:OE1	2.16	0.98
1:A:522:PRO:HA	1:A:666:ARG:HE	1.25	0.98
28:X:15:DA:H61	29:Y:79:DC:N4	1.60	0.98
1:A:930:LEU:HD22	1:A:934:LEU:CD1	1.93	0.98
2:B:880:LEU:O	2:B:881:GLU:CB	2.08	0.98
25:1:1:MET:HE1	26:2:440:LEU:HD13	1.44	0.98
5:E:64:HIS:NE2	5:E:69:THR:CA	2.27	0.98
18:R:195:PRO:CB	18:R:199:LYS:CB	2.42	0.97
27:3:173:GLN:HA	27:3:176:ASN:HD21	1.28	0.97
8:H:85:ALA:C	8:H:87:GLN:H	1.70	0.97
22:V:516:PRO:HA	25:1:15:ALA:O	1.62	0.97
26:2:118:LEU:CD2	27:3:39:ASP:O	2.12	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:HIS:HE2	5:E:69:THR:CB	1.76	0.97
16:P:297:LYS:HB3	16:P:298:PRO:HD2	1.43	0.97
2:B:958:CYS:SG	2:B:959:GLU:N	2.37	0.97
26:2:196:ILE:HD11	26:2:210:ALA:HB2	1.45	0.97
27:3:165:LYS:HD2	27:3:195:VAL:HG22	1.44	0.97
18:R:164:GLY:HA3	18:R:203:PHE:CZ	1.95	0.97
22:V:321:GLU:CD	23:W:499:ASN:CA	2.37	0.97
1:A:930:LEU:CD2	1:A:934:LEU:HD13	1.93	0.97
22:V:523:VAL:CG1	25:1:20:LEU:CD2	2.43	0.97
26:2:176:ALA:HB1	26:2:178:LEU:HD13	1.47	0.96
23:W:584:TYR:CD1	23:W:594:ALA:HB2	1.99	0.96
26:2:100:LEU:HD11	26:2:119:ARG:HG3	1.46	0.96
23:W:59:TYR:CE1	23:W:62:ALA:HB1	2.01	0.96
27:3:59:VAL:CB	27:3:71:TYR:CD1	2.48	0.96
27:3:133:LEU:HD23	27:3:177:PHE:CD1	2.01	0.96
13:M:182:ALA:HB1	20:T:152:ASN:OD1	1.66	0.96
23:W:209:TYR:HH	23:W:233:PHE:HA	1.31	0.95
26:2:211:GLN:HA	26:2:261:PHE:CZ	2.02	0.95
25:1:2:VAL:CG1	26:2:422:LEU:HD11	1.96	0.95
1:A:1158:LEU:CD2	1:A:1308:TYR:HE2	1.77	0.95
1:A:926:ASN:HB3	1:A:931:ARG:HH11	1.19	0.95
1:A:263:ALA:HB1	1:A:272:ASN:C	1.91	0.95
17:Q:105:TYR:CE1	18:R:234:GLU:OE2	2.17	0.95
2:B:225:LEU:O	2:B:227:ASN:N	2.00	0.95
10:J:64:PRO:C	10:J:66:GLU:H	1.71	0.95
25:1:18:GLN:HB2	25:1:44:PHE:HE2	1.26	0.95
26:2:118:LEU:HD11	27:3:43:VAL:CG2	1.95	0.95
26:2:35:TYR:CE1	26:2:62:LEU:HG	2.02	0.94
22:V:321:GLU:OE2	23:W:500:ASP:N	2.00	0.94
25:1:1:MET:HB3	26:2:413:LEU:CG	1.98	0.94
26:2:117:ASN:N	27:3:104:LEU:HD21	1.83	0.94
1:A:426:ARG:O	13:M:39:LEU:O	1.83	0.94
1:A:133:SER:OG	1:A:136:GLN:CB	2.16	0.94
3:C:212:ASP:C	3:C:214:ASP:H	1.74	0.94
13:M:94:ASP:O	13:M:96:PHE:N	2.01	0.94
1:A:1158:LEU:HD11	1:A:1308:TYR:HD2	0.83	0.94
5:E:45:GLY:O	5:E:46:ASP:O	1.86	0.94
9:I:102:ALA:O	9:I:104:ALA:N	2.00	0.94
17:Q:113:ARG:HH22	18:R:218:LYS:HE3	1.25	0.94
21:U:256:THR:CB	21:U:272:THR:HG21	1.93	0.94
23:W:696:TRP:CD1	23:W:697:ILE:HG12	2.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:645:GLU:OE1	2:B:649:ASN:ND2	2.00	0.94
5:E:64:HIS:HD2	5:E:69:THR:H	1.16	0.94
5:E:64:HIS:HD2	5:E:67:ASP:O	1.50	0.94
17:Q:105:TYR:CD1	18:R:234:GLU:CD	2.45	0.94
2:B:91:ILE:CG2	20:T:141:LEU:HD12	1.97	0.93
22:V:515:SER:CB	22:V:539:ASN:HD21	1.80	0.93
25:1:9:LEU:HD22	25:1:51:ASN:HD22	1.33	0.93
21:U:256:THR:CB	21:U:272:THR:HG22	1.96	0.93
27:3:187:GLN:HG3	27:3:189:ILE:HG12	1.51	0.93
17:Q:105:TYR:HE1	18:R:234:GLU:OE2	1.49	0.93
22:V:366:ASN:HD21	22:V:613:THR:HG23	1.31	0.93
26:2:118:LEU:HD23	27:3:42:MET:HB2	1.50	0.93
22:V:631:GLY:O	22:V:632:SER:CB	2.14	0.93
26:2:29:GLY:CA	27:3:25:GLN:HG3	1.98	0.93
1:A:930:LEU:CB	1:A:934:LEU:HB2	1.99	0.93
1:A:1158:LEU:CD2	1:A:1308:TYR:CE2	2.51	0.93
16:P:205:ARG:O	16:P:206:GLU:O	1.86	0.93
26:2:177:GLN:HA	26:2:220:LEU:CD2	1.99	0.93
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.02	0.92
26:2:31:LEU:CD2	27:3:33:THR:N	2.30	0.92
27:3:190:LEU:HA	27:3:210:THR:HG22	1.50	0.92
25:1:13:ASP:OD2	25:1:17:LYS:HB3	1.69	0.92
27:3:11:LEU:HD22	27:3:160:ARG:HG2	1.51	0.92
1:A:1110:ALA:HB2	21:U:256:THR:CG2	1.98	0.92
1:A:1112:VAL:O	21:U:252:LYS:CB	2.17	0.92
2:B:132:VAL:HG21	2:B:141:GLN:HG2	1.50	0.92
27:3:165:LYS:HE3	27:3:200:SER:CB	2.00	0.92
17:Q:112:ARG:CD	18:R:237:LEU:CD1	2.48	0.92
18:R:195:PRO:HG2	18:R:199:LYS:HB3	1.07	0.92
1:A:516:GLN:HA	1:A:520:MET:HE2	1.52	0.92
1:A:47:THR:HG23	1:A:53:LYS:CG	1.97	0.92
5:E:64:HIS:NE2	5:E:69:THR:C	2.27	0.92
27:3:133:LEU:HD13	27:3:133:LEU:H	1.33	0.92
1:A:199:TYR:OH	13:M:93:PHE:HE2	1.35	0.92
27:3:58:ALA:C	27:3:71:TYR:CZ	2.48	0.92
25:1:8:VAL:HG11	25:1:45:VAL:CG1	1.99	0.91
1:A:355:MET:SD	2:B:1091:ARG:NH1	2.43	0.91
18:R:163:LEU:O	18:R:164:GLY:C	2.13	0.91
26:2:29:GLY:H	27:3:25:GLN:HG3	1.13	0.91
1:A:263:ALA:C	1:A:264:VAL:HG13	1.93	0.91
16:P:206:GLU:CB	16:P:207:PRO:HD2	1.98	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:154:LEU:CD2	18:R:163:LEU:HD23	2.00	0.91
5:E:64:HIS:HE1	5:E:69:THR:O	1.46	0.91
8:H:74:GLU:C	8:H:75:TYR:CD1	2.49	0.91
25:1:1:MET:HB3	26:2:413:LEU:HB3	1.52	0.91
3:C:7:PRO:O	3:C:8:THR:OG1	1.87	0.91
22:V:325:ARG:HH21	23:W:499:ASN:HB2	1.32	0.91
26:2:81:LYS:CE	26:2:93:LEU:HD21	2.00	0.91
26:2:118:LEU:HD22	27:3:39:ASP:CG	1.94	0.91
26:2:159:VAL:HG22	26:2:160:LEU:HD12	1.51	0.91
24:0:54:ARG:HG3	27:3:182:PHE:CZ	2.05	0.91
17:Q:23:ARG:HH21	18:R:206:LYS:CB	1.76	0.91
27:3:137:LEU:CB	27:3:180:VAL:HG11	2.01	0.91
1:A:197:GLU:OE1	13:M:93:PHE:CD2	2.24	0.91
18:R:195:PRO:CB	18:R:199:LYS:HB3	1.99	0.91
23:W:59:TYR:CE1	23:W:62:ALA:CB	2.52	0.90
23:W:430:ASN:HB3	23:W:431:PRO:HD2	1.54	0.90
22:V:516:PRO:CD	22:V:706:LYS:HZ3	1.84	0.90
27:3:58:ALA:HA	27:3:71:TYR:CE2	2.05	0.90
27:3:165:LYS:HG3	27:3:203:LEU:HD12	1.52	0.90
17:Q:180:PHE:CE1	18:R:213:ASP:HA	2.07	0.90
21:U:227:GLU:O	21:U:228:MET:CE	2.19	0.90
26:2:29:GLY:N	27:3:25:GLN:CG	2.32	0.90
26:2:81:LYS:HD2	26:2:89:LEU:HD21	1.52	0.90
1:A:609:HIS:N	1:A:610:PRO:HD2	1.83	0.90
1:A:1110:ALA:HB1	21:U:256:THR:CG2	2.01	0.89
22:V:315:VAL:HG13	23:W:500:ASP:CA	2.03	0.89
22:V:612:ASP:OD2	22:V:635:GLN:CD	2.16	0.89
24:0:98:GLN:OE1	27:3:209:ILE:HA	1.70	0.89
1:A:544:ALA:HB2	1:A:680:LEU:HD22	1.53	0.89
17:Q:101:ASN:C	17:Q:103:VAL:H	1.78	0.89
13:M:10:LEU:C	13:M:12:ARG:H	1.78	0.89
25:1:47:ALA:CB	25:1:50:VAL:HB	2.03	0.89
27:3:177:PHE:CE2	27:3:181:ILE:HD11	2.08	0.89
18:R:195:PRO:HG2	18:R:199:LYS:HB2	0.89	0.88
26:2:160:LEU:HB3	26:2:206:LEU:HD11	1.52	0.88
2:B:90:GLN:HE21	20:T:141:LEU:CA	1.80	0.88
22:V:615:PHE:O	22:V:616:ASP:C	2.17	0.88
25:1:8:VAL:HG11	25:1:45:VAL:HG13	1.55	0.88
26:2:29:GLY:H	27:3:25:GLN:CG	1.85	0.88
18:R:204:ASN:ND2	18:R:205:ASP:N	2.20	0.88
3:C:275:ASN:ND2	11:K:31:CYS:SG	2.46	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:105:TYR:HE1	18:R:234:GLU:CD	1.79	0.88
1:A:156:GLY:HA2	1:A:181:HIS:CG	2.07	0.88
22:V:523:VAL:CG1	25:1:20:LEU:HD23	2.03	0.88
26:2:117:ASN:CB	27:3:42:MET:CE	2.51	0.88
26:2:160:LEU:CA	26:2:206:LEU:HD11	2.04	0.88
27:3:71:TYR:CD2	27:3:72:PRO:HD2	2.07	0.88
17:Q:20:TYR:HE2	18:R:210:PHE:CB	1.70	0.88
17:Q:113:ARG:HH21	18:R:218:LYS:HE3	1.10	0.88
25:1:4:VAL:HG11	26:2:412:PHE:HD2	1.36	0.88
26:2:163:MET:SD	26:2:196:ILE:HG21	2.14	0.88
27:3:177:PHE:CD2	27:3:181:ILE:HD11	2.08	0.88
3:C:5:ASN:O	3:C:7:PRO:CD	2.20	0.88
23:W:696:TRP:CD1	23:W:697:ILE:CG1	2.57	0.88
26:2:243:SER:CB	26:2:258:LEU:HD22	2.04	0.88
27:3:70:LEU:HD13	27:3:115:ILE:HD11	1.55	0.88
27:3:165:LYS:HE3	27:3:200:SER:HB2	1.56	0.88
1:A:201:GLU:CA	1:A:212:LYS:O	2.19	0.87
17:Q:70:LYS:O	17:Q:102:VAL:HG11	1.74	0.87
1:A:197:GLU:OE1	13:M:93:PHE:CE2	2.28	0.87
1:A:263:ALA:HB1	1:A:272:ASN:HB3	1.56	0.87
9:I:102:ALA:C	9:I:104:ALA:H	1.82	0.87
13:M:92:SER:O	13:M:93:PHE:O	1.91	0.87
13:M:178:LYS:C	20:T:154:LYS:HE3	1.98	0.87
26:2:218:GLN:HB3	26:2:264:HIS:HD2	1.38	0.87
27:3:59:VAL:HG11	27:3:71:TYR:HD1	1.39	0.87
9:I:85:PRO:O	9:I:86:CYS:O	1.93	0.87
2:B:875:GLU:O	2:B:876:ASN:HB2	1.73	0.87
26:2:218:GLN:HB3	26:2:264:HIS:CD2	2.08	0.87
27:3:59:VAL:CG1	27:3:70:LEU:HB2	2.03	0.87
26:2:28:PRO:HD2	27:3:25:GLN:NE2	1.90	0.87
26:2:45:PHE:HB2	26:2:51:LEU:HD13	1.56	0.87
26:2:118:LEU:HD11	27:3:43:VAL:HG22	1.56	0.87
26:2:160:LEU:CD2	26:2:206:LEU:HD21	2.04	0.87
22:V:366:ASN:ND2	22:V:613:THR:HG23	1.86	0.87
2:B:132:VAL:HG23	2:B:141:GLN:HB3	1.56	0.87
3:C:6:GLN:HB2	11:K:104:ARG:HH12	0.72	0.87
25:1:1:MET:HB3	26:2:413:LEU:CB	2.04	0.87
25:1:28:ALA:CB	25:1:31:LYS:HD2	2.04	0.87
26:2:117:ASN:OD1	27:3:108:ASN:CB	2.23	0.87
17:Q:20:TYR:CE2	18:R:210:PHE:HB2	2.10	0.87
23:W:37:HIS:CE1	23:W:454:VAL:HG13	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:164:GLY:HA2	18:R:203:PHE:CE2	2.09	0.87
23:W:59:TYR:CG	23:W:62:ALA:HB2	2.10	0.87
13:M:16:PRO:HG2	13:M:39:LEU:HD21	1.54	0.86
21:U:251:ALA:O	21:U:253:THR:N	2.07	0.86
26:2:48:LEU:HB3	26:2:49:PRO:HD3	1.57	0.86
27:3:14:VAL:HG21	27:3:163:VAL:HG22	1.57	0.86
26:2:138:PRO:HG3	26:2:189:GLU:HG3	1.57	0.86
27:3:64:ILE:HG13	27:3:123:ASP:HB3	1.57	0.86
17:Q:23:ARG:HH22	18:R:206:LYS:C	1.45	0.86
17:Q:23:ARG:HH22	18:R:206:LYS:HB3	1.03	0.86
26:2:160:LEU:CB	26:2:206:LEU:HD11	2.04	0.86
27:3:178:MET:HE2	27:3:202:LEU:CD1	2.05	0.86
9:I:103:ARG:C	9:I:105:GLU:N	2.32	0.86
17:Q:113:ARG:HH22	18:R:218:LYS:CE	1.79	0.86
27:3:69:PHE:CZ	27:3:139:LYS:HB3	2.10	0.86
17:Q:113:ARG:HH21	18:R:218:LYS:CE	1.70	0.86
26:2:117:ASN:OD1	27:3:108:ASN:CG	2.18	0.86
26:2:224:GLN:HB2	26:2:268:PHE:CZ	2.09	0.86
2:B:225:LEU:C	2:B:227:ASN:N	2.27	0.86
26:2:171:VAL:HG22	26:2:213:TRP:CA	2.06	0.86
26:2:211:GLN:HG3	26:2:257:SER:CB	2.05	0.86
27:3:100:LYS:HB3	27:3:103:LEU:HD13	1.58	0.86
9:I:61:GLU:O	9:I:63:ASP:N	2.07	0.86
26:2:81:LYS:CD	26:2:89:LEU:HD21	2.05	0.86
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.09	0.86
8:H:65:TYR:CE2	8:H:70:LEU:HB2	2.10	0.85
16:P:206:GLU:HG3	16:P:236:LYS:HZ2	0.99	0.85
21:U:227:GLU:O	21:U:228:MET:CB	2.19	0.85
23:W:59:TYR:CD2	23:W:62:ALA:HB2	2.11	0.85
25:1:1:MET:O	26:2:413:LEU:CG	2.21	0.85
25:1:2:VAL:HG13	26:2:422:LEU:CD1	2.03	0.85
27:3:124:ILE:HD13	27:3:125:LYS:N	1.91	0.85
26:2:118:LEU:CD2	27:3:42:MET:HB2	2.06	0.85
26:2:159:VAL:HG22	26:2:160:LEU:H	1.40	0.85
17:Q:23:ARG:HH21	18:R:206:LYS:CA	1.76	0.85
26:2:78:GLU:O	26:2:81:LYS:HG2	1.77	0.85
26:2:81:LYS:CD	26:2:93:LEU:HD21	2.07	0.85
27:3:190:LEU:HA	27:3:210:THR:CG2	2.05	0.85
25:1:1:MET:SD	26:2:415:GLN:O	2.34	0.85
27:3:59:VAL:HG12	27:3:71:TYR:CG	2.07	0.85
21:U:256:THR:O	21:U:272:THR:CG2	2.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:631:GLY:O	22:V:632:SER:HB2	1.76	0.85
27:3:160:ARG:HB3	27:3:190:LEU:HD21	1.57	0.85
27:3:184:ALA:HA	27:3:187:GLN:HG2	1.57	0.85
26:2:221:GLN:HG2	26:2:268:PHE:CZ	2.11	0.84
29:Y:24:DC:H2''	29:Y:25:DT:H71	0.87	0.84
18:R:151:LEU:CD1	18:R:163:LEU:CD2	2.54	0.84
25:1:19:PHE:O	25:1:23:LEU:HG	1.75	0.84
27:3:49:LEU:CB	27:3:101:TYR:HB3	2.05	0.84
27:3:49:LEU:HB3	27:3:101:TYR:CB	2.05	0.84
1:A:274:ASP:O	1:A:277:THR:N	2.10	0.84
1:A:574:VAL:O	8:H:74:GLU:HA	1.78	0.84
2:B:492:ASP:O	29:Y:45:DT:C2'	2.25	0.84
18:R:164:GLY:CA	18:R:203:PHE:CE2	2.60	0.84
25:1:2:VAL:CG1	26:2:422:LEU:CD1	2.55	0.84
26:2:177:GLN:HA	26:2:220:LEU:HD21	1.56	0.84
26:2:221:GLN:NE2	26:2:230:LEU:HB2	1.93	0.84
23:W:696:TRP:NE1	23:W:697:ILE:HG12	1.91	0.84
26:2:118:LEU:CD2	27:3:39:ASP:HA	2.08	0.84
26:2:176:ALA:CB	26:2:178:LEU:HD13	2.07	0.84
1:A:79:THR:HG21	13:M:43:ASP:OD1	1.77	0.84
8:H:65:TYR:HE2	8:H:70:LEU:HB2	1.40	0.84
26:2:167:PRO:O	26:2:171:VAL:HG23	1.76	0.84
22:V:523:VAL:CG1	25:1:20:LEU:HD21	2.04	0.84
26:2:118:LEU:HD12	26:2:119:ARG:N	1.92	0.84
26:2:159:VAL:HG22	26:2:160:LEU:CD1	2.08	0.84
27:3:178:MET:HE2	27:3:202:LEU:HD12	1.57	0.84
1:A:264:VAL:HG23	1:A:272:ASN:OD1	1.78	0.84
1:A:621:ILE:O	1:A:623:PRO:N	2.11	0.84
5:E:64:HIS:HE2	5:E:69:THR:CA	1.87	0.83
18:R:151:LEU:HD11	18:R:163:LEU:HD21	1.58	0.83
26:2:160:LEU:HD23	26:2:206:LEU:CD2	2.07	0.83
17:Q:52:LEU:HB3	17:Q:54:PHE:HD2	1.43	0.83
13:M:10:LEU:O	13:M:12:ARG:N	2.09	0.83
13:M:89:GLY:O	13:M:90:ALA:CB	2.25	0.83
26:2:229:ASP:O	26:2:233:ILE:HG12	1.78	0.83
27:3:196:LEU:HD21	27:3:223:LEU:CD2	2.08	0.83
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.13	0.83
26:2:160:LEU:O	26:2:164:VAL:HG23	1.79	0.83
1:A:273:GLN:NE2	13:M:79:ASP:OD2	2.11	0.83
2:B:874:PRO:O	2:B:876:ASN:N	2.10	0.83
9:I:89:CYS:HB3	9:I:119:CYS:SG	2.17	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:516:PRO:CG	25:1:15:ALA:HB1	1.96	0.83
26:2:57:MET:HA	26:2:60:LEU:CD1	2.09	0.83
22:V:516:PRO:HG3	25:1:15:ALA:HB2	1.57	0.83
1:A:931:ARG:HA	1:A:931:ARG:NE	1.93	0.83
22:V:315:VAL:HG12	23:W:500:ASP:HB2	1.54	0.83
1:A:932:ARG:HD2	1:A:943:LEU:HD21	0.84	0.83
26:2:259:LEU:HD12	26:2:260:ASN:N	1.94	0.83
25:1:47:ALA:HB2	25:1:50:VAL:HB	1.61	0.82
25:1:52:VAL:HG23	25:1:53:LEU:HD12	1.59	0.82
1:A:608:THR:C	1:A:610:PRO:CD	2.50	0.82
27:3:12:VAL:HG21	27:3:161:ILE:HG12	1.61	0.82
20:T:141:LEU:O	20:T:143:GLN:OE1	1.96	0.82
25:1:9:LEU:HB2	25:1:51:ASN:HD21	1.43	0.82
1:A:375:ILE:HG21	1:A:666:ARG:CZ	2.08	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
25:1:59:GLU:OE1	26:2:402:ARG:NH1	2.13	0.82
17:Q:68:GLY:O	18:R:226:ASP:HB3	1.79	0.82
27:3:216:LYS:H	27:3:216:LYS:HD2	1.43	0.82
12:L:17:TYR:CE1	12:L:46:LYS:CG	2.47	0.82
26:2:37:HIS:HB3	26:2:38:PRO:HD3	1.61	0.82
27:3:57:LEU:HD23	27:3:58:ALA:N	1.91	0.82
22:V:516:PRO:HA	25:1:15:ALA:C	2.03	0.81
1:A:926:ASN:CG	1:A:931:ARG:NH1	2.38	0.81
22:V:427:MET:O	22:V:432:THR:O	1.98	0.81
25:1:52:VAL:CG2	25:1:53:LEU:HD12	2.09	0.81
26:2:174:ASP:OD1	26:2:179:LEU:HD12	1.80	0.81
26:2:175:LEU:HB3	26:2:216:MET:SD	2.20	0.81
18:R:204:ASN:ND2	18:R:205:ASP:H	1.78	0.81
26:2:30:VAL:H	27:3:25:GLN:HB3	1.44	0.81
26:2:86:SER:HB3	26:2:140:LYS:HE2	1.60	0.81
2:B:761:THR:H	2:B:764:MET:HE3	1.44	0.81
8:H:65:TYR:CD2	8:H:70:LEU:HD22	2.16	0.81
17:Q:113:ARG:NH2	18:R:218:LYS:CD	2.43	0.81
1:A:1290:SER:HB3	2:B:250:SER:CB	2.11	0.81
23:W:59:TYR:CD1	23:W:62:ALA:HB2	2.16	0.81
25:1:9:LEU:CD1	25:1:48:GLU:HA	2.09	0.81
26:2:174:ASP:O	26:2:220:LEU:HD23	1.79	0.81
27:3:58:ALA:C	27:3:71:TYR:CE1	2.58	0.81
1:A:264:VAL:HG23	1:A:272:ASN:CG	2.05	0.81
5:E:46:ASP:O	5:E:48:PRO:CD	2.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:SER:O	5:E:50:GLU:O	1.96	0.81
17:Q:184:ILE:HD13	18:R:218:LYS:NZ	1.94	0.81
26:2:177:GLN:CD	26:2:220:LEU:HD22	2.06	0.81
27:3:12:VAL:CG2	27:3:161:ILE:HG12	2.10	0.81
25:1:50:VAL:HG12	25:1:54:GLN:HG2	1.62	0.81
26:2:31:LEU:CD1	27:3:33:THR:HG22	1.96	0.81
1:A:1113:SER:CB	1:A:1309:MET:SD	2.69	0.81
1:A:1312:PRO:HB3	1:A:1334:TRP:CZ3	2.16	0.81
2:B:226:GLU:OE2	2:B:617:ASP:HB2	1.81	0.81
2:B:566:LYS:HD3	2:B:573:TRP:HE1	1.47	0.80
25:1:34:ILE:HG22	25:1:46:ILE:HD11	1.63	0.80
27:3:144:ILE:CD1	27:3:147:MET:HE3	2.11	0.80
26:2:42:LEU:HD12	26:2:59:MET:CE	2.11	0.80
26:2:256:ASP:O	26:2:259:LEU:HG	1.82	0.80
2:B:132:VAL:HG21	2:B:141:GLN:CG	2.10	0.80
5:E:64:HIS:CD2	5:E:67:ASP:O	2.34	0.80
17:Q:113:ARG:NH1	18:R:218:LYS:HG3	1.96	0.80
26:2:35:TYR:CD1	26:2:62:LEU:HG	2.16	0.80
1:A:47:THR:CG2	1:A:53:LYS:HG2	2.01	0.80
26:2:117:ASN:HB3	27:3:42:MET:HE3	1.62	0.80
27:3:214:TYR:O	27:3:215:LEU:HD23	1.82	0.80
27:3:11:LEU:CD2	27:3:160:ARG:HG2	2.12	0.80
1:A:926:ASN:CB	1:A:931:ARG:HH11	1.78	0.80
1:A:1115:LYS:O	1:A:1116:ASN:O	2.00	0.80
16:P:298:PRO:O	16:P:300:ILE:CD1	2.30	0.80
17:Q:113:ARG:HH22	18:R:218:LYS:CD	1.93	0.80
26:2:205:LEU:O	26:2:209:PRO:HD2	1.81	0.80
27:3:121:LYS:O	27:3:124:ILE:HB	1.81	0.80
13:M:7:LEU:HD21	13:M:10:LEU:HD13	1.63	0.80
26:2:93:LEU:HA	26:2:96:TRP:CD1	2.17	0.80
27:3:165:LYS:HE2	27:3:167:ALA:O	1.81	0.80
26:2:251:VAL:HG11	26:2:254:MET:HG3	1.62	0.79
1:A:1304:ILE:O	1:A:1307:VAL:CG2	2.30	0.79
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.05	0.79
22:V:674:THR:CG2	26:2:392:ARG:CZ	2.59	0.79
25:1:13:ASP:OD2	25:1:17:LYS:CB	2.31	0.79
26:2:30:VAL:HG23	27:3:25:GLN:HB3	0.80	0.79
27:3:14:VAL:CG2	27:3:163:VAL:HG22	2.13	0.79
27:3:64:ILE:HG23	27:3:128:HIS:CD2	2.17	0.79
3:C:5:ASN:C	3:C:7:PRO:HD3	2.07	0.79
29:Y:24:DC:H2"	29:Y:25:DT:C5	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:41:LYS:HG3	5:E:46:ASP:OD2	1.80	0.79
26:2:117:ASN:CG	27:3:42:MET:CE	2.55	0.79
26:2:224:GLN:HB2	26:2:268:PHE:CE2	2.17	0.79
27:3:222:SER:O	27:3:225:GLN:HG2	1.83	0.79
28:X:15:DA:N6	29:Y:79:DC:N4	2.24	0.79
25:1:1:MET:HA	26:2:414:SER:H	1.46	0.79
25:1:38:ILE:HA	25:1:44:PHE:HD1	1.48	0.79
24:0:54:ARG:NE	27:3:182:PHE:HE1	1.73	0.78
26:2:52:ALA:O	26:2:56:VAL:HG13	1.81	0.78
26:2:234:LEU:O	26:2:234:LEU:HD23	1.83	0.78
17:Q:69:ASP:HA	18:R:226:ASP:OD1	1.83	0.78
26:2:211:GLN:CG	26:2:257:SER:HB3	2.13	0.78
27:3:58:ALA:HA	27:3:71:TYR:CZ	2.17	0.78
26:2:181:GLN:OE1	26:2:229:ASP:HB2	1.83	0.78
27:3:151:VAL:HG12	27:3:155:GLN:O	1.84	0.78
5:E:55:ARG:NH1	5:E:107:GLN:OE1	2.17	0.78
25:1:34:ILE:CG2	25:1:46:ILE:HD11	2.13	0.78
27:3:57:LEU:C	27:3:71:TYR:CZ	2.61	0.78
26:2:34:LEU:O	26:2:38:PRO:HD2	1.84	0.78
26:2:118:LEU:CG	27:3:39:ASP:OD1	2.32	0.78
26:2:189:GLU:HB2	26:2:190:PRO:HD3	1.66	0.78
10:J:64:PRO:C	10:J:66:GLU:N	2.39	0.78
25:1:1:MET:CB	26:2:413:LEU:CB	2.60	0.78
25:1:1:MET:HB3	26:2:413:LEU:HD23	1.65	0.78
26:2:77:LYS:HD3	26:2:78:GLU:N	1.97	0.78
27:3:208:ASP:OD1	27:3:209:ILE:HG13	1.83	0.78
1:A:79:THR:HG21	13:M:43:ASP:CG	2.08	0.78
26:2:159:VAL:HG13	26:2:161:HIS:N	1.96	0.78
26:2:203:PHE:CD2	26:2:205:LEU:HD23	2.18	0.78
26:2:207:ASP:O	26:2:211:GLN:HG2	1.84	0.78
1:A:485:ASN:OD1	1:A:486:LEU:N	2.16	0.78
2:B:490:GLY:O	2:B:491:ARG:HB2	1.84	0.78
26:2:163:MET:CE	26:2:206:LEU:HD12	2.14	0.78
27:3:57:LEU:C	27:3:71:TYR:CE2	2.61	0.78
17:Q:184:ILE:CD1	18:R:218:LYS:NZ	2.47	0.77
22:V:516:PRO:CD	25:1:15:ALA:HB3	2.10	0.77
26:2:53:LYS:O	26:2:56:VAL:HG22	1.84	0.77
26:2:196:ILE:CD1	26:2:210:ALA:HB2	2.13	0.77
27:3:185:GLN:HA	27:3:185:GLN:HE21	1.48	0.77
27:3:147:MET:O	27:3:151:VAL:HG23	1.84	0.77
27:3:185:GLN:NE2	27:3:210:THR:HA	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:674:THR:CG2	26:2:392:ARG:NH2	2.43	0.77
25:1:10:ILE:CG2	26:2:407:VAL:HG21	2.15	0.77
26:2:118:LEU:CD1	27:3:39:ASP:OD1	2.31	0.77
26:2:208:THR:HG23	26:2:209:PRO:HD3	1.66	0.77
21:U:256:THR:C	21:U:272:THR:HG22	2.09	0.77
25:1:1:MET:HG3	26:2:415:GLN:O	1.84	0.77
26:2:117:ASN:HD21	27:3:108:ASN:HB3	1.47	0.77
1:A:930:LEU:CD2	1:A:934:LEU:CD1	2.60	0.77
25:1:1:MET:HE3	26:2:415:GLN:C	2.10	0.77
25:1:38:ILE:HG22	25:1:44:PHE:CD1	2.18	0.77
26:2:190:PRO:O	26:2:194:PRO:HD2	1.82	0.77
25:1:2:VAL:CG1	26:2:456:LYS:CG	2.53	0.77
26:2:117:ASN:CG	27:3:42:MET:HE2	2.09	0.77
26:2:42:LEU:HD21	26:2:55:TRP:CB	2.10	0.77
2:B:897:ARG:O	2:B:900:GLU:CG	2.32	0.77
25:1:25:GLU:CD	25:1:35:ILE:HG12	2.09	0.77
17:Q:112:ARG:CZ	18:R:237:LEU:HD11	2.14	0.77
22:V:516:PRO:CB	22:V:706:LYS:NZ	2.48	0.77
4:D:48:ASN:HD22	4:D:57:LEU:HG	1.48	0.77
8:H:74:GLU:O	8:H:75:TYR:CE1	2.38	0.77
19:S:49:ARG:NH1	19:S:96:GLN:O	2.18	0.77
1:A:551:ARG:CD	1:A:625:ASP:OD2	2.25	0.76
9:I:103:ARG:O	9:I:105:GLU:CA	2.33	0.76
26:2:179:LEU:HB3	26:2:184:LEU:HD11	1.65	0.76
13:M:182:ALA:HB1	20:T:152:ASN:CG	2.09	0.76
1:A:270:ALA:O	1:A:272:ASN:N	2.18	0.76
2:B:492:ASP:O	29:Y:45:DT:H2'	1.83	0.76
26:2:221:GLN:HE22	26:2:230:LEU:HB2	1.47	0.76
26:2:208:THR:HG23	26:2:209:PRO:CD	2.16	0.76
26:2:211:GLN:HA	26:2:261:PHE:HZ	1.49	0.76
26:2:218:GLN:NE2	26:2:265:LEU:HA	2.00	0.76
27:3:147:MET:HE1	27:3:157:MET:SD	2.25	0.76
27:3:190:LEU:HD23	27:3:190:LEU:H	1.51	0.76
1:A:298:ALA:HB1	1:A:303:ILE:HD11	1.67	0.76
25:1:1:MET:CE	26:2:440:LEU:HD13	2.16	0.76
1:A:133:SER:O	1:A:134:LYS:C	2.21	0.76
17:Q:180:PHE:CE1	18:R:212:VAL:C	2.62	0.76
27:3:58:ALA:N	27:3:71:TYR:CZ	2.51	0.76
1:A:926:ASN:CG	1:A:931:ARG:HH11	1.93	0.76
26:2:86:SER:HB3	26:2:140:LYS:CE	2.16	0.76
27:3:172:LEU:HD13	27:3:172:LEU:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:875:GLU:OE2	2:B:875:GLU:HA	1.85	0.76
23:W:298:ALA:HA	23:W:421:PHE:CD2	2.21	0.76
26:2:44:VAL:HG13	26:2:45:PHE:CD1	2.20	0.76
2:B:897:ARG:O	2:B:900:GLU:HG3	1.86	0.76
13:M:178:LYS:HB3	20:T:154:LYS:HD3	1.68	0.76
25:1:1:MET:HB3	26:2:413:LEU:CD2	2.15	0.76
26:2:127:LYS:N	26:2:178:LEU:HD23	2.01	0.76
1:A:1290:SER:CB	2:B:250:SER:CB	2.62	0.75
18:R:151:LEU:HD13	18:R:163:LEU:HD21	1.64	0.75
25:1:1:MET:SD	26:2:413:LEU:HB3	2.25	0.75
13:M:16:PRO:HD2	13:M:39:LEU:CD2	2.16	0.75
24:0:54:ARG:HB2	27:3:209:ILE:CG2	2.14	0.75
26:2:234:LEU:CD2	26:2:237:LEU:HD12	2.14	0.75
28:X:70:DG:N2	29:Y:25:DT:O2	2.19	0.75
9:I:102:ALA:C	9:I:104:ALA:N	2.38	0.75
27:3:14:VAL:CG2	27:3:163:VAL:HA	2.16	0.75
22:V:321:GLU:HG2	23:W:499:ASN:CB	2.07	0.75
27:3:11:LEU:HD22	27:3:160:ARG:CG	2.16	0.75
26:2:243:SER:HB3	26:2:258:LEU:HD22	1.69	0.75
27:3:148:ASN:CB	27:3:157:MET:HE2	2.17	0.75
12:L:27:GLU:HB2	12:L:37:ARG:HH12	1.51	0.75
18:R:151:LEU:HD13	18:R:163:LEU:CD2	2.16	0.75
26:2:118:LEU:HD22	27:3:39:ASP:HA	1.65	0.75
27:3:133:LEU:HD23	27:3:177:PHE:HD1	1.49	0.75
8:H:65:TYR:CZ	8:H:70:LEU:HD13	2.22	0.75
9:I:84:HIS:CG	9:I:85:PRO:HD3	1.80	0.75
26:2:180:SER:O	26:2:184:LEU:HG	1.87	0.74
27:3:38:ILE:O	27:3:41:VAL:HG12	1.87	0.74
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.18	0.74
20:T:152:ASN:O	20:T:154:LYS:N	2.20	0.74
26:2:163:MET:HE2	26:2:206:LEU:CD1	2.15	0.74
27:3:8:LEU:HD23	27:3:54:SER:HB3	1.68	0.74
2:B:92:TYR:HA	20:T:141:LEU:CD1	2.10	0.74
25:1:24:ASP:OD2	25:1:57:VAL:HG11	1.85	0.74
26:2:35:TYR:CD2	26:2:62:LEU:HB3	2.22	0.74
13:M:94:ASP:HB2	13:M:99:SER:H	1.53	0.74
22:V:444:HIS:O	22:V:447:PRO:HD2	1.86	0.74
23:W:430:ASN:HB3	23:W:431:PRO:CD	2.17	0.74
25:1:38:ILE:H	25:1:38:ILE:HD13	1.51	0.74
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.68	0.74
9:I:103:ARG:O	9:I:104:ALA:C	2.30	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:100:LEU:CD1	26:2:119:ARG:HG3	2.16	0.74
26:2:132:ASP:O	26:2:135:GLN:HG2	1.88	0.74
18:R:195:PRO:HG2	18:R:199:LYS:C	2.12	0.74
23:W:73:CYS:HB2	23:W:209:TYR:CZ	2.22	0.74
25:1:1:MET:HB2	26:2:418:PHE:CB	2.18	0.74
2:B:490:GLY:O	2:B:491:ARG:CB	2.36	0.74
22:V:415:HIS:HA	22:V:421:TRP:CD1	2.22	0.74
26:2:51:LEU:HD23	26:2:51:LEU:O	1.87	0.74
26:2:53:LYS:HE3	26:2:95:ILE:HD11	1.67	0.74
27:3:24:LYS:O	27:3:25:GLN:O	2.06	0.74
27:3:59:VAL:CA	27:3:71:TYR:CE1	2.70	0.74
22:V:516:PRO:HG2	22:V:706:LYS:CE	2.17	0.74
26:2:196:ILE:HD11	26:2:210:ALA:CB	2.17	0.74
27:3:33:THR:HG23	27:3:36:LYS:N	1.98	0.74
29:Y:63:DG:H3'	29:Y:64:DC:H2'	1.67	0.74
1:A:932:ARG:HG3	1:A:943:LEU:HD11	1.70	0.74
17:Q:187:ILE:CD1	18:R:210:PHE:O	2.29	0.74
22:V:522:TYR:HE2	25:1:62:ASP:CG	1.96	0.74
26:2:160:LEU:HA	26:2:206:LEU:HD11	1.70	0.73
1:A:263:ALA:O	1:A:264:VAL:CB	2.36	0.73
1:A:890:ARG:HH21	1:A:1023:VAL:HG13	1.51	0.73
13:M:11:PRO:C	13:M:12:ARG:HG2	2.07	0.73
22:V:523:VAL:HG21	25:1:20:LEU:HG	1.68	0.73
25:1:34:ILE:HD13	25:1:54:GLN:OE1	1.88	0.73
9:I:84:HIS:CG	9:I:85:PRO:CD	2.59	0.73
17:Q:112:ARG:CZ	18:R:237:LEU:CD1	2.66	0.73
26:2:118:LEU:HD21	27:3:39:ASP:C	2.12	0.73
2:B:175:ASN:HD21	10:J:64:PRO:HG2	1.52	0.73
14:N:347:ASN:ND2	14:N:375:GLU:OE2	2.21	0.73
18:R:225:VAL:CG1	18:R:227:SER:HB2	2.05	0.73
2:B:838:GLN:HB3	2:B:890:ARG:HA	1.70	0.73
25:1:1:MET:HG2	26:2:413:LEU:C	2.14	0.73
26:2:237:LEU:O	26:2:240:LEU:HD13	1.88	0.73
27:3:141:LEU:O	27:3:144:ILE:HG22	1.88	0.73
2:B:793:SER:HA	2:B:944:THR:O	1.89	0.73
26:2:251:VAL:HG11	26:2:254:MET:CG	2.18	0.73
2:B:492:ASP:O	29:Y:45:DT:H2''	1.88	0.73
22:V:667:THR:HA	25:1:62:ASP:OD1	1.89	0.73
27:3:226:TYR:HA	27:3:230:VAL:HG23	1.71	0.73
18:R:163:LEU:O	18:R:164:GLY:O	2.06	0.73
26:2:172:SER:HA	26:2:175:LEU:CD2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:214:TYR:HE2	27:3:216:LYS:HE2	1.53	0.73
17:Q:188:TYR:HA	17:Q:191:LEU:HD13	1.70	0.73
25:1:9:LEU:HD22	25:1:51:ASN:ND2	2.04	0.73
23:W:298:ALA:HA	23:W:421:PHE:HD2	1.52	0.73
26:2:117:ASN:ND2	27:3:42:MET:HE1	2.04	0.73
26:2:199:ALA:HB3	26:2:202:GLN:NE2	2.02	0.73
26:2:218:GLN:HE22	26:2:265:LEU:HA	1.54	0.73
26:2:243:SER:HB2	26:2:258:LEU:HD22	1.71	0.73
14:N:320:VAL:HB	16:P:236:LYS:HE3	1.71	0.72
25:1:1:MET:HG3	26:2:418:PHE:HB2	1.69	0.72
21:U:256:THR:HB	21:U:272:THR:HG22	1.64	0.72
22:V:611:GLY:HA2	22:V:615:PHE:HB3	1.71	0.72
25:1:1:MET:C	26:2:413:LEU:HG	2.12	0.72
2:B:132:VAL:CG2	2:B:141:GLN:CG	2.66	0.72
14:N:317:GLU:HG3	16:P:235:ARG:HG2	1.71	0.72
22:V:689:VAL:HB	26:2:391:ILE:HD11	1.70	0.72
23:W:59:TYR:CD2	23:W:62:ALA:CB	2.70	0.72
26:2:175:LEU:HD22	26:2:216:MET:SD	2.29	0.72
27:3:111:ILE:HG13	27:3:112:VAL:N	2.02	0.72
1:A:264:VAL:CG2	1:A:272:ASN:CG	2.63	0.72
1:A:264:VAL:CG2	1:A:272:ASN:ND2	2.51	0.72
1:A:274:ASP:O	1:A:276:LEU:N	2.22	0.72
24:O:76:LEU:O	24:O:77:LYS:O	2.07	0.72
26:2:60:LEU:HD11	26:2:95:ILE:HB	1.71	0.72
17:Q:23:ARG:HH21	18:R:206:LYS:N	1.86	0.72
26:2:41:CYS:O	26:2:44:VAL:HG12	1.88	0.72
26:2:118:LEU:HD22	27:3:39:ASP:CA	2.19	0.72
26:2:134:SER:O	26:2:138:PRO:HD2	1.89	0.72
22:V:504:LYS:HB3	22:V:654:GLU:O	1.90	0.72
26:2:117:ASN:HB3	27:3:42:MET:CE	2.18	0.72
1:A:18:ILE:HB	1:A:1460:LEU:HD21	1.70	0.72
1:A:79:THR:CG2	13:M:43:ASP:OD1	2.37	0.72
17:Q:68:GLY:O	18:R:226:ASP:CB	2.38	0.72
25:1:28:ALA:HB3	25:1:31:LYS:HB2	1.71	0.72
27:3:12:VAL:HG23	27:3:161:ILE:HG23	1.70	0.72
1:A:932:ARG:HG3	1:A:943:LEU:CD1	2.19	0.72
1:A:1211:LEU:HD11	1:A:1258:ARG:HG3	1.72	0.72
4:D:96:GLU:OE1	4:D:121:ARG:NH1	2.23	0.72
11:K:111:ASP:O	11:K:113:GLN:N	2.19	0.72
22:V:516:PRO:HB2	22:V:706:LYS:HZ1	1.54	0.72
23:W:73:CYS:C	23:W:209:TYR:CE2	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:5:LEU:HD21	26:2:408:LEU:HD13	0.87	0.72
26:2:35:TYR:CG	26:2:62:LEU:HD12	2.25	0.72
27:3:69:PHE:CE1	27:3:139:LYS:HD2	2.25	0.72
27:3:144:ILE:HG12	27:3:147:MET:HE3	1.71	0.72
27:3:217:VAL:HG13	27:3:226:TYR:CZ	2.24	0.72
2:B:1006:VAL:HG23	2:B:1010:LYS:HB2	1.72	0.72
12:L:19:CYS:SG	12:L:20:GLY:N	2.63	0.72
13:M:16:PRO:CD	13:M:39:LEU:CD2	2.67	0.72
26:2:117:ASN:HB2	27:3:104:LEU:HD11	1.71	0.72
26:2:42:LEU:HD12	26:2:59:MET:HE1	1.71	0.72
8:H:65:TYR:CE2	8:H:70:LEU:CB	2.73	0.71
17:Q:19:LYS:O	17:Q:22:ILE:HG13	1.88	0.71
25:1:2:VAL:HG12	26:2:422:LEU:HD13	1.72	0.71
25:1:13:ASP:OD1	25:1:14:PRO:HD2	1.89	0.71
27:3:222:SER:HB2	27:3:226:TYR:HE2	1.55	0.71
1:A:199:TYR:HH	13:M:93:PHE:HE2	0.99	0.71
17:Q:23:ARG:NH2	18:R:206:LYS:N	2.38	0.71
2:B:73:HIS:O	2:B:75:SER:N	2.22	0.71
5:E:3:ASP:HB2	5:E:50:GLU:OE1	1.90	0.71
16:P:206:GLU:C	16:P:208:ARG:H	1.98	0.71
26:2:118:LEU:CD2	27:3:39:ASP:CA	2.68	0.71
26:2:171:VAL:HG12	26:2:216:MET:SD	2.31	0.71
3:C:134:ASN:C	3:C:136:ASP:OD1	2.33	0.71
12:L:35:ARG:HH12	12:L:42:ARG:HH21	1.39	0.71
27:3:66:GLU:CA	27:3:132:LEU:HD12	2.13	0.71
1:A:1304:ILE:O	1:A:1307:VAL:HG22	1.90	0.71
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.73	0.71
23:W:209:TYR:OH	23:W:234:ASP:N	2.23	0.71
23:W:209:TYR:HE1	23:W:233:PHE:CD1	2.08	0.71
25:1:1:MET:HE2	26:2:413:LEU:O	1.90	0.71
27:3:165:LYS:HG3	27:3:203:LEU:CD1	2.20	0.71
17:Q:20:TYR:HE2	18:R:210:PHE:HB2	1.50	0.71
22:V:648:LYS:O	22:V:650:MET:N	2.24	0.71
26:2:30:VAL:H	27:3:25:GLN:CB	2.04	0.71
5:E:64:HIS:NE2	5:E:69:THR:O	2.19	0.71
15:O:79:VAL:HG21	15:O:93:VAL:HG12	1.72	0.71
24:0:54:ARG:CD	27:3:182:PHE:CE1	2.60	0.71
26:2:86:SER:CB	26:2:140:LYS:HE2	2.20	0.71
18:R:195:PRO:HB2	18:R:199:LYS:CB	2.21	0.71
18:R:204:ASN:CG	18:R:205:ASP:H	1.98	0.71
26:2:126:GLY:C	26:2:178:LEU:HD23	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:THR:CB	1:A:610:PRO:HD2	2.20	0.71
17:Q:42:CYS:HB3	17:Q:95:ASN:HD21	1.54	0.71
27:3:18:ASN:CG	27:3:20:ILE:HD13	2.15	0.71
3:C:7:PRO:O	3:C:8:THR:CB	2.39	0.70
25:1:1:MET:HG2	26:2:413:LEU:HB3	1.71	0.70
8:H:66:GLU:O	8:H:67:ASP:HB2	1.89	0.70
22:V:515:SER:HB3	22:V:539:ASN:ND2	2.05	0.70
23:W:589:GLU:O	23:W:594:ALA:HB1	1.91	0.70
27:3:177:PHE:CZ	27:3:203:LEU:HD23	2.27	0.70
1:A:206:ASN:O	1:A:207:GLU:CB	2.33	0.70
20:T:8:ASP:OD2	20:T:10:THR:OG1	2.08	0.70
27:3:133:LEU:HD22	27:3:134:ALA:H	1.56	0.70
2:B:812:ARG:HD3	2:B:814:TYR:OH	1.92	0.70
27:3:33:THR:HG22	27:3:36:LYS:HB2	1.73	0.70
2:B:285:LEU:HD21	2:B:298:MET:HE3	1.73	0.70
17:Q:184:ILE:CD1	18:R:218:LYS:HZ1	2.01	0.70
20:T:155:PRO:O	20:T:157:ALA:N	2.17	0.70
26:2:218:GLN:CD	26:2:265:LEU:HA	2.17	0.70
27:3:51:MET:HE3	27:3:52:ASN:ND2	2.07	0.70
16:P:267:PRO:HB2	16:P:337:LYS:HD2	1.73	0.70
26:2:218:GLN:OE1	26:2:265:LEU:HA	1.92	0.70
1:A:263:ALA:CB	1:A:272:ASN:HB3	2.21	0.70
17:Q:184:ILE:HG12	18:R:211:SER:HB2	1.74	0.70
25:1:8:VAL:HG11	25:1:45:VAL:HG12	1.74	0.70
25:1:13:ASP:CG	25:1:14:PRO:CD	2.58	0.70
25:1:29:LEU:HD23	25:1:30:GLY:N	2.06	0.70
26:2:189:GLU:HA	26:2:192:GLU:HG2	1.72	0.70
14:N:32:ASP:HB3	14:N:34:VAL:HG23	1.73	0.70
23:W:584:TYR:HD1	23:W:594:ALA:HB2	1.51	0.70
1:A:298:ALA:O	17:Q:60:ARG:NE	2.24	0.70
16:P:206:GLU:OE2	16:P:206:GLU:HA	1.91	0.70
18:R:201:LEU:HB3	18:R:203:PHE:HE1	1.57	0.70
18:R:202:PHE:C	18:R:203:PHE:CD1	2.70	0.70
24:0:100:PRO:CG	27:3:208:ASP:OD2	2.39	0.70
1:A:643:LYS:NZ	21:U:299:LYS:O	2.22	0.70
1:A:1158:LEU:HD21	1:A:1308:TYR:CD2	2.25	0.70
1:A:1307:VAL:O	1:A:1308:TYR:HB3	1.91	0.70
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.24	0.70
23:W:696:TRP:CD1	23:W:697:ILE:HG13	2.25	0.70
26:2:31:LEU:CD1	27:3:33:THR:HG21	2.22	0.70
1:A:505:LEU:O	2:B:1106:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:GLU:HG2	3:C:228:ARG:HG3	1.73	0.69
25:1:2:VAL:HG12	26:2:456:LYS:HE2	1.74	0.69
25:1:18:GLN:CB	25:1:44:PHE:HE2	2.01	0.69
27:3:162:LEU:HA	27:3:192:ASP:OD1	1.92	0.69
5:E:64:HIS:CD2	5:E:68:PRO:C	2.70	0.69
23:W:59:TYR:CE1	23:W:62:ALA:HB2	2.26	0.69
26:2:130:SER:O	26:2:133:THR:HG22	1.92	0.69
26:2:163:MET:O	26:2:167:PRO:HD2	1.91	0.69
1:A:931:ARG:C	1:A:933:THR:H	1.99	0.69
2:B:429:PHE:H	20:T:160:GLN:HG2	1.55	0.69
27:3:144:ILE:CG1	27:3:147:MET:HE3	2.23	0.69
2:B:721:ARG:HG3	2:B:939:HIS:O	1.91	0.69
22:V:516:PRO:HB2	22:V:706:LYS:NZ	2.08	0.69
24:0:54:ARG:NE	27:3:182:PHE:CD1	2.60	0.69
25:1:1:MET:CG	26:2:415:GLN:O	2.41	0.69
26:2:185:MET:SD	26:2:232:GLU:HB2	2.31	0.69
1:A:79:THR:CG2	13:M:43:ASP:CG	2.65	0.69
1:A:1319:LYS:HE2	1:A:1333:GLU:OE2	1.93	0.69
18:R:127:ASN:HD21	18:R:140:LYS:HD3	1.57	0.69
22:V:674:THR:OG1	26:2:392:ARG:NE	2.25	0.69
26:2:118:LEU:HD11	27:3:43:VAL:HG23	1.75	0.69
26:2:163:MET:CE	26:2:206:LEU:HB3	2.23	0.69
26:2:211:GLN:HA	26:2:261:PHE:CE1	2.28	0.69
27:3:69:PHE:CZ	27:3:139:LYS:HD2	2.27	0.69
2:B:92:TYR:HD1	20:T:141:LEU:CD2	2.04	0.69
19:S:115:LYS:HB2	19:S:143:TRP:HB3	1.73	0.69
25:1:53:LEU:HD12	25:1:53:LEU:H	1.57	0.69
26:2:181:GLN:HG3	26:2:229:ASP:CG	2.18	0.69
1:A:138:LYS:NZ	1:A:1441:GLU:OE2	2.25	0.69
1:A:156:GLY:HA2	1:A:181:HIS:CD2	2.26	0.69
2:B:92:TYR:CD1	20:T:141:LEU:HD21	2.20	0.69
2:B:905:ASP:OD2	2:B:922:ARG:NH2	2.22	0.69
18:R:193:ASN:ND2	18:R:197:LYS:O	2.22	0.69
25:1:34:ILE:HG12	25:1:50:VAL:CG1	2.18	0.69
26:2:81:LYS:HD2	26:2:89:LEU:CD2	2.20	0.69
26:2:140:LYS:HD3	26:2:162:PHE:HE1	1.58	0.69
1:A:269:SER:O	1:A:270:ALA:HB3	1.92	0.69
1:A:608:THR:OG1	1:A:610:PRO:HG2	1.93	0.69
3:C:56:SER:HG	3:C:158:GLU:H	1.39	0.69
13:M:89:GLY:O	13:M:90:ALA:HB2	1.93	0.69
22:V:321:GLU:CD	23:W:499:ASN:N	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:612:ASP:CG	22:V:635:GLN:CD	2.60	0.69
25:1:4:VAL:CG1	26:2:411:GLN:O	2.39	0.69
27:3:215:LEU:HD12	27:3:230:VAL:CG1	2.23	0.69
13:M:238:LYS:HD2	13:M:299:LEU:HA	1.75	0.68
13:M:178:LYS:HZ2	20:T:156:VAL:HG11	1.57	0.68
22:V:516:PRO:CA	25:1:15:ALA:O	2.40	0.68
25:1:55:GLU:OE2	26:2:402:ARG:HG3	1.93	0.68
26:2:81:LYS:HE3	26:2:93:LEU:CD2	2.20	0.68
26:2:176:ALA:HB1	26:2:178:LEU:CD1	2.23	0.68
1:A:1291:ASN:OD1	2:B:250:SER:OG	2.09	0.68
13:M:7:LEU:CD2	13:M:10:LEU:HD13	2.23	0.68
26:2:48:LEU:CB	26:2:49:PRO:HD3	2.19	0.68
27:3:34:LEU:O	27:3:34:LEU:HD13	1.92	0.68
22:V:516:PRO:HB3	25:1:15:ALA:CB	2.04	0.68
26:2:251:VAL:HG12	26:2:254:MET:H	1.58	0.68
27:3:24:LYS:HE2	27:3:220:MET:SD	2.34	0.68
1:A:471:GLY:O	1:A:521:VAL:HG23	1.93	0.68
2:B:274:ARG:NH1	2:B:281:ASP:OD1	2.25	0.68
25:1:10:ILE:HG21	26:2:407:VAL:HG21	1.76	0.68
29:Y:24:DC:C2'	29:Y:25:DT:H73	2.23	0.68
1:A:263:ALA:CA	1:A:272:ASN:O	2.41	0.68
3:C:272:LEU:HD21	11:K:84:GLN:HG2	1.74	0.68
17:Q:68:GLY:O	18:R:226:ASP:CG	2.35	0.68
18:R:164:GLY:CA	18:R:203:PHE:HZ	1.87	0.68
18:R:202:PHE:O	18:R:203:PHE:CD1	2.46	0.68
1:A:1304:ILE:O	1:A:1307:VAL:N	2.27	0.68
27:3:114:GLU:O	27:3:118:LEU:HD23	1.92	0.68
26:2:170:ALA:HB1	26:2:213:TRP:CZ3	2.29	0.68
27:3:18:ASN:CG	27:3:64:ILE:HD11	2.19	0.68
1:A:202:TRP:H	1:A:212:LYS:HA	1.58	0.68
1:A:487:SER:HB2	1:A:673:GLN:HE22	1.59	0.68
17:Q:113:ARG:CD	18:R:222:SER:CB	2.72	0.68
17:Q:180:PHE:CZ	18:R:212:VAL:C	2.71	0.68
23:W:584:TYR:CE1	23:W:614:TYR:O	2.46	0.68
26:2:211:GLN:HB3	26:2:261:PHE:HE1	1.59	0.68
27:3:159:SER:OG	27:3:189:ILE:HD12	1.94	0.68
1:A:1052:ARG:NH1	1:A:1056:GLU:OE1	2.27	0.68
17:Q:113:ARG:NH2	18:R:218:LYS:CG	2.57	0.68
26:2:199:ALA:CB	26:2:202:GLN:HE22	2.02	0.68
8:H:17:PRO:O	8:H:19:GLY:N	2.27	0.67
17:Q:184:ILE:HG12	18:R:211:SER:CB	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PRO:HD2	1:A:62:GLN:HG2	1.75	0.67
1:A:199:TYR:OH	13:M:93:PHE:HZ	1.69	0.67
1:A:455:ILE:HD13	1:A:520:MET:HE1	1.76	0.67
26:2:118:LEU:HD13	27:3:39:ASP:OD1	1.92	0.67
17:Q:109:HIS:CE1	18:R:233:ILE:HG21	2.30	0.67
25:1:39:ASP:OD1	25:1:43:VAL:HB	1.94	0.67
1:A:201:GLU:CG	1:A:212:LYS:HB3	2.25	0.67
11:K:82:SER:OG	11:K:84:GLN:OE1	2.12	0.67
23:W:419:GLU:CB	23:W:420:PRO:CD	2.45	0.67
27:3:187:GLN:HG3	27:3:189:ILE:CG1	2.24	0.67
27:3:187:GLN:CG	27:3:189:ILE:HG12	2.24	0.67
1:A:67:ARG:NH2	13:M:45:VAL:O	2.28	0.67
22:V:667:THR:HA	25:1:62:ASP:CG	2.19	0.67
26:2:56:VAL:O	26:2:60:LEU:HG	1.94	0.67
26:2:172:SER:O	26:2:175:LEU:HD23	1.95	0.67
27:3:111:ILE:O	27:3:115:ILE:HD13	1.94	0.67
5:E:64:HIS:CD2	5:E:68:PRO:HA	2.29	0.67
9:I:61:GLU:C	9:I:63:ASP:N	2.52	0.67
21:U:226:GLU:HA	21:U:226:GLU:OE2	1.93	0.67
2:B:685:LYS:HD2	2:B:691:SER:HA	1.77	0.67
22:V:325:ARG:HH21	23:W:499:ASN:CB	1.95	0.67
17:Q:101:ASN:O	17:Q:103:VAL:N	2.28	0.67
18:R:195:PRO:HB2	18:R:199:LYS:HB3	1.77	0.67
22:V:516:PRO:CD	22:V:706:LYS:NZ	2.54	0.67
26:2:181:GLN:CD	26:2:229:ASP:HB2	2.19	0.67
27:3:217:VAL:HG13	27:3:226:TYR:CE2	2.30	0.67
1:A:932:ARG:CG	1:A:943:LEU:HD21	2.25	0.67
1:A:1154:ALA:HB1	1:A:1310:HIS:HE1	1.59	0.67
1:A:1471:PHE:CE1	6:F:64:ARG:HD3	2.30	0.67
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.60	0.67
