



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 09:00 PM UTC

PDB ID : 5IY7 / pdb_00005iy7
EMDB ID : EMD-8132
Title : Human holo-PIC in the open state
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on : 2016-03-24
Resolution : 8.60 Å(reported)

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

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

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:

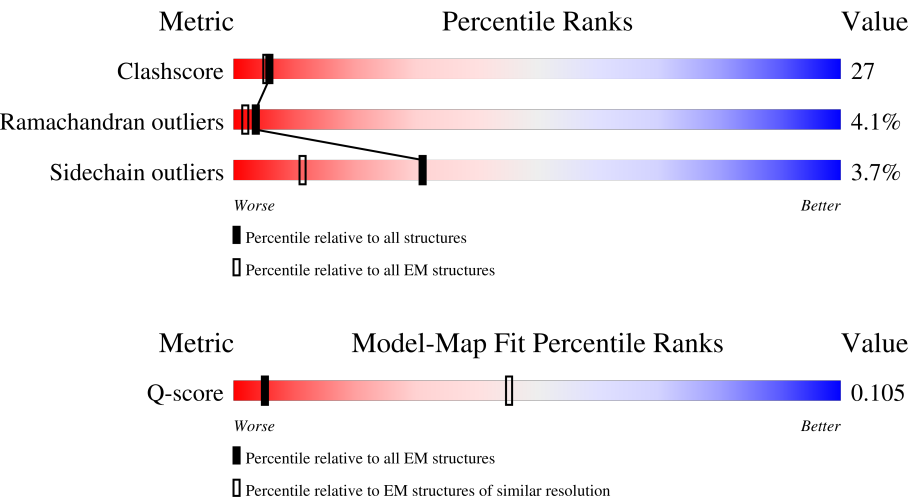
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 8.60 Å.

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



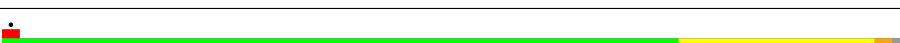
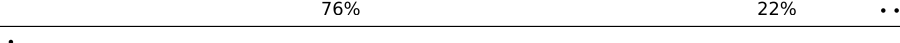
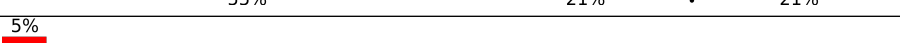
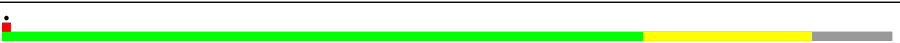
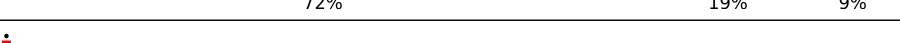
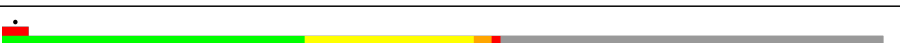
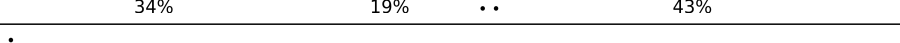
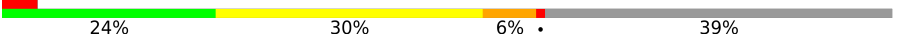
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	292 (8.10 - 9.10)

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	46% 23% • • 26%
2	B	1174	58% 35% 5% • •
3	C	275	69% 25% 6%
4	D	142	5% 82% 8% 9%

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	77	
29	Y	77	

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called 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	77	Total	C	N	O	P	0	0
			1591	753	303	459	76		