26:2:56:VAL:HG11	26:2:91:SER:HB2	1.77	0.67
2:B:1062:ARG:HH21	2:B:1065:GLY:H	1.41	0.67
24:0:97:ASP:C	27:3:208:ASP:HB2	2.12	0.67
27:3:130:GLU:HB2	27:3:173:GLN:NE2	2.09	0.67
2:B:57:ARG:NH1	2:B:537:GLN:OE1	2.27	0.66
1:A:729:PRO:HG2	21:U:250:MET:HB2	1.76	0.66
1:A:1158:LEU:CG	1:A:1308:TYR:CD2	2.78	0.66
7:G:10:GLU:HB3	7:G:67:LEU:HD11	1.77	0.66
9:I:104:ALA:O	9:I:105:GLU:C	2.37	0.66
26:2:160:LEU:HD12	26:2:160:LEU:H	1.60	0.66
27:3:59:VAL:N	27:3:71:TYR:CD1	2.63	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:207:CYS:SG	27:3:214:TYR:HB2	2.34	0.66
1:A:426:ARG:HD2	13:M:40:VAL:HG21	1.77	0.66
1:A:609:HIS:N	1:A:610:PRO:HD3	2.07	0.66
3:C:148:ILE:HG13	10:J:5:VAL:HG22	1.77	0.66
18:R:195:PRO:CB	18:R:199:LYS:HB2	2.14	0.66
28:X:14:DA:H2''	28:X:15:DA:C8	2.30	0.66
17:Q:184:ILE:HD11	18:R:218:LYS:HZ2	1.61	0.66
22:V:366:ASN:ND2	22:V:613:THR:HG22	1.93	0.66
25:1:1:MET:HE3	26:2:415:GLN:CA	2.24	0.66
26:2:117:ASN:HD21	27:3:108:ASN:CA	2.05	0.66
27:3:146:ARG:O	27:3:149:LYS:HG2	1.95	0.66
1:A:199:TYR:CE2	13:M:93:PHE:HZ	2.14	0.66
5:E:29:THR:HB	5:E:32:GLU:HG3	1.77	0.66
25:1:8:VAL:HG12	25:1:9:LEU:N	2.10	0.66
26:2:218:GLN:CG	26:2:268:PHE:HB3	2.26	0.66
2:B:91:ILE:HG23	20:T:141:LEU:CD1	2.20	0.66
13:M:10:LEU:C	13:M:12:ARG:N	2.46	0.66
27:3:45:GLY:O	27:3:49:LEU:HD23	1.96	0.66
17:Q:180:PHE:CE1	18:R:213:ASP:CA	2.75	0.66
20:T:177:ARG:N	20:T:178:ALA:O	2.27	0.66
1:A:549:THR:O	1:A:589:LYS:NZ	2.27	0.66
17:Q:141:ALA:HB1	17:Q:152:PHE:HE2	1.60	0.66
18:R:204:ASN:CG	18:R:205:ASP:N	2.53	0.66
1:A:1309:MET:HG3	1:A:1309:MET:O	1.95	0.66
9:I:65:LEU:O	9:I:122:ARG:NH2	2.29	0.66
25:1:59:GLU:OE2	26:2:402:ARG:CZ	2.41	0.66
26:2:30:VAL:CB	27:3:25:GLN:O	2.34	0.66
26:2:117:ASN:CB	27:3:42:MET:HE3	2.22	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
26:2:171:VAL:HG13	26:2:216:MET:CB	2.26	0.66
26:2:189:GLU:HA	26:2:192:GLU:CG	2.26	0.66
1:A:926:ASN:CB	1:A:931:ARG:HH12	2.04	0.65
2:B:132:VAL:HG23	2:B:141:GLN:CB	2.26	0.65
12:L:35:ARG:NH1	12:L:42:ARG:HE	1.94	0.65
25:1:35:ILE:HG22	25:1:46:ILE:HD12	1.78	0.65
27:3:106:SER:O	27:3:110:VAL:HG23	1.97	0.65
21:U:284:PRO:O	21:U:286:THR:N	2.28	0.65
25:1:1:MET:SD	26:2:419:GLU:HB2	2.37	0.65
25:1:10:ILE:HG22	26:2:407:VAL:HG21	1.79	0.65
8:H:72:ASP:O	8:H:73:GLY:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:355:CYS:HG	22:V:381:TRP:CD1	2.14	0.65
22:V:631:GLY:O	22:V:632:SER:HB3	1.96	0.65
26:2:270:LEU:HD23	26:2:273:GLN:HE21	1.62	0.65
27:3:137:LEU:HB3	27:3:180:VAL:CG1	2.20	0.65
1:A:541:THR:O	1:A:545:VAL:HG23	1.97	0.65
1:A:929:ALA:O	1:A:930:LEU:HB2	1.95	0.65
1:A:930:LEU:HD23	1:A:934:LEU:CA	2.27	0.65
16:P:206:GLU:HG2	16:P:236:LYS:HZ1	1.57	0.65
23:W:696:TRP:HD1	23:W:697:ILE:HG13	1.62	0.65
26:2:57:MET:HA	26:2:60:LEU:HD11	1.77	0.65
26:2:236:PHE:CZ	26:2:262:LEU:HD22	2.32	0.65
1:A:42:LYS:HE3	1:A:56:GLY:HA3	1.79	0.65
1:A:1022:ILE:HG23	1:A:1023:VAL:HG23	1.77	0.65
1:A:1319:LYS:HG2	1:A:1333:GLU:OE2	1.96	0.65
25:1:34:ILE:CG1	25:1:50:VAL:HG11	2.21	0.65
1:A:358:ARG:HH21	2:B:1076:GLU:HA	1.62	0.65
26:2:28:PRO:CA	27:3:25:GLN:C	2.69	0.65
26:2:45:PHE:HB2	26:2:51:LEU:CD1	2.26	0.65
2:B:73:HIS:C	2:B:75:SER:H	2.04	0.65
18:R:195:PRO:O	18:R:196:ASP:HB3	1.95	0.65
27:3:184:ALA:CA	27:3:187:GLN:HG2	2.25	0.65
1:A:623:PRO:C	1:A:625:ASP:H	2.04	0.65
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.79	0.65
4:D:26:PHE:HZ	7:G:42:TYR:HA	1.60	0.65
26:2:117:ASN:ND2	27:3:42:MET:CE	2.60	0.65
1:A:190:ARG:NH2	28:X:58:DT:OP2	2.29	0.65
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.32	0.65
8:H:146:LYS:O	8:H:148:LEU:N	2.29	0.65
13:M:86:LYS:NZ	28:X:40:DT:C4	2.64	0.65
26:2:192:GLU:HG3	26:2:193:PRO:CD	2.19	0.65
27:3:17:ALA:CB	27:3:63:HIS:HD2	2.10	0.65
27:3:33:THR:CG2	27:3:36:LYS:HB2	2.26	0.65
27:3:59:VAL:HB	27:3:71:TYR:CD1	2.25	0.65
27:3:130:GLU:HB2	27:3:173:GLN:HE22	1.61	0.65
1:A:912:SER:H	1:A:1327:GLU:HB3	1.61	0.64
5:E:41:LYS:HG3	5:E:46:ASP:CG	2.22	0.64
26:2:266:ARG:O	26:2:270:LEU:HB2	1.97	0.64
1:A:367:ILE:HG13	1:A:496:PHE:HD1	1.62	0.64
16:P:167:ASN:ND2	29:Y:79:DC:O2	2.26	0.64
18:R:195:PRO:CG	18:R:199:LYS:C	2.69	0.64
26:2:160:LEU:HB3	26:2:206:LEU:CD1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:211:GLN:CB	26:2:261:PHE:HE1	2.11	0.64
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.78	0.64
22:V:426:VAL:HG13	22:V:427:MET:H	1.63	0.64
25:1:35:ILE:HG22	25:1:46:ILE:CD1	2.27	0.64
26:2:173:GLN:CD	26:2:179:LEU:HD21	2.21	0.64
27:3:14:VAL:HG22	27:3:163:VAL:HA	1.78	0.64
9:I:63:ASP:OD1	9:I:66:THR:OG1	2.16	0.64
23:W:581:LEU:HD21	23:W:608:ILE:HG21	1.78	0.64
27:3:192:ASP:HB2	27:3:231:PHE:CE1	2.32	0.64
1:A:608:THR:HB	1:A:610:PRO:CD	2.28	0.64
1:A:1117:VAL:O	1:A:1118:THR:C	2.40	0.64
9:I:84:HIS:H	9:I:84:HIS:CD2	2.13	0.64
12:L:35:ARG:HH12	12:L:42:ARG:HE	1.44	0.64
18:R:225:VAL:HG12	18:R:227:SER:CB	2.06	0.64
26:2:159:VAL:HG11	26:2:161:HIS:HD2	1.62	0.64
26:2:202:GLN:HE21	26:2:202:GLN:H	1.44	0.64
1:A:1309:MET:O	1:A:1311:LEU:HD12	1.97	0.64
20:T:20:LEU:HD23	20:T:113:ARG:HG2	1.79	0.64
22:V:366:ASN:ND2	22:V:613:THR:HG21	2.05	0.64
26:2:42:LEU:CD2	26:2:55:TRP:HB2	2.13	0.64
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.78	0.64
2:B:906:GLN:HG2	12:L:45:TYR:OH	1.98	0.64
2:B:1062:ARG:HH12	2:B:1075:MET:H	1.45	0.64
18:R:154:LEU:CD2	18:R:163:LEU:CD2	2.73	0.64
26:2:220:LEU:O	26:2:220:LEU:HD13	1.98	0.64
27:3:64:ILE:HB	27:3:123:ASP:OD2	1.98	0.64
27:3:70:LEU:HD13	27:3:115:ILE:CD1	2.28	0.64
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.79	0.64
23:W:59:TYR:CZ	23:W:62:ALA:HB2	2.29	0.64
27:3:58:ALA:CA	27:3:71:TYR:OH	2.39	0.64
1:A:640:LEU:HD23	1:A:645:LEU:HD11	1.79	0.64
5:E:46:ASP:C	5:E:48:PRO:HD3	2.20	0.64
8:H:137:VAL:HG22	8:H:138:ASP:H	1.63	0.64
17:Q:25:PHE:O	18:R:219:LEU:HD21	1.98	0.64
1:A:51:ARG:H	1:A:52:PRO:HD2	1.61	0.64
2:B:761:THR:H	2:B:764:MET:CE	2.11	0.64
2:B:823:PHE:HA	13:M:140:ASN:HD21	1.63	0.64
13:M:16:PRO:CD	13:M:39:LEU:HD23	2.27	0.64
22:V:517:GLU:HB2	22:V:713:LEU:HD22	1.79	0.64
25:1:59:GLU:CD	26:2:402:ARG:NH1	2.56	0.64
26:2:117:ASN:CG	27:3:108:ASN:ND2	2.50	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:181:ALA:HA	18:R:184:ALA:HB3	1.80	0.63
26:2:100:LEU:HG	26:2:119:ARG:NE	2.13	0.63
26:2:177:GLN:OE1	26:2:220:LEU:HD22	1.98	0.63
27:3:17:ALA:HB1	27:3:63:HIS:HD2	1.63	0.63
27:3:131:THR:O	27:3:133:LEU:HD13	1.97	0.63
27:3:144:ILE:HD13	27:3:147:MET:HE3	1.80	0.63
17:Q:113:ARG:HD2	18:R:222:SER:CB	2.28	0.63
26:2:117:ASN:ND2	27:3:108:ASN:CA	2.57	0.63
27:3:160:ARG:NH2	27:3:190:LEU:HD12	2.13	0.63
1:A:1246:ILE:HD11	1:A:1258:ARG:HD2	1.81	0.63
16:P:297:LYS:O	16:P:299:ARG:N	2.26	0.63
18:R:212:VAL:O	18:R:213:ASP:CG	2.41	0.63
25:1:38:ILE:HB	25:1:44:PHE:HE1	1.63	0.63
7:G:78:ARG:NH1	7:G:79:PRO:O	2.31	0.63
26:2:28:PRO:HA	27:3:33:THR:HB	1.81	0.63
26:2:60:LEU:HD11	26:2:95:ILE:CB	2.29	0.63
27:3:149:LYS:HG3	27:3:150:GLU:N	2.12	0.63
27:3:214:TYR:CE2	27:3:216:LYS:HE2	2.32	0.63
1:A:108:ARG:NH1	1:A:145:TYR:OH	2.32	0.63
25:1:2:VAL:HG12	26:2:422:LEU:CD1	2.27	0.63
16:P:165:LEU:HD23	16:P:168:ILE:HD11	1.80	0.63
2:B:747:LEU:HD11	2:B:810:PHE:CZ	2.34	0.63
25:1:35:ILE:HA	25:1:46:ILE:HG13	1.80	0.63
26:2:35:TYR:CZ	26:2:62:LEU:HG	2.34	0.63
26:2:140:LYS:HG2	26:2:162:PHE:CE1	2.33	0.63
26:2:258:LEU:HG	26:2:262:LEU:CD2	2.28	0.63
1:A:285:LYS:HE3	13:M:80:LEU:HD23	1.80	0.63
17:Q:105:TYR:CE1	18:R:234:GLU:OE1	2.40	0.63
22:V:516:PRO:CB	22:V:706:LYS:HZ1	2.11	0.63
26:2:123:LEU:O	26:2:123:LEU:HD23	1.99	0.63
26:2:173:GLN:HG2	26:2:179:LEU:HG	1.81	0.63
27:3:64:ILE:CG1	27:3:123:ASP:HB3	2.29	0.63
27:3:70:LEU:CD1	27:3:115:ILE:HD11	2.27	0.63
1:A:930:LEU:HD23	1:A:934:LEU:HA	1.79	0.62
2:B:223:SER:OG	2:B:232:THR:O	2.17	0.62
27:3:134:ALA:HB2	27:3:176:ASN:OD1	1.99	0.62
27:3:205:GLN:O	27:3:208:ASP:CG	2.42	0.62
3:C:56:SER:OG	3:C:158:GLU:N	2.21	0.62
6:F:48:ASN:ND2	6:F:51:ARG:O	2.26	0.62
26:2:89:LEU:HD23	26:2:89:LEU:O	1.99	0.62
26:2:93:LEU:HA	26:2:96:TRP:HD1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:165:LYS:O	27:3:165:LYS:HD3	1.98	0.62
1:A:265:VAL:HA	1:A:272:ASN:HB2	1.80	0.62
2:B:588:ARG:NH1	2:B:669:GLU:OE2	2.31	0.62
12:L:16:ILE:HG21	12:L:47:LYS:HD2	1.81	0.62
1:A:455:ILE:HG21	1:A:520:MET:HE1	1.81	0.62
1:A:673:GLN:O	1:A:677:ASN:HB2	1.98	0.62
1:A:931:ARG:O	1:A:933:THR:N	2.33	0.62
2:B:80:GLU:O	2:B:82:PRO:HD3	1.98	0.62
5:E:64:HIS:CD2	5:E:68:PRO:CA	2.81	0.62
13:M:90:ALA:HB2	13:M:100:LYS:HE3	1.80	0.62
18:R:195:PRO:CD	18:R:199:LYS:HB2	2.25	0.62
23:W:584:TYR:CG	23:W:594:ALA:HB2	2.34	0.62
25:1:18:GLN:NE2	25:1:44:PHE:HZ	1.97	0.62
25:1:38:ILE:HB	25:1:44:PHE:CE1	2.35	0.62
25:1:50:VAL:HA	25:1:53:LEU:HD13	1.82	0.62
1:A:924:TYR:O	1:A:926:ASN:ND2	2.32	0.62
2:B:749:HIS:CD2	2:B:810:PHE:CD1	2.88	0.62
13:M:7:LEU:HD21	13:M:10:LEU:CD1	2.29	0.62
19:S:48:GLU:OE1	19:S:101:ARG:NH2	2.33	0.62
23:W:59:TYR:CE2	23:W:62:ALA:HB2	2.22	0.62
27:3:133:LEU:HD22	27:3:134:ALA:N	2.14	0.62
1:A:931:ARG:CZ	1:A:931:ARG:HA	2.29	0.62
5:E:84:ILE:HD11	28:X:65:DG:P	2.39	0.62
14:N:318:ASP:OD1	16:P:239:ARG:NH2	2.32	0.62
15:O:84:VAL:HG23	15:O:85:THR:HG23	1.81	0.62
17:Q:60:ARG:O	17:Q:64:ASN:ND2	2.28	0.62
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.62	0.62
25:1:47:ALA:HB1	25:1:50:VAL:HB	1.81	0.62
1:A:133:SER:O	1:A:135:GLY:N	2.33	0.62
17:Q:109:HIS:HE1	18:R:233:ILE:HG21	1.64	0.62
23:W:209:TYR:OH	23:W:233:PHE:C	2.42	0.62
26:2:189:GLU:O	26:2:193:PRO:HD2	2.00	0.62
17:Q:113:ARG:CZ	18:R:218:LYS:HG3	2.29	0.62
22:V:325:ARG:HH21	23:W:499:ASN:CG	2.08	0.62
25:1:8:VAL:O	26:2:407:VAL:HG12	1.99	0.62
26:2:31:LEU:CG	27:3:33:THR:HB	2.28	0.62
26:2:46:ARG:CD	26:2:85:GLU:HB2	2.30	0.62
2:B:998:ASP:OD1	2:B:999:ALA:N	2.32	0.62
5:E:46:ASP:C	5:E:48:PRO:CD	2.73	0.62
8:H:108:ALA:O	8:H:110:THR:N	2.32	0.62
24:0:100:PRO:HG3	27:3:208:ASP:OD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:197:THR:HG21	26:2:239:GLN:CD	2.25	0.62
2:B:132:VAL:CG2	2:B:141:GLN:HB3	2.28	0.62
2:B:249:LYS:O	2:B:249:LYS:HG2	1.98	0.62
25:1:1:MET:HG2	26:2:414:SER:N	2.15	0.62
26:2:44:VAL:HG13	26:2:45:PHE:HD1	1.59	0.62
27:3:9:ASN:O	27:3:56:LYS:HD3	1.99	0.62
1:A:622:SER:C	1:A:624:GLY:N	2.58	0.61
2:B:898:THR:O	2:B:900:GLU:HG3	2.00	0.61
21:U:243:GLU:CD	21:U:246:ARG:HH12	2.08	0.61
23:W:59:TYR:OH	23:W:63:TYR:CE2	2.52	0.61
26:2:218:GLN:HG2	26:2:268:PHE:HB3	1.82	0.61
27:3:18:ASN:O	27:3:21:TRP:HD1	1.83	0.61
2:B:1144:THR:O	2:B:1146:ILE:N	2.33	0.61
15:O:75:VAL:HG22	15:O:94:LYS:HG2	1.81	0.61
26:2:117:ASN:CG	27:3:108:ASN:CG	2.65	0.61
27:3:190:LEU:H	27:3:190:LEU:CD2	2.11	0.61
1:A:1316:ASN:ND2	1:A:1318:LYS:HE3	2.14	0.61
1:A:1319:LYS:HB3	1:A:1331:LEU:HB3	1.81	0.61
3:C:154:ARG:HD3	10:J:65:LEU:HD11	1.81	0.61
14:N:319:ASP:C	14:N:321:SER:H	2.08	0.61
16:P:205:ARG:O	16:P:206:GLU:C	2.42	0.61
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.64	0.61
25:1:1:MET:HB2	26:2:418:PHE:HB3	1.81	0.61
26:2:30:VAL:CG2	27:3:25:GLN:CB	2.48	0.61
26:2:60:LEU:CD1	26:2:95:ILE:HB	2.31	0.61
28:X:32:DT:H4'	28:X:33:DT:H5'	1.82	0.61
2:B:42:GLN:HG2	2:B:43:GLN:N	2.15	0.61
2:B:380:ARG:NE	2:B:609:GLU:OE2	2.34	0.61
23:W:584:TYR:HB2	23:W:594:ALA:HB2	1.81	0.61
1:A:199:TYR:CZ	13:M:93:PHE:CZ	2.87	0.61
1:A:344:LYS:HA	1:A:1435:THR:HG21	1.82	0.61
2:B:1040:GLN:H	2:B:1040:GLN:CD	2.08	0.61
16:P:206:GLU:CG	16:P:236:LYS:HZ2	1.70	0.61
16:P:298:PRO:O	16:P:299:ARG:C	2.43	0.61
23:W:37:HIS:CE1	23:W:454:VAL:CG1	2.83	0.61
27:3:184:ALA:HA	27:3:187:GLN:CG	2.29	0.61
1:A:1158:LEU:CG	1:A:1308:TYR:CE2	2.83	0.61
2:B:78:VAL:O	2:B:78:VAL:HG12	2.00	0.61
13:M:50:SER:O	13:M:53:ARG:HB2	2.01	0.61
27:3:46:ASN:CG	27:3:104:LEU:HD22	2.25	0.61
1:A:685:HIS:HB3	2:B:784:SER:OG	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:ILE:HG13	1:A:885:GLN:HG3	1.82	0.61
1:A:1158:LEU:HD13	1:A:1336:LEU:HD22	1.81	0.61
1:A:1177:TYR:OH	9:I:28:GLU:OE2	2.14	0.61
26:2:251:VAL:CG1	26:2:254:MET:HG3	2.30	0.61
27:3:100:LYS:HG3	27:3:101:TYR:N	2.16	0.61
1:A:1112:VAL:O	21:U:252:LYS:HB2	1.99	0.61
2:B:247:ALA:O	19:S:169:LYS:NZ	2.25	0.61
24:0:77:LYS:H	24:0:77:LYS:HD2	1.66	0.61
2:B:513:GLU:CD	2:B:707:CYS:HB2	2.26	0.61
2:B:823:PHE:HA	13:M:140:ASN:ND2	2.16	0.61
8:H:66:GLU:HA	8:H:66:GLU:OE2	2.00	0.61
18:R:163:LEU:O	18:R:163:LEU:HD12	2.01	0.61
22:V:368:ALA:O	22:V:371:VAL:HG22	2.00	0.61
27:3:24:LYS:O	27:3:25:GLN:C	2.44	0.61
2:B:529:MET:SD	2:B:623:ARG:HB2	2.41	0.61
10:J:64:PRO:O	10:J:66:GLU:N	2.34	0.61
26:2:203:PHE:HD2	26:2:205:LEU:HD23	1.64	0.61
26:2:236:PHE:CE2	26:2:262:LEU:HD13	2.36	0.61
27:3:8:LEU:HA	27:3:54:SER:HB3	1.83	0.61
1:A:379:GLY:HA2	1:A:475:ARG:O	2.01	0.60
7:G:52:ASP:H	7:G:72:TYR:HA	1.64	0.60
16:P:153:THR:N	16:P:326:GLU:OE2	2.34	0.60
25:1:13:ASP:OD1	25:1:14:PRO:CD	2.48	0.60
26:2:30:VAL:HG12	26:2:34:LEU:HD23	1.82	0.60
26:2:56:VAL:HG11	26:2:91:SER:CB	2.31	0.60
1:A:265:VAL:C	1:A:272:ASN:OD1	2.44	0.60
1:A:786:ALA:O	1:A:826:SER:HB3	2.00	0.60
1:A:1304:ILE:O	1:A:1307:VAL:HG23	2.00	0.60
1:A:930:LEU:HB3	1:A:934:LEU:CB	2.23	0.60
2:B:968:ASN:OD1	2:B:969:PRO:HD2	2.00	0.60
24:0:55:LEU:HD12	27:3:178:MET:CE	2.31	0.60
25:1:1:MET:HA	26:2:414:SER:N	2.15	0.60
27:3:58:ALA:CA	27:3:71:TYR:CE2	2.76	0.60
1:A:95:PHE:N	1:A:311:GLN:OE1	2.31	0.60
2:B:874:PRO:C	2:B:876:ASN:H	2.08	0.60
12:L:17:TYR:CD1	12:L:46:LYS:HG3	2.29	0.60
13:M:91:ALA:O	13:M:93:PHE:N	2.35	0.60
25:1:10:ILE:C	25:1:10:ILE:HD13	2.26	0.60
27:3:143:TYR:O	27:3:146:ARG:HG2	2.01	0.60
2:B:333:GLU:OE1	19:S:53:ASN:ND2	2.27	0.60
5:E:64:HIS:CG	5:E:68:PRO:HA	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:65:LEU:HD22	9:I:122:ARG:HG2	1.82	0.60
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.67	0.60
17:Q:52:LEU:HB3	17:Q:54:PHE:CD2	2.32	0.60
23:W:73:CYS:CB	23:W:209:TYR:CZ	2.84	0.60
26:2:42:LEU:HD12	26:2:59:MET:HE3	1.83	0.60
27:3:21:TRP:O	27:3:24:LYS:HB2	2.02	0.60
27:3:196:LEU:CD2	27:3:223:LEU:HD23	2.25	0.60
25:1:1:MET:HA	26:2:413:LEU:HA	1.83	0.60
1:A:26:LEU:HD23	2:B:1168:ALA:HB2	1.84	0.60
1:A:622:SER:C	1:A:624:GLY:H	2.04	0.60
1:A:1196:TYR:OH	1:A:1247:PHE:O	2.12	0.60
2:B:898:THR:O	2:B:900:GLU:N	2.35	0.60
9:I:80:ARG:HD3	9:I:95:VAL:HG12	1.83	0.60
18:R:118:TRP:NE1	18:R:122:GLU:OE1	2.34	0.60
27:3:42:MET:HE2	27:3:108:ASN:CG	2.27	0.60
28:X:70:DG:N2	29:Y:25:DT:C2	2.70	0.60
2:B:676:ALA:HB2	2:B:693:TYR:CD1	2.36	0.60
2:B:790:GLN:HA	2:B:968:ASN:HD22	1.67	0.60
23:W:419:GLU:O	23:W:420:PRO:O	2.19	0.60
26:2:259:LEU:HD12	26:2:259:LEU:C	2.27	0.60
27:3:222:SER:HB2	27:3:226:TYR:CE2	2.37	0.60
1:A:201:GLU:HG3	1:A:212:LYS:HB3	1.84	0.60
2:B:489:ILE:HG21	2:B:522:LEU:HD13	1.83	0.60
23:W:209:TYR:CE1	23:W:233:PHE:CD1	2.89	0.60
23:W:584:TYR:HB2	23:W:594:ALA:CB	2.32	0.60
26:2:28:PRO:HD2	27:3:25:GLN:CD	2.26	0.60
26:2:30:VAL:HG23	27:3:25:GLN:HB2	1.74	0.60
26:2:164:VAL:HG13	26:2:209:PRO:HG2	1.83	0.60
29:Y:24:DC:C2	29:Y:25:DT:O4	2.55	0.60
1:A:575:PRO:HG2	1:A:594:LEU:HD11	1.83	0.59
1:A:1431:SER:CB	1:A:1459:MET:HE1	2.32	0.59
27:3:213:LEU:HD23	27:3:230:VAL:HG12	1.84	0.59
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.84	0.59
26:2:196:ILE:HA	26:2:202:GLN:OE1	2.02	0.59
26:2:202:GLN:NE2	26:2:202:GLN:H	2.00	0.59
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.84	0.59
13:M:90:ALA:HB2	13:M:100:LYS:CE	2.31	0.59
26:2:83:GLN:OE1	26:2:83:GLN:HA	2.01	0.59
26:2:159:VAL:HG13	26:2:160:LEU:N	2.17	0.59
9:I:61:GLU:O	9:I:62:VAL:C	2.46	0.59
17:Q:24:GLY:HA2	18:R:209:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:195:PRO:HG3	18:R:199:LYS:HB3	1.72	0.59
26:2:206:LEU:HD22	26:2:206:LEU:N	2.17	0.59
27:3:110:VAL:O	27:3:114:GLU:HG2	2.02	0.59
27:3:160:ARG:HB3	27:3:190:LEU:CD2	2.32	0.59
1:A:200:ALA:O	1:A:213:LYS:HA	2.03	0.59
1:A:263:ALA:HB1	1:A:272:ASN:CB	2.32	0.59
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.35	0.59
23:W:584:TYR:CE2	23:W:614:TYR:HB2	2.37	0.59
25:1:53:LEU:HD12	25:1:53:LEU:N	2.18	0.59
27:3:14:VAL:HG23	27:3:163:VAL:HA	1.84	0.59
28:X:49:DT:H3'	28:X:50:DT:H5''	1.83	0.59
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.85	0.59
2:B:873:LEU:HB3	2:B:874:PRO:CD	2.31	0.59
7:G:110:ARG:NH2	7:G:118:GLU:OE2	2.36	0.59
9:I:105:GLU:HB3	9:I:107:ALA:CB	2.33	0.59
20:T:129:ARG:HA	20:T:132:ILE:HD12	1.84	0.59
1:A:415:GLY:C	1:A:449:HIS:HD2	2.11	0.59
1:A:540:ASP:CB	2:B:790:GLN:HE21	2.15	0.59
1:A:932:ARG:HB2	1:A:943:LEU:HD11	1.85	0.59
1:A:1127:LEU:HD21	1:A:1381:GLU:HB3	1.84	0.59
17:Q:98:THR:HG22	17:Q:100:VAL:H	1.67	0.59
17:Q:113:ARG:NH2	18:R:218:LYS:HE2	2.11	0.59
1:A:199:TYR:CZ	13:M:93:PHE:HZ	2.19	0.59
1:A:261:ARG:C	1:A:263:ALA:H	2.11	0.59
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.66	0.59
1:A:926:ASN:OD1	1:A:931:ARG:NH1	2.35	0.59
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.83	0.59
2:B:841:ARG:NH2	2:B:893:SER:O	2.35	0.59
6:F:88:ASP:OD2	6:F:91:LEU:N	2.35	0.59
7:G:145:LEU:HD13	7:G:161:GLY:HA3	1.84	0.59
12:L:17:TYR:CD1	12:L:46:LYS:HA	2.37	0.59
13:M:218:PHE:HD1	13:M:277:ILE:HG22	1.67	0.59
23:W:37:HIS:ND1	23:W:454:VAL:HG13	2.16	0.59
24:0:54:ARG:C	27:3:209:ILE:HD11	2.25	0.59
24:0:77:LYS:C	24:0:79:ASN:H	2.03	0.59
26:2:44:VAL:HG13	26:2:45:PHE:N	2.17	0.59
26:2:118:LEU:CD2	27:3:39:ASP:C	2.72	0.59
26:2:160:LEU:HD12	26:2:160:LEU:N	2.18	0.59
26:2:203:PHE:CE2	26:2:205:LEU:HD23	2.38	0.59
1:A:354:LEU:O	1:A:357:LYS:HE2	2.02	0.59
1:A:386:ALA:O	1:A:449:HIS:ND1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:ARG:CD	1:A:943:LEU:CD2	2.50	0.59
1:A:998:PRO:HA	1:A:1059:ARG:HG2	1.85	0.59
2:B:216:ALA:HB2	2:B:241:ALA:HB2	1.84	0.59
25:1:29:LEU:HD23	25:1:29:LEU:C	2.27	0.59
26:2:217:LEU:HD23	26:2:233:ILE:CD1	2.32	0.59
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.38	0.59
17:Q:112:ARG:HD3	18:R:237:LEU:CD1	2.22	0.59
25:1:22:TYR:O	25:1:25:GLU:HB3	2.03	0.59
25:1:34:ILE:O	25:1:46:ILE:HG13	2.03	0.59
27:3:173:GLN:CA	27:3:176:ASN:HD21	2.10	0.59
28:X:15:DA:N1	29:Y:79:DC:N3	2.51	0.59
2:B:78:VAL:O	2:B:79:GLU:C	2.45	0.58
2:B:921:ILE:HG13	2:B:921:ILE:O	2.03	0.58
17:Q:25:PHE:CD1	18:R:210:PHE:CZ	2.90	0.58
21:U:250:MET:O	21:U:251:ALA:HB2	2.02	0.58
22:V:321:GLU:CD	23:W:499:ASN:C	2.71	0.58
26:2:30:VAL:CB	27:3:25:GLN:HB3	2.33	0.58
26:2:171:VAL:HG13	26:2:216:MET:HB2	1.83	0.58
27:3:71:TYR:CG	27:3:72:PRO:HD2	2.19	0.58
27:3:131:THR:CG2	27:3:133:LEU:HD12	2.33	0.58
27:3:169:ASP:CG	27:3:202:LEU:HD23	2.28	0.58
27:3:174:TYR:CE1	27:3:178:MET:HE3	2.37	0.58
27:3:215:LEU:CD1	27:3:230:VAL:HG13	2.32	0.58
1:A:608:THR:CA	1:A:610:PRO:HD2	2.31	0.58
8:H:74:GLU:C	8:H:75:TYR:HD1	2.07	0.58
23:W:419:GLU:HB3	23:W:420:PRO:HD3	1.82	0.58
26:2:215:PHE:CD2	26:2:264:HIS:HB2	2.38	0.58
26:2:220:LEU:HD13	26:2:220:LEU:C	2.29	0.58
27:3:131:THR:HG23	27:3:133:LEU:CD1	2.33	0.58
3:C:6:GLN:O	11:K:104:ARG:NH1	2.35	0.58
25:1:2:VAL:HB	26:2:456:LYS:HD3	1.85	0.58
25:1:18:GLN:HB2	25:1:44:PHE:CZ	2.37	0.58
26:2:35:TYR:CB	26:2:62:LEU:HD12	2.33	0.58
26:2:177:GLN:HE22	26:2:220:LEU:HA	1.68	0.58
27:3:169:ASP:CB	27:3:202:LEU:HD23	2.33	0.58
1:A:1307:VAL:O	1:A:1307:VAL:HG12	2.03	0.58
10:J:63:ALA:CB	10:J:64:PRO:HD3	2.18	0.58
16:P:171:THR:HG22	16:P:220:VAL:HG13	1.85	0.58
27:3:190:LEU:HD23	27:3:190:LEU:N	2.18	0.58
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.04	0.58
3:C:85:SER:HB2	3:C:166:LYS:HE3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:133:GLN:N	5:E:133:GLN:OE1	2.36	0.58
12:L:17:TYR:HE1	12:L:46:LYS:CD	2.14	0.58
25:1:2:VAL:CG1	26:2:456:LYS:CD	2.82	0.58
25:1:38:ILE:H	25:1:38:ILE:CD1	2.16	0.58
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.84	0.58
1:A:641:CYS:SG	1:A:643:LYS:N	2.77	0.58
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.04	0.58
2:B:798:ARG:HD3	2:B:950:ARG:HG2	1.86	0.58
26:2:118:LEU:HD12	26:2:118:LEU:C	2.29	0.58
1:A:865:ILE:HG13	1:A:866:LYS:N	2.17	0.58
1:A:927:GLU:O	1:A:929:ALA:N	2.37	0.58
25:1:34:ILE:HG22	25:1:46:ILE:CD1	2.32	0.58
1:A:244:ARG:HD2	1:A:245:PRO:HD2	1.85	0.58
5:E:52:ARG:HG3	5:E:54:ARG:HG3	1.85	0.58
6:F:88:ASP:CG	6:F:91:LEU:H	2.12	0.58
24:0:77:LYS:C	24:0:79:ASN:N	2.56	0.58
26:2:62:LEU:HD13	26:2:62:LEU:C	2.28	0.58
27:3:71:TYR:HD2	27:3:72:PRO:HD2	1.68	0.58
1:A:264:VAL:O	1:A:266:MET:N	2.36	0.58
1:A:1029:LEU:H	5:E:162:ARG:NH1	2.02	0.58
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.37	0.58
11:K:63:VAL:HB	11:K:71:ILE:HG22	1.86	0.58
13:M:47:ASP:C	13:M:49:GLY:N	2.59	0.58
25:1:1:MET:HB3	26:2:413:LEU:HG	1.83	0.58
26:2:236:PHE:CZ	26:2:258:LEU:HD11	2.39	0.58
27:3:14:VAL:HG23	27:3:163:VAL:HG13	1.86	0.58
1:A:606:HIS:CG	1:A:607:SER:N	2.72	0.57
1:A:931:ARG:C	1:A:933:THR:N	2.62	0.57
1:A:1102:MET:HG2	21:U:277:GLN:HB2	1.85	0.57
1:A:1319:LYS:CG	1:A:1333:GLU:CD	2.77	0.57
2:B:819:SER:HB3	2:B:821:LYS:HG3	1.84	0.57
3:C:60:HIS:NE2	3:C:63:PHE:HB2	2.18	0.57
21:U:257:GLN:NE2	21:U:257:GLN:HA	2.19	0.57
26:2:30:VAL:N	27:3:25:GLN:HB3	2.19	0.57
27:3:16:ASP:O	27:3:21:TRP:NE1	2.27	0.57
27:3:59:VAL:CB	27:3:71:TYR:HE1	1.95	0.57
1:A:537:ILE:HG13	1:A:672:ILE:HD13	1.86	0.57
2:B:839:GLY:HA3	2:B:891:ASP:HB3	1.86	0.57
8:H:1:MET:HE1	8:H:85:ALA:HB2	1.86	0.57
17:Q:25:PHE:CD1	18:R:210:PHE:HZ	2.23	0.57
25:1:8:VAL:HG12	25:1:9:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:82:ALA:HA	26:2:89:LEU:HD11	1.85	0.57
27:3:21:TRP:CD2	27:3:34:LEU:HD23	2.39	0.57
2:B:812:ARG:HH22	29:Y:52:DT:P	2.26	0.57
3:C:154:ARG:HB3	10:J:65:LEU:CD2	2.34	0.57
8:H:108:ALA:O	8:H:109:ALA:C	2.47	0.57
27:3:216:LYS:H	27:3:216:LYS:CD	2.13	0.57
1:A:608:THR:CB	1:A:610:PRO:CD	2.83	0.57
2:B:438:ARG:NE	2:B:442:ASP:OD2	2.31	0.57
13:M:16:PRO:CG	13:M:39:LEU:HD21	2.30	0.57
22:V:315:VAL:HG12	23:W:500:ASP:CB	2.17	0.57
2:B:230:ARG:HD2	2:B:405:ARG:HH12	1.69	0.57
2:B:255:ARG:NE	2:B:307:GLU:OE2	2.38	0.57
2:B:1029:TYR:CE1	2:B:1036:LYS:HG2	2.39	0.57
5:E:84:ILE:HD11	28:X:64:DC:H3'	1.87	0.57
12:L:27:GLU:OE1	12:L:27:GLU:HA	2.04	0.57
23:W:584:TYR:CB	23:W:594:ALA:HB2	2.33	0.57
24:O:109:THR:HB	24:O:144:SER:H	1.67	0.57
25:1:18:GLN:CD	25:1:44:PHE:HZ	2.12	0.57
27:3:215:LEU:HD12	27:3:230:VAL:HG13	1.85	0.57
2:B:290:TYR:CE2	2:B:562:ALA:HA	2.39	0.57
17:Q:113:ARG:CD	18:R:222:SER:HB2	2.34	0.57
25:1:1:MET:CG	26:2:418:PHE:HB2	2.35	0.57
1:A:789:GLY:HA2	1:A:822:PHE:CE1	2.40	0.57
1:A:1281:ASP:O	1:A:1285:LEU:N	2.35	0.57
2:B:690:CYS:SG	2:B:691:SER:N	2.76	0.57
12:L:35:ARG:HH12	12:L:42:ARG:NH2	2.02	0.57
27:3:44:LEU:HD13	27:3:44:LEU:C	2.30	0.57
27:3:144:ILE:HG12	27:3:147:MET:CE	2.34	0.57
27:3:172:LEU:HD13	27:3:172:LEU:C	2.29	0.57
27:3:223:LEU:HD11	27:3:227:LEU:HD11	1.87	0.57
29:Y:39:DG:H2'	29:Y:40:DT:C6	2.40	0.57
1:A:601:ASN:HD21	1:A:632:ASN:H	1.52	0.57
2:B:223:SER:HB2	2:B:349:PRO:HD2	1.87	0.57
17:Q:105:TYR:CD1	18:R:234:GLU:HB2	2.40	0.57
17:Q:180:PHE:HE1	18:R:212:VAL:C	2.12	0.57
1:A:1312:PRO:HB3	1:A:1334:TRP:HZ3	1.65	0.57
2:B:1062:ARG:NH1	2:B:1074:PRO:HB3	2.19	0.57
27:3:187:GLN:NE2	27:3:189:ILE:HG13	2.20	0.57
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	1.86	0.57
2:B:857:GLY:HA2	2:B:903:ILE:HD11	1.86	0.57
2:B:1069:ILE:HD11	13:M:45:VAL:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:214:GLU:OE1	18:R:217:GLN:NE2	2.32	0.57
26:2:185:MET:HB2	26:2:229:ASP:OD1	2.04	0.57
27:3:19:PRO:HG2	27:3:123:ASP:O	2.05	0.57
1:A:274:ASP:OD2	1:A:276:LEU:HB3	2.05	0.56
18:R:142:LYS:HD3	18:R:145:VAL:HG23	1.87	0.56
25:1:9:LEU:CB	25:1:51:ASN:HD21	2.14	0.56
25:1:1:MET:CB	26:2:418:PHE:HB2	2.35	0.56
26:2:60:LEU:HD11	26:2:95:ILE:CG2	2.35	0.56
27:3:57:LEU:HD23	27:3:58:ALA:C	2.31	0.56
1:A:305:GLU:OE1	13:M:102:GLN:NE2	2.38	0.56
1:A:623:PRO:O	1:A:625:ASP:N	2.38	0.56
1:A:1128:ILE:HG23	1:A:1414:ILE:HD11	1.87	0.56
2:B:232:THR:OG1	2:B:233:SER:N	2.38	0.56
12:L:16:ILE:HG21	12:L:47:LYS:CD	2.35	0.56
13:M:47:ASP:O	13:M:48:VAL:C	2.47	0.56
13:M:60:ALA:HB1	29:Y:54:DA:H2	1.70	0.56
13:M:178:LYS:HB3	20:T:154:LYS:CD	2.35	0.56
13:M:179:GLU:HG3	20:T:154:LYS:HE2	1.87	0.56
21:U:256:THR:HB	21:U:272:THR:CB	2.35	0.56
22:V:428:GLU:OE1	22:V:460:ALA:HA	2.05	0.56
22:V:514:MET:SD	22:V:537:ASN:ND2	2.78	0.56
25:1:52:VAL:HG22	25:1:53:LEU:HD12	1.87	0.56
26:2:117:ASN:HB2	27:3:104:LEU:CD1	2.35	0.56
27:3:42:MET:SD	27:3:111:ILE:HD13	2.46	0.56
27:3:178:MET:SD	27:3:181:ILE:HD12	2.46	0.56
27:3:195:VAL:HG21	27:3:214:TYR:OH	2.05	0.56
2:B:499:ARG:NH2	2:B:522:LEU:HD11	2.20	0.56
3:C:5:ASN:ND2	3:C:25:ASN:HD21	2.03	0.56
3:C:136:ASP:OD1	3:C:136:ASP:N	2.36	0.56
25:1:31:LYS:O	25:1:32:LYS:HB2	2.06	0.56
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.86	0.56
1:A:1431:SER:HB2	1:A:1459:MET:HE1	1.86	0.56
2:B:1040:GLN:CD	2:B:1040:GLN:N	2.63	0.56
17:Q:112:ARG:NE	18:R:237:LEU:HD12	2.13	0.56
1:A:832:THR:N	1:A:835:GLU:OE1	2.25	0.56
26:2:130:SER:HB2	26:2:173:GLN:OE1	2.06	0.56
27:3:223:LEU:O	27:3:223:LEU:HD13	2.06	0.56
29:Y:24:DC:N1	29:Y:25:DT:C4	2.74	0.56
1:A:522:PRO:CA	1:A:666:ARG:HE	2.10	0.56
12:L:35:ARG:NH1	12:L:42:ARG:HH21	2.04	0.56
13:M:89:GLY:O	13:M:90:ALA:HB3	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:113:ARG:CZ	18:R:218:LYS:CG	2.84	0.56
25:1:1:MET:HB2	26:2:418:PHE:HB2	1.88	0.56
1:A:265:VAL:O	1:A:272:ASN:OD1	2.23	0.56
1:A:1097:GLU:O	1:A:1100:THR:OG1	2.23	0.56
2:B:555:GLU:OE1	19:S:124:TYR:OH	2.18	0.56
3:C:133:ARG:CA	3:C:136:ASP:OD2	2.42	0.56
13:M:183:VAL:HG12	20:T:152:ASN:HD21	1.70	0.56
25:1:36:GLN:HB3	25:1:45:VAL:HG12	1.88	0.56
1:A:293:ASN:OD1	1:A:298:ALA:HA	2.06	0.56
1:A:1223:ASP:OD1	1:A:1224:ARG:NH1	2.39	0.56
26:2:47:GLU:HG3	26:2:48:LEU:N	2.20	0.56
26:2:160:LEU:H	26:2:160:LEU:CD1	2.18	0.56
1:A:625:ASP:O	1:A:638:GLY:HA2	2.06	0.56
1:A:632:ASN:CA	1:A:992:LYS:HD2	2.36	0.56
5:E:6:GLU:OE2	5:E:9:ARG:NH1	2.39	0.56
11:K:16:GLU:OE1	11:K:36:ASN:ND2	2.39	0.56
19:S:46:ARG:NH2	20:T:2:ALA:O	2.39	0.56
26:2:181:GLN:HA	26:2:181:GLN:HE21	1.70	0.56
26:2:423:ALA:HA	26:2:426:ARG:HE	1.70	0.56
1:A:207:GLU:O	1:A:209:SER:N	2.39	0.55
1:A:1222:THR:HB	21:U:241:THR:HG21	1.88	0.55
22:V:520:ARG:NE	22:V:521:GLU:OE2	2.29	0.55
27:3:44:LEU:HD13	27:3:44:LEU:O	2.06	0.55
1:A:263:ALA:C	1:A:264:VAL:CG1	2.65	0.55
1:A:522:PRO:HB3	1:A:666:ARG:CG	2.36	0.55
1:A:621:ILE:C	1:A:623:PRO:N	2.64	0.55
3:C:6:GLN:O	3:C:7:PRO:C	2.45	0.55
8:H:65:TYR:CE2	8:H:70:LEU:HD13	2.40	0.55
26:2:206:LEU:HD22	26:2:206:LEU:H	1.71	0.55
27:3:210:THR:HG22	27:3:210:THR:O	2.04	0.55
28:X:47:DT:H3'	28:X:48:DT:H5''	1.88	0.55
28:X:53:DA:H2'	28:X:54:DA:C8	2.40	0.55
1:A:121:SER:HA	1:A:126:ILE:HG21	1.87	0.55
1:A:936:GLU:HA	1:A:1002:SER:HB2	1.89	0.55
10:J:63:ALA:N	10:J:64:PRO:CD	2.69	0.55
17:Q:153:ARG:HH11	17:Q:158:HIS:HB3	1.72	0.55
18:R:154:LEU:HD23	18:R:163:LEU:CD2	2.24	0.55
21:U:256:THR:CA	21:U:272:THR:HG22	2.36	0.55
2:B:529:MET:HG2	2:B:530:ALA:N	2.22	0.55
8:H:64:LEU:H	8:H:70:LEU:HD21	1.71	0.55
8:H:106:THR:O	8:H:108:ALA:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:ASP:C	3:C:214:ASP:N	2.43	0.55
9:I:61:GLU:C	9:I:63:ASP:H	2.13	0.55
23:W:209:TYR:HH	23:W:233:PHE:CA	2.09	0.55
27:3:165:LYS:HD3	27:3:165:LYS:C	2.31	0.55
1:A:61:ARG:HB3	1:A:72:GLN:HE21	1.71	0.55
1:A:1316:ASN:CG	1:A:1318:LYS:HE2	2.31	0.55
2:B:529:MET:HE2	2:B:624:PRO:HD2	1.88	0.55
22:V:504:LYS:HD2	22:V:654:GLU:O	2.07	0.55
25:1:52:VAL:HG23	25:1:53:LEU:N	2.21	0.55
1:A:624:GLY:O	1:A:626:THR:N	2.35	0.55
1:A:1143:LEU:HD11	1:A:1336:LEU:HG	1.88	0.55
2:B:360:LYS:HG3	2:B:553:LEU:HD23	1.88	0.55
5:E:84:ILE:HG23	28:X:64:DC:OP1	2.05	0.55
9:I:85:PRO:C	9:I:86:CYS:O	2.49	0.55
26:2:53:LYS:CE	26:2:95:ILE:HD11	2.35	0.55
2:B:1094:GLN:NE2	2:B:1102:PHE:HD2	2.04	0.55
3:C:70:LEU:HD23	10:J:5:VAL:O	2.07	0.55
19:S:31:PHE:HB2	20:T:92:THR:HB	1.89	0.55
21:U:291:CYS:SG	21:U:293:GLU:HB2	2.46	0.55
1:A:522:PRO:HB3	1:A:666:ARG:HG3	1.89	0.55
1:A:1109:TYR:HE2	1:A:1113:SER:H	1.55	0.55
2:B:1076:GLU:HB2	13:M:54:THR:OG1	2.06	0.55
5:E:94:MET:HB2	5:E:99:ILE:HD11	1.88	0.55
20:T:58:LEU:HD23	20:T:63:ALA:HB2	1.87	0.55
26:2:29:GLY:H	27:3:25:GLN:CD	2.15	0.55
13:M:52:TRP:CD1	13:M:52:TRP:O	2.60	0.55
16:P:239:ARG:NH1	16:P:242:GLN:OE1	2.40	0.55
17:Q:102:VAL:HG23	17:Q:102:VAL:O	2.06	0.55
22:V:638:GLN:O	22:V:642:ARG:HG2	2.07	0.55
25:1:34:ILE:HG23	25:1:50:VAL:HG11	1.89	0.55
26:2:123:LEU:CD2	26:2:178:LEU:HD11	2.37	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	1.89	0.55
2:B:914:GLU:OE1	2:B:914:GLU:N	2.40	0.54
22:V:516:PRO:HD2	22:V:706:LYS:NZ	2.22	0.54
24:0:54:ARG:CG	27:3:182:PHE:CZ	2.80	0.54
24:0:54:ARG:CB	27:3:209:ILE:HG23	2.25	0.54
24:0:77:LYS:HD2	24:0:77:LYS:N	2.21	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
27:3:58:ALA:C	27:3:71:TYR:OH	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:82:PRO:HG2	20:T:117:ARG:HB2	1.89	0.54
25:1:3:ASN:CB	26:2:412:PHE:O	2.54	0.54
1:A:1161:LEU:HD23	1:A:1307:VAL:CG1	2.38	0.54
4:D:90:LYS:HE3	4:D:130:ILE:HD11	1.88	0.54
5:E:15:LYS:NZ	5:E:33:LEU:O	2.31	0.54
5:E:64:HIS:NE2	5:E:69:THR:OG1	1.98	0.54
26:2:117:ASN:HD22	27:3:42:MET:HE1	1.69	0.54
1:A:30:GLU:CD	1:A:33:ARG:HH21	2.16	0.54
17:Q:113:ARG:HD2	18:R:222:SER:HB3	1.90	0.54
27:3:64:ILE:HG23	27:3:128:HIS:CG	2.42	0.54
1:A:932:ARG:CG	1:A:943:LEU:HD11	2.36	0.54
13:M:193:ARG:NH1	29:Y:75:DC:OP1	2.41	0.54
20:T:142:SER:O	20:T:144:GLN:HG3	2.08	0.54
27:3:133:LEU:H	27:3:133:LEU:CD1	2.10	0.54
1:A:299:ALA:HA	17:Q:60:ARG:NH2	2.23	0.54
25:1:25:GLU:HG2	25:1:32:LYS:HA	1.89	0.54
26:2:214:TYR:CD2	26:2:261:PHE:CD2	2.95	0.54
27:3:100:LYS:O	27:3:103:LEU:HB2	2.08	0.54
1:A:156:GLY:HA2	1:A:181:HIS:ND1	2.23	0.54
1:A:297:GLY:HA3	17:Q:57:LYS:HB3	1.90	0.54
1:A:1114:ALA:HB3	1:A:1309:MET:HE1	1.89	0.54
25:1:34:ILE:HG21	25:1:54:GLN:CD	2.32	0.54
26:2:211:GLN:HB3	26:2:261:PHE:CE1	2.40	0.54
26:2:222:THR:HG23	26:2:222:THR:O	2.07	0.54
27:3:223:LEU:HD13	27:3:223:LEU:C	2.33	0.54
1:A:1163:HIS:ND1	1:A:1302:GLU:O	2.41	0.54
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.72	0.54
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.90	0.54
19:S:46:ARG:HB2	19:S:101:ARG:HB2	1.89	0.54
26:2:159:VAL:CG1	26:2:161:HIS:H	2.06	0.54
26:2:199:ALA:HB1	26:2:201:PHE:CD2	2.43	0.54
1:A:389:THR:HG21	1:A:417:LYS:HD2	1.90	0.54
1:A:521:VAL:HB	1:A:522:PRO:HD3	1.90	0.54
2:B:109:MET:HG3	2:B:174:LEU:HD11	1.89	0.54
2:B:733:MET:HE1	2:B:1054:MET:SD	2.47	0.54
5:E:67:ASP:O	5:E:69:THR:N	2.41	0.54
6:F:56:TYR:CE1	6:F:124:ILE:HB	2.43	0.54
19:S:172:ASN:OD1	19:S:173:HIS:N	2.37	0.54
25:1:1:MET:CE	26:2:415:GLN:C	2.80	0.54
26:2:37:HIS:HB3	26:2:38:PRO:CD	2.35	0.54
2:B:248:LYS:HA	19:S:169:LYS:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:ASN:CA	3:C:136:ASP:OD1	2.56	0.54
3:C:147:ASP:O	10:J:16:ASN:HB3	2.08	0.54
12:L:27:GLU:HB2	12:L:37:ARG:NH1	2.22	0.54
23:W:428:ILE:HA	23:W:430:ASN:ND2	2.23	0.54
1:A:629:VAL:HG21	1:A:637:MET:HE3	1.89	0.53
1:A:1319:LYS:HG2	1:A:1333:GLU:CD	2.33	0.53
3:C:82:LEU:HD23	3:C:167:LYS:HB2	1.90	0.53
8:H:60:ILE:HD11	8:H:123:MET:HE1	1.90	0.53
26:2:86:SER:O	26:2:90:LEU:HD13	2.08	0.53
1:A:34:MET:SD	2:B:1124:ILE:HG21	2.48	0.53
1:A:729:PRO:CG	21:U:250:MET:HB2	2.38	0.53
5:E:64:HIS:HD2	5:E:67:ASP:C	2.15	0.53
26:2:159:VAL:HG22	26:2:160:LEU:N	2.16	0.53
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.43	0.53
1:A:894:ASP:OD1	1:A:895:GLY:N	2.40	0.53
2:B:132:VAL:CG2	2:B:141:GLN:CB	2.86	0.53
2:B:834:ARG:HB3	2:B:840:MET:HE2	1.91	0.53
3:C:30:VAL:HG22	11:K:45:ILE:HD11	1.90	0.53
3:C:47:ILE:H	3:C:47:ILE:HD12	1.73	0.53
6:F:102:ILE:HG22	6:F:104:ILE:HG12	1.89	0.53
18:R:195:PRO:HB2	18:R:199:LYS:CG	2.38	0.53
26:2:138:PRO:O	26:2:139:ASP:HB2	2.08	0.53
1:A:930:LEU:HD23	1:A:934:LEU:CB	2.39	0.53
13:M:90:ALA:CB	13:M:100:LYS:HE3	2.37	0.53
13:M:179:GLU:N	20:T:154:LYS:HE3	2.22	0.53
22:V:667:THR:HA	25:1:62:ASP:OD2	2.07	0.53
26:2:30:VAL:O	26:2:34:LEU:HD23	2.09	0.53
26:2:211:GLN:HE21	26:2:257:SER:CB	2.21	0.53
27:3:15:VAL:HG23	27:3:15:VAL:O	2.08	0.53
27:3:105:THR:HG23	27:3:106:SER:N	2.23	0.53
27:3:191:ILE:N	27:3:210:THR:HG21	2.24	0.53
1:A:929:ALA:O	1:A:930:LEU:CB	2.57	0.53
17:Q:180:PHE:CZ	18:R:213:ASP:N	2.76	0.53
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.44	0.53
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.91	0.53
1:A:1309:MET:O	1:A:1311:LEU:CD1	2.56	0.53
2:B:490:GLY:O	2:B:491:ARG:CG	2.56	0.53
2:B:1078:ARG:NH1	29:Y:50:DA:O3'	2.41	0.53
5:E:91:CYS:HA	5:E:94:MET:HE3	1.90	0.53
6:F:69:ARG:HG3	6:F:102:ILE:HD12	1.91	0.53
17:Q:68:GLY:C	18:R:226:ASP:CG	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:125:ALA:HB1	17:Q:138:ASP:HB3	1.91	0.53
22:V:523:VAL:CB	25:1:20:LEU:HD23	2.38	0.53
26:2:141:HIS:HA	26:2:162:PHE:CE2	2.43	0.53
27:3:34:LEU:HD13	27:3:34:LEU:C	2.33	0.53
27:3:106:SER:O	27:3:109:GLU:HG3	2.08	0.53
27:3:160:ARG:NH2	27:3:192:ASP:HB3	2.23	0.53
1:A:467:MET:SD	1:A:524:MET:HB3	2.49	0.53
2:B:1163:MET:HA	2:B:1168:ALA:H	1.73	0.53
18:R:80:LYS:HD3	20:T:188:PHE:HE2	1.74	0.53
19:S:51:LEU:HD21	19:S:54:LYS:HD3	1.90	0.53
19:S:115:LYS:NZ	19:S:117:GLY:O	2.28	0.53
26:2:160:LEU:CG	26:2:206:LEU:HD21	2.39	0.53
26:2:234:LEU:HD23	26:2:234:LEU:C	2.34	0.53
27:3:10:LEU:HD21	27:3:143:TYR:CE2	2.44	0.53
1:A:859:TYR:OH	1:A:863:ARG:NH2	2.41	0.53
2:B:91:ILE:HD11	2:B:124:LEU:HD21	1.89	0.53
14:N:332:GLU:HB2	15:O:92:LYS:O	2.09	0.53
14:N:359:ASN:ND2	14:N:364:ASP:OD1	2.38	0.53
27:3:204:GLN:HG2	27:3:214:TYR:CZ	2.44	0.53
1:A:542:LEU:HD21	1:A:642:LYS:HB2	1.91	0.53
5:E:14:ARG:O	5:E:17:ILE:HG13	2.09	0.53
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.43	0.53
14:N:314:LEU:HD21	16:P:250:PHE:HB2	1.90	0.53
20:T:93:LEU:HB2	20:T:110:VAL:HB	1.91	0.53
26:2:81:LYS:HG3	26:2:82:ALA:N	2.21	0.53
2:B:598:VAL:C	2:B:600:GLU:H	2.16	0.53
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.42	0.53
26:2:241:SER:O	26:2:245:LEU:HD23	2.09	0.53
1:A:48:GLU:O	1:A:50:GLY:N	2.41	0.52
9:I:84:HIS:CD2	9:I:84:HIS:N	2.77	0.52
9:I:119:CYS:HB3	9:I:121:HIS:HB2	1.90	0.52
1:A:930:LEU:CD2	1:A:934:LEU:HB2	2.40	0.52
8:H:74:GLU:O	8:H:75:TYR:CG	2.57	0.52
17:Q:75:ARG:HH21	17:Q:95:ASN:HD22	1.57	0.52
1:A:255:VAL:HG13	1:A:280:LEU:HD21	1.91	0.52
1:A:263:ALA:O	1:A:264:VAL:CG2	2.58	0.52
1:A:790:GLN:CD	1:A:797:ARG:HG2	2.34	0.52
2:B:852:GLY:O	2:B:868:GLY:N	2.30	0.52
6:F:73:ILE:HD11	6:F:96:GLU:OE2	2.08	0.52
9:I:61:GLU:O	9:I:63:ASP:HB2	2.10	0.52
13:M:13:VAL:HG12	13:M:20:ASP:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:196:LYS:NZ	28:X:13:DT:OP1	2.41	0.52
21:U:279:ARG:NH1	21:U:280:SER:O	2.43	0.52
26:2:138:PRO:HG3	26:2:189:GLU:CG	2.35	0.52
27:3:10:LEU:HD21	27:3:143:TYR:CD2	2.44	0.52
1:A:1316:ASN:ND2	1:A:1318:LYS:CE	2.72	0.52
8:H:85:ALA:C	8:H:87:GLN:N	2.38	0.52
13:M:178:LYS:HG2	20:T:156:VAL:HG12	1.92	0.52
27:3:22:TRP:O	27:3:25:GLN:NE2	2.40	0.52
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.90	0.52
2:B:931:ILE:HD11	2:B:947:ILE:HA	1.92	0.52
2:B:1022:LEU:HD11	2:B:1023:ARG:NH1	2.24	0.52
13:M:178:LYS:HB3	20:T:154:LYS:CE	2.40	0.52
17:Q:25:PHE:HD1	18:R:210:PHE:CZ	2.27	0.52
20:T:155:PRO:C	20:T:157:ALA:H	2.14	0.52
20:T:191:PHE:HZ	20:T:237:PRO:HG3	1.74	0.52
25:1:35:ILE:O	25:1:35:ILE:HG13	2.08	0.52
1:A:364:ARG:HB2	2:B:1084:LEU:HD11	1.91	0.52
1:A:484:LEU:HD12	1:A:484:LEU:O	2.08	0.52
17:Q:101:ASN:C	17:Q:103:VAL:N	2.43	0.52
20:T:208:GLN:HE21	20:T:213:LEU:HB2	1.74	0.52
22:V:516:PRO:HD2	22:V:706:LYS:HZ3	1.67	0.52
22:V:611:GLY:HA2	22:V:615:PHE:CB	2.38	0.52
26:2:192:GLU:CG	26:2:193:PRO:HD2	2.23	0.52
26:2:221:GLN:CD	26:2:230:LEU:HB2	2.34	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
1:A:201:GLU:HA	1:A:212:LYS:C	2.23	0.52
1:A:265:VAL:HA	1:A:272:ASN:CB	2.28	0.52
1:A:926:ASN:CB	1:A:931:ARG:CZ	2.61	0.52
2:B:529:MET:HG3	2:B:624:PRO:HD2	1.91	0.52
3:C:267:ILE:HG13	3:C:272:LEU:HB3	1.92	0.52
5:E:64:HIS:CB	5:E:68:PRO:HA	2.39	0.52
5:E:149:VAL:HG23	5:E:192:LYS:HB3	1.92	0.52
17:Q:105:TYR:HD1	18:R:234:GLU:HB2	1.75	0.52
1:A:133:SER:HG	1:A:136:GLN:HB2	1.64	0.52
1:A:263:ALA:O	1:A:264:VAL:HG22	2.10	0.52
1:A:274:ASP:O	1:A:275:ASP:C	2.53	0.52
1:A:621:ILE:O	1:A:621:ILE:HG22	2.10	0.52
1:A:890:ARG:NH2	1:A:1023:VAL:HG13	2.23	0.52
2:B:322:GLY:O	2:B:326:ALA:N	2.34	0.52
2:B:483:ARG:NH1	2:B:527:ALA:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:ASN:H	3:C:136:ASP:CG	2.16	0.52
5:E:151:MET:HE2	5:E:155:GLU:HB3	1.91	0.52
6:F:79:VAL:HG12	6:F:81:VAL:H	1.74	0.52
9:I:84:HIS:ND1	9:I:85:PRO:HD3	2.20	0.52
18:R:212:VAL:O	18:R:213:ASP:OD2	2.28	0.52
26:2:193:PRO:HB2	26:2:194:PRO:HD3	1.92	0.52
27:3:222:SER:HB3	27:3:225:GLN:HG2	1.92	0.52
2:B:552:ASN:OD1	2:B:553:LEU:N	2.43	0.52
12:L:35:ARG:HH12	12:L:42:ARG:NE	2.07	0.52
27:3:10:LEU:HD22	27:3:147:MET:HG2	1.92	0.52
3:C:7:PRO:HA	3:C:25:ASN:O	2.09	0.52
17:Q:25:PHE:HA	18:R:219:LEU:HD13	1.90	0.52
20:T:12:ALA:HB2	20:T:106:LEU:HD13	1.90	0.52
24:0:77:LYS:HG2	24:0:225:GLU:OE2	2.09	0.52
27:3:165:LYS:HZ1	27:3:200:SER:H	1.58	0.52
27:3:226:TYR:O	27:3:230:VAL:HB	2.10	0.52
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.92	0.51
13:M:94:ASP:O	13:M:97:GLY:N	2.42	0.51
14:N:366:ILE:O	15:O:54:ASN:ND2	2.44	0.51
17:Q:141:ALA:HB1	17:Q:152:PHE:CE2	2.44	0.51
20:T:177:ARG:N	20:T:178:ALA:HB3	2.24	0.51
25:1:59:GLU:CD	26:2:402:ARG:HH12	2.13	0.51
27:3:133:LEU:HD13	27:3:133:LEU:N	2.14	0.51
27:3:141:LEU:HG	27:3:187:GLN:HE22	1.75	0.51
1:A:604:ARG:HG3	1:A:606:HIS:CE1	2.45	0.51
1:A:678:ASN:O	1:A:681:LEU:HB3	2.10	0.51
1:A:790:GLN:NE2	1:A:797:ARG:HG2	2.25	0.51
1:A:972:THR:HA	1:A:1320:ILE:HG21	1.91	0.51
2:B:72:GLN:HE22	2:B:80:GLU:H	1.58	0.51
2:B:326:ALA:HB2	2:B:338:TYR:HE2	1.76	0.51
2:B:363:TYR:CD2	2:B:553:LEU:HD21	2.45	0.51
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.75	0.51
22:V:689:VAL:CB	26:2:391:ILE:HD11	2.39	0.51
26:2:30:VAL:H	27:3:25:GLN:CG	2.23	0.51
26:2:257:SER:O	26:2:261:PHE:HD1	1.93	0.51
27:3:64:ILE:HG21	27:3:128:HIS:CB	2.40	0.51
2:B:50:PHE:O	2:B:54:SER:HB2	2.11	0.51
2:B:976:MET:O	2:B:978:ILE:N	2.41	0.51
20:T:166:GLU:HA	20:T:169:LYS:HE3	1.93	0.51
25:1:4:VAL:HG11	26:2:412:PHE:CD2	2.29	0.51
27:3:42:MET:CG	27:3:111:ILE:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:65:DG:H2''	28:X:66:DA:O4'	2.10	0.51
1:A:126:ILE:HD13	1:A:129:ILE:HD12	1.92	0.51
2:B:386:ASP:OD2	2:B:502:HIS:HB2	2.09	0.51
2:B:553:LEU:HB2	2:B:573:TRP:HZ3	1.75	0.51
2:B:675:LEU:HD11	2:B:697:GLU:OE2	2.09	0.51
2:B:891:ASP:OD1	2:B:892:CYS:N	2.44	0.51
2:B:1072:ARG:HG3	2:B:1072:ARG:O	2.10	0.51
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.46	0.51
25:1:8:VAL:CG1	25:1:45:VAL:HG13	2.35	0.51
26:2:31:LEU:HD13	27:3:33:THR:HG22	1.86	0.51
26:2:160:LEU:HB3	26:2:206:LEU:HD21	1.93	0.51
27:3:14:VAL:HG23	27:3:14:VAL:O	2.09	0.51
27:3:100:LYS:HG3	27:3:101:TYR:H	1.74	0.51
9:I:58:ILE:C	9:I:60:HIS:H	2.19	0.51
23:W:209:TYR:CZ	23:W:233:PHE:HA	2.39	0.51
29:Y:24:DC:C1'	29:Y:25:DT:C5	2.93	0.51
2:B:62:ALA:N	2:B:63:PRO:HD3	2.25	0.51
2:B:226:GLU:OE2	2:B:617:ASP:CB	2.57	0.51
2:B:499:ARG:CZ	2:B:522:LEU:HD11	2.41	0.51
2:B:907:VAL:HG13	2:B:921:ILE:HG22	1.93	0.51
3:C:154:ARG:HH11	10:J:65:LEU:HD11	1.75	0.51
5:E:52:ARG:NH2	5:E:54:ARG:HD3	2.26	0.51
5:E:172:ARG:HD3	5:E:210:GLN:HG2	1.92	0.51
17:Q:109:HIS:CE1	18:R:233:ILE:CG2	2.93	0.51
23:W:73:CYS:O	23:W:209:TYR:CE2	2.64	0.51
23:W:584:TYR:HB2	23:W:591:GLY:HA3	1.92	0.51
25:1:4:VAL:HG12	26:2:411:GLN:C	2.30	0.51
27:3:100:LYS:HB3	27:3:103:LEU:CD1	2.37	0.51
27:3:121:LYS:HD3	27:3:121:LYS:N	2.25	0.51
2:B:992:ASN:ND2	2:B:1018:TYR:CD2	2.74	0.51
3:C:5:ASN:C	3:C:7:PRO:CD	2.77	0.51
8:H:95:LYS:HB2	8:H:139:SER:HA	1.92	0.51
12:L:36:CYS:HB2	12:L:44:MET:HE1	1.93	0.51
16:P:294:ARG:NH1	28:X:14:DA:OP1	2.28	0.51
20:T:177:ARG:H	20:T:178:ALA:HB3	1.76	0.51
26:2:207:ASP:OD2	26:2:254:MET:HE2	2.10	0.51
27:3:131:THR:HG23	27:3:133:LEU:HD12	1.92	0.51
27:3:165:LYS:HE3	27:3:200:SER:OG	2.09	0.51
1:A:469:MET:HE3	2:B:1094:GLN:OE1	2.11	0.51
1:A:818:GLU:H	1:A:818:GLU:CD	2.19	0.51
2:B:716:HIS:CE1	2:B:1007:ASN:HD21	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:749:HIS:CD2	2:B:810:PHE:HD1	2.27	0.51
2:B:1101:GLN:HE22	6:F:64:ARG:HG2	1.76	0.51
10:J:66:GLU:HG3	12:L:23:HIS:CG	2.46	0.51
17:Q:17:LEU:HD21	17:Q:191:LEU:HB3	1.93	0.51
17:Q:25:PHE:CD2	18:R:219:LEU:CD1	2.94	0.51
23:W:581:LEU:C	23:W:581:LEU:HD13	2.36	0.51
26:2:46:ARG:HD3	26:2:85:GLU:HB2	1.93	0.51
26:2:179:LEU:CB	26:2:184:LEU:HD11	2.40	0.51
26:2:236:PHE:CZ	26:2:262:LEU:CD2	2.94	0.51
29:Y:45:DT:H5''	29:Y:46:DC:H5''	1.92	0.51
1:A:375:ILE:HG21	1:A:666:ARG:NH1	2.26	0.51
2:B:1060:HIS:HB2	2:B:1078:ARG:HE	1.75	0.51
3:C:60:HIS:CD2	3:C:63:PHE:HB2	2.45	0.51
10:J:52:HIS:HE1	10:J:54:ASP:HA	1.75	0.51
26:2:57:MET:HA	26:2:60:LEU:CG	2.41	0.51
26:2:236:PHE:CE1	26:2:261:PHE:CB	2.94	0.51
27:3:12:VAL:HG12	27:3:58:ALA:HB3	1.92	0.51
1:A:201:GLU:HG3	1:A:212:LYS:CB	2.41	0.51
1:A:1161:LEU:HD23	1:A:1307:VAL:HG11	1.93	0.51
2:B:240:LEU:O	2:B:253:GLY:HA2	2.11	0.51
2:B:380:ARG:HE	2:B:609:GLU:CD	2.19	0.51
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.93	0.51
19:S:26:TYR:CD1	20:T:97:THR:HG22	2.46	0.51
22:V:516:PRO:CA	25:1:15:ALA:C	2.82	0.51
26:2:35:TYR:CD1	26:2:35:TYR:N	2.79	0.51
26:2:51:LEU:CD2	26:2:55:TRP:CD1	2.94	0.51
26:2:215:PHE:CE2	26:2:264:HIS:HB2	2.46	0.51
28:X:19:DG:N2	29:Y:76:DC:O2	2.44	0.51
1:A:1407:CYS:SG	1:A:1408:ARG:N	2.84	0.50
12:L:17:TYR:CE1	12:L:46:LYS:CB	2.94	0.50
19:S:26:TYR:HD1	20:T:97:THR:HG22	1.77	0.50
24:0:55:LEU:HD12	27:3:178:MET:HE3	1.93	0.50
26:2:199:ALA:HB1	26:2:201:PHE:CE2	2.47	0.50
28:X:42:DT:H2''	28:X:43:DT:H5''	1.92	0.50
1:A:261:ARG:HD2	1:A:277:THR:OG1	2.12	0.50
1:A:893:GLU:HG2	5:E:203:TYR:CD1	2.47	0.50
1:A:1167:ARG:HA	1:A:1293:LEU:HD22	1.94	0.50
2:B:309:PHE:CZ	9:I:40:ARG:HB2	2.46	0.50
13:M:10:LEU:N	13:M:11:PRO:CD	2.74	0.50
19:S:15:VAL:HA	20:T:42:LYS:HG2	1.93	0.50
28:X:44:DT:H3'	28:X:45:DT:H5''	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:62:DC:H1'	29:Y:63:DG:H4'	1.93	0.50
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	1.92	0.50
2:B:796:MET:HE1	2:B:935:PHE:CE2	2.46	0.50
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.93	0.50
14:N:323:GLU:HG2	14:N:325:GLY:HA3	1.94	0.50
21:U:286:THR:HG21	21:U:299:LYS:HD2	1.93	0.50
23:W:430:ASN:CB	23:W:431:PRO:CD	2.85	0.50
26:2:236:PHE:CE2	26:2:262:LEU:CD1	2.94	0.50
1:A:1319:LYS:HG3	1:A:1333:GLU:CD	2.36	0.50
2:B:939:HIS:NE2	2:B:980:HIS:HA	2.26	0.50
3:C:49:TRP:CZ3	12:L:54:VAL:HG21	2.46	0.50
9:I:65:LEU:CA	9:I:122:ARG:HE	2.23	0.50
26:2:30:VAL:CG1	26:2:34:LEU:HD23	2.40	0.50
26:2:93:LEU:CD2	26:2:96:TRP:HE1	2.25	0.50
1:A:48:GLU:O	1:A:49:GLY:C	2.53	0.50
1:A:334:ARG:NH2	13:M:66:ARG:O	2.44	0.50
15:O:64:THR:HG22	15:O:75:VAL:HB	1.92	0.50
17:Q:25:PHE:O	18:R:219:LEU:CD2	2.59	0.50
17:Q:188:TYR:HD1	17:Q:191:LEU:HD22	1.77	0.50
20:T:217:LEU:HB3	20:T:233:TRP:CE3	2.46	0.50
21:U:251:ALA:C	21:U:253:THR:N	2.69	0.50
26:2:223:ALA:O	26:2:224:GLN:HB3	2.12	0.50
26:2:231:VAL:O	26:2:234:LEU:HB3	2.11	0.50
1:A:11:SER:O	2:B:1135:TYR:OH	2.27	0.50
2:B:92:TYR:CD1	20:T:141:LEU:CD2	2.90	0.50
2:B:867:ILE:O	2:B:893:SER:HB2	2.11	0.50
2:B:906:GLN:HB3	12:L:45:TYR:HE1	1.75	0.50
3:C:116:THR:HB	3:C:146:ASP:HB2	1.93	0.50
27:3:108:ASN:O	27:3:111:ILE:HG12	2.12	0.50
27:3:187:GLN:O	27:3:188:ASN:HB2	2.12	0.50
1:A:366:VAL:O	1:A:481:THR:HB	2.12	0.50
1:A:623:PRO:C	1:A:625:ASP:N	2.68	0.50
1:A:673:GLN:O	1:A:677:ASN:CB	2.60	0.50
2:B:1092:ASP:HA	2:B:1095:ILE:HD12	1.94	0.50
11:K:111:ASP:C	11:K:113:GLN:H	2.15	0.50
13:M:47:ASP:C	13:M:49:GLY:H	2.14	0.50
13:M:276:ASP:HA	20:T:153:TYR:CE1	2.47	0.50
18:R:195:PRO:O	18:R:196:ASP:CB	2.59	0.50
25:1:1:MET:HA	26:2:413:LEU:CA	2.42	0.50
25:1:2:VAL:HG12	26:2:456:LYS:HG2	1.79	0.50
26:2:214:TYR:CB	26:2:261:PHE:CE2	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:29:DC:H2''	28:X:30:DG:H5'	1.94	0.50
2:B:295:PRO:HB2	9:I:11:PHE:HD2	1.77	0.50
2:B:483:ARG:HG3	2:B:526:LEU:HB3	1.94	0.50
2:B:728:MET:HE2	2:B:942:LYS:HG2	1.93	0.50
16:P:256:GLN:O	16:P:316:LYS:NZ	2.32	0.50
17:Q:95:ASN:OD1	17:Q:96:TYR:N	2.45	0.50
22:V:667:THR:CA	25:1:62:ASP:OD1	2.59	0.50
23:W:209:TYR:HH	23:W:234:ASP:H	1.58	0.50
26:2:81:LYS:CE	26:2:89:LEU:HD21	2.42	0.50
26:2:188:THR:HG23	26:2:189:GLU:N	2.27	0.50
27:3:12:VAL:CG2	27:3:161:ILE:HA	2.42	0.50
2:B:455:ASP:O	2:B:457:LYS:N	2.40	0.50
2:B:855:ALA:HB2	12:L:46:LYS:HE2	1.93	0.50
13:M:86:LYS:NZ	28:X:40:DT:N3	2.60	0.50
13:M:178:LYS:HB3	20:T:154:LYS:HE3	1.93	0.50
17:Q:153:ARG:HD3	17:Q:158:HIS:HB3	1.94	0.50
23:W:325:THR:HG22	23:W:329:PHE:CE2	2.47	0.50
25:1:45:VAL:CG2	26:2:409:TYR:CE2	2.95	0.50
26:2:35:TYR:CD1	26:2:62:LEU:CD1	2.95	0.50
26:2:140:LYS:CG	26:2:162:PHE:CE1	2.94	0.50
26:2:181:GLN:HE22	26:2:220:LEU:HD12	1.76	0.50
27:3:12:VAL:HG23	27:3:12:VAL:O	2.10	0.50
27:3:60:ILE:HG22	27:3:61:ALA:N	2.26	0.50
27:3:64:ILE:CG2	27:3:128:HIS:HB3	2.42	0.50
25:1:1:MET:HE1	26:2:440:LEU:CD1	2.31	0.49
27:3:12:VAL:HG22	27:3:161:ILE:HA	1.94	0.49
28:X:13:DT:H2''	28:X:14:DA:H8	1.77	0.49
1:A:205:VAL:HG23	1:A:205:VAL:O	2.12	0.49
1:A:604:ARG:HG3	1:A:606:HIS:HE1	1.76	0.49
17:Q:23:ARG:HD3	18:R:207:SER:O	2.12	0.49
23:W:116:CYS:SG	23:W:191:PRO:HD2	2.51	0.49
25:1:2:VAL:HG23	25:1:2:VAL:O	2.11	0.49
26:2:77:LYS:CD	26:2:78:GLU:HG3	2.41	0.49
27:3:202:LEU:HD22	27:3:202:LEU:N	2.27	0.49
27:3:217:VAL:CG1	27:3:226:TYR:CE2	2.95	0.49
28:X:52:DG:H2''	28:X:53:DA:O4'	2.11	0.49
1:A:267:GLN:O	1:A:268:GLY:C	2.55	0.49
1:A:269:SER:O	1:A:270:ALA:CB	2.58	0.49
5:E:45:GLY:C	5:E:46:ASP:O	2.55	0.49
7:G:97:LEU:HB3	7:G:108:ILE:HB	1.93	0.49
14:N:312:GLU:C	14:N:314:LEU:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:315:VAL:CG1	23:W:500:ASP:HB3	2.26	0.49
26:2:51:LEU:HD23	26:2:51:LEU:C	2.37	0.49
27:3:59:VAL:HG13	27:3:59:VAL:O	2.12	0.49
27:3:178:MET:HE2	27:3:202:LEU:HD13	1.93	0.49
27:3:216:LYS:O	27:3:216:LYS:HG2	2.11	0.49
1:A:362:SER:OG	2:B:1084:LEU:HB2	2.11	0.49
1:A:1158:LEU:HD11	1:A:1308:TYR:CG	2.32	0.49
1:A:1162:GLU:OE2	1:A:1308:TYR:CZ	2.65	0.49
1:A:1471:PHE:HE1	6:F:64:ARG:HD3	1.77	0.49
7:G:63:ARG:C	7:G:65:PHE:H	2.20	0.49
13:M:245:VAL:HG12	13:M:291:LEU:HD23	1.92	0.49
18:R:225:VAL:HG12	18:R:225:VAL:O	2.13	0.49
23:W:494:ILE:HD11	23:W:680:ALA:HB2	1.93	0.49
26:2:199:ALA:CB	26:2:201:PHE:CE2	2.95	0.49
26:2:245:LEU:HD22	26:2:245:LEU:N	2.27	0.49
27:3:24:LYS:HE2	27:3:196:LEU:HB3	1.93	0.49
28:X:45:DT:H4'	28:X:45:DT:OP1	2.12	0.49
29:Y:24:DC:C2'	29:Y:25:DT:C5	2.88	0.49
26:2:57:MET:HA	26:2:60:LEU:HG	1.93	0.49
26:2:426:ARG:HD2	26:2:444:THR:CG2	2.43	0.49
27:3:53:ARG:HA	27:3:101:TYR:HE1	1.78	0.49
27:3:137:LEU:CD1	27:3:177:PHE:CE1	2.95	0.49
27:3:220:MET:N	27:3:221:PRO:HD2	2.28	0.49
1:A:197:GLU:CD	13:M:93:PHE:CE2	2.90	0.49
1:A:560:VAL:HG21	1:A:586:TRP:CE3	2.48	0.49
1:A:624:GLY:C	1:A:626:THR:H	2.20	0.49
1:A:862:ARG:HG3	2:B:1089:MET:HE2	1.95	0.49
3:C:49:TRP:O	3:C:163:ALA:HA	2.12	0.49
5:E:64:HIS:ND1	5:E:70:ASP:O	2.46	0.49
24:0:55:LEU:N	27:3:209:ILE:HD11	2.28	0.49
26:2:29:GLY:CA	27:3:25:GLN:CG	2.82	0.49
26:2:236:PHE:CZ	26:2:258:LEU:CD1	2.95	0.49
27:3:42:MET:HE2	27:3:108:ASN:CB	2.42	0.49
27:3:166:ALA:O	27:3:198:SER:HB2	2.13	0.49
27:3:215:LEU:HD12	27:3:230:VAL:CG2	2.42	0.49
1:A:358:ARG:NH2	2:B:1076:GLU:HA	2.25	0.49
1:A:1158:LEU:CD2	1:A:1308:TYR:CD2	2.90	0.49
7:G:158:PHE:N	7:G:158:PHE:CD1	2.80	0.49
18:R:80:LYS:HB2	20:T:188:PHE:CE2	2.47	0.49
20:T:175:ARG:HE	28:X:21:DG:P	2.36	0.49
23:W:624:PRO:O	23:W:656:ALA:HB1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:28:PRO:HA	27:3:33:THR:CB	2.41	0.49
26:2:203:PHE:CE2	26:2:205:LEU:CD2	2.96	0.49
27:3:107:ALA:O	27:3:111:ILE:HG23	2.11	0.49
27:3:174:TYR:HD1	27:3:202:LEU:HD11	1.78	0.49
27:3:195:VAL:HG23	27:3:214:TYR:CE1	2.48	0.49
1:A:524:MET:N	1:A:524:MET:SD	2.82	0.49
1:A:1307:VAL:O	1:A:1308:TYR:CB	2.51	0.49
2:B:677:MET:HG3	2:B:678:THR:HG23	1.95	0.49
3:C:169:PHE:CE1	3:C:171:LYS:HB3	2.48	0.49
22:V:516:PRO:HG2	22:V:706:LYS:HE2	1.91	0.49
26:2:181:GLN:HE21	26:2:181:GLN:CA	2.23	0.49
27:3:10:LEU:CD2	27:3:143:TYR:HE2	2.25	0.49
27:3:21:TRP:HA	27:3:24:LYS:CG	2.41	0.49
27:3:177:PHE:CZ	27:3:203:LEU:CD2	2.95	0.49
1:A:263:ALA:C	1:A:264:VAL:HG22	2.37	0.49
2:B:474:THR:HG23	2:B:732:ALA:O	2.13	0.49
2:B:871:VAL:HG13	2:B:890:ARG:HB2	1.95	0.49
7:G:1:MET:N	7:G:78:ARG:O	2.45	0.49
17:Q:23:ARG:CZ	18:R:207:SER:O	2.48	0.49
22:V:321:GLU:HG3	23:W:499:ASN:HB3	1.70	0.49
26:2:77:LYS:HD3	26:2:78:GLU:HG3	1.94	0.49
28:X:46:DT:H2'	28:X:47:DT:C5	2.48	0.49
2:B:72:GLN:HE22	2:B:80:GLU:N	2.11	0.49
2:B:812:ARG:NH2	29:Y:52:DT:OP1	2.38	0.49
2:B:935:PHE:CE1	2:B:1050:ARG:HG3	2.48	0.49
2:B:1132:THR:HG23	2:B:1133:HIS:ND1	2.27	0.49
3:C:135:ARG:O	3:C:136:ASP:O	2.31	0.49
4:D:30:GLU:O	7:G:3:TYR:HA	2.13	0.49
24:0:54:ARG:CB	27:3:209:ILE:CG2	2.87	0.49
26:2:42:LEU:HD22	26:2:52:ALA:HA	1.95	0.49
26:2:189:GLU:CA	26:2:192:GLU:HG2	2.41	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:CE2	2.95	0.49
27:3:160:ARG:HE	27:3:190:LEU:HG	1.78	0.49
29:Y:24:DC:C2	29:Y:25:DT:N3	2.81	0.49
1:A:201:GLU:HG2	1:A:212:LYS:HB3	1.93	0.48
2:B:333:GLU:CD	19:S:53:ASN:HD21	2.17	0.48
2:B:566:LYS:HD3	2:B:573:TRP:NE1	2.23	0.48
2:B:1124:ILE:HG22	2:B:1126:ALA:H	1.78	0.48
12:L:19:CYS:HB3	12:L:22:CYS:SG	2.53	0.48
16:P:293:TYR:HD2	16:P:302:LEU:HD13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:44:LYS:HG3	17:Q:47:ASP:H	1.76	0.48
26:2:89:LEU:HD23	26:2:93:LEU:HG	1.94	0.48
26:2:159:VAL:N	26:2:162:PHE:HB3	2.28	0.48
26:2:166:SER:HB3	26:2:167:PRO:CD	2.43	0.48
26:2:251:VAL:HG11	26:2:254:MET:SD	2.53	0.48
27:3:216:LYS:HD2	27:3:216:LYS:N	2.22	0.48
1:A:261:ARG:HB2	1:A:274:ASP:HB3	1.95	0.48
1:A:1138:SER:OG	1:A:1139:LEU:N	2.46	0.48
2:B:873:LEU:CB	2:B:874:PRO:HD3	2.41	0.48
17:Q:188:TYR:CE1	18:R:210:PHE:HB2	2.48	0.48
26:2:60:LEU:CD1	26:2:95:ILE:CG2	2.91	0.48
26:2:133:THR:HG23	26:2:134:SER:N	2.29	0.48
26:2:198:SER:OG	26:2:238:PHE:HE2	1.96	0.48
1:A:522:PRO:HA	1:A:666:ARG:NE	2.09	0.48
2:B:80:GLU:O	2:B:82:PRO:CD	2.61	0.48
2:B:513:GLU:HG3	2:B:726:SER:HB3	1.94	0.48
2:B:761:THR:N	2:B:764:MET:HE3	2.22	0.48
5:E:48:PRO:O	5:E:52:ARG:NH1	2.45	0.48
10:J:6:ARG:HA	10:J:13:ILE:HA	1.95	0.48
11:K:47:LYS:HD2	11:K:61:TYR:HD1	1.78	0.48
17:Q:69:ASP:HA	18:R:226:ASP:CG	2.37	0.48
23:W:73:CYS:HB2	23:W:209:TYR:CE1	2.48	0.48
23:W:596:LEU:HG	23:W:597:LEU:N	2.27	0.48
24:0:209:THR:HA	24:0:219:TYR:CD1	2.48	0.48
25:1:45:VAL:HG21	26:2:409:TYR:CE2	2.48	0.48
26:2:90:LEU:CD2	26:2:140:LYS:HD3	2.42	0.48
28:X:50:DT:H4'	28:X:50:DT:OP1	2.13	0.48
1:A:455:ILE:HD13	1:A:520:MET:CE	2.43	0.48
1:A:1162:GLU:HA	1:A:1307:VAL:HB	1.96	0.48
1:A:1319:LYS:HA	1:A:1319:LYS:HD3	1.69	0.48
2:B:464:ALA:HB1	13:M:62:LYS:NZ	2.28	0.48
2:B:747:LEU:HD11	2:B:810:PHE:HZ	1.79	0.48
2:B:798:ARG:O	2:B:801:VAL:HG22	2.14	0.48
9:I:57:LYS:O	9:I:58:ILE:HG12	2.13	0.48
13:M:91:ALA:O	13:M:92:SER:C	2.55	0.48
19:S:124:TYR:HB3	20:T:20:LEU:HD11	1.95	0.48
24:0:55:LEU:HD12	27:3:178:MET:HE1	1.95	0.48
25:1:3:ASN:HB2	26:2:412:PHE:O	2.12	0.48
26:2:176:ALA:O	26:2:177:GLN:HB2	2.12	0.48
2:B:324:ARG:NH1	19:S:162:GLU:OE2	2.46	0.48
2:B:489:ILE:HG13	2:B:490:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:873:LEU:CB	2:B:874:PRO:CD	2.90	0.48
2:B:1028:LEU:C	2:B:1029:TYR:HD1	2.21	0.48
2:B:1060:HIS:CE1	2:B:1078:ARG:HG3	2.48	0.48
18:R:167:LEU:HD22	18:R:200:ILE:HB	1.96	0.48
23:W:285:TYR:CE1	23:W:403:PHE:CZ	3.01	0.48
27:3:174:TYR:HE1	27:3:178:MET:HE3	1.77	0.48
1:A:632:ASN:HA	1:A:992:LYS:HD2	1.96	0.48
2:B:418:TYR:CD1	2:B:434:ALA:HB2	2.48	0.48
2:B:626:LEU:HG	2:B:698:ILE:HG22	1.95	0.48
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.78	0.48
17:Q:184:ILE:HD11	18:R:218:LYS:NZ	2.19	0.48
23:W:37:HIS:NE2	23:W:454:VAL:CG1	2.76	0.48
25:1:38:ILE:CG2	25:1:44:PHE:CE1	2.96	0.48
26:2:35:TYR:CE2	26:2:62:LEU:CB	2.96	0.48
27:3:21:TRP:CG	27:3:34:LEU:HD23	2.48	0.48
1:A:53:LYS:HE3	1:A:59:ASP:HB3	1.95	0.48
2:B:124:LEU:HD23	2:B:149:ILE:HD11	1.95	0.48
2:B:356:PHE:O	19:S:116:GLY:HA2	2.13	0.48
2:B:726:SER:O	2:B:730:LYS:HE2	2.14	0.48
2:B:796:MET:O	2:B:948:GLN:HA	2.14	0.48
2:B:1101:GLN:NE2	6:F:64:ARG:CG	2.77	0.48
3:C:154:ARG:HB3	10:J:65:LEU:CD1	2.43	0.48
14:N:319:ASP:C	14:N:321:SER:N	2.72	0.48
17:Q:164:ASP:O	17:Q:166:SER:N	2.45	0.48
22:V:504:LYS:CB	22:V:654:GLU:O	2.59	0.48
23:W:73:CYS:HB3	23:W:209:TYR:CG	2.48	0.48
25:1:34:ILE:HG22	25:1:46:ILE:CG1	2.44	0.48
26:2:178:LEU:HD12	26:2:178:LEU:N	2.28	0.48
1:A:202:TRP:O	1:A:203:LYS:O	2.32	0.48
1:A:578:ALA:HB3	1:A:587:THR:HG23	1.96	0.48
1:A:1276:VAL:HG12	1:A:1279:MET:HB2	1.93	0.48
2:B:213:SER:HA	2:B:242:ARG:HD2	1.96	0.48
2:B:1000:THR:HG23	2:B:1001:PRO:HD2	1.96	0.48
5:E:13:ILE:HG22	5:E:136:LEU:HA	1.94	0.48
13:M:30:GLY:HA2	13:M:44:ARG:HG2	1.96	0.48
18:R:119:LEU:HA	18:R:123:ALA:HB3	1.95	0.48
22:V:370:SER:O	22:V:374:TRP:HD1	1.96	0.48
26:2:211:GLN:HE21	26:2:257:SER:HB3	1.78	0.48
1:A:187:TYR:HB2	1:A:205:VAL:HG21	1.95	0.48
18:R:195:PRO:HB2	18:R:199:LYS:HG3	1.95	0.48
20:T:81:HIS:HB3	20:T:116:CYS:SG	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:514:MET:SD	22:V:537:ASN:CG	2.97	0.48
23:W:73:CYS:CB	23:W:209:TYR:CE1	2.97	0.48
25:1:21:LEU:N	25:1:21:LEU:HD23	2.29	0.48
26:2:211:GLN:CA	26:2:261:PHE:CE1	2.95	0.48
29:Y:52:DT:H2''	29:Y:53:DG:O4'	2.13	0.48
1:A:932:ARG:CB	1:A:943:LEU:HD11	2.43	0.48
1:A:1263:ASN:HB2	1:A:1268:LYS:HD2	1.96	0.48
2:B:94:SER:OG	2:B:95:LYS:N	2.47	0.48
9:I:105:GLU:HB3	9:I:107:ALA:HB2	1.94	0.48
10:J:63:ALA:CB	10:J:64:PRO:CD	2.90	0.48
16:P:156:SER:O	16:P:158:SER:N	2.47	0.48
23:W:28:LEU:HD13	23:W:28:LEU:C	2.38	0.48
23:W:263:LEU:C	23:W:263:LEU:HD23	2.39	0.48
24:0:165:ARG:HB2	24:0:193:LYS:O	2.14	0.48
25:1:53:LEU:H	25:1:53:LEU:CD1	2.26	0.48
26:2:218:GLN:HG2	26:2:268:PHE:CB	2.44	0.48
26:2:236:PHE:CD1	26:2:261:PHE:HB3	2.49	0.48
27:3:124:ILE:O	27:3:127:GLN:HB2	2.14	0.48
27:3:226:TYR:CA	27:3:230:VAL:HG23	2.42	0.48
1:A:265:VAL:HG23	1:A:266:MET:H	1.79	0.47
1:A:686:THR:OG1	1:A:687:ILE:N	2.46	0.47
2:B:810:PHE:CD2	2:B:927:ARG:NH2	2.81	0.47
9:I:41:ASN:HA	19:S:177:MET:HE1	1.95	0.47
21:U:248:HIS:O	21:U:252:LYS:NZ	2.47	0.47
25:1:38:ILE:HG22	25:1:44:PHE:CE1	2.48	0.47
26:2:170:ALA:CB	26:2:213:TRP:CZ3	2.95	0.47
27:3:10:LEU:CD1	27:3:56:LYS:HG2	2.44	0.47
27:3:34:LEU:HD22	27:3:37:CYS:SG	2.54	0.47
28:X:82:DG:N2	29:Y:13:DC:C2	2.81	0.47
29:Y:24:DC:O2	29:Y:25:DT:N3	2.47	0.47
1:A:375:ILE:HG23	1:A:375:ILE:HD12	1.54	0.47
2:B:718:GLN:HB2	2:B:976:MET:HE3	1.96	0.47
5:E:71:GLN:HE21	5:E:99:ILE:HG22	1.79	0.47
8:H:65:TYR:CG	8:H:70:LEU:HD22	2.49	0.47
10:J:40:LEU:HD11	10:J:49:LEU:HD13	1.97	0.47
16:P:206:GLU:C	16:P:208:ARG:N	2.67	0.47
17:Q:105:TYR:CD1	18:R:234:GLU:CB	2.97	0.47
22:V:361:CYS:HB3	22:V:405:VAL:HG21	1.96	0.47
22:V:522:TYR:CE2	25:1:62:ASP:CG	2.69	0.47
25:1:43:VAL:HG12	25:1:44:PHE:N	2.28	0.47
26:2:203:PHE:CD2	26:2:204:LEU:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:124:ILE:HD13	27:3:124:ILE:C	2.38	0.47
27:3:165:LYS:NZ	27:3:200:SER:H	2.12	0.47
1:A:274:ASP:C	1:A:276:LEU:N	2.72	0.47
2:B:184:TYR:HE2	2:B:191:GLU:HG2	1.79	0.47
2:B:422:PHE:CD1	2:B:422:PHE:C	2.91	0.47
2:B:875:GLU:O	2:B:876:ASN:CB	2.49	0.47
2:B:947:ILE:HG12	2:B:948:GLN:N	2.29	0.47
3:C:169:PHE:HE1	3:C:171:LYS:HB3	1.78	0.47
9:I:60:HIS:C	9:I:62:VAL:N	2.71	0.47
16:P:297:LYS:C	16:P:299:ARG:N	2.71	0.47
20:T:229:HIS:CD2	28:X:28:DG:H21	2.33	0.47
27:3:10:LEU:HA	27:3:56:LYS:HG2	1.96	0.47
1:A:426:ARG:HB3	13:M:40:VAL:HG22	1.94	0.47
1:A:807:LEU:HB3	1:A:809:HIS:HD2	1.78	0.47
2:B:348:LEU:HD13	2:B:364:PHE:HD2	1.79	0.47
3:C:184:PHE:HD1	3:C:231:TYR:CE1	2.33	0.47
10:J:43:TYR:HA	10:J:46:ARG:HB2	1.95	0.47
14:N:360:LEU:HD11	15:O:81:PHE:HD2	1.79	0.47
20:T:80:GLU:O	20:T:119:ALA:HB2	2.14	0.47
23:W:73:CYS:HB3	23:W:209:TYR:CD1	2.50	0.47
26:2:205:LEU:HD22	26:2:205:LEU:N	2.30	0.47
26:2:236:PHE:HE2	26:2:262:LEU:CD1	2.27	0.47
1:A:880:ARG:HG2	1:A:886:VAL:HA	1.97	0.47
2:B:177:CYS:HB3	2:B:180:ASP:HB2	1.95	0.47
17:Q:184:ILE:HD11	18:R:213:ASP:OD1	2.14	0.47
26:2:117:ASN:CB	27:3:42:MET:HE1	2.42	0.47
26:2:138:PRO:HD3	26:2:189:GLU:CD	2.40	0.47
27:3:160:ARG:HB2	27:3:190:LEU:HG	1.96	0.47
27:3:216:LYS:O	27:3:218:PRO:HD3	2.14	0.47
1:A:275:ASP:OD1	1:A:276:LEU:N	2.47	0.47
1:A:1065:PHE:CE2	1:A:1069:LEU:HD11	2.49	0.47
1:A:1304:ILE:C	1:A:1307:VAL:HG22	2.32	0.47
2:B:728:MET:HE1	2:B:940:GLY:C	2.39	0.47
3:C:69:GLY:HA3	12:L:57:ALA:HB1	1.95	0.47
15:O:77:ASN:OD1	15:O:78:ASP:N	2.48	0.47
18:R:151:LEU:HB3	18:R:154:LEU:HB3	1.97	0.47
25:1:50:VAL:CG1	25:1:54:GLN:HG2	2.41	0.47
25:1:57:VAL:CG2	25:1:61:MET:HE3	2.44	0.47
1:A:608:THR:HB	1:A:610:PRO:HD2	1.92	0.47
1:A:612:ASP:O	1:A:613:GLU:C	2.57	0.47
1:A:1319:LYS:O	1:A:1321:ILE:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:ILE:HD12	1:A:1329:LYS:O	2.14	0.47
1:A:1472:ASP:HB2	6:F:107:ARG:HB3	1.97	0.47
2:B:950:ARG:HB2	2:B:952:GLU:OE1	2.15	0.47
2:B:957:THR:O	2:B:960:GLY:N	2.36	0.47
3:C:75:SER:HB3	3:C:79:VAL:HB	1.96	0.47
3:C:86:ARG:HH22	11:K:10:PHE:HE1	1.62	0.47
3:C:262:GLN:HG3	11:K:18:LYS:HG2	1.95	0.47
5:E:129:GLN:OE1	5:E:130:PHE:N	2.47	0.47
8:H:65:TYR:CE2	8:H:70:LEU:HD22	2.49	0.47
13:M:16:PRO:HD2	13:M:39:LEU:HD22	1.96	0.47
19:S:122:THR:HA	20:T:24:PRO:HA	1.96	0.47
20:T:155:PRO:C	20:T:157:ALA:N	2.73	0.47
24:O:77:LYS:HA	24:O:77:LYS:HE3	1.96	0.47
26:2:100:LEU:HD11	26:2:119:ARG:CG	2.31	0.47
26:2:118:LEU:HD21	27:3:39:ASP:OD1	1.95	0.47
26:2:163:MET:HE1	26:2:206:LEU:HB3	1.94	0.47
27:3:12:VAL:CG2	27:3:161:ILE:HG23	2.43	0.47
27:3:34:LEU:HD13	27:3:38:ILE:HG12	1.95	0.47
27:3:70:LEU:HD22	27:3:114:GLU:CB	2.44	0.47
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.96	0.47
8:H:93:TYR:HE1	8:H:140:ARG:HA	1.79	0.47
8:H:108:ALA:C	8:H:110:THR:N	2.72	0.47
13:M:300:PHE:HD2	13:M:306:PHE:HE1	1.62	0.47
25:1:9:LEU:N	25:1:9:LEU:HD12	2.30	0.47
25:1:38:ILE:CG2	25:1:44:PHE:CD1	2.94	0.47
26:2:89:LEU:CD2	26:2:93:LEU:HG	2.44	0.47
1:A:620:HIS:O	1:A:621:ILE:C	2.54	0.47
1:A:889:LEU:HD21	5:E:206:TYR:HE1	1.80	0.47
1:A:926:ASN:OD1	1:A:932:ARG:HG2	2.15	0.47
2:B:239:MET:HE2	2:B:372:LEU:HD21	1.97	0.47
2:B:628:VAL:HG21	2:B:682:LEU:HD11	1.97	0.47
2:B:972:ILE:O	2:B:976:MET:N	2.48	0.47
2:B:1091:ARG:O	2:B:1095:ILE:HG13	2.14	0.47
10:J:66:GLU:HG3	12:L:23:HIS:CE1	2.49	0.47
13:M:75:LEU:HD22	13:M:139:ASN:OD1	2.14	0.47
20:T:168:LYS:C	20:T:170:LYS:H	2.22	0.47
26:2:51:LEU:HD21	26:2:55:TRP:CD1	2.50	0.47
27:3:137:LEU:HD11	27:3:177:PHE:CE1	2.50	0.47
1:A:367:ILE:HA	1:A:482:PHE:O	2.15	0.47
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.79	0.47
1:A:878:THR:HG1	1:A:880:ARG:HE	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:LEU:HD13	1:A:1043:ILE:HD11	1.96	0.47
1:A:1163:HIS:H	1:A:1307:VAL:HG21	1.80	0.47
2:B:81:PRO:HD2	2:B:135:GLU:HG3	1.97	0.47
3:C:35:ARG:HG2	3:C:36:ARG:N	2.30	0.47
13:M:16:PRO:HG2	13:M:39:LEU:CD2	2.38	0.47
14:N:25:VAL:HG11	15:O:36:VAL:HG13	1.97	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
26:2:46:ARG:CD	26:2:85:GLU:CB	2.93	0.47
26:2:85:GLU:O	26:2:89:LEU:HB2	2.14	0.47
27:3:56:LYS:HD3	27:3:56:LYS:N	2.30	0.47
27:3:64:ILE:HG21	27:3:128:HIS:HB3	1.97	0.47
2:B:470:LEU:HD11	2:B:478:THR:HG23	1.96	0.46
9:I:98:GLN:O	9:I:100:HIS:N	2.48	0.46
17:Q:173:ALA:O	17:Q:177:LEU:HD23	2.15	0.46
21:U:223:MET:O	21:U:226:GLU:O	2.33	0.46
25:1:38:ILE:HA	25:1:44:PHE:CD1	2.37	0.46
25:1:38:ILE:O	25:1:38:ILE:HG12	2.15	0.46
26:2:93:LEU:CA	26:2:96:TRP:CD1	2.94	0.46
26:2:201:PHE:CD1	26:2:202:GLN:N	2.83	0.46
1:A:1408:ARG:O	1:A:1410:HIS:N	2.48	0.46
2:B:1062:ARG:HH12	2:B:1075:MET:N	2.11	0.46
3:C:157:GLN:CG	10:J:65:LEU:HB3	2.45	0.46
10:J:63:ALA:N	10:J:64:PRO:HD2	2.30	0.46
13:M:16:PRO:CG	13:M:39:LEU:CD2	2.93	0.46
20:T:125:MET:O	20:T:129:ARG:N	2.41	0.46
22:V:689:VAL:CG2	26:2:391:ILE:CD1	2.92	0.46
25:1:38:ILE:CB	25:1:44:PHE:CE1	2.98	0.46
25:1:53:LEU:O	25:1:57:VAL:HG12	2.15	0.46
26:2:211:GLN:CB	26:2:261:PHE:CE1	2.95	0.46
1:A:156:GLY:HA2	1:A:181:HIS:CE1	2.50	0.46
1:A:525:ILE:HG12	1:A:666:ARG:NH2	2.30	0.46
1:A:1130:ILE:HG21	1:A:1411:LEU:HD13	1.98	0.46
2:B:422:PHE:HD1	2:B:428:ASP:H	1.62	0.46
2:B:954:MET:HE2	2:B:963:PRO:O	2.15	0.46
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.49	0.46
20:T:198:ASN:OD1	20:T:199:LEU:N	2.49	0.46
25:1:10:ILE:HG12	25:1:43:VAL:CG1	2.45	0.46
27:3:131:THR:HG23	27:3:133:LEU:HD13	1.95	0.46
27:3:177:PHE:O	27:3:181:ILE:HG13	2.15	0.46
1:A:264:VAL:HG23	1:A:272:ASN:ND2	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:THR:CB	1:A:610:PRO:HG2	2.45	0.46
1:A:1185:VAL:HG21	9:I:51:SER:OG	2.16	0.46
3:C:154:ARG:HB3	10:J:65:LEU:HD22	1.96	0.46
13:M:94:ASP:CG	13:M:97:GLY:O	2.49	0.46
16:P:298:PRO:O	16:P:300:ILE:N	2.48	0.46
21:U:215:ILE:HG23	21:U:219:LEU:HD23	1.97	0.46
25:1:40:ASP:HB2	25:1:43:VAL:H	1.81	0.46
26:2:96:TRP:CH2	26:2:97:HIS:CE1	3.03	0.46
1:A:261:ARG:HB2	1:A:274:ASP:CB	2.45	0.46
1:A:451:CYS:SG	1:A:452:ASP:N	2.88	0.46
1:A:1171:ALA:O	9:I:59:THR:HG23	2.15	0.46
2:B:960:GLY:O	2:B:962:THR:N	2.48	0.46
3:C:76:ASP:OD1	3:C:243:THR:HG21	2.15	0.46
18:R:116:LYS:HA	18:R:119:LEU:HD12	1.98	0.46
19:S:135:PHE:HD1	19:S:135:PHE:HA	1.66	0.46
22:V:613:THR:O	22:V:614:SER:HB2	2.14	0.46
26:2:35:TYR:CD1	26:2:62:LEU:CG	2.92	0.46
26:2:223:ALA:C	26:2:225:SER:H	2.24	0.46
26:2:240:LEU:HD12	26:2:240:LEU:N	2.30	0.46
27:3:10:LEU:HB2	27:3:56:LYS:HE3	1.97	0.46
29:Y:16:DA:H2'	29:Y:17:DG:C8	2.50	0.46
1:A:963:ARG:O	1:A:967:ARG:HG3	2.16	0.46
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	1.96	0.46
2:B:282:ARG:HD2	9:I:21:ASN:HD21	1.80	0.46
2:B:676:ALA:HB2	2:B:693:TYR:CG	2.50	0.46
4:D:40:LEU:HD13	7:G:75:ILE:HD11	1.97	0.46
7:G:55:GLY:HA3	7:G:69:PRO:HG2	1.97	0.46
10:J:3:ILE:HD13	10:J:18:TRP:CD2	2.50	0.46
11:K:39:ASP:OD1	11:K:39:ASP:N	2.37	0.46
23:W:37:HIS:CG	23:W:454:VAL:HG13	2.50	0.46
27:3:196:LEU:HB3	27:3:220:MET:SD	2.56	0.46
1:A:425:ASP:CG	13:M:39:LEU:CD1	2.82	0.46
1:A:557:ARG:HB3	1:A:557:ARG:HH11	1.79	0.46
2:B:526:LEU:HA	2:B:526:LEU:HD12	1.48	0.46
2:B:964:ASP:O	2:B:965:ILE:HG13	2.14	0.46
3:C:149:LEU:HD21	3:C:152:LYS:HG3	1.98	0.46
4:D:70:ARG:NE	7:G:142:GLU:OE2	2.43	0.46
22:V:325:ARG:NH2	23:W:499:ASN:CG	2.62	0.46
22:V:325:ARG:HH22	23:W:499:ASN:HB2	0.64	0.46
25:1:2:VAL:HG12	26:2:456:LYS:CE	2.44	0.46
26:2:214:TYR:CE1	26:2:233:ILE:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:15:VAL:HG12	27:3:164:ILE:HD12	1.97	0.46
27:3:69:PHE:HE1	27:3:139:LYS:HD2	1.77	0.46
28:X:73:DG:C2	28:X:74:DT:C2	3.04	0.46
1:A:49:GLY:O	1:A:52:PRO:HD2	2.16	0.46
1:A:79:THR:HG23	13:M:43:ASP:CG	2.40	0.46
1:A:117:LEU:HB2	1:A:232:GLU:HG2	1.96	0.46
1:A:619:LYS:HD3	1:A:619:LYS:HA	1.47	0.46
2:B:223:SER:OG	2:B:233:SER:HB2	2.15	0.46
2:B:1066:PRO:HB2	2:B:1075:MET:HG3	1.97	0.46
5:E:41:LYS:HG3	5:E:46:ASP:HB2	1.98	0.46
9:I:29:ASP:OD2	9:I:32:ASN:ND2	2.37	0.46
19:S:127:PHE:HB2	20:T:19:TRP:HB2	1.98	0.46
22:V:519:TYR:CE2	25:1:20:LEU:HG	2.51	0.46
23:W:623:VAL:HG23	23:W:681:ASP:HB2	1.98	0.46
25:1:13:ASP:OD2	25:1:17:LYS:HB2	2.13	0.46
25:1:18:GLN:CD	25:1:44:PHE:CZ	2.92	0.46
26:2:81:LYS:CG	26:2:82:ALA:N	2.79	0.46
26:2:96:TRP:CZ2	26:2:97:HIS:NE2	2.83	0.46
26:2:170:ALA:C	26:2:213:TRP:CZ3	2.94	0.46
26:2:171:VAL:HG13	26:2:216:MET:HB3	1.98	0.46
27:3:10:LEU:N	27:3:56:LYS:HE3	2.31	0.46
27:3:25:GLN:HA	27:3:25:GLN:NE2	2.31	0.46
1:A:117:LEU:H	1:A:232:GLU:CD	2.24	0.46
2:B:180:ASP:OD1	2:B:181:PRO:HD2	2.16	0.46
2:B:508:MET:HE2	2:B:670:GLU:OE1	2.16	0.46
2:B:529:MET:HE2	2:B:624:PRO:CD	2.46	0.46
2:B:802:ASP:C	2:B:804:GLY:H	2.24	0.46
13:M:183:VAL:HG12	20:T:152:ASN:ND2	2.31	0.46
17:Q:185:GLU:HB3	17:Q:186:PRO:HD3	1.97	0.46
18:R:80:LYS:HG2	18:R:108:HIS:HE1	1.81	0.46
26:2:171:VAL:CG2	26:2:213:TRP:HA	2.19	0.46
26:2:187:SER:OG	26:2:190:PRO:HD2	2.16	0.46
27:3:125:LYS:C	27:3:127:GLN:H	2.24	0.46
1:A:734:ARG:HH12	9:I:104:ALA:HB1	1.81	0.46
1:A:1026:ASP:O	1:A:1031:ARG:NH2	2.49	0.46
1:A:1158:LEU:O	1:A:1162:GLU:HG3	2.16	0.46
2:B:1101:GLN:HE22	6:F:64:ARG:CG	2.29	0.46
8:H:85:ALA:HB1	8:H:88:PHE:CZ	2.51	0.46
15:O:80:GLU:HG3	15:O:89:LYS:HG2	1.98	0.46
17:Q:104:LYS:HE3	17:Q:105:TYR:CZ	2.50	0.46
17:Q:170:LYS:O	17:Q:174:ARG:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:315:VAL:CG1	23:W:500:ASP:CG	2.80	0.46
25:1:57:VAL:HG13	25:1:58:GLY:N	2.31	0.46
27:3:64:ILE:CG2	27:3:128:HIS:CG	2.99	0.46
29:Y:25:DT:H2"	29:Y:26:DG:C8	2.51	0.46
1:A:42:LYS:NZ	1:A:43:TYR:O	2.49	0.45
1:A:365:THR:HG22	2:B:1059:ILE:HG22	1.97	0.45
1:A:511:THR:HG21	2:B:1105:GLU:OE2	2.16	0.45
1:A:621:ILE:O	1:A:623:PRO:CD	2.64	0.45
1:A:1163:HIS:H	1:A:1307:VAL:CG2	2.29	0.45
2:B:422:PHE:CD1	2:B:427:LYS:HA	2.50	0.45
23:W:420:PRO:O	23:W:421:PHE:CG	2.68	0.45
25:1:54:GLN:O	25:1:57:VAL:HG12	2.16	0.45
26:2:211:GLN:CD	26:2:261:PHE:CE1	2.94	0.45
27:3:8:LEU:HD23	27:3:54:SER:CB	2.42	0.45
28:X:77:DC:H2"	28:X:78:DT:H72	1.98	0.45
1:A:1408:ARG:HH22	1:A:1421:ARG:HB2	1.81	0.45
1:A:1431:SER:HB3	1:A:1459:MET:HE1	1.97	0.45
2:B:964:ASP:OD1	2:B:964:ASP:N	2.47	0.45
3:C:133:ARG:HA	3:C:136:ASP:CG	2.33	0.45
13:M:157:ASP:OD2	13:M:185:ARG:NH2	2.49	0.45
17:Q:112:ARG:NH2	18:R:237:LEU:O	2.50	0.45
17:Q:113:ARG:NH2	18:R:218:LYS:HG3	2.29	0.45
17:Q:180:PHE:CE1	18:R:213:ASP:N	2.84	0.45
18:R:123:ALA:O	18:R:127:ASN:HB2	2.16	0.45
22:V:517:GLU:CB	22:V:713:LEU:HD22	2.46	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	2.47	0.45
26:2:217:LEU:CD2	26:2:233:ILE:HD11	2.45	0.45
26:2:236:PHE:CD1	26:2:239:GLN:CD	2.95	0.45
27:3:9:ASN:C	27:3:56:LYS:HE3	2.41	0.45
27:3:228:LEU:HD23	27:3:228:LEU:C	2.41	0.45
1:A:119:VAL:HG21	1:A:147:LEU:HD21	1.97	0.45
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.52	0.45
1:A:804:HIS:NE2	9:I:100:HIS:HA	2.31	0.45
1:A:873:VAL:HG22	1:A:1083:PRO:HA	1.99	0.45
2:B:809:VAL:HG23	2:B:924:ARG:HG3	1.99	0.45
2:B:1001:PRO:HB2	2:B:1002:PHE:CE1	2.51	0.45
3:C:148:ILE:HG12	3:C:149:LEU:N	2.28	0.45
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.52	0.45
10:J:3:ILE:HG13	10:J:52:HIS:CD2	2.51	0.45
20:T:3:GLU:H	20:T:3:GLU:CD	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:256:THR:HB	21:U:272:THR:HB	1.99	0.45
27:3:64:ILE:CG2	27:3:128:HIS:CB	2.94	0.45
27:3:141:LEU:C	27:3:144:ILE:HG22	2.41	0.45
29:Y:54:DA:H3'	29:Y:55:DG:H5''	1.97	0.45
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.90	0.45
1:A:196:LEU:HG	1:A:325:LEU:HD21	1.98	0.45
1:A:529:GLN:HG3	1:A:1094:SER:HB3	1.98	0.45
1:A:610:PRO:HB3	1:A:626:THR:CG2	2.47	0.45
2:B:573:TRP:O	2:B:573:TRP:HE3	2.00	0.45
9:I:73:SER:HA	9:I:95:VAL:HG21	1.97	0.45
17:Q:36:ILE:HG23	17:Q:39:ARG:NH2	2.32	0.45
17:Q:187:ILE:HG21	18:R:210:PHE:O	2.16	0.45
26:2:123:LEU:HD23	26:2:123:LEU:C	2.42	0.45
26:2:203:PHE:CG	26:2:204:LEU:N	2.85	0.45
27:3:33:THR:HG22	27:3:36:LYS:CB	2.44	0.45
27:3:190:LEU:HA	27:3:210:THR:HG21	1.91	0.45
1:A:948:ILE:HG23	1:A:1007:ILE:HD11	1.99	0.45
1:A:1451:MET:CE	1:A:1456:GLU:HB3	2.47	0.45
2:B:109:MET:O	2:B:112:GLU:N	2.50	0.45
2:B:1062:ARG:HH21	2:B:1065:GLY:N	2.10	0.45
4:D:140:PHE:CZ	4:D:142:TYR:HB3	2.52	0.45
5:E:84:ILE:CD1	28:X:65:DG:OP1	2.64	0.45
5:E:91:CYS:HA	5:E:94:MET:HG2	1.98	0.45
8:H:85:ALA:CB	8:H:88:PHE:CE2	2.99	0.45
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.51	0.45
13:M:52:TRP:CD1	13:M:52:TRP:C	2.92	0.45
16:P:204:ILE:HD12	16:P:206:GLU:HB2	1.98	0.45
25:1:2:VAL:HG11	26:2:456:LYS:CB	2.44	0.45
27:3:148:ASN:CG	27:3:157:MET:HE2	2.42	0.45
1:A:48:GLU:C	1:A:50:GLY:N	2.73	0.45
1:A:787:VAL:HG23	1:A:824:GLU:C	2.42	0.45
1:A:1119:LEU:HD13	1:A:1388:PHE:CG	2.52	0.45