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

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

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

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

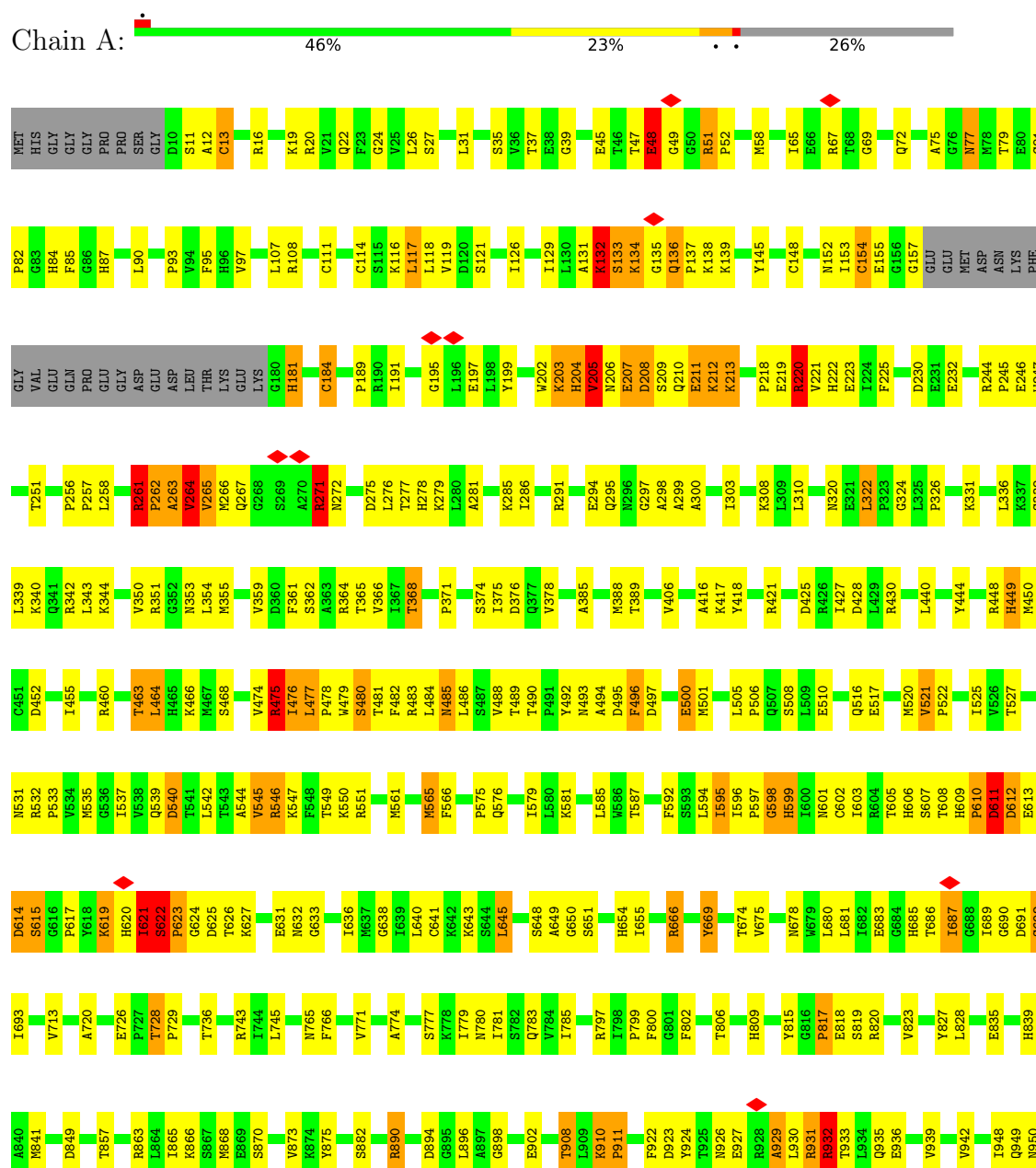
- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

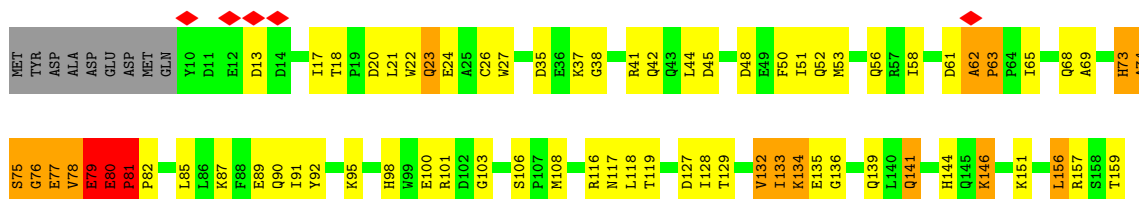
Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Zn	0
			2	2	
31	B	2	Total	Zn	0
			2	2	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	
31	Q	1	Total	Zn	0
			1	1	
31	U	1	Total	Zn	0
			1	1	