1:A:1163:HIS:N	1:A:1307:VAL:HG21	2.31	0.45
2:B:496:ALA:HB3	2:B:498:PRO:HD2	1.99	0.45
2:B:1068:GLN:HB3	13:M:51:GLU:HB3	1.99	0.45
3:C:275:ASN:ND2	11:K:23:LYS:HA	2.31	0.45
7:G:107:PHE:CZ	17:Q:127:PHE:HZ	2.34	0.45
9:I:75:ASP:HA	9:I:76:PRO:HD3	1.87	0.45
14:N:333:ASN:HB3	14:N:359:ASN:O	2.16	0.45
16:P:263:ASP:OD1	16:P:264:VAL:N	2.49	0.45
21:U:194:ARG:HD3	21:U:194:ARG:HA	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:514:MET:HE2	22:V:664:SER:HB3	1.99	0.45
26:2:84:GLU:OE1	26:2:84:GLU:HA	2.15	0.45
26:2:189:GLU:CB	26:2:190:PRO:HD3	2.43	0.45
27:3:121:LYS:HD3	27:3:121:LYS:H	1.80	0.45
1:A:271:ARG:O	1:A:272:ASN:OD1	2.34	0.45
1:A:576:GLN:HG3	1:A:577:PRO:HD2	1.97	0.45
1:A:1189:ASP:O	1:A:1192:TRP:N	2.48	0.45
2:B:41:ARG:HD2	2:B:41:ARG:HA	1.36	0.45
2:B:531:TYR:CD2	2:B:532:ILE:N	2.85	0.45
13:M:17:ASN:CG	13:M:18:HIS:HD1	2.23	0.45
19:S:166:ARG:HH11	19:S:166:ARG:CG	2.28	0.45
26:2:30:VAL:CG1	26:2:34:LEU:CD2	2.94	0.45
26:2:35:TYR:HB2	26:2:62:LEU:HD12	1.99	0.45
26:2:130:SER:HB2	26:2:179:LEU:HD23	1.98	0.45
26:2:203:PHE:CD2	26:2:205:LEU:CD2	2.95	0.45
27:3:42:MET:CG	27:3:111:ILE:CD1	2.95	0.45
28:X:48:DT:OP1	28:X:48:DT:H4'	2.16	0.45
1:A:197:GLU:CD	13:M:93:PHE:CD2	2.93	0.45
1:A:522:PRO:HG3	1:A:666:ARG:HG3	1.99	0.45
1:A:893:GLU:O	5:E:200:ALA:HB2	2.17	0.45
1:A:931:ARG:O	1:A:933:THR:HG23	2.16	0.45
1:A:1468:THR:HA	6:F:60:TYR:HB3	1.98	0.45
2:B:91:ILE:HD11	2:B:124:LEU:HD11	1.98	0.45
5:E:52:ARG:NH2	5:E:54:ARG:HH11	2.15	0.45
9:I:11:PHE:HE1	9:I:54:TYR:HA	1.81	0.45
9:I:41:ASN:HB2	19:S:153:ARG:HD2	1.99	0.45
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.99	0.45
11:K:5:PRO:HB2	11:K:7:PHE:CE2	2.52	0.45
13:M:7:LEU:CG	13:M:10:LEU:HD13	2.46	0.45
14:N:313:PRO:HD2	16:P:250:PHE:HB3	1.98	0.45
27:3:219:GLN:OE1	27:3:219:GLN:HA	2.17	0.45
28:X:65:DG:C6	28:X:66:DA:C2	3.05	0.45
29:Y:34:DC:H1'	29:Y:35:DG:OP2	2.16	0.45
12:L:26:ASN:OD1	12:L:36:CYS:HA	2.17	0.45
15:O:7:ARG:HB3	15:O:16:GLN:NE2	2.32	0.45
23:W:37:HIS:NE2	23:W:454:VAL:HG11	2.32	0.45
26:2:217:LEU:CD2	26:2:233:ILE:CD1	2.95	0.45
1:A:26:LEU:O	1:A:26:LEU:HD12	2.17	0.45
1:A:540:ASP:CB	2:B:790:GLN:NE2	2.79	0.45
1:A:1139:LEU:HB3	1:A:1338:THR:OG1	2.16	0.45
2:B:1078:ARG:C	2:B:1080:ARG:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:171:ILE:HG12	18:R:177:ASN:H	1.82	0.45
26:2:35:TYR:CD2	26:2:62:LEU:CB	2.95	0.45
27:3:148:ASN:ND2	27:3:157:MET:HG3	2.32	0.45
29:Y:58:DC:H1'	29:Y:59:DG:C4	2.51	0.45
1:A:208:ASP:OD1	1:A:209:SER:N	2.38	0.44
1:A:599:HIS:O	1:A:992:LYS:NZ	2.50	0.44
1:A:1103:THR:HG23	1:A:1106:THR:OG1	2.17	0.44
1:A:1103:THR:HG21	1:A:1119:LEU:HG	1.99	0.44
1:A:1128:ILE:HD12	1:A:1414:ILE:HD11	1.98	0.44
2:B:289:ILE:HG12	2:B:291:ASP:H	1.82	0.44
5:E:84:ILE:CD1	28:X:65:DG:P	3.04	0.44
7:G:44:PHE:HE2	7:G:104:MET:HB2	1.83	0.44
23:W:37:HIS:CD2	23:W:454:VAL:CG1	3.00	0.44
24:0:100:PRO:HG2	27:3:208:ASP:OD2	2.17	0.44
26:2:89:LEU:HD23	26:2:89:LEU:C	2.42	0.44
26:2:123:LEU:CD2	26:2:178:LEU:CD1	2.95	0.44
26:2:140:LYS:HD3	26:2:162:PHE:CE1	2.47	0.44
27:3:71:TYR:CG	27:3:71:TYR:O	2.70	0.44
1:A:1029:LEU:H	5:E:162:ARG:HH12	1.66	0.44
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.56	0.44
1:A:1435:THR:OG1	1:A:1436:VAL:N	2.49	0.44
2:B:74:ALA:HB2	20:T:201:ASP:CG	2.42	0.44
2:B:598:VAL:O	2:B:600:GLU:N	2.49	0.44
5:E:11:TRP:CE3	5:E:37:LEU:HD13	2.51	0.44
6:F:61:GLU:CD	6:F:108:ARG:HH21	2.25	0.44
8:H:71:ASP:OD1	8:H:71:ASP:N	2.48	0.44
10:J:3:ILE:HG22	10:J:15:GLY:HA2	1.99	0.44
17:Q:25:PHE:CE1	18:R:210:PHE:CZ	3.05	0.44
17:Q:128:LYS:HG3	17:Q:129:CYS:N	2.32	0.44
17:Q:188:TYR:CE2	18:R:211:SER:HB3	2.52	0.44
20:T:121:SER:OG	20:T:122:GLU:N	2.50	0.44
22:V:370:SER:O	22:V:374:TRP:CD1	2.71	0.44
26:2:28:PRO:CD	27:3:25:GLN:NE2	2.72	0.44
1:A:426:ARG:HB3	13:M:40:VAL:CG2	2.48	0.44
1:A:460:ARG:HB3	1:A:501:MET:HE3	1.98	0.44
1:A:1112:VAL:HG12	21:U:254:GLY:HA2	2.00	0.44
1:A:1310:HIS:O	21:U:252:LYS:HD3	2.16	0.44
2:B:1055:VAL:HG13	2:B:1056:ASP:N	2.33	0.44
3:C:85:SER:CB	3:C:166:LYS:HE3	2.46	0.44
9:I:105:GLU:HB3	9:I:107:ALA:HB3	1.98	0.44
18:R:157:GLN:HG3	18:R:159:ASP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:134:PRO:HG2	21:U:174:GLU:HG2	1.99	0.44
24:0:106:ILE:HD11	24:0:127:HIS:HB3	2.00	0.44
24:0:165:ARG:HD3	24:0:194:ILE:HG12	2.00	0.44
26:2:258:LEU:HG	26:2:262:LEU:HD21	1.99	0.44
1:A:415:GLY:O	1:A:449:HIS:HD2	2.00	0.44
1:A:1117:VAL:O	1:A:1118:THR:O	2.35	0.44
1:A:1371:ILE:HD13	1:A:1409:GLY:O	2.17	0.44
8:H:96:VAL:HG22	8:H:116:VAL:HG13	2.00	0.44
9:I:25:TYR:HD2	9:I:40:ARG:HG3	1.82	0.44
16:P:317:VAL:HG12	16:P:319:ALA:H	1.82	0.44
17:Q:188:TYR:CE1	18:R:210:PHE:CG	3.04	0.44
19:S:18:VAL:HG22	19:S:137:ALA:HB3	1.98	0.44
21:U:243:GLU:O	21:U:247:GLU:N	2.46	0.44
25:1:59:GLU:CD	26:2:402:ARG:CZ	2.89	0.44
26:2:159:VAL:HG22	26:2:160:LEU:HD13	1.95	0.44
27:3:65:GLN:O	27:3:132:LEU:HD11	2.18	0.44
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.99	0.44
1:A:672:ILE:HD13	1:A:672:ILE:HG21	1.74	0.44
1:A:1429:LYS:HB2	1:A:1438:VAL:HG21	2.00	0.44
11:K:53:ASP:OD1	11:K:54:PRO:HD2	2.18	0.44
12:L:56:ASP:N	12:L:56:ASP:OD1	2.46	0.44
19:S:128:THR:HG22	19:S:136:GLU:HB3	1.98	0.44
19:S:177:MET:HE3	19:S:177:MET:HB3	1.83	0.44
22:V:444:HIS:O	22:V:447:PRO:CD	2.61	0.44
22:V:647:LYS:O	22:V:648:LYS:O	2.35	0.44
23:W:73:CYS:CB	23:W:209:TYR:CE2	3.01	0.44
25:1:7:GLY:C	25:1:8:VAL:HG23	2.43	0.44
26:2:219:TYR:CD1	26:2:219:TYR:C	2.95	0.44
27:3:228:LEU:HD23	27:3:228:LEU:O	2.18	0.44
2:B:836:THR:C	2:B:886:ARG:HA	2.42	0.44
2:B:899:SER:O	2:B:901:THR:N	2.51	0.44
2:B:926:VAL:HG23	2:B:926:VAL:O	2.17	0.44
2:B:934:LYS:HE2	2:B:942:LYS:HD2	1.98	0.44
5:E:3:ASP:O	5:E:6:GLU:HB2	2.18	0.44
9:I:84:HIS:HB2	9:I:85:PRO:HD3	0.96	0.44
13:M:60:ALA:HB1	29:Y:54:DA:C2	2.51	0.44
13:M:178:LYS:NZ	20:T:156:VAL:HG11	2.31	0.44
18:R:148:LYS:HD3	18:R:174:ALA:HB2	2.00	0.44
20:T:194:HIS:N	20:T:197:TYR:OH	2.50	0.44
21:U:260:LEU:HB3	21:U:261:PHE:H	1.61	0.44
25:1:21:LEU:O	25:1:24:ASP:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:159:VAL:HG12	26:2:161:HIS:HB2	1.99	0.44
27:3:33:THR:CG2	27:3:36:LYS:H	2.04	0.44
27:3:59:VAL:N	27:3:71:TYR:CZ	2.69	0.44
1:A:186:ARG:HH11	1:A:208:ASP:HB2	1.82	0.44
1:A:1407:CYS:SG	1:A:1408:ARG:HG2	2.58	0.44
2:B:783:ALA:HB2	2:B:1041:ILE:CG2	2.48	0.44
3:C:31:ALA:HB1	3:C:184:PHE:HE1	1.81	0.44
13:M:70:SER:C	13:M:72:ASN:H	2.25	0.44
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.99	0.44
25:1:1:MET:SD	26:2:419:GLU:N	2.90	0.44
26:2:164:VAL:HG13	26:2:209:PRO:CG	2.45	0.44
26:2:206:LEU:CD2	26:2:206:LEU:H	2.31	0.44
27:3:124:ILE:O	27:3:124:ILE:HG23	2.18	0.44
27:3:160:ARG:HE	27:3:160:ARG:HB2	1.58	0.44
27:3:160:ARG:CB	27:3:190:LEU:CD2	2.95	0.44
27:3:184:ALA:C	27:3:187:GLN:HG2	2.43	0.44
1:A:270:ALA:C	1:A:272:ASN:N	2.75	0.44
7:G:18:PHE:HA	7:G:22:LEU:HD13	2.00	0.44
7:G:116:GLU:O	7:G:130:THR:HA	2.16	0.44
9:I:92:LYS:HG3	9:I:93:GLU:HG2	1.99	0.44
13:M:37:CYS:SG	13:M:38:GLY:N	2.91	0.44
18:R:88:ARG:NH1	18:R:97:LEU:HD11	2.33	0.44
18:R:212:VAL:C	18:R:213:ASP:CG	2.86	0.44
20:T:128:LYS:O	20:T:132:ILE:N	2.44	0.44
25:1:11:GLU:HG2	26:2:404:THR:OG1	2.17	0.44
25:1:21:LEU:HB3	25:1:54:GLN:NE2	2.33	0.44
25:1:34:ILE:CG2	25:1:50:VAL:HG11	2.48	0.44
26:2:35:TYR:CD1	26:2:62:LEU:HD12	2.52	0.44
26:2:189:GLU:HB2	26:2:190:PRO:CD	2.43	0.44
26:2:221:GLN:HG2	26:2:268:PHE:HZ	1.75	0.44
27:3:60:ILE:HG23	27:3:68:ARG:O	2.17	0.44
27:3:144:ILE:O	27:3:144:ILE:HD13	2.17	0.44
1:A:1156:ASP:OD1	1:A:1225:LYS:NZ	2.40	0.44
2:B:1072:ARG:HD3	2:B:1153:TYR:CD2	2.53	0.44
3:C:59:LEU:HD12	3:C:59:LEU:HA	1.73	0.44
22:V:282:LYS:HE3	22:V:482:PHE:CD1	2.53	0.44
23:W:73:CYS:HB3	23:W:209:TYR:CD2	2.52	0.44
26:2:214:TYR:OH	26:2:265:LEU:HD13	2.18	0.44
27:3:165:LYS:HZ1	27:3:200:SER:N	2.15	0.44
28:X:51:DC:H2'	28:X:52:DG:C4	2.53	0.44
1:A:865:ILE:HD12	2:B:1092:ASP:OD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:ASN:CA	1:A:931:ARG:NH1	2.73	0.43
1:A:931:ARG:NE	1:A:931:ARG:CA	2.74	0.43
1:A:1316:ASN:CG	1:A:1318:LYS:CE	2.91	0.43
2:B:17:ILE:HG23	2:B:18:THR:HG23	2.00	0.43
2:B:271:ILE:HD12	2:B:311:ILE:HD11	2.00	0.43
13:M:25:GLU:OE1	13:M:44:ARG:NH2	2.36	0.43
16:P:288:PHE:CD1	16:P:289:PRO:HD2	2.54	0.43
17:Q:100:VAL:O	17:Q:103:VAL:HG23	2.18	0.43
25:1:13:ASP:CB	25:1:14:PRO:HD2	2.46	0.43
26:2:60:LEU:CD1	26:2:95:ILE:CB	2.95	0.43
26:2:117:ASN:CA	27:3:104:LEU:HD21	2.47	0.43
26:2:236:PHE:HZ	26:2:258:LEU:HD11	1.83	0.43
26:2:270:LEU:HD23	26:2:270:LEU:C	2.42	0.43
27:3:222:SER:HB3	27:3:225:GLN:CD	2.43	0.43
1:A:514:GLU:OE1	2:B:1099:ALA:HB1	2.18	0.43
1:A:614:ASP:OD2	21:U:267:LYS:HG3	2.17	0.43
2:B:106:SER:HB2	2:B:107:PRO:HD2	2.00	0.43
2:B:759:VAL:CG1	2:B:999:ALA:HB2	2.48	0.43
3:C:71:ILE:HG22	3:C:148:ILE:HG21	2.00	0.43
10:J:35:LEU:HD13	10:J:46:ARG:HG2	2.00	0.43
13:M:57:ASN:HA	29:Y:51:DC:N4	2.33	0.43
16:P:329:TYR:N	16:P:330:PRO:HD2	2.34	0.43
22:V:519:TYR:HA	22:V:522:TYR:HB3	2.00	0.43
24:0:60:HIS:CE1	24:0:159:MET:SD	3.11	0.43
25:1:3:ASN:HB3	26:2:412:PHE:O	2.18	0.43
26:2:117:ASN:ND2	27:3:104:LEU:O	2.52	0.43
26:2:166:SER:HB3	26:2:167:PRO:HD3	2.00	0.43
27:3:64:ILE:HB	27:3:123:ASP:CG	2.43	0.43
1:A:779:ILE:O	1:A:783:GLN:HG3	2.19	0.43
2:B:936:ALA:O	2:B:1049:GLN:N	2.42	0.43
2:B:1029:TYR:N	2:B:1029:TYR:CD1	2.85	0.43
9:I:58:ILE:O	9:I:59:THR:OG1	2.36	0.43
16:P:297:LYS:C	16:P:299:ARG:H	2.19	0.43
17:Q:113:ARG:CD	18:R:222:SER:HB3	2.46	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
27:3:178:MET:O	27:3:182:PHE:HD2	2.01	0.43
27:3:187:GLN:CD	27:3:189:ILE:HG13	2.43	0.43
1:A:270:ALA:O	1:A:271:ARG:C	2.58	0.43
1:A:866:LYS:HG2	1:A:1432:PHE:CD1	2.54	0.43
1:A:1162:GLU:OE2	1:A:1308:TYR:CE2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:GLU:HG2	3:C:228:ARG:CG	2.46	0.43
3:C:71:ILE:CG2	3:C:148:ILE:HG21	2.48	0.43
6:F:102:ILE:CG2	6:F:104:ILE:HG12	2.49	0.43
8:H:10:PHE:CE2	8:H:39:LEU:HD13	2.54	0.43
8:H:34:SER:O	8:H:36:LYS:HG3	2.19	0.43
9:I:65:LEU:HA	9:I:122:ARG:HE	1.83	0.43
15:O:80:GLU:OE2	15:O:82:ARG:NE	2.44	0.43
17:Q:126:SER:O	17:Q:164:ASP:HB2	2.18	0.43
20:T:138:PRO:HG2	20:T:140:ARG:HH22	1.83	0.43
21:U:139:SER:O	21:U:143:LYS:HG2	2.19	0.43
22:V:514:MET:HE3	25:1:16:MET:CE	2.48	0.43
25:1:4:VAL:HG22	25:1:5:LEU:N	2.33	0.43
26:2:61:PHE:CE1	26:2:99:GLN:NE2	2.85	0.43
26:2:94:ARG:HD2	26:2:95:ILE:CD1	2.47	0.43
26:2:117:ASN:ND2	27:3:108:ASN:N	2.65	0.43
26:2:127:LYS:CA	26:2:178:LEU:HD23	2.48	0.43
26:2:218:GLN:HE22	26:2:265:LEU:CA	2.28	0.43
26:2:224:GLN:N	26:2:268:PHE:HZ	2.16	0.43
27:3:33:THR:CG2	27:3:36:LYS:CB	2.95	0.43
28:X:77:DC:C2'	28:X:78:DT:H72	2.48	0.43
1:A:199:TYR:HE2	13:M:93:PHE:HZ	1.64	0.43
1:A:924:TYR:CE2	1:A:949:GLN:HG2	2.54	0.43
1:A:987:ILE:HD13	1:A:1058:PHE:CD2	2.53	0.43
1:A:1290:SER:HB2	2:B:250:SER:CB	2.47	0.43
2:B:461:GLN:H	2:B:461:GLN:CD	2.26	0.43
2:B:783:ALA:HB2	2:B:1041:ILE:HG21	2.01	0.43
2:B:952:GLU:CD	2:B:952:GLU:H	2.26	0.43
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	2.00	0.43
3:C:6:GLN:HA	3:C:7:PRO:HD2	1.78	0.43
10:J:4:PRO:O	10:J:14:VAL:HG12	2.18	0.43
21:U:200:ASP:OD2	21:U:203:ASN:N	2.52	0.43
22:V:524:ALA:HB2	25:1:23:LEU:HD13	1.99	0.43
22:V:666:ASP:CB	25:1:17:LYS:HZ3	2.30	0.43
23:W:107:LEU:HB2	23:W:175:TYR:CZ	2.54	0.43
26:2:87:THR:C	26:2:89:LEU:H	2.27	0.43
26:2:214:TYR:HB3	26:2:261:PHE:CE2	2.54	0.43
26:2:223:ALA:H	26:2:268:PHE:HE1	1.64	0.43
26:2:243:SER:HB3	26:2:258:LEU:CD2	2.45	0.43
26:2:270:LEU:HA	26:2:273:GLN:HG3	2.00	0.43
27:3:121:LYS:H	27:3:121:LYS:CD	2.32	0.43
27:3:178:MET:HA	27:3:181:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:PRO:HD3	13:M:92:SER:OG	2.18	0.43
1:A:894:ASP:OD1	1:A:894:ASP:C	2.62	0.43
2:B:758:LEU:HA	2:B:758:LEU:HD23	1.68	0.43
2:B:967:ILE:HD12	2:B:968:ASN:H	1.83	0.43
4:D:26:PHE:CE2	7:G:78:ARG:HG2	2.53	0.43
8:H:11:ASP:HB2	8:H:55:LYS:HG2	2.00	0.43
13:M:27:TYR:HD1	13:M:46:ILE:HG21	1.84	0.43
14:N:376:TRP:HD1	15:O:62:LEU:O	2.01	0.43
19:S:100:LEU:HD23	19:S:110:PHE:CD2	2.50	0.43
20:T:229:HIS:HD2	28:X:28:DG:H21	1.65	0.43
22:V:405:VAL:HG12	22:V:406:ALA:H	1.83	0.43
25:1:25:GLU:OE2	25:1:35:ILE:HG12	2.18	0.43
26:2:215:PHE:CE2	26:2:264:HIS:ND1	2.86	0.43
26:2:409:TYR:CD2	26:2:443:VAL:HG22	2.54	0.43
1:A:15:LEU:HD12	2:B:1148:LEU:O	2.19	0.43
1:A:133:SER:C	1:A:135:GLY:N	2.75	0.43
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.49	0.43
5:E:41:LYS:HG3	5:E:46:ASP:CB	2.48	0.43
16:P:178:LEU:HB3	16:P:183:ILE:HD11	2.00	0.43
20:T:82:PRO:HD2	20:T:117:ARG:O	2.19	0.43
22:V:519:TYR:HB3	25:1:16:MET:HG3	2.00	0.43
25:1:8:VAL:CG1	25:1:9:LEU:N	2.80	0.43
25:1:50:VAL:HG12	25:1:50:VAL:O	2.18	0.43
26:2:236:PHE:CE1	26:2:239:GLN:NE2	2.87	0.43
27:3:184:ALA:O	27:3:187:GLN:HG2	2.19	0.43
1:A:388:MET:HE2	1:A:388:MET:HB3	1.82	0.43
1:A:505:LEU:HD23	1:A:507:GLN:HE22	1.84	0.43
2:B:51:ILE:HA	2:B:51:ILE:HD13	1.75	0.43
2:B:90:GLN:NE2	20:T:141:LEU:CA	2.56	0.43
5:E:47:LYS:HD3	5:E:47:LYS:HA	1.63	0.43
17:Q:137:THR:OG1	17:Q:139:LEU:HG	2.18	0.43
1:A:156:GLY:O	1:A:180:GLY:HA2	2.19	0.43
1:A:1128:ILE:HD13	1:A:1128:ILE:HA	1.80	0.43
2:B:52:GLN:HB2	2:B:160:TYR:OH	2.19	0.43
9:I:50:ASN:OD1	9:I:51:SER:N	2.51	0.43
14:N:354:LYS:C	14:N:355:ASP:O	2.62	0.43
17:Q:113:ARG:HD3	18:R:222:SER:HB2	1.99	0.43
21:U:133:ALA:HA	21:U:134:PRO:HD3	1.89	0.43
22:V:615:PHE:O	22:V:615:PHE:CG	2.70	0.43
1:A:264:VAL:HB	13:M:52:TRP:CE3	2.53	0.43
1:A:271:ARG:O	1:A:272:ASN:CB	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:HIS:O	1:A:610:PRO:O	2.36	0.43
2:B:132:VAL:CG2	2:B:141:GLN:HG3	2.48	0.43
2:B:975:ARG:C	2:B:976:MET:HG3	2.42	0.43
2:B:1162:LEU:O	2:B:1167:ILE:HB	2.18	0.43
3:C:125:PRO:C	3:C:127:VAL:H	2.27	0.43
13:M:184:SER:OG	13:M:185:ARG:N	2.52	0.43
18:R:151:LEU:HD12	18:R:163:LEU:HD21	1.86	0.43
20:T:59:ASN:OD1	20:T:60:GLU:N	2.52	0.43
23:W:584:TYR:CB	23:W:591:GLY:HA3	2.48	0.43
26:2:117:ASN:HD21	27:3:108:ASN:N	2.16	0.43
26:2:201:PHE:CD1	26:2:201:PHE:C	2.96	0.43
1:A:231:GLU:OE1	1:A:231:GLU:N	2.41	0.42
1:A:937:ASP:O	1:A:940:LYS:HD2	2.19	0.42
1:A:1175:ILE:HG23	1:A:1285:LEU:HD23	2.01	0.42
2:B:25:ALA:HA	2:B:28:ILE:HD12	2.01	0.42
2:B:285:LEU:HD22	9:I:16:PHE:HZ	1.84	0.42
8:H:65:TYR:CD1	8:H:65:TYR:N	2.87	0.42
14:N:347:ASN:HB3	16:P:208:ARG:HH11	1.84	0.42
20:T:26:TYR:CE2	20:T:127:LEU:HD21	2.54	0.42
26:2:34:LEU:N	26:2:34:LEU:HD22	2.33	0.42
27:3:141:LEU:HA	27:3:144:ILE:HG22	2.01	0.42
1:A:199:TYR:CE2	13:M:93:PHE:CZ	3.02	0.42
1:A:212:LYS:HE2	1:A:212:LYS:H	1.84	0.42
3:C:73:LEU:O	3:C:238:SER:HB3	2.20	0.42
5:E:56:THR:N	5:E:78:GLU:OE2	2.52	0.42
16:P:297:LYS:HA	16:P:297:LYS:HD2	1.76	0.42
18:R:166:ILE:HG22	18:R:168:LEU:H	1.84	0.42
23:W:416:ILE:HA	23:W:434:HIS:O	2.19	0.42
25:1:20:LEU:C	25:1:20:LEU:HD13	2.44	0.42
26:2:172:SER:C	26:2:175:LEU:HD23	2.43	0.42
27:3:111:ILE:HG13	27:3:112:VAL:H	1.83	0.42
27:3:229:TRP:CD1	27:3:229:TRP:C	2.96	0.42
29:Y:70:DC:H2"	29:Y:71:DA:C8	2.54	0.42
1:A:666:ARG:HD3	1:A:666:ARG:HA	1.79	0.42
1:A:766:PHE:CD1	1:A:781:ILE:HD11	2.54	0.42
1:A:799:PRO:O	1:A:806:THR:HG22	2.19	0.42
1:A:954:ARG:HD3	1:A:954:ARG:HA	1.84	0.42
1:A:1154:ALA:HB1	1:A:1310:HIS:CE1	2.46	0.42
1:A:1301:ILE:HG13	1:A:1302:GLU:HG2	2.01	0.42
2:B:230:ARG:HB2	2:B:405:ARG:CZ	2.50	0.42
4:D:48:ASN:ND2	4:D:57:LEU:HG	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:GLY:O	5:E:65:ASN:HA	2.19	0.42
10:J:66:GLU:HG3	12:L:23:HIS:ND1	2.34	0.42
12:L:26:ASN:ND2	12:L:44:MET:SD	2.92	0.42
13:M:178:LYS:HD3	20:T:154:LYS:HD3	2.00	0.42
13:M:245:VAL:HB	13:M:248:ARG:HB2	2.01	0.42
21:U:226:GLU:HB3	21:U:227:GLU:H	1.57	0.42
22:V:514:MET:HB3	25:1:16:MET:SD	2.59	0.42
26:2:57:MET:CA	26:2:60:LEU:HG	2.49	0.42
26:2:230:LEU:C	26:2:230:LEU:HD13	2.44	0.42
27:3:154:ASN:CG	27:3:155:GLN:H	2.26	0.42
1:A:1251:ASN:HB3	21:U:234:LYS:HE2	2.01	0.42
1:A:1389:ASP:O	21:U:297:ARG:NH2	2.53	0.42
2:B:906:GLN:HB3	12:L:45:TYR:CE1	2.53	0.42
2:B:1027:VAL:HG12	2:B:1029:TYR:HE1	1.84	0.42
5:E:121:MET:HG2	5:E:127:LEU:HD13	2.00	0.42
6:F:105:ILE:HG22	6:F:119:GLY:HA2	2.00	0.42
7:G:108:ILE:HG21	7:G:163:LEU:HG	2.01	0.42
7:G:117:MET:HG2	7:G:128:TYR:HB3	2.00	0.42
21:U:250:MET:O	21:U:251:ALA:CB	2.68	0.42
26:2:203:PHE:HD2	26:2:205:LEU:H	1.65	0.42
27:3:128:HIS:NE2	27:3:130:GLU:CG	2.82	0.42
27:3:137:LEU:HD12	27:3:177:PHE:CE1	2.54	0.42
1:A:392:GLU:OE1	1:A:448:ARG:NE	2.45	0.42
1:A:922:PHE:HA	1:A:1052:ARG:HD3	2.01	0.42
2:B:510:CYS:SG	2:B:511:PRO:HD2	2.60	0.42
2:B:1029:TYR:CD1	2:B:1036:LYS:HG2	2.54	0.42
9:I:105:GLU:OE1	9:I:105:GLU:HA	2.18	0.42
12:L:17:TYR:HD1	12:L:46:LYS:HA	1.83	0.42
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.84	0.42
13:M:263:GLN:HA	13:M:268:LYS:HG2	2.01	0.42
26:2:133:THR:CG2	26:2:134:SER:N	2.83	0.42
26:2:140:LYS:CD	26:2:162:PHE:HE1	2.29	0.42
27:3:9:ASN:OD1	27:3:158:LYS:HB3	2.19	0.42
27:3:14:VAL:CG2	27:3:163:VAL:HG13	2.48	0.42
27:3:42:MET:SD	27:3:111:ILE:CD1	3.07	0.42
27:3:160:ARG:CZ	27:3:190:LEU:CD1	2.97	0.42
2:B:192:LYS:HE2	2:B:449:ALA:O	2.20	0.42
2:B:198:GLU:OE2	2:B:391:LYS:HD3	2.20	0.42
3:C:74:ILE:O	3:C:128:ILE:HG13	2.19	0.42
3:C:225:LYS:O	3:C:227:GLU:HG2	2.19	0.42
8:H:81:ARG:HA	8:H:82:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:146:LYS:C	8:H:148:LEU:H	2.21	0.42
10:J:64:PRO:HG3	12:L:21:GLU:OE2	2.19	0.42
13:M:178:LYS:HG2	20:T:156:VAL:CG1	2.48	0.42
13:M:179:GLU:HA	20:T:154:LYS:HZ1	1.85	0.42
18:R:113:LEU:HA	18:R:116:LYS:HE3	2.01	0.42
25:1:1:MET:HE3	26:2:415:GLN:N	2.35	0.42
26:2:188:THR:CG2	26:2:189:GLU:N	2.83	0.42
26:2:236:PHE:CE1	26:2:261:PHE:HB3	2.54	0.42
27:3:159:SER:HG	27:3:189:ILE:HD12	1.85	0.42
1:A:43:TYR:O	1:A:45:GLU:N	2.49	0.42
1:A:376:ASP:HB3	1:A:521:VAL:HB	2.00	0.42
1:A:455:ILE:HG12	1:A:473:ARG:HG2	2.02	0.42
1:A:999:ARG:CZ	8:H:99:ILE:HG21	2.49	0.42
2:B:72:GLN:NE2	2:B:80:GLU:N	2.67	0.42
2:B:155:MET:HB2	2:B:185:PHE:CE1	2.54	0.42
2:B:613:ARG:HD3	2:B:615:TYR:OH	2.19	0.42
3:C:67:ARG:NH1	3:C:150:ILE:HA	2.35	0.42
5:E:50:GLU:C	5:E:52:ARG:N	2.77	0.42
9:I:66:THR:O	9:I:68:ILE:HG22	2.20	0.42
13:M:46:ILE:O	13:M:46:ILE:HG13	2.19	0.42
19:S:51:LEU:HG	19:S:54:LYS:HB2	2.00	0.42
26:2:77:LYS:HD3	26:2:78:GLU:CG	2.50	0.42
29:Y:24:DC:C6	29:Y:25:DT:H73	2.55	0.42
29:Y:57:DA:H5''	29:Y:58:DC:H2'	2.02	0.42
1:A:22:GLN:OE1	1:A:1448:SER:OG	2.32	0.42
1:A:486:LEU:HD12	1:A:486:LEU:HA	1.79	0.42
2:B:1124:ILE:HD11	2:B:1170:ARG:HD3	2.00	0.42
8:H:13:LYS:HE2	8:H:31:GLU:HB2	2.02	0.42
9:I:99:SER:OG	9:I:100:HIS:N	2.52	0.42
10:J:6:ARG:HG2	10:J:13:ILE:HG22	2.01	0.42
17:Q:54:PHE:CD1	18:R:194:ARG:HG2	2.55	0.42
20:T:124:TYR:O	20:T:127:LEU:HB3	2.19	0.42
22:V:426:VAL:C	22:V:427:MET:O	2.51	0.42
22:V:518:PHE:CD1	22:V:713:LEU:HD13	2.55	0.42
26:2:35:TYR:CG	26:2:62:LEU:CD1	2.99	0.42
26:2:89:LEU:CD2	26:2:89:LEU:C	2.93	0.42
27:3:144:ILE:HG13	27:3:159:SER:OG	2.20	0.42
27:3:197:ASP:O	27:3:198:SER:HB3	2.20	0.42
27:3:202:LEU:N	27:3:202:LEU:CD2	2.83	0.42
27:3:217:VAL:HG12	27:3:218:PRO:O	2.20	0.42
28:X:77:DC:H2''	28:X:78:DT:C7	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:PRO:CG	1:A:594:LEU:HD11	2.48	0.42
1:A:1218:ARG:HG2	21:U:237:ARG:NH2	2.34	0.42
2:B:588:ARG:NH2	2:B:663:GLU:OE1	2.51	0.42
2:B:623:ARG:NH2	2:B:675:LEU:HD21	2.35	0.42
2:B:730:LYS:HB2	2:B:730:LYS:HE3	1.92	0.42
2:B:958:CYS:C	2:B:960:GLY:N	2.78	0.42
3:C:45:ILE:HD11	3:C:82:LEU:HD22	2.00	0.42
13:M:65:SER:O	13:M:67:VAL:N	2.53	0.42
17:Q:112:ARG:CG	18:R:237:LEU:HD11	2.37	0.42
22:V:689:VAL:CG2	26:2:391:ILE:HD13	2.50	0.42
26:2:159:VAL:HG11	26:2:161:HIS:CD2	2.49	0.42
26:2:160:LEU:CD1	26:2:160:LEU:N	2.82	0.42
27:3:8:LEU:CD2	27:3:54:SER:HB3	2.45	0.42
27:3:133:LEU:CD2	27:3:134:ALA:N	2.82	0.42
27:3:215:LEU:HD23	27:3:215:LEU:HA	1.89	0.42
27:3:221:PRO:C	27:3:223:LEU:H	2.27	0.42
28:X:33:DT:H2''	28:X:34:DT:C5	2.54	0.42
1:A:203:LYS:CE	1:A:203:LYS:HA	2.47	0.42
1:A:203:LYS:HA	1:A:203:LYS:NZ	2.35	0.42
1:A:672:ILE:HG23	1:A:673:GLN:N	2.35	0.42
1:A:728:THR:HG23	1:A:736:THR:HG23	2.02	0.42
1:A:792:ASN:OD1	1:A:792:ASN:N	2.53	0.42
1:A:924:TYR:OH	1:A:952:LEU:HD12	2.19	0.42
2:B:203:ASN:O	2:B:571:GLY:HA3	2.20	0.42
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.54	0.42
9:I:84:HIS:HB3	9:I:92:LYS:CB	2.49	0.42
17:Q:28:ILE:HA	17:Q:31:ALA:HB3	2.02	0.42
22:V:514:MET:HE2	22:V:667:THR:HG21	2.01	0.42
25:1:1:MET:HG2	26:2:413:LEU:CB	2.47	0.42
26:2:118:LEU:HD23	27:3:42:MET:CB	2.35	0.42
26:2:123:LEU:CD2	26:2:123:LEU:C	2.93	0.42
26:2:202:GLN:HE21	26:2:202:GLN:N	2.15	0.42
28:X:69:DA:C2	29:Y:26:DG:N2	2.88	0.42
1:A:48:GLU:OE1	1:A:48:GLU:N	2.53	0.41
1:A:930:LEU:HD23	1:A:934:LEU:HB2	2.00	0.41
2:B:281:ASP:CG	9:I:22:ASN:HD22	2.27	0.41
2:B:343:LEU:O	2:B:347:MET:HB3	2.20	0.41
8:H:69:THR:HG22	8:H:140:ARG:NH1	2.35	0.41
8:H:81:ARG:C	8:H:83:SER:H	2.28	0.41
17:Q:30:HIS:O	17:Q:34:LEU:HB2	2.20	0.41
18:R:181:ALA:O	18:R:185:LEU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:8:ASP:CG	20:T:10:THR:HG1	2.24	0.41
22:V:315:VAL:HG13	23:W:500:ASP:HB2	0.42	0.41
25:1:1:MET:N	26:2:418:PHE:CB	2.83	0.41
26:2:170:ALA:C	26:2:213:TRP:HZ3	2.27	0.41
26:2:204:LEU:HD23	26:2:254:MET:HE3	2.02	0.41
27:3:105:THR:CG2	27:3:106:SER:N	2.82	0.41
28:X:43:DT:H2'	28:X:44:DT:C6	2.55	0.41
29:Y:70:DC:H2''	29:Y:71:DA:H8	1.85	0.41
1:A:244:ARG:HA	1:A:245:PRO:HD3	1.87	0.41
1:A:612:ASP:O	1:A:613:GLU:O	2.38	0.41
1:A:630:VAL:HG12	1:A:635:LEU:CD1	2.51	0.41
1:A:660:MET:HE3	1:A:664:ILE:HD13	2.03	0.41
1:A:779:ILE:O	1:A:782:SER:HB2	2.20	0.41
2:B:187:ILE:HG22	2:B:188:ASN:OD1	2.20	0.41
2:B:202:THR:OG1	2:B:226:GLU:OE1	2.38	0.41
2:B:710:ILE:HD13	2:B:710:ILE:HA	1.87	0.41
13:M:92:SER:O	13:M:93:PHE:C	2.59	0.41
17:Q:113:ARG:HD2	18:R:222:SER:CA	2.49	0.41
20:T:191:PHE:CZ	20:T:237:PRO:HG3	2.54	0.41
20:T:229:HIS:CD2	29:Y:67:DC:H1'	2.55	0.41
21:U:252:LYS:C	21:U:253:THR:HG22	2.44	0.41
23:W:15:ASP:HA	23:W:100:GLU:OE2	2.21	0.41
23:W:25:MET:SD	23:W:58:ALA:HB2	2.59	0.41
26:2:171:VAL:CG1	26:2:216:MET:SD	3.06	0.41
27:3:100:LYS:HB2	27:3:100:LYS:HE2	1.89	0.41
27:3:228:LEU:C	27:3:228:LEU:CD2	2.93	0.41
1:A:413:TYR:OH	1:A:451:CYS:HA	2.21	0.41
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.50	0.41
2:B:235:ILE:CD1	2:B:261:PRO:HD3	2.50	0.41
2:B:602:SER:OG	2:B:620:ARG:NH1	2.54	0.41
2:B:899:SER:C	2:B:901:THR:H	2.27	0.41
2:B:1008:VAL:HG13	2:B:1009:GLN:N	2.35	0.41
5:E:64:HIS:CE1	5:E:70:ASP:C	2.99	0.41
7:G:14:HIS:HA	7:G:15:PRO:HD3	1.94	0.41
13:M:15:CYS:HA	13:M:16:PRO:HD3	1.75	0.41
17:Q:113:ARG:HH21	18:R:218:LYS:HE2	1.67	0.41
19:S:111:LYS:O	19:S:146:PHE:HA	2.20	0.41
20:T:93:LEU:HD11	20:T:113:ARG:HD2	2.01	0.41
22:V:519:TYR:CE2	22:V:523:VAL:HG21	2.54	0.41
26:2:47:GLU:HG3	26:2:48:LEU:H	1.83	0.41
26:2:270:LEU:C	26:2:270:LEU:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:69:PHE:HZ	27:3:139:LYS:HD2	1.80	0.41
1:A:1319:LYS:HG3	1:A:1333:GLU:OE1	2.20	0.41
2:B:629:GLU:O	2:B:631:GLN:N	2.53	0.41
2:B:1022:LEU:CD1	2:B:1023:ARG:HG3	2.50	0.41
8:H:1:MET:CE	8:H:85:ALA:HB2	2.51	0.41
9:I:81:THR:HG22	9:I:94:ALA:O	2.19	0.41
10:J:2:ILE:HA	10:J:2:ILE:HD12	1.82	0.41
13:M:27:TYR:CD1	13:M:46:ILE:HG21	2.56	0.41
22:V:523:VAL:HG21	25:1:20:LEU:CG	2.43	0.41
26:2:42:LEU:HD23	26:2:42:LEU:HA	1.78	0.41
27:3:14:VAL:HG22	27:3:162:LEU:O	2.21	0.41
27:3:18:ASN:ND2	27:3:64:ILE:HD11	2.35	0.41
27:3:69:PHE:HZ	27:3:139:LYS:HB3	1.73	0.41
29:Y:24:DC:O2	29:Y:25:DT:C4	2.68	0.41
29:Y:50:DA:H2''	29:Y:51:DC:O5'	2.20	0.41
1:A:375:ILE:HG13	1:A:666:ARG:NH1	2.36	0.41
1:A:460:ARG:NH2	1:A:499:ASP:HB3	2.35	0.41
1:A:570:TRP:CZ3	1:A:572:GLY:HA2	2.56	0.41
2:B:347:MET:CE	2:B:365:LEU:HD13	2.51	0.41
2:B:470:LEU:HD23	2:B:472:ARG:HH11	1.86	0.41
2:B:721:ARG:HA	2:B:721:ARG:NE	2.34	0.41
2:B:816:GLU:OE1	2:B:894:THR:OG1	2.31	0.41
2:B:1071:ASN:O	2:B:1072:ARG:HG2	2.19	0.41
18:R:77:VAL:HG21	18:R:111:ILE:HD11	2.02	0.41
20:T:166:GLU:HA	20:T:169:LYS:CE	2.50	0.41
23:W:420:PRO:O	23:W:431:PRO:HB3	2.20	0.41
26:2:176:ALA:HB3	26:2:178:LEU:HD13	1.97	0.41
26:2:206:LEU:CD2	26:2:206:LEU:N	2.84	0.41
27:3:11:LEU:CD1	27:3:48:HIS:NE2	2.82	0.41
27:3:41:VAL:HG13	27:3:42:MET:N	2.34	0.41
1:A:286:ILE:HG13	1:A:287:ASN:N	2.36	0.41
1:A:413:TYR:C	1:A:415:GLY:H	2.28	0.41
1:A:597:PRO:HB2	1:A:660:MET:HG3	2.01	0.41
1:A:734:ARG:HH22	9:I:104:ALA:HB1	1.86	0.41
2:B:552:ASN:O	2:B:555:GLU:HG2	2.20	0.41
2:B:598:VAL:C	2:B:600:GLU:N	2.78	0.41
2:B:838:GLN:OE1	2:B:886:ARG:NH1	2.53	0.41
2:B:1101:GLN:NE2	6:F:64:ARG:HG3	2.36	0.41
7:G:144:ARG:HE	7:G:171:VAL:HG11	1.86	0.41
8:H:92:MET:CE	8:H:143:LEU:HD23	2.51	0.41
9:I:29:ASP:CG	9:I:32:ASN:HD22	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:65:LEU:CB	9:I:122:ARG:HE	2.33	0.41
13:M:11:PRO:HD2	13:M:13:VAL:HG22	2.01	0.41
13:M:179:GLU:HA	20:T:154:LYS:NZ	2.36	0.41
14:N:324:GLU:OE1	16:P:188:ARG:NH1	2.40	0.41
15:O:63:ASN:HD22	15:O:63:ASN:C	2.29	0.41
17:Q:180:PHE:HZ	18:R:213:ASP:N	2.15	0.41
17:Q:184:ILE:HG12	18:R:211:SER:HB3	2.02	0.41
25:1:4:VAL:CG1	26:2:412:PHE:HD2	2.20	0.41
25:1:43:VAL:CG1	25:1:44:PHE:N	2.83	0.41
26:2:93:LEU:HD23	26:2:96:TRP:HE1	1.85	0.41
26:2:221:GLN:O	26:2:268:PHE:CE1	2.74	0.41
27:3:64:ILE:CB	27:3:123:ASP:HB3	2.50	0.41
1:A:244:ARG:HG3	1:A:246:GLU:CD	2.45	0.41
1:A:375:ILE:HA	1:A:375:ILE:HD13	1.69	0.41
1:A:457:ILE:HD13	1:A:470:MET:C	2.46	0.41
1:A:478:PRO:O	1:A:479:TRP:HB2	2.19	0.41
1:A:932:ARG:HG3	1:A:943:LEU:CD2	2.50	0.41
1:A:1191:GLU:O	1:A:1194:ASN:ND2	2.54	0.41
1:A:1191:GLU:HA	1:A:1194:ASN:ND2	2.35	0.41
1:A:1320:ILE:HD11	1:A:1328:PHE:HB3	2.03	0.41
2:B:1022:LEU:HD11	2:B:1023:ARG:CZ	2.51	0.41
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.86	0.41
18:R:88:ARG:HH21	18:R:95:HIS:HB3	1.85	0.41
20:T:229:HIS:NE2	28:X:28:DG:N3	2.60	0.41
22:V:390:CYS:SG	22:V:399:LYS:HE3	2.61	0.41
26:2:118:LEU:HD21	27:3:42:MET:HB2	1.99	0.41
28:X:11:DT:H6	28:X:11:DT:H2'	1.71	0.41
1:A:128:ASP:O	1:A:132:LYS:HB2	2.21	0.41
2:B:430:ASN:CG	2:B:433:LEU:HG	2.45	0.41
2:B:544:PHE:HD1	2:B:544:PHE:HA	1.78	0.41
2:B:1142:ASN:ND2	2:B:1145:GLN:HG2	2.36	0.41
5:E:45:GLY:O	5:E:48:PRO:HD3	2.21	0.41
8:H:85:ALA:CB	8:H:88:PHE:CZ	3.04	0.41
9:I:66:THR:O	9:I:68:ILE:N	2.47	0.41
19:S:125:TYR:CD1	19:S:139:PRO:HA	2.56	0.41
23:W:212:LEU:C	23:W:212:LEU:HD13	2.46	0.41
25:1:52:VAL:CG2	25:1:53:LEU:N	2.83	0.41
26:2:62:LEU:C	26:2:62:LEU:CD1	2.94	0.41
26:2:236:PHE:CD2	26:2:236:PHE:C	2.94	0.41
27:3:59:VAL:CA	27:3:71:TYR:CD1	3.03	0.41
27:3:109:GLU:HG3	27:3:110:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:146:ARG:HG3	27:3:147:MET:N	2.35	0.41
1:A:36:VAL:HG11	1:A:72:GLN:HE22	1.85	0.41
1:A:202:TRP:H	1:A:212:LYS:CA	2.29	0.41
1:A:209:SER:O	1:A:210:GLN:HG2	2.21	0.41
1:A:482:PHE:HE2	1:A:501:MET:O	2.03	0.41
1:A:522:PRO:CG	1:A:666:ARG:HG3	2.50	0.41
1:A:1194:ASN:O	1:A:1197:TYR:HD2	2.04	0.41
1:A:1376:LYS:HD2	1:A:1376:LYS:HA	1.80	0.41
2:B:33:TYR:CE1	2:B:37:LYS:HG3	2.55	0.41
2:B:51:ILE:HB	2:B:160:TYR:CE2	2.56	0.41
2:B:193:VAL:HG21	2:B:482:LEU:HD23	2.02	0.41
2:B:721:ARG:CG	2:B:939:HIS:O	2.66	0.41
2:B:800:ALA:O	2:B:805:PHE:HB2	2.20	0.41
2:B:897:ARG:O	2:B:900:GLU:HG2	2.19	0.41
2:B:1001:PRO:HB2	2:B:1002:PHE:CD1	2.55	0.41
3:C:25:ASN:HA	3:C:227:GLU:OE1	2.21	0.41
3:C:47:ILE:HD12	3:C:47:ILE:N	2.34	0.41
5:E:39:GLU:O	5:E:43:GLN:N	2.51	0.41
11:K:82:SER:HA	11:K:83:PRO:HD3	1.85	0.41
12:L:35:ARG:HH12	12:L:42:ARG:CZ	2.34	0.41
13:M:16:PRO:HD3	13:M:39:LEU:HD23	2.00	0.41
20:T:175:ARG:HB3	20:T:208:GLN:HA	2.02	0.41
22:V:321:GLU:OE1	23:W:499:ASN:HB3	1.73	0.41
22:V:518:PHE:HB2	25:1:16:MET:SD	2.61	0.41
23:W:428:ILE:HA	23:W:430:ASN:HD21	1.85	0.41
25:1:7:GLY:C	25:1:8:VAL:CG2	2.94	0.41
25:1:31:LYS:C	25:1:33:PHE:H	2.28	0.41
25:1:52:VAL:O	25:1:56:ARG:HG2	2.21	0.41
26:2:174:ASP:OD2	26:2:213:TRP:CZ3	2.74	0.41
27:3:34:LEU:C	27:3:34:LEU:CD1	2.94	0.41
27:3:167:ALA:C	27:3:198:SER:HG	2.28	0.41
27:3:191:ILE:H	27:3:210:THR:HG21	1.85	0.41
27:3:222:SER:HB3	27:3:225:GLN:CG	2.51	0.41
29:Y:80:DT:H6	29:Y:80:DT:H2'	1.72	0.41
1:A:124:PRO:HA	1:A:127:LYS:HE3	2.02	0.41
1:A:685:HIS:ND1	1:A:686:THR:N	2.69	0.41
2:B:628:VAL:HG23	2:B:632:LYS:C	2.45	0.41
2:B:776:ILE:HG21	2:B:776:ILE:HD13	1.73	0.41
2:B:778:SER:O	2:B:1045:PRO:HA	2.21	0.41
2:B:797:ASN:C	2:B:797:ASN:OD1	2.62	0.41
2:B:931:ILE:CD1	2:B:947:ILE:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:PRO:HA	3:C:25:ASN:HB3	2.03	0.41
17:Q:128:LYS:HE3	17:Q:133:SER:HA	2.03	0.41
22:V:366:ASN:HD22	22:V:613:THR:CG2	2.20	0.41
25:1:39:ASP:OD2	26:2:434:GLU:OE2	2.39	0.41
27:3:222:SER:HB3	27:3:225:GLN:OE1	2.21	0.41
1:A:426:ARG:O	13:M:39:LEU:C	2.59	0.40
1:A:818:GLU:HG2	1:A:819:SER:N	2.36	0.40
3:C:154:ARG:CD	10:J:65:LEU:HD11	2.49	0.40
7:G:99:THR:HG21	7:G:143:ILE:HD11	2.03	0.40
9:I:12:VAL:HG11	9:I:15:ARG:HH21	1.85	0.40
22:V:297:PHE:CG	22:V:298:ARG:N	2.89	0.40
26:2:93:LEU:CA	26:2:96:TRP:HD1	2.31	0.40
26:2:236:PHE:HZ	26:2:258:LEU:CD1	2.34	0.40
27:3:18:ASN:OD1	27:3:19:PRO:HD2	2.21	0.40
27:3:114:GLU:OE1	27:3:114:GLU:HA	2.21	0.40
1:A:51:ARG:H	1:A:52:PRO:CD	2.33	0.40
1:A:522:PRO:O	1:A:525:ILE:HG13	2.21	0.40
1:A:1419:VAL:HG11	1:A:1432:PHE:CE2	2.57	0.40
2:B:699:HIS:CE1	2:B:701:SER:OG	2.74	0.40
3:C:19:VAL:HB	3:C:241:PRO:HB2	2.02	0.40
8:H:115:TYR:HE1	8:H:124:ARG:HG3	1.85	0.40
22:V:450:MET:HG3	28:X:75:DG:H3'	2.04	0.40
22:V:678:ARG:NH1	26:2:392:ARG:HH12	2.19	0.40
25:1:10:ILE:HG23	25:1:10:ILE:O	2.21	0.40
26:2:51:LEU:CD2	26:2:51:LEU:C	2.94	0.40
26:2:236:PHE:HZ	26:2:262:LEU:CD2	2.35	0.40
27:3:17:ALA:CB	27:3:63:HIS:CD2	2.99	0.40
27:3:44:LEU:C	27:3:44:LEU:CD1	2.94	0.40
27:3:187:GLN:CG	27:3:189:ILE:CG1	2.94	0.40
1:A:133:SER:O	1:A:136:GLN:N	2.37	0.40
1:A:540:ASP:O	1:A:544:ALA:N	2.41	0.40
1:A:626:THR:OG1	1:A:627:LYS:N	2.54	0.40
1:A:837:PHE:HB2	2:B:506:TRP:CZ3	2.56	0.40
1:A:937:ASP:HB2	1:A:1002:SER:O	2.22	0.40
2:B:254:GLN:HG3	2:B:303:PRO:CG	2.50	0.40
2:B:290:TYR:HE2	2:B:562:ALA:HA	1.83	0.40
2:B:363:TYR:CG	2:B:553:LEU:HD21	2.56	0.40
2:B:520:VAL:O	2:B:520:VAL:HG13	2.20	0.40
2:B:854:ILE:HD12	2:B:904:VAL:HG21	2.02	0.40
2:B:1060:HIS:CD2	2:B:1078:ARG:HD2	2.56	0.40
3:C:47:ILE:HB	3:C:69:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:62:LYS:O	11:K:64:PRO:HD3	2.21	0.40
12:L:17:TYR:O	12:L:26:ASN:HB2	2.22	0.40
13:M:107:MET:HG3	13:M:108:SER:H	1.86	0.40
13:M:178:LYS:O	20:T:154:LYS:HE3	2.21	0.40
14:N:337:CYS:HB2	14:N:355:ASP:O	2.22	0.40
16:P:246:PHE:HA	16:P:247:PRO:HD3	1.95	0.40
17:Q:23:ARG:CD	18:R:207:SER:O	2.70	0.40
19:S:126:ILE:O	19:S:138:PHE:N	2.50	0.40
22:V:516:PRO:HB3	25:1:15:ALA:O	2.22	0.40
22:V:593:LEU:HD11	22:V:615:PHE:CZ	2.56	0.40
23:W:233:PHE:HB2	23:W:456:ILE:HG22	2.02	0.40
25:1:20:LEU:O	25:1:24:ASP:N	2.48	0.40
26:2:93:LEU:O	26:2:96:TRP:CD1	2.74	0.40
26:2:117:ASN:CG	27:3:42:MET:HE1	2.38	0.40
27:3:42:MET:HG2	27:3:111:ILE:CD1	2.52	0.40
27:3:60:ILE:CG2	27:3:61:ALA:N	2.84	0.40
28:X:24:DG:H2'	28:X:25:DG:C8	2.56	0.40
1:A:386:ALA:O	1:A:449:HIS:CE1	2.74	0.40
1:A:1158:LEU:HG	1:A:1308:TYR:CE2	2.57	0.40
1:A:1310:HIS:HE2	1:A:1334:TRP:CG	2.40	0.40
2:B:197:GLN:NE2	2:B:466:VAL:HG22	2.36	0.40
2:B:278:PHE:HZ	2:B:359:THR:HG22	1.85	0.40
2:B:385:ARG:HH11	2:B:497:LYS:HE3	1.87	0.40
2:B:854:ILE:H	2:B:854:ILE:HG12	1.63	0.40
2:B:873:LEU:H	2:B:874:PRO:HD2	1.86	0.40
2:B:985:LEU:HD12	2:B:985:LEU:HA	1.93	0.40
5:E:64:HIS:HB3	5:E:68:PRO:HA	2.04	0.40
8:H:91:VAL:HG13	8:H:144:LEU:HD12	2.04	0.40
13:M:52:TRP:C	13:M:54:THR:H	2.29	0.40
17:Q:28:ILE:HD12	18:R:192:VAL:HG12	2.03	0.40
19:S:112:GLY:HA2	19:S:145:ASN:O	2.22	0.40
26:2:34:LEU:CD2	26:2:34:LEU:N	2.84	0.40
26:2:94:ARG:HD2	26:2:95:ILE:HD13	2.02	0.40
26:2:100:LEU:CG	26:2:119:ARG:HE	2.22	0.40
26:2:181:GLN:HA	26:2:181:GLN:NE2	2.35	0.40
1:A:865:ILE:HD12	2:B:1092:ASP:CG	2.45	0.40
1:A:930:LEU:CD2	1:A:934:LEU:CB	2.98	0.40
1:A:1176:TYR:HE2	1:A:1213:ARG:NH1	2.20	0.40
1:A:1421:ARG:HA	1:A:1421:ARG:HD3	2.01	0.40
2:B:548:TRP:O	2:B:549:SER:OG	2.35	0.40
2:B:759:VAL:HG13	2:B:999:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:ASP:C	3:C:148:ILE:H	2.29	0.40
3:C:189:ASP:OD1	3:C:189:ASP:N	2.53	0.40
8:H:2:ALA:HB1	8:H:63:THR:HG23	2.03	0.40
15:O:66:ARG:N	15:O:73:THR:O	2.54	0.40
17:Q:77:ARG:HB3	17:Q:93:PHE:HB3	2.03	0.40
26:2:399:ASP:OD1	26:2:402:ARG:NH1	2.55	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%)	1266 (87%)	119 (8%)	65 (4%)	2	17
2	B	1163/1174 (99%)	1004 (86%)	109 (9%)	50 (4%)	2	17
3	C	273/275 (99%)	241 (88%)	22 (8%)	10 (4%)	2	20
4	D	127/142 (89%)	120 (94%)	7 (6%)	0	100	100
5	E	208/210 (99%)	191 (92%)	8 (4%)	9 (4%)	2	17
6	F	84/127 (66%)	80 (95%)	4 (5%)	0	100	100
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
8	H	148/150 (99%)	116 (78%)	14 (10%)	18 (12%)	0	4
9	I	123/125 (98%)	91 (74%)	20 (16%)	12 (10%)	0	7
10	J	65/67 (97%)	54 (83%)	5 (8%)	6 (9%)	0	8
11	K	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	14	51
12	L	44/58 (76%)	32 (73%)	9 (20%)	3 (7%)	1	11
13	M	308/316 (98%)	262 (85%)	28 (9%)	18 (6%)	1	14
14	N	109/376 (29%)	97 (89%)	9 (8%)	3 (3%)	4	24
15	O	97/109 (89%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	183/339 (54%)	170 (93%)	7 (4%)	6 (3%)	3	21
17	Q	176/439 (40%)	159 (90%)	7 (4%)	10 (6%)	1	14
18	R	163/291 (56%)	141 (86%)	14 (9%)	8 (5%)	1	16
19	S	134/517 (26%)	119 (89%)	11 (8%)	4 (3%)	3	23
20	T	218/249 (88%)	187 (86%)	19 (9%)	12 (6%)	1	15
21	U	168/301 (56%)	143 (85%)	17 (10%)	8 (5%)	2	16
22	V	473/782 (60%)	400 (85%)	45 (10%)	28 (6%)	1	13
23	W	661/760 (87%)	571 (86%)	67 (10%)	23 (4%)	3	20
24	0	186/395 (47%)	168 (90%)	13 (7%)	5 (3%)	4	25
25	1	60/71 (84%)	53 (88%)	5 (8%)	2 (3%)	3	21
26	2	264/462 (57%)	246 (93%)	14 (5%)	4 (2%)	8	40
27	3	187/308 (61%)	176 (94%)	9 (5%)	2 (1%)	11	46
All	All	7356/10302 (71%)	6450 (88%)	599 (8%)	307 (4%)	3	17