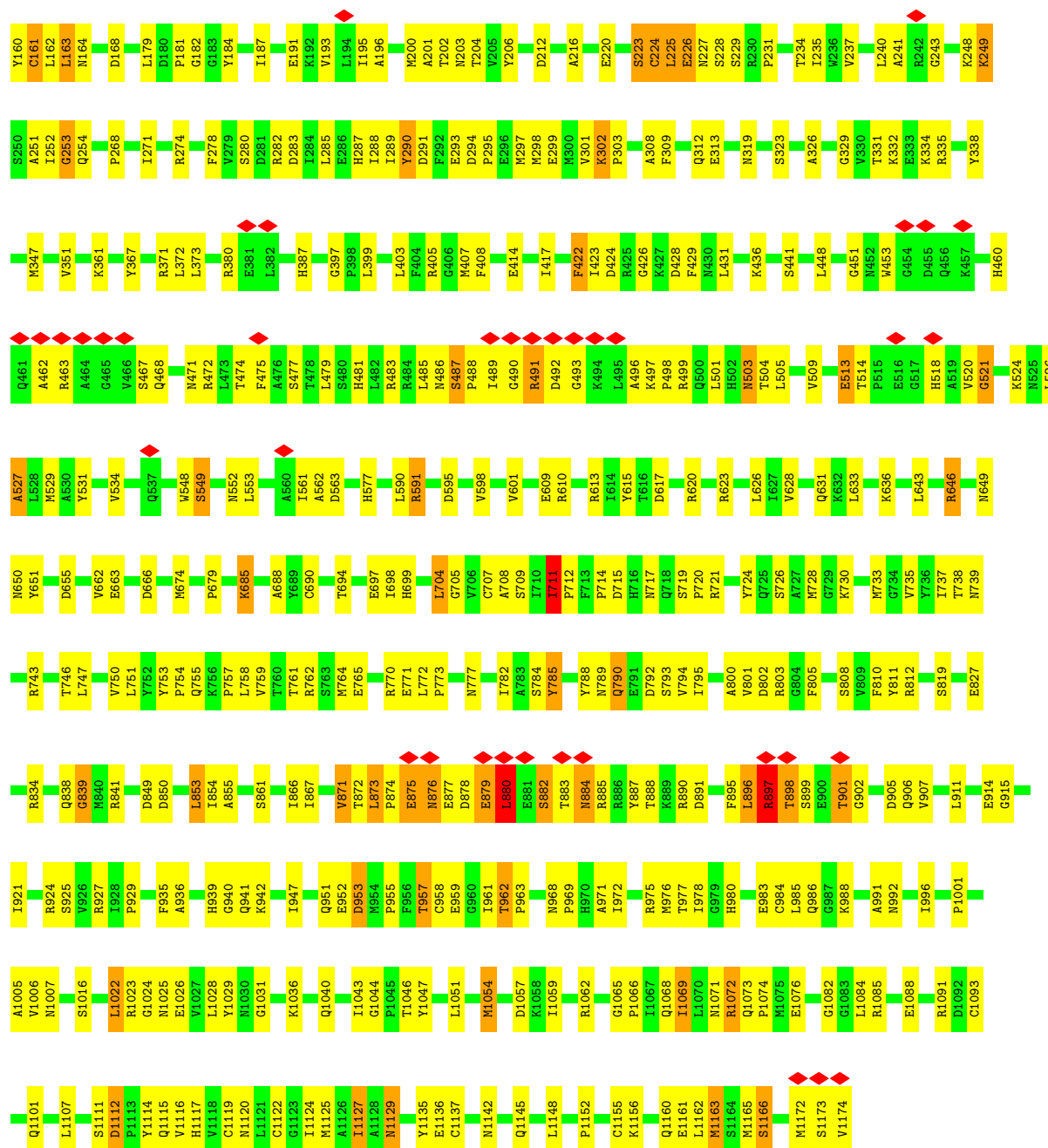
3 Residue-property plots

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

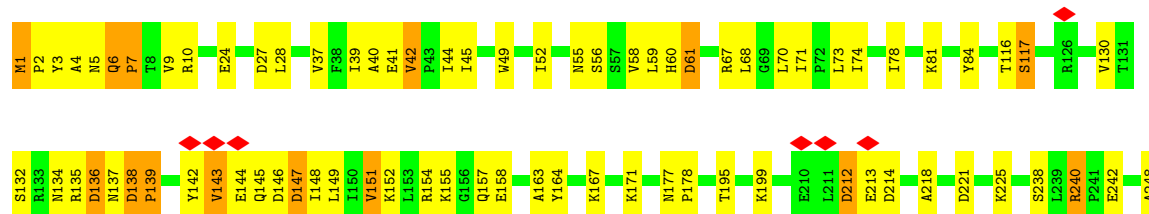
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





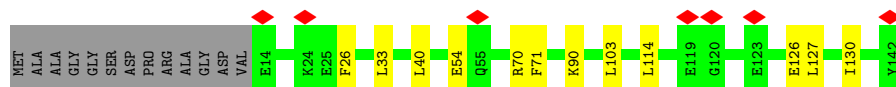
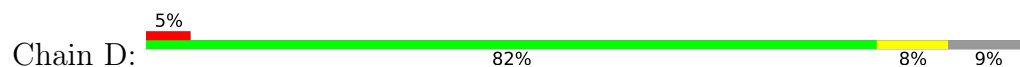


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

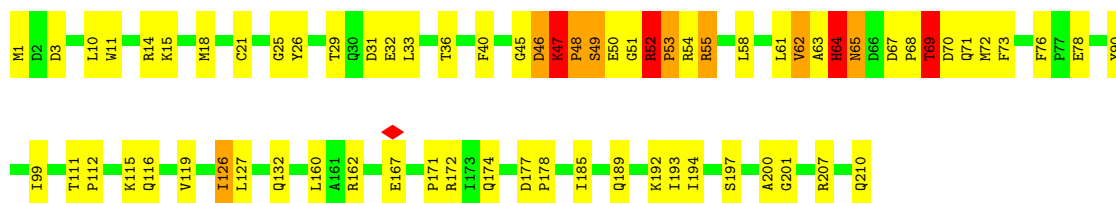




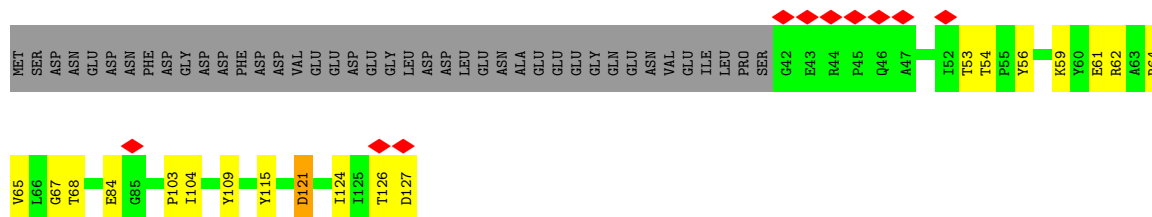
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



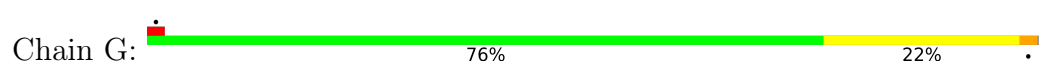
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5



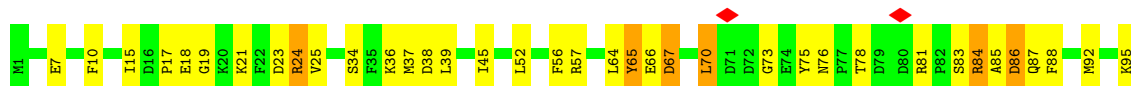
- Molecule 6: DNA-directed RNA polymerase II subunit RPB6