All (307) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	133	SER
1	A	203	LYS
1	A	208	ASP
1	A	264	VAL
1	A	265	VAL
1	A	272	ASN
1	A	275	ASP
1	A	531	ASN
1	A	607	SER
1	A	610	PRO
1	A	622	SER
1	A	623	PRO
1	A	931	ARG
1	A	932	ARG
1	A	1087	VAL
1	A	1116	ASN
1	A	1200	PRO
1	A	1307	VAL
2	B	74	ALA
2	B	226	GLU

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Mol	Chain	Res	Type
2	B	231	PRO
2	B	452	ASN
2	B	460	HIS
2	B	491	ARG
2	B	513	GLU
2	B	526	LEU
2	B	876	ASN
2	B	881	GLU
2	B	898	THR
2	B	1108	PHE
3	C	6	GLN
3	C	7	PRO
3	C	8	THR
3	C	136	ASP
3	C	137	ASN
3	C	213	GLU
5	E	46	ASP
5	E	47	LYS
5	E	50	GLU
5	E	64	HIS
5	E	65	ASN
5	E	68	PRO
8	H	18	GLU
8	H	67	ASP
8	H	73	GLY
8	H	74	GLU
8	H	86	ASP
9	I	85	PRO
9	I	86	CYS
9	I	99	SER
9	I	104	ALA
9	I	105	GLU
9	I	106	ASP
10	J	2	ILE
11	K	112	LYS
13	M	48	VAL
13	M	90	ALA
13	M	92	SER
13	M	93	PHE
13	M	94	ASP
13	M	95	GLU
14	N	355	ASP