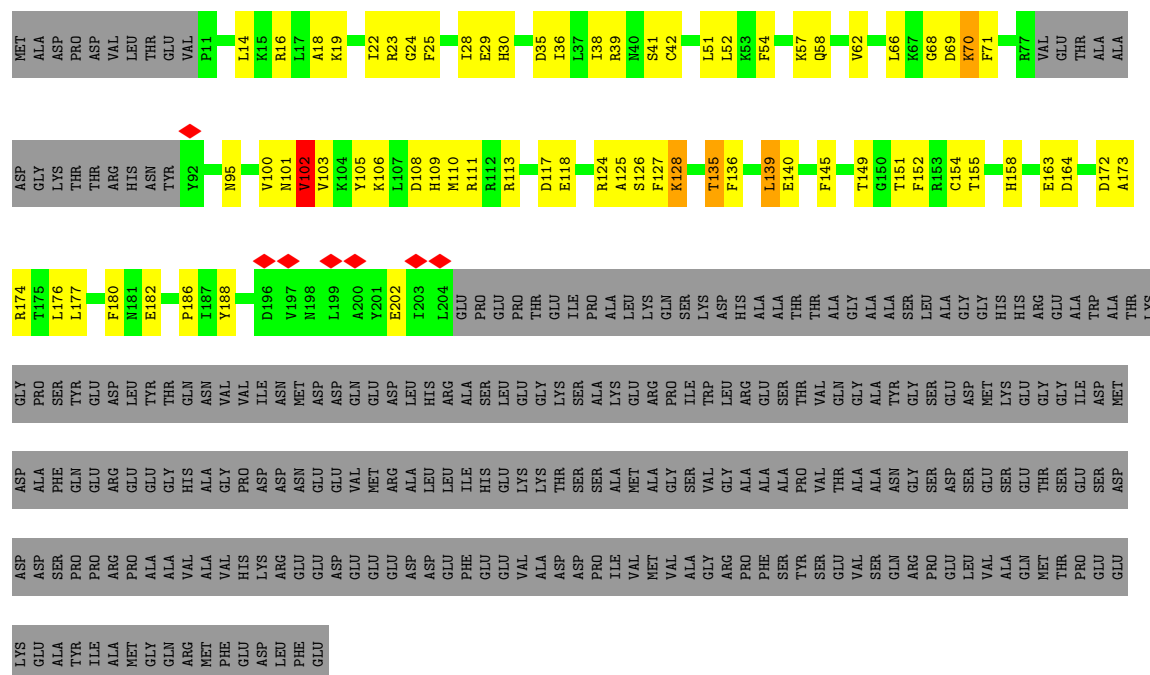


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

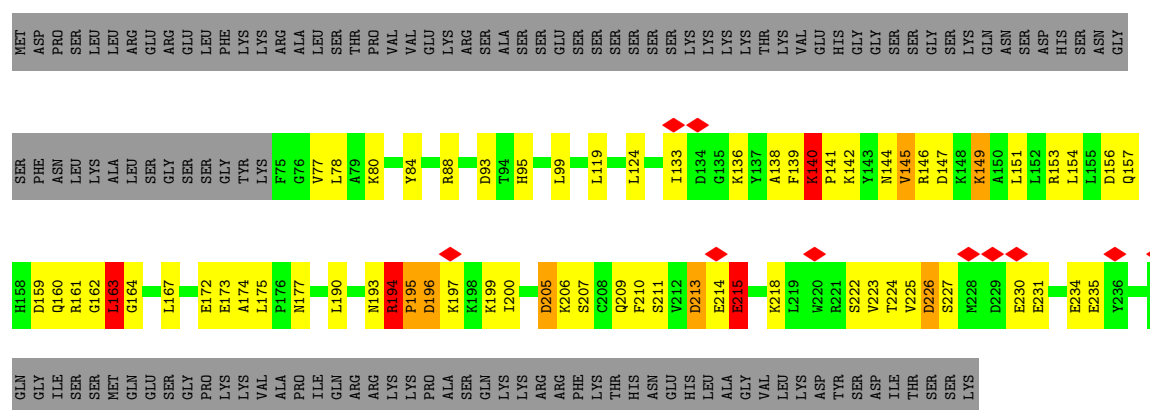
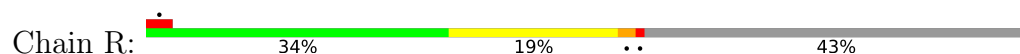


- Molecule 8: DNA-directed RNA polymerase II subunit RPB8

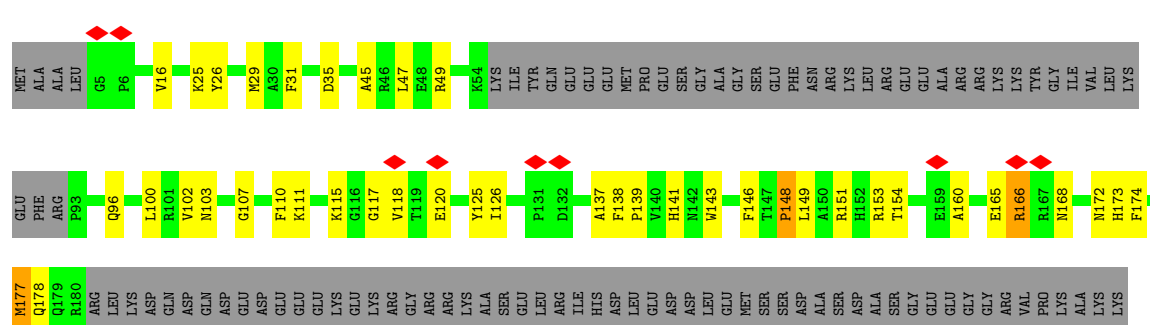


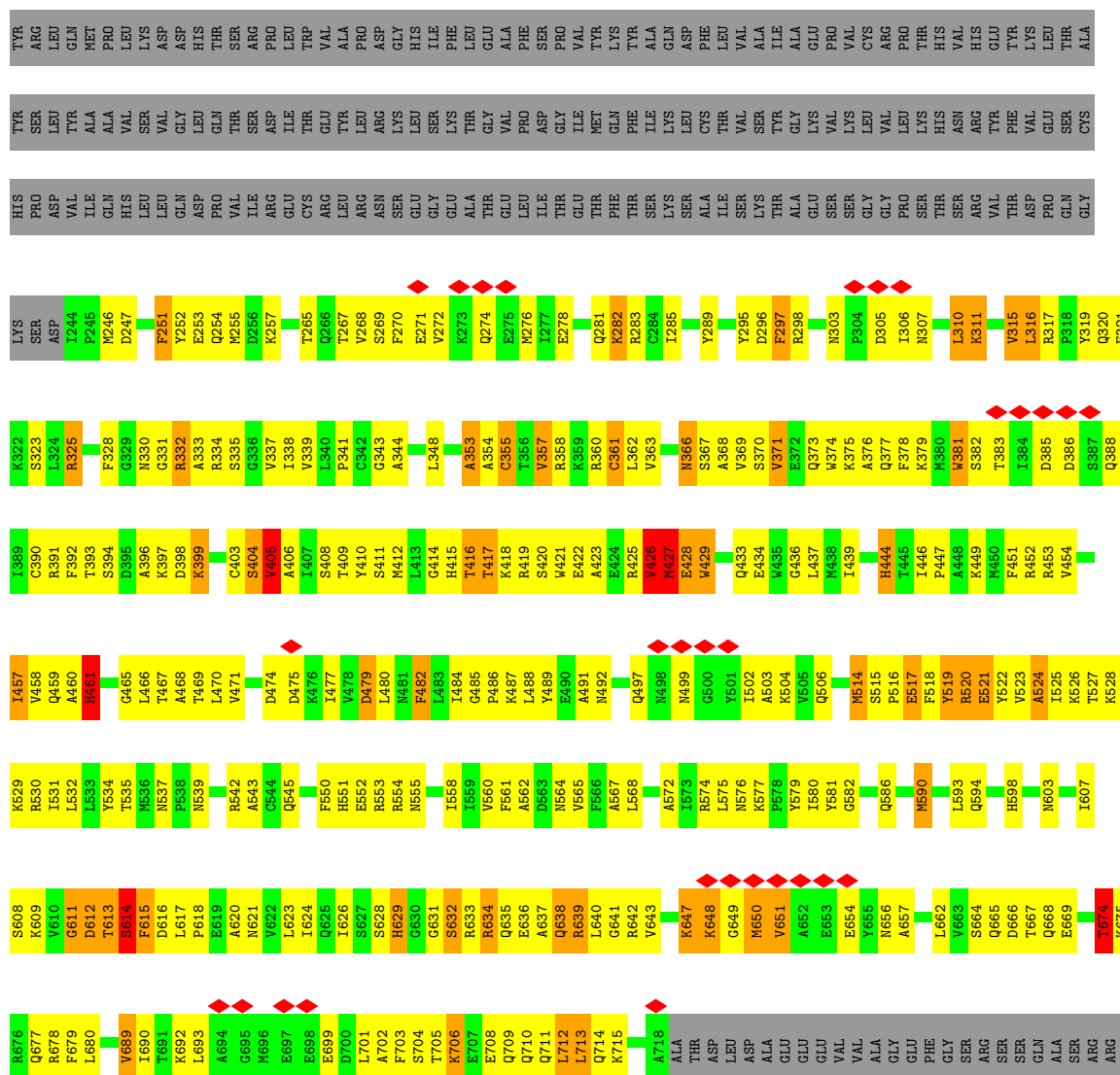


• Molecule 18: Transcription initiation factor IIE subunit beta

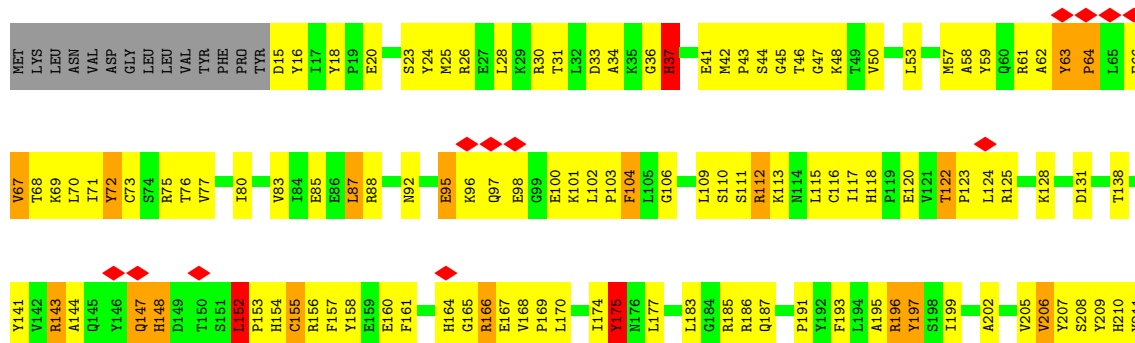


• Molecule 19: General transcription factor IIF subunit 1

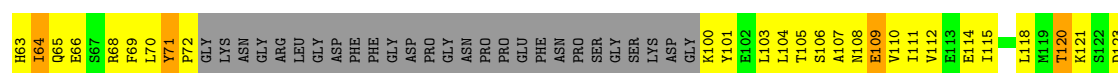


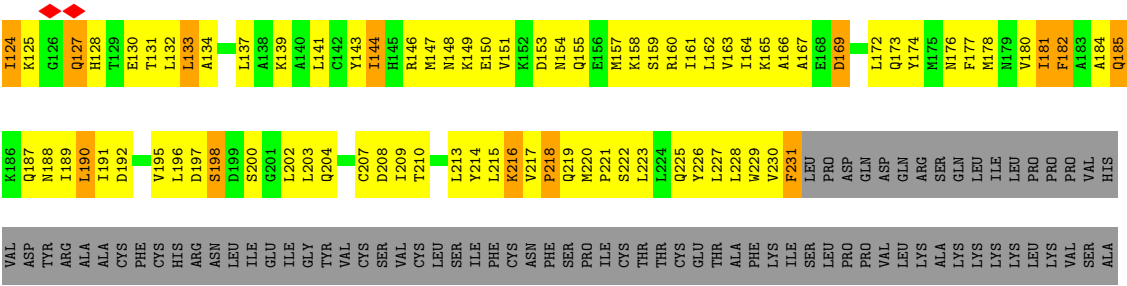


• Molecule 23: TFIIF basal transcription factor complex helicase XPD subunit

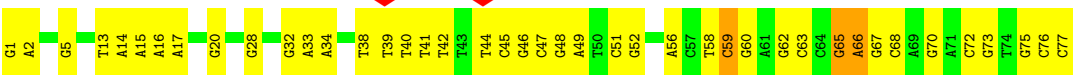


WORLDWIDE
PDB
PROTEIN DATA BANK

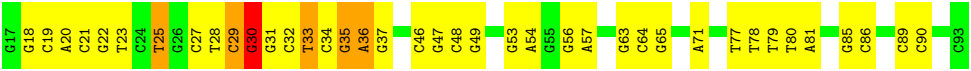




• Molecule 28: SCP-X



• Molecule 29: SCP-Y



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59271	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	503.03998, 503.03998, 503.03998	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.65	2/11727 (0.0%)	1.15	67/15833 (0.4%)
2	B	0.72	5/9503 (0.1%)	1.18	76/12831 (0.6%)
3	C	0.64	0/2259	1.18	20/3073 (0.7%)
4	D	0.34	0/1077	0.88	1/1446 (0.1%)