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Mol	Chain	Res	Type
16	P	206	GLU
16	P	297	LYS
16	P	299	ARG
17	Q	102	VAL
17	Q	126	SER
18	R	195	PRO
18	R	226	ASP
18	R	228	MET
19	S	160	ALA
20	T	124	TYR
20	T	151	THR
20	T	153	TYR
20	T	156	VAL
20	T	180	LYS
21	U	228	MET
21	U	251	ALA
21	U	252	LYS
21	U	253	THR
21	U	258	THR
21	U	285	MET
21	U	300	PHE
22	V	385	ASP
22	V	427	MET
22	V	461	HIS
22	V	491	ALA
22	V	499	ASN
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

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Mol	Chain	Res	Type
26	2	49	PRO
27	3	120	THR
1	A	51	ARG
1	A	66	GLU
1	A	263	ALA
1	A	613	GLU
1	A	624	GLY
1	A	625	ASP
1	A	912	SER
1	A	926	ASN
1	A	928	ARG
1	A	935	GLN
1	A	1305	SER
1	A	1409	GLY
2	B	79	GLU
2	B	249	LYS
2	B	456	GLN
2	B	599	SER
2	B	705	GLY
2	B	875	GLU
2	B	879	GLU
2	B	899	SER
2	B	1145	GLN
3	C	143	VAL
3	C	272	LEU
5	E	124	LYS
8	H	109	ALA
8	H	111	ARG
8	H	139	SER
9	I	62	VAL
9	I	103	ARG
10	J	41	LYS
10	J	65	LEU
12	L	16	ILE
12	L	27	GLU
13	M	12	ARG
13	M	53	ARG
13	M	66	ARG
13	M	91	ALA
13	M	110	SER
14	N	320	VAL
16	P	157	GLU

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Mol	Chain	Res	Type
16	P	208	ARG
17	Q	101	ASN
17	Q	125	ALA
17	Q	158	HIS
18	R	163	LEU
18	R	164	GLY
18	R	223	VAL
18	R	224	THR
20	T	169	LYS
20	T	178	ALA
22	V	254	GLN
22	V	404	SER
22	V	460	ALA
23	W	124	LEU
23	W	408	SER
23	W	646	ILE
26	2	223	ALA
26	2	231	VAL
1	A	54	LEU
1	A	134	LYS
1	A	156	GLY
1	A	195	GLY
1	A	274	ASP
1	A	614	ASP
1	A	724	GLU
1	A	1085	GLU
1	A	1265	ASP
1	A	1274	GLU
1	A	1299	GLN
1	A	1316	ASN
2	B	63	PRO
2	B	242	ARG
2	B	548	TRP
2	B	630	LYS
2	B	691	SER
2	B	839	GLY
2	B	873	LEU
2	B	892	CYS
2	B	1136	GLU
8	H	21	LYS
8	H	35	PHE
8	H	66	GLU

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Mol	Chain	Res	Type
8	H	70	LEU
8	H	138	ASP
8	H	140	ARG
8	H	148	LEU
9	I	118	HIS
13	M	14	THR
13	M	101	TYR
14	N	325	GLY
17	Q	40	ASN
17	Q	100	VAL
17	Q	164	ASP
17	Q	165	GLU
19	S	156	THR
22	V	343	GLY
23	W	147	GLN
23	W	155	CYS
23	W	509	GLU
27	3	198	SER
1	A	44	PRO
1	A	62	GLN
1	A	75	ALA
1	A	184	CYS
1	A	205	VAL
1	A	206	ASN
1	A	210	GLN
1	A	726	GLU
1	A	894	ASP
1	A	930	LEU
1	A	1103	THR
1	A	1118	THR
2	B	80	GLU
2	B	427	LYS
2	B	527	ALA
2	B	823	PHE
3	C	217	GLN
5	E	27	LEU
8	H	22	PHE
8	H	149	ALA
12	L	45	TYR
13	M	40	VAL
13	M	56	SER
13	M	71	GLN

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Mol	Chain	Res	Type
17	Q	25	PHE
18	R	207	SER
19	S	154	THR
20	T	141	LEU
20	T	154	LYS
21	U	225	ALA
22	V	310	LEU
22	V	428	GLU
22	V	436	GLY
22	V	475	ASP
22	V	502	ILE
22	V	629	HIS
1	A	56	GLY
1	A	1271	GLU
2	B	232	THR
2	B	511	PRO
2	B	631	GLN
2	B	803	ARG
2	B	886	ARG
2	B	900	GLU
9	I	67	GLN
10	J	5	VAL
16	P	162	VAL
20	T	148	VAL
22	V	470	LEU
22	V	650	MET
23	W	152	LEU
23	W	551	SER
24	O	79	ASN
26	2	430	VAL
1	A	132	LYS
1	A	299	ALA
1	A	1414	ILE
2	B	61	ASP
2	B	685	LYS
2	B	884	ASN
2	B	1069	ILE
9	I	58	ILE
10	J	6	ARG
13	M	11	PRO
19	S	121	ASN
20	T	171	GLU

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Mol	Chain	Res	Type
22	V	582	GLY
23	W	36	GLY
23	W	111	SER
23	W	345	ARG
23	W	697	ILE
1	A	1275	VAL
9	I	117	PRO
22	V	311	LYS
22	V	651	VAL
23	W	174	ILE
1	A	182	GLY
2	B	136	GLY
2	B	330	VAL
2	B	561	ILE
22	V	426	VAL
22	V	457	ILE
23	W	495	ILE
24	0	216	GLY
1	A	1312	PRO
2	B	253	GLY
5	E	48	PRO
8	H	82	PRO
10	J	64	PRO
22	V	405	VAL
25	1	2	VAL
2	B	81	PRO
2	B	931	ILE
3	C	151	VAL
20	T	38	GLY
1	A	55	GLY
1	A	371	PRO
13	M	38	GLY
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%)	1225 (96%)	54 (4%)	26	48
2	B	1020/1028 (99%)	977 (96%)	43 (4%)	26	48
3	C	252/252 (100%)	246 (98%)	6 (2%)	43	64
4	D	119/126 (94%)	119 (100%)	0	100	100
5	E	192/192 (100%)	186 (97%)	6 (3%)	35	56
6	F	74/111 (67%)	72 (97%)	2 (3%)	39	61
7	G	152/153 (99%)	151 (99%)	1 (1%)	76	81
8	H	131/131 (100%)	124 (95%)	7 (5%)	20	41
9	I	112/112 (100%)	106 (95%)	6 (5%)	20	41
10	J	56/56 (100%)	49 (88%)	7 (12%)	4	16
11	K	106/106 (100%)	103 (97%)	3 (3%)	38	60
12	L	43/55 (78%)	41 (95%)	2 (5%)	23	45
13	M	263/268 (98%)	254 (97%)	9 (3%)	32	54
14	N	105/324 (32%)	104 (99%)	1 (1%)	68	78
15	O	90/98 (92%)	89 (99%)	1 (1%)	65	76
16	P	159/293 (54%)	156 (98%)	3 (2%)	50	67
17	Q	164/373 (44%)	153 (93%)	11 (7%)	15	36
18	R	150/261 (58%)	144 (96%)	6 (4%)	28	49
19	S	121/448 (27%)	118 (98%)	3 (2%)	42	63
20	T	196/218 (90%)	192 (98%)	4 (2%)	48	66
21	U	148/266 (56%)	139 (94%)	9 (6%)	17	38
22	V	422/688 (61%)	405 (96%)	17 (4%)	28	49
23	W	577/664 (87%)	545 (94%)	32 (6%)	19	41
24	0	171/352 (49%)	163 (95%)	8 (5%)	23	45
25	1	56/64 (88%)	51 (91%)	5 (9%)	9	28
26	2	238/399 (60%)	229 (96%)	9 (4%)	29	50
27	3	171/272 (63%)	161 (94%)	10 (6%)	18	40
All	All	6567/9058 (72%)	6302 (96%)	265 (4%)	29	49

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU

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Mol	Chain	Res	Type
1	A	117	LEU
1	A	132	LYS
1	A	146	ASP
1	A	203	LYS
1	A	204	HIS
1	A	211	GLU
1	A	212	LYS
1	A	227	ARG
1	A	271	ARG
1	A	272	ASN
1	A	436	SER
1	A	463	THR
1	A	484	LEU
1	A	488	VAL
1	A	524	MET
1	A	534	VAL
1	A	538	VAL
1	A	545	VAL
1	A	557	ARG
1	A	562	ASN
1	A	607	SER
1	A	613	GLU
1	A	619	LYS
1	A	621	ILE
1	A	625	ASP
1	A	644	SER
1	A	687	ILE
1	A	691	ASP
1	A	792	ASN
1	A	818	GLU
1	A	849	ASP
1	A	853	LYS
1	A	864	LEU
1	A	873	VAL
1	A	908	THR
1	A	930	LEU
1	A	931	ARG
1	A	932	ARG
1	A	954	ARG
1	A	1036	ASN
1	A	1128	ILE
1	A	1160	ARG

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Mol	Chain	Res	Type
1	A	1165	THR
1	A	1203	ASP
1	A	1282	ASP
1	A	1298	LEU
1	A	1305	SER
1	A	1306	LYS
1	A	1308	TYR
1	A	1311	LEU
1	A	1318	LYS
1	A	1341	VAL
1	A	1485	GLU
2	B	41	ARG
2	B	57	ARG
2	B	61	ASP
2	B	67	LEU
2	B	73	HIS
2	B	80	GLU
2	B	129	THR
2	B	132	VAL
2	B	224	CYS
2	B	225	LEU
2	B	226	GLU
2	B	250	SER
2	B	269	ILE
2	B	302	LYS
2	B	330	VAL
2	B	371	ARG
2	B	388	TYR
2	B	416	ARG
2	B	422	PHE
2	B	448	LEU
2	B	485	LEU
2	B	604	ILE
2	B	621	ILE
2	B	628	VAL
2	B	655	ASP
2	B	667	THR
2	B	711	ILE
2	B	733	MET
2	B	735	VAL
2	B	737	ILE
2	B	747	LEU

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Mol	Chain	Res	Type
2	B	784	SER
2	B	853	LEU
2	B	875	GLU
2	B	880	LEU
2	B	881	GLU
2	B	921	ILE
2	B	958	CYS
2	B	961	ILE
2	B	1022	LEU
2	B	1035	ARG
2	B	1071	ASN
2	B	1092	ASP
3	C	6	GLN
3	C	35	ARG
3	C	58	VAL
3	C	70	LEU
3	C	136	ASP
3	C	148	ILE
5	E	38	GLU
5	E	47	LYS
5	E	64	HIS
5	E	113	SER
5	E	191	VAL
5	E	205	THR
6	F	54	THR
6	F	64	ARG
7	G	158	PHE
8	H	65	TYR
8	H	66	GLU
8	H	74	GLU
8	H	84	ARG
8	H	107	GLU
8	H	116	VAL
8	H	144	LEU
9	I	28	GLU
9	I	60	HIS
9	I	61	GLU
9	I	84	HIS
9	I	103	ARG
9	I	105	GLU
10	J	3	ILE
10	J	7	CYS