5	E	0.52	0/1753	1.09	10/2368 (0.4%)
6	F	0.57	0/700	1.02	4/946 (0.4%)
7	G	0.35	0/1382	0.95	9/1874 (0.5%)
8	H	0.44	0/1227	0.91	1/1654 (0.1%)
9	I	0.40	0/1038	1.18	13/1407 (0.9%)
10	J	0.69	0/542	1.27	3/730 (0.4%)
11	K	0.52	0/956	1.04	7/1294 (0.5%)
12	L	0.49	0/394	0.91	0/524
13	M	0.45	0/2429	1.04	11/3281 (0.3%)
14	N	0.34	0/945	0.97	7/1274 (0.5%)
15	O	0.32	0/816	0.81	0/1105
16	P	0.37	0/1489	1.01	3/2005 (0.1%)
17	Q	0.38	0/1507	1.03	4/2023 (0.2%)
18	R	0.53	0/1380	1.17	5/1854 (0.3%)
19	S	0.33	0/1167	0.80	0/1576
20	T	0.43	0/1817	1.07	13/2445 (0.5%)
21	U	0.45	0/1358	1.05	5/1820 (0.3%)
22	V	1.87	75/3931 (1.9%)	2.32	241/5298 (4.5%)
23	W	2.03	128/5460 (2.3%)	2.41	346/7390 (4.7%)
24	0	2.09	34/1506 (2.3%)	2.31	74/2038 (3.6%)
25	1	1.29	1/496 (0.2%)	1.79	13/669 (1.9%)
26	2	1.23	0/2243	1.70	41/3024 (1.4%)
27	3	1.26	0/1548	1.55	15/2090 (0.7%)
28	X	0.64	3/1788 (0.2%)	1.01	16/2762 (0.6%)
29	Y	0.62	0/1746	1.09	25/2690 (0.9%)
All	All	1.01	248/64184 (0.4%)	1.43	1030/87324 (1.2%)

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

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

All (248) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	9.58	1.63	1.53
23	W	465	ASP	CA-C	9.18	1.64	1.52
22	V	590	MET	CA-C	8.93	1.64	1.52
22	V	376	ALA	CA-C	8.57	1.63	1.52
24	0	142	GLU	CA-C	8.51	1.60	1.52
22	V	255	MET	N-CA	8.44	1.54	1.47
23	W	237	HIS	CE1-NE2	8.35	1.41	1.32
24	0	122	GLY	N-CA	8.13	1.55	1.45
24	0	235	HIS	CE1-NE2	7.92	1.40	1.32
24	0	186	ILE	N-CA	7.78	1.55	1.46
23	W	670	GLY	CA-C	7.71	1.59	1.52
23	W	302	ASP	CA-C	7.67	1.62	1.53
22	V	289	TYR	N-CA	7.59	1.54	1.46
23	W	606	GLU	CA-CB	7.54	1.65	1.53
22	V	554	ARG	NE-CZ	7.40	1.41	1.33
24	0	135	VAL	N-CA	7.34	1.55	1.46
24	0	112	LYS	N-CA	7.33	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	168	VAL	CA-CB	7.31	1.58	1.54
23	W	566	LEU	CA-C	7.29	1.61	1.52
22	V	391	ARG	CZ-NH2	-7.27	1.24	1.33
22	V	417	THR	CA-C	7.25	1.62	1.52
23	W	556	GLY	N-CA	7.24	1.52	1.45
24	O	203	ALA	CA-C	7.20	1.61	1.52
23	W	706	LEU	CA-C	7.14	1.62	1.52
23	W	521	GLY	N-CA	7.13	1.55	1.45
23	W	272	ARG	CA-CB	7.12	1.64	1.53
24	O	169	ILE	CA-CB	7.08	1.63	1.54
22	V	626	ILE	N-CA	7.07	1.55	1.46
23	W	327	GLU	CA-C	7.02	1.61	1.52
23	W	546	GLU	C-N	6.92	1.43	1.33
23	W	531	VAL	C-N	6.89	1.39	1.33
23	W	272	ARG	N-CA	6.80	1.54	1.45
23	W	429	ALA	CA-C	6.70	1.61	1.52
23	W	615	GLY	N-CA	6.70	1.51	1.44
23	W	474	HIS	CD2-NE2	-6.69	1.30	1.37
24	O	188	THR	N-CA	6.67	1.54	1.46
22	V	353	ALA	C-N	6.60	1.42	1.33
23	W	115	LEU	N-CA	6.60	1.54	1.46
23	W	698	GLN	N-CA	6.60	1.54	1.46
22	V	382	SER	N-CA	6.58	1.54	1.46
22	V	425	ARG	C-O	-6.57	1.16	1.24
24	O	202	SER	CA-C	6.57	1.62	1.53
23	W	674	TYR	N-CA	6.57	1.54	1.45
22	V	706	LYS	N-CA	-6.56	1.38	1.46
23	W	683	ARG	CZ-NH2	-6.54	1.25	1.33
24	O	171	PHE	CA-C	6.52	1.60	1.52
24	O	96	PHE	CA-C	6.51	1.61	1.52
23	W	494	ILE	C-O	-6.50	1.17	1.24
2	B	947	ILE	CA-CB	-6.47	1.50	1.55
23	W	522	ASN	CA-C	6.46	1.61	1.52
23	W	321	GLY	N-CA	6.45	1.54	1.45
23	W	291	GLY	CA-C	6.43	1.59	1.52
22	V	479	ASP	N-CA	-6.37	1.38	1.46
1	A	474	VAL	C-O	-6.36	1.15	1.24
22	V	453	ARG	CZ-NH2	-6.35	1.25	1.33
23	W	245	ASP	N-CA	6.35	1.53	1.46
23	W	301	THR	N-CA	6.31	1.54	1.45
22	V	348	LEU	C-O	-6.30	1.16	1.24
22	V	712	LEU	CA-C	6.27	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	414	GLY	CA-C	6.26	1.58	1.51
23	W	265	THR	N-CA	6.24	1.54	1.46
23	W	608	ILE	CA-CB	6.22	1.63	1.54
22	V	618	PRO	C-O	6.20	1.31	1.23
23	W	693	LEU	CA-CB	6.19	1.61	1.54
23	W	523	LEU	N-CA	6.19	1.53	1.46
24	O	142	GLU	CA-CB	-6.19	1.46	1.54
23	W	47	GLY	N-CA	6.14	1.54	1.45
23	W	67	VAL	N-CA	6.14	1.54	1.46
22	V	332	ARG	CA-C	6.12	1.60	1.52
23	W	685	ALA	N-CA	6.12	1.53	1.46
24	O	128	ILE	CA-C	6.12	1.60	1.52
23	W	490	LEU	CA-C	6.11	1.59	1.52
23	W	69	LYS	CA-C	6.09	1.60	1.52
23	W	18	TYR	CA-CB	6.09	1.63	1.53
23	W	158	TYR	N-CA	6.07	1.54	1.46
22	V	609	LYS	N-CA	6.05	1.54	1.46
24	O	199	ILE	C-N	6.04	1.41	1.33
23	W	492	PRO	CA-C	6.02	1.59	1.52