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Mol	Chain	Res	Type
10	J	14	VAL
10	J	47	ARG
10	J	54	ASP
10	J	59	LEU
10	J	65	LEU
11	K	39	ASP
11	K	48	SER
11	K	63	VAL
12	L	16	ILE
12	L	27	GLU
13	M	10	LEU
13	M	40	VAL
13	M	43	ASP
13	M	47	ASP
13	M	48	VAL
13	M	110	SER
13	M	111	ASP
13	M	133	ASN
13	M	282	ASP
14	N	20	ASP
15	O	88	ILE
16	P	180	LEU
16	P	206	GLU
16	P	297	LYS
17	Q	17	LEU
17	Q	72	ILE
17	Q	76	MET
17	Q	135	THR
17	Q	138	ASP
17	Q	151	THR
17	Q	159	THR
17	Q	171	LYS
17	Q	177	LEU
17	Q	184	ILE
17	Q	191	LEU
18	R	163	LEU
18	R	169	GLU
18	R	205	ASP
18	R	206	LYS
18	R	209	GLN
18	R	228	MET
19	S	135	PHE

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Mol	Chain	Res	Type
19	S	166	ARG
19	S	177	MET
20	T	141	LEU
20	T	148	VAL
20	T	154	LYS
20	T	183	VAL
21	U	194	ARG
21	U	226	GLU
21	U	248	HIS
21	U	252	LYS
21	U	253	THR
21	U	257	GLN
21	U	260	LEU
21	U	276	VAL
21	U	299	LYS
22	V	246	MET
22	V	271	GLU
22	V	332	ARG
22	V	362	LEU
22	V	371	VAL
22	V	427	MET
22	V	429	TRP
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	568	LEU
22	V	581	TYR
22	V	590	MET
22	V	614	SER
23	W	37	HIS
23	W	64	PRO
23	W	87	LEU
23	W	95	GLU
23	W	101	LYS
23	W	112	ARG
23	W	122	THR
23	W	123	PRO
23	W	152	LEU
23	W	166	ARG

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Mol	Chain	Res	Type
23	W	196	ARG
23	W	263	LEU
23	W	283	ASP
23	W	288	LEU
23	W	307	ASN
23	W	309	VAL
23	W	327	GLU
23	W	333	LEU
23	W	346	VAL
23	W	425	THR
23	W	461	LEU
23	W	523	LEU
23	W	533	ASP
23	W	554	GLU
23	W	581	LEU
23	W	596	LEU
23	W	610	PHE
23	W	620	MET
23	W	647	ARG
23	W	664	VAL
23	W	669	ARG
23	W	676	LEU
24	0	77	LYS
24	0	103	GLN
24	0	125	ARG
24	0	174	LEU
24	0	202	SER
24	0	218	THR
24	0	222	ILE
24	0	223	LEU
25	1	10	ILE
25	1	16	MET
25	1	18	GLN
25	1	21	LEU
25	1	38	ILE
26	2	77	LYS
26	2	181	GLN
26	2	202	GLN
26	2	402	ARG
26	2	407	VAL
26	2	421	LEU
26	2	426	ARG

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Mol	Chain	Res	Type
26	2	430	VAL
26	2	452	LYS
27	3	24	LYS
27	3	25	GLN
27	3	56	LYS
27	3	109	GLU
27	3	124	ILE
27	3	133	LEU
27	3	144	ILE
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 (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	122	ASN
1	A	181	HIS
1	A	222	HIS
1	A	273	GLN
1	A	296	ASN
1	A	410	ASN
1	A	504	HIS
1	A	507	GLN
1	A	529	GLN
1	A	632	ASN
1	A	673	GLN
1	A	746	ASN
1	A	757	GLN
1	A	780	ASN
1	A	783	GLN
1	A	989	ASN
1	A	1101	GLN
1	A	1194	ASN
1	A	1445	HIS
2	B	72	GLN
2	B	90	GLN
2	B	98	HIS
2	B	175	ASN
2	B	370	HIS
2	B	460	HIS

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Mol	Chain	Res	Type
2	B	790	GLN
2	B	817	GLN
2	B	842	HIS
2	B	941	GLN
2	B	1101	GLN
3	C	5	ASN
3	C	275	ASN
4	D	48	ASN
6	F	46	GLN
7	G	24	ASN
7	G	91	GLN
9	I	21	ASN
9	I	22	ASN
9	I	41	ASN
9	I	45	GLN
9	I	84	HIS
10	J	52	HIS
11	K	29	ASN
11	K	89	ASN
12	L	26	ASN
13	M	71	GLN
13	M	102	GLN
13	M	116	ASN
13	M	140	ASN
13	M	144	GLN
13	M	227	GLN
16	P	189	ASN
17	Q	101	ASN
17	Q	109	HIS
18	R	204	ASN
19	S	121	ASN
20	T	30	GLN
20	T	81	HIS
21	U	203	ASN
22	V	281	GLN
22	V	366	ASN
22	V	377	GLN
22	V	459	GLN
22	V	537	ASN
22	V	539	ASN
22	V	621	ASN
22	V	665	GLN

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Mol	Chain	Res	Type
22	V	677	GLN
23	W	187	GLN
23	W	316	GLN
23	W	328	HIS
23	W	430	ASN
23	W	499	ASN
24	0	60	HIS
25	1	51	ASN
26	2	97	HIS
26	2	161	HIS
26	2	181	GLN
26	2	202	GLN
26	2	221	GLN
26	2	239	GLN
26	2	263	GLN
26	2	273	GLN
26	2	411	GLN
26	2	458	GLN
27	3	25	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

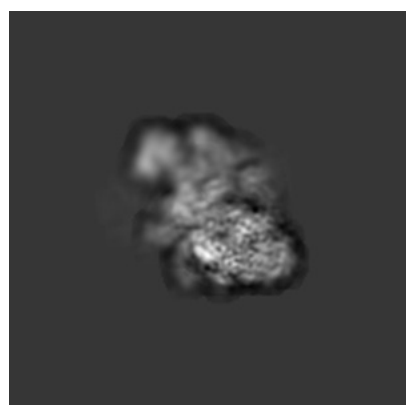
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8133. These allow visual inspection of the internal detail of the map and identification of artifacts.

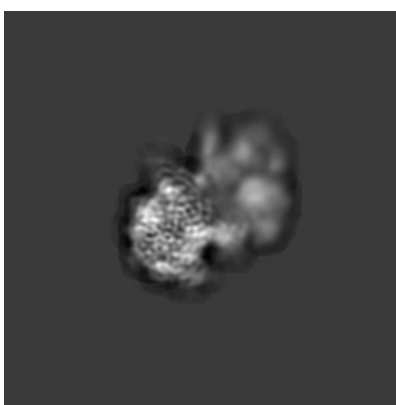
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

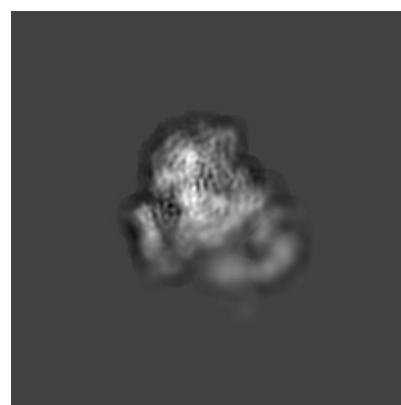
6.1.1 Primary map



X



Y

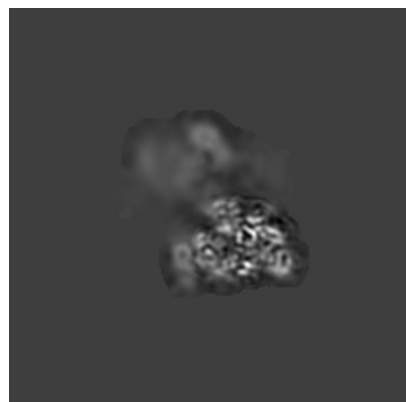


Z

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

6.2 Central slices [i](#)

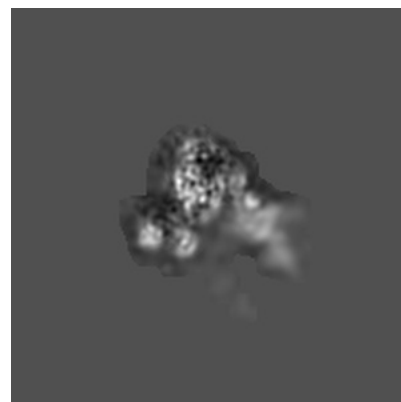
6.2.1 Primary map



X Index: 96



Y Index: 96

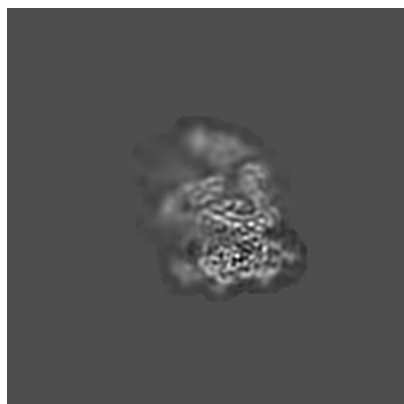


Z Index: 96

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

6.3 Largest variance slices [i](#)

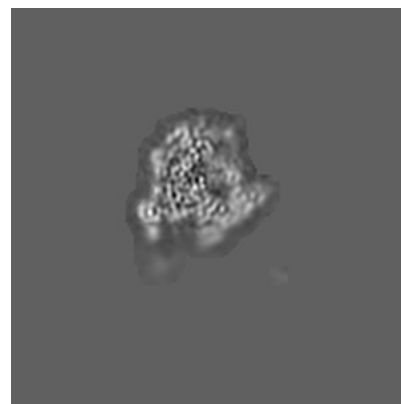
6.3.1 Primary map



X Index: 87



Y Index: 96

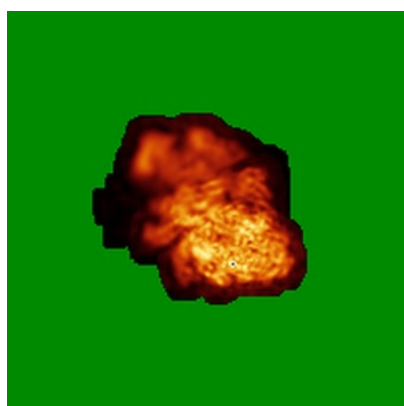


Z Index: 75

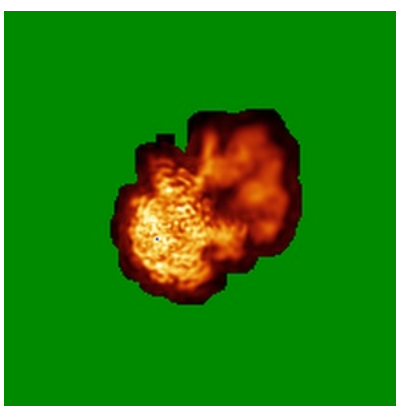
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

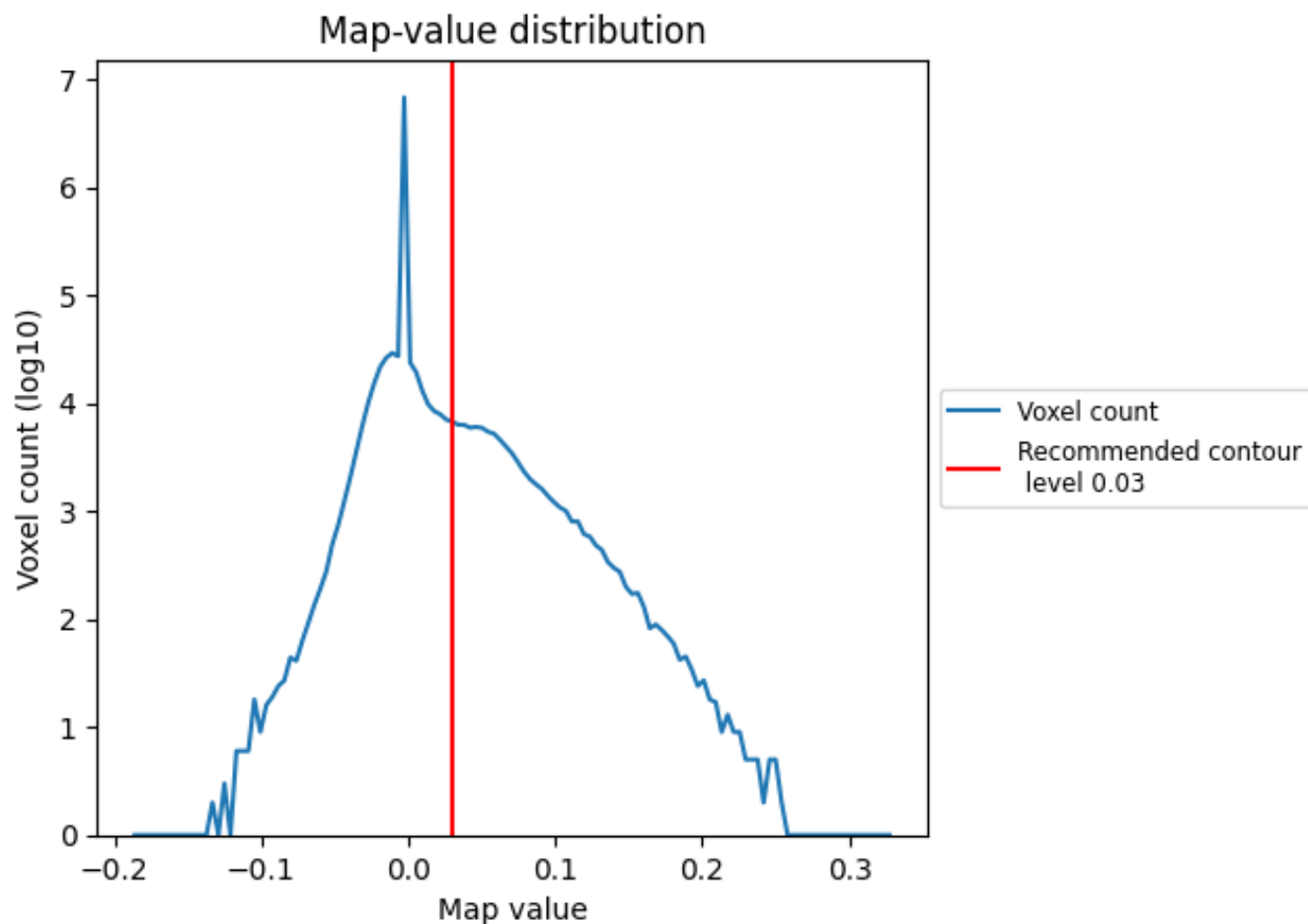
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

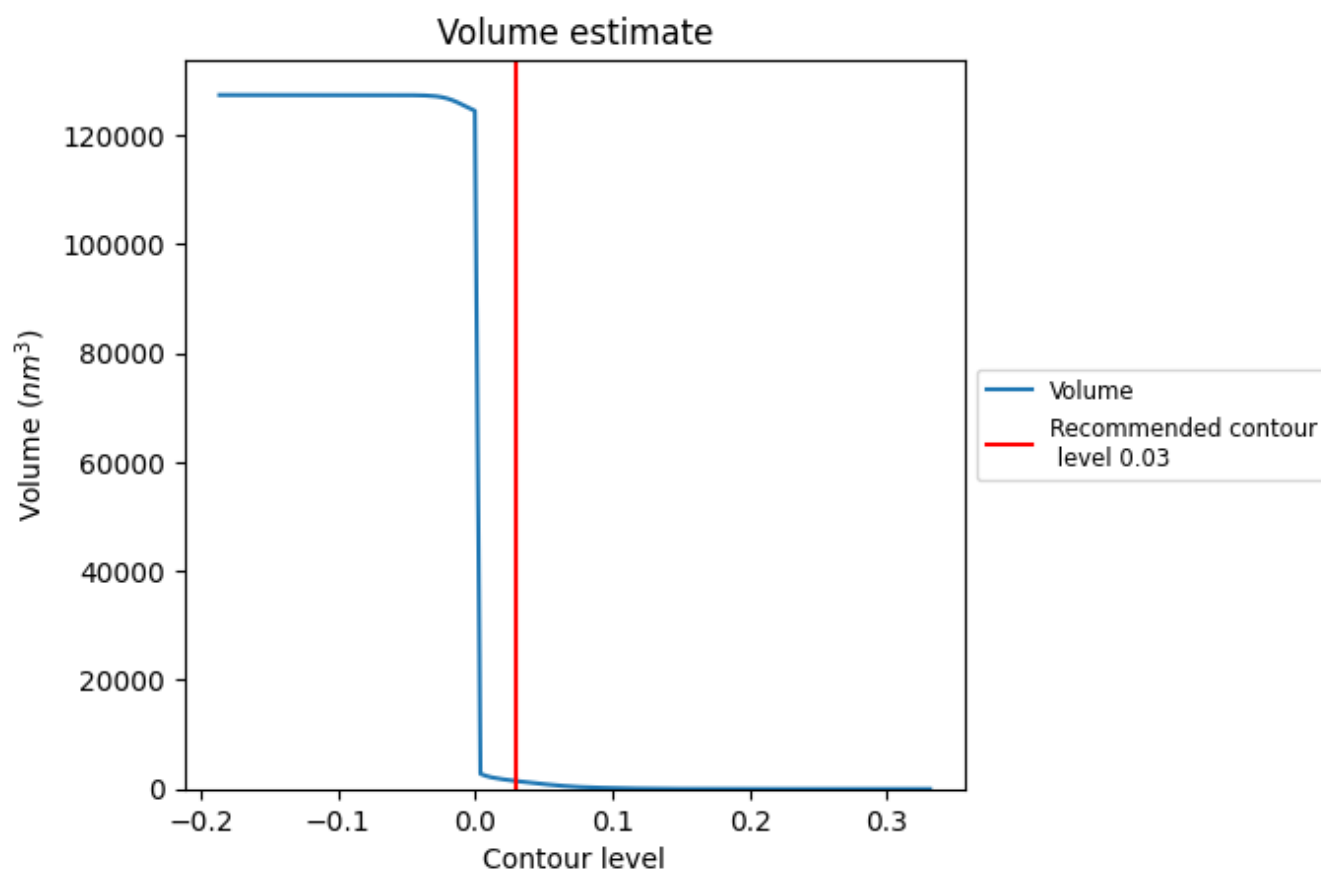
This section contains the results of statistical analysis of the map.

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.

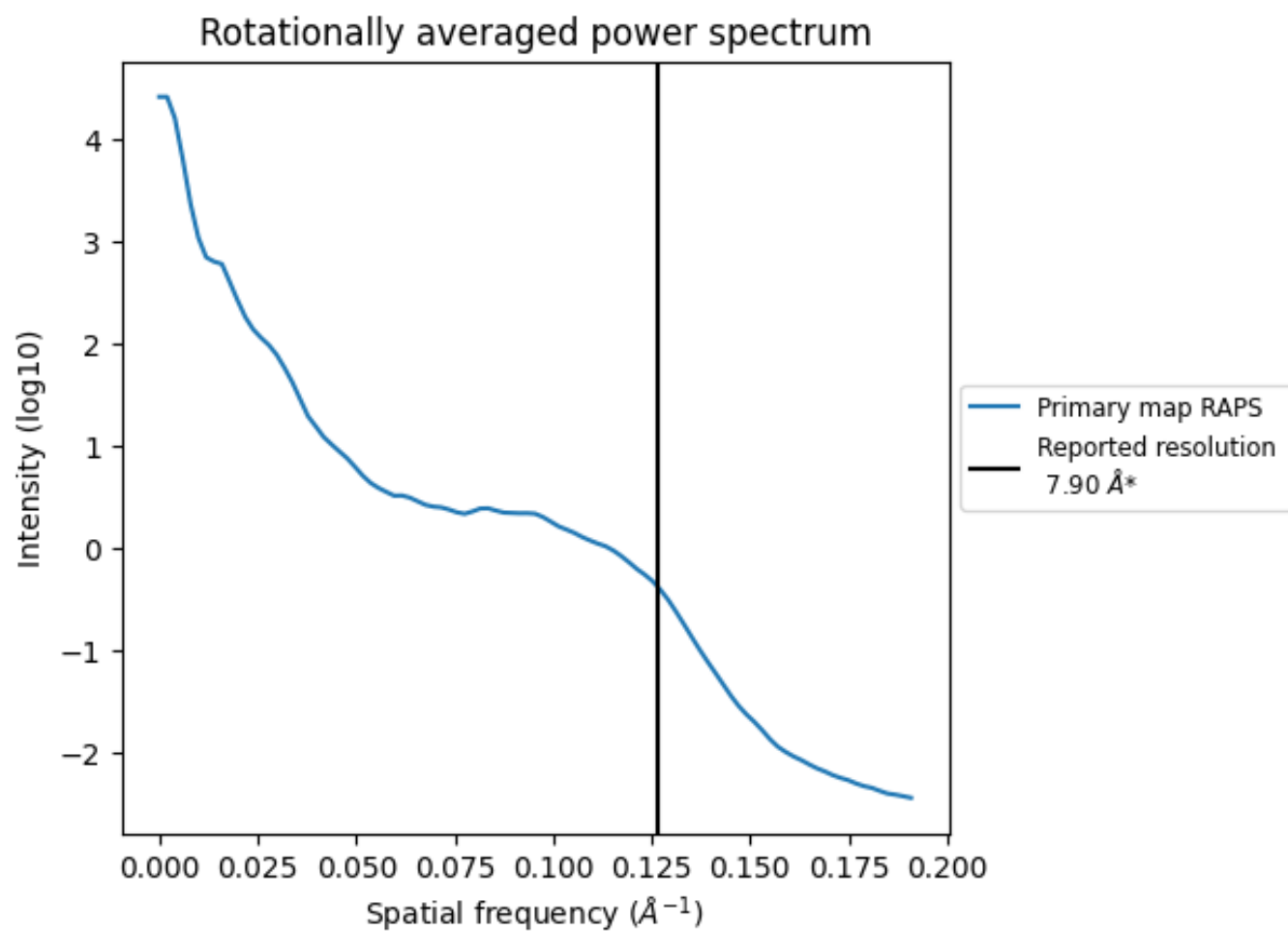
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1447 nm³; this corresponds to an approximate mass of 1307 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 ⓘ

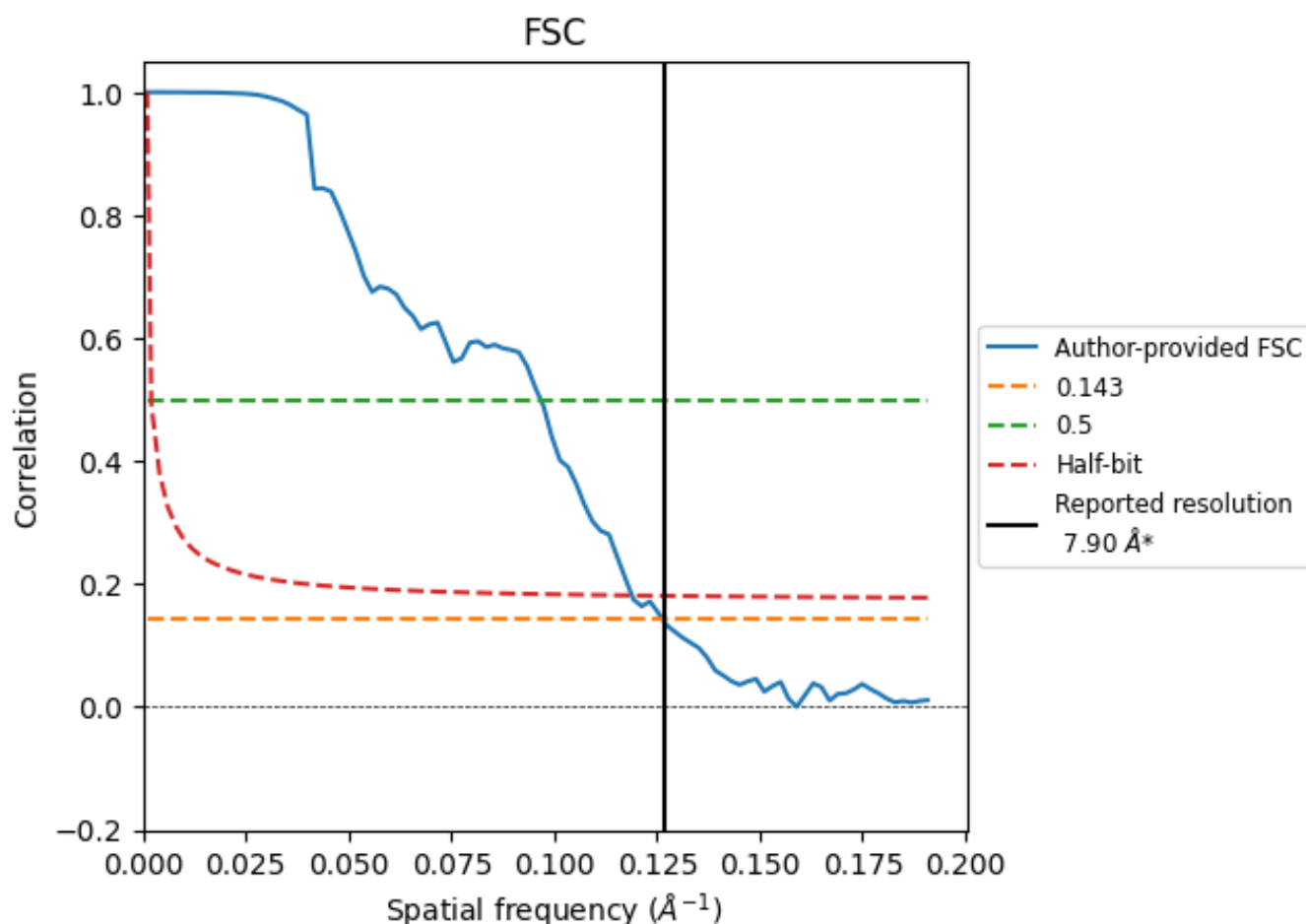


*Reported resolution corresponds to spatial frequency of 0.127 Å⁻¹

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 0.127 Å⁻¹

8.2 Resolution estimates [i](#)

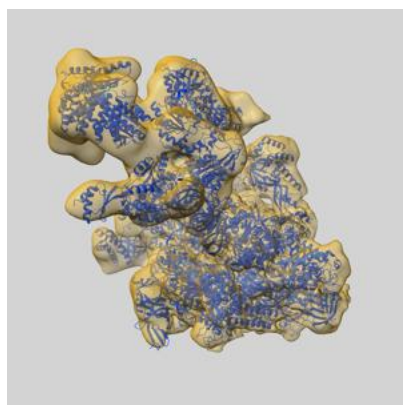
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.90	-	-
Author-provided FSC curve	7.92	10.34	8.41
Unmasked-calculated*	-	-	-

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

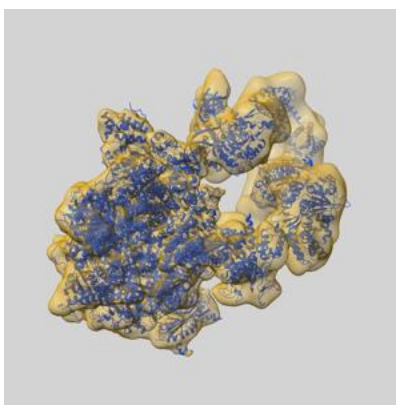
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8133 and PDB model 5IY8. Per-residue inclusion information can be found in section 3 on page 9.

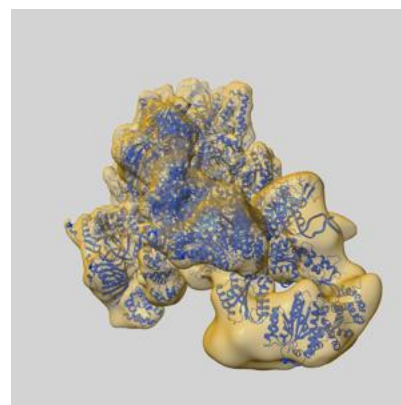
9.1 Map-model overlay [i](#)



X



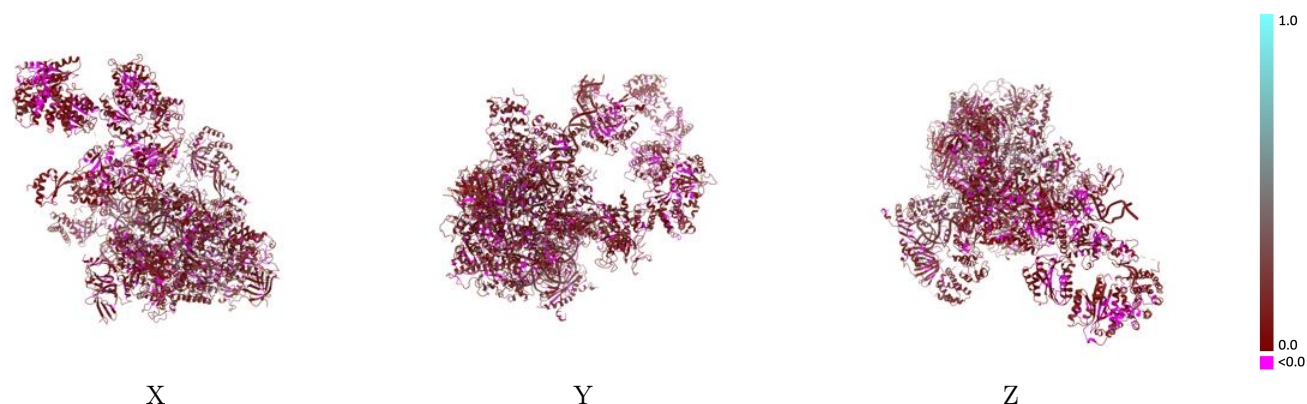
Y



Z

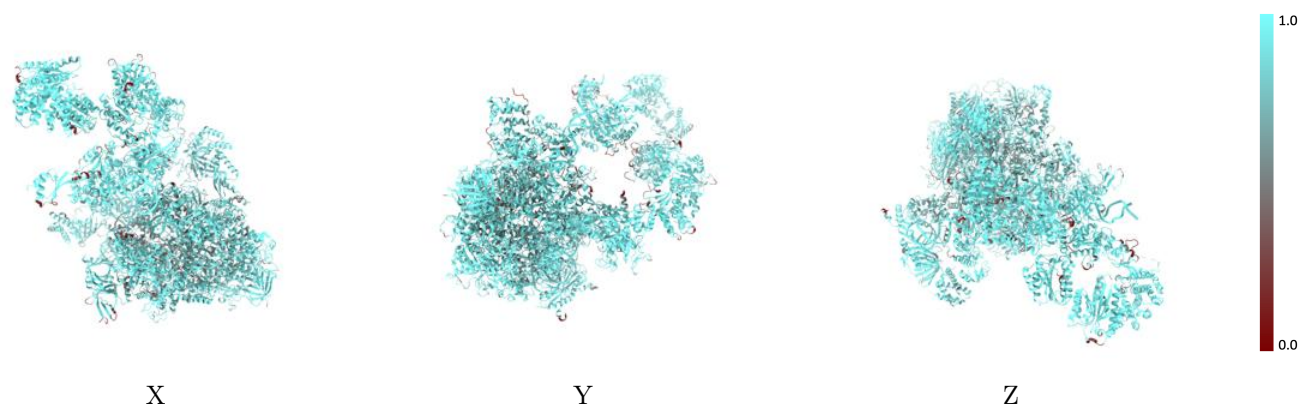
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



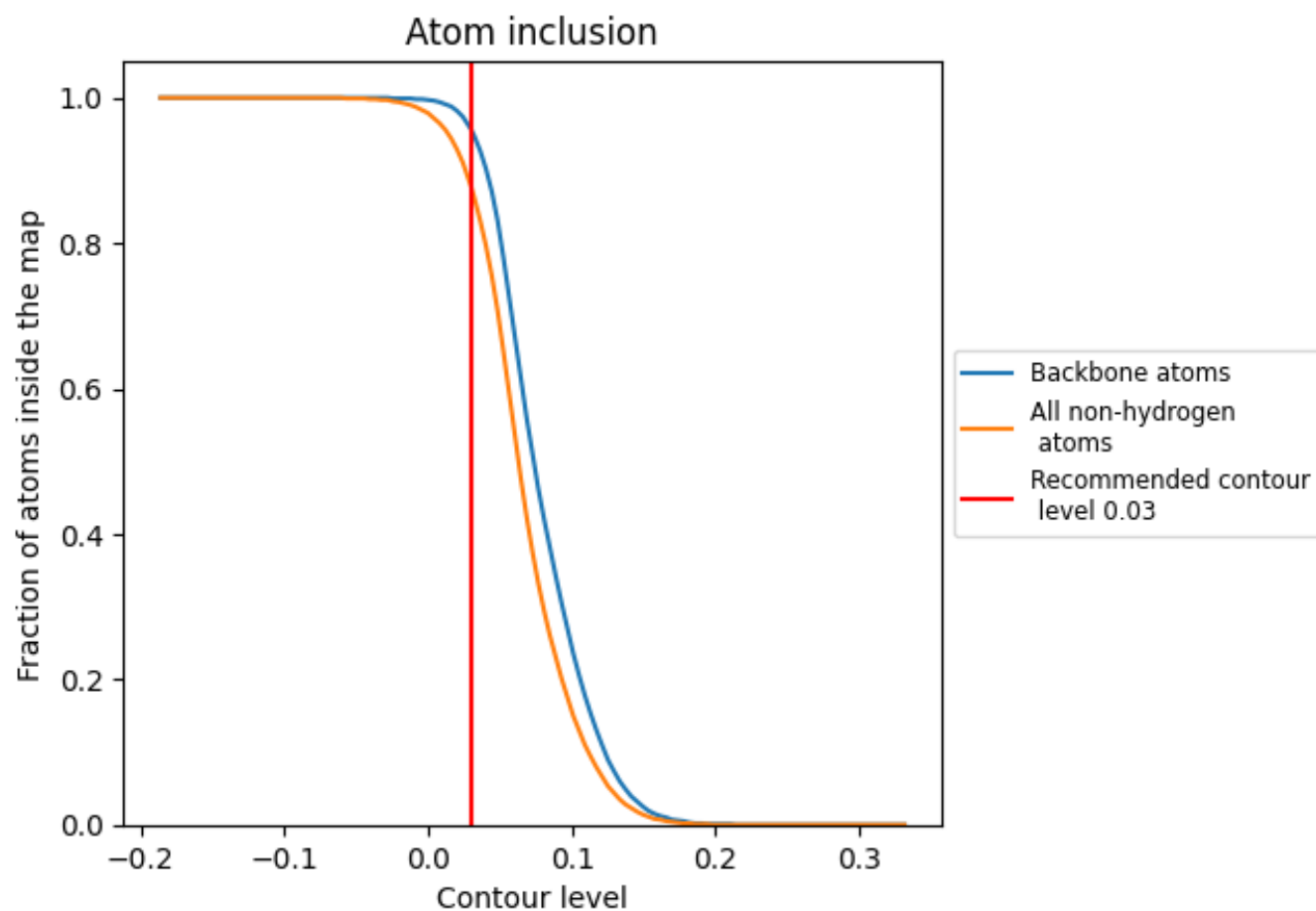
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 88% 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	 0.8770	 0.1110
0	 0.9370	 0.0560
1	 0.8030	 0.0740
2	 0.9410	 0.0800
3	 0.9390	 0.0510
A	 0.8480	 0.1330
B	 0.8160	 0.1230
C	 0.9330	 0.1240
D	 0.9200	 0.1280
E	 0.8760	 0.1360
F	 0.7920	 0.1280
G	 0.9410	 0.1240
H	 0.9230	 0.1230
I	 0.9090	 0.1190
J	 0.7790	 0.1220
K	 0.9240	 0.1450
L	 0.9190	 0.1400
M	 0.8620	 0.1310
N	 0.9410	 0.1170
O	 0.9350	 0.1020
P	 0.9480	 0.1110
Q	 0.9150	 0.1060
R	 0.9060	 0.1180
S	 0.8060	 0.0790
T	 0.8500	 0.1040
U	 0.7180	 0.0980
V	 0.9220	 0.0660
W	 0.9010	 0.0680
X	 0.8780	 0.1520
Y	 0.9200	 0.1610