23	W	511	ARG	NE-CZ	-6.01	1.26	1.33
23	W	701	LEU	N-CA	6.01	1.54	1.46
23	W	83	VAL	CA-C	6.00	1.60	1.52
23	W	491	CYS	N-CA	5.99	1.52	1.46
22	V	620	ALA	N-CA	5.99	1.54	1.46
22	V	383	THR	CB-OG1	-5.99	1.34	1.43
2	B	794	VAL	CA-CB	5.98	1.63	1.54
22	V	647	LYS	CA-C	5.98	1.60	1.52
23	W	698	GLN	CA-C	5.96	1.60	1.52
28	X	56	DA	O3'-P	-5.96	1.52	1.61
22	V	325	ARG	CZ-NH1	-5.95	1.24	1.32
23	W	559	GLU	C-O	-5.94	1.16	1.23
24	O	171	PHE	N-CA	-5.93	1.39	1.46
22	V	633	ARG	CZ-NH1	-5.91	1.24	1.32
23	W	244	ILE	CA-CB	5.90	1.61	1.54
23	W	632	ILE	N-CA	5.90	1.53	1.46
22	V	252	TYR	CA-CB	5.89	1.62	1.53
22	V	638	GLN	N-CA	5.87	1.53	1.46
22	V	306	ILE	N-CA	-5.87	1.39	1.46
22	V	269	SER	N-CA	5.87	1.53	1.46
22	V	551	HIS	CA-C	5.84	1.60	1.52
23	W	666	ARG	NE-CZ	-5.83	1.26	1.33
23	W	242	VAL	N-CA	5.82	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	VAL	CA-CB	5.82	1.61	1.54
22	V	690	ILE	CA-CB	5.82	1.61	1.54
22	V	468	ALA	N-CA	5.80	1.53	1.46
23	W	237	HIS	CA-C	5.80	1.60	1.52
22	V	629	HIS	CE1-NE2	5.78	1.38	1.32
23	W	648	GLU	C-N	5.78	1.41	1.33
23	W	705	ASN	C-O	-5.78	1.16	1.24
23	W	152	LEU	N-CA	5.76	1.54	1.46
24	O	162	HIS	CA-C	5.76	1.60	1.52
23	W	508	PHE	CA-CB	5.76	1.57	1.53
23	W	106	GLY	CA-C	5.75	1.56	1.51
24	O	207	VAL	CA-CB	5.75	1.61	1.54
23	W	42	MET	CA-C	5.74	1.60	1.52
23	W	448	PHE	CA-C	5.73	1.60	1.52
23	W	334	ARG	CZ-NH2	-5.72	1.26	1.33
22	V	332	ARG	CZ-NH2	-5.72	1.26	1.33
22	V	565	VAL	N-CA	5.68	1.53	1.46
23	W	160	GLU	CA-C	5.66	1.60	1.52
23	W	343	ARG	CA-C	5.66	1.60	1.52
24	O	147	ASN	CA-C	5.66	1.60	1.52
22	V	657	ALA	CA-C	5.65	1.59	1.52
23	W	600	ALA	N-CA	5.64	1.53	1.46
22	V	437	LEU	C-N	5.64	1.41	1.33
23	W	286	ARG	CZ-NH2	-5.64	1.26	1.33
23	W	256	LEU	C-N	-5.63	1.26	1.33
23	W	703	ASP	CA-C	5.63	1.60	1.53
23	W	645	GLN	N-CA	5.60	1.53	1.46
28	X	66	DA	C1'-N9	5.59	1.57	1.46
24	O	131	LEU	CA-C	5.59	1.60	1.52
23	W	155	CYS	C-N	5.59	1.43	1.34
22	V	461	HIS	CG-CD2	5.58	1.42	1.35
24	O	190	LYS	N-CA	5.57	1.53	1.46
22	V	252	TYR	C-N	5.55	1.41	1.33
22	V	392	PHE	C-N	5.54	1.38	1.33
22	V	474	ASP	N-CA	5.54	1.53	1.46
22	V	560	VAL	N-CA	-5.53	1.39	1.46
23	W	283	ASP	CA-CB	5.53	1.61	1.53
22	V	452	ARG	CZ-NH2	-5.52	1.26	1.33
22	V	639	ARG	N-CA	5.52	1.52	1.46
23	W	663	CYS	N-CA	-5.51	1.39	1.46
25	1	47	ALA	CA-C	-5.51	1.48	1.53
23	W	291	GLY	C-N	5.50	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	640	LEU	CA-C	5.49	1.59	1.52
23	W	331	GLY	N-CA	-5.46	1.39	1.45
24	O	195	ARG	CA-CB	5.46	1.61	1.53
23	W	110	SER	CA-CB	5.45	1.63	1.53
23	W	693	LEU	N-CA	5.44	1.51	1.45
22	V	323	SER	CA-C	5.42	1.59	1.52
23	W	77	VAL	CA-C	5.42	1.57	1.52
23	W	405	THR	N-CA	5.41	1.52	1.46
23	W	552	TRP	C-O	-5.39	1.17	1.24
23	W	185	ARG	CA-CB	5.38	1.61	1.53
24	O	136	ASP	N-CA	5.38	1.52	1.46
22	V	626	ILE	CB-CG1	5.38	1.64	1.53
22	V	705	THR	CB-OG1	-5.37	1.35	1.43
23	W	592	ARG	CD-NE	5.36	1.53	1.46
23	W	48	LYS	N-CA	5.35	1.52	1.46
22	V	310	LEU	CA-C	5.33	1.59	1.52
22	V	296	ASP	CA-C	5.33	1.59	1.52
22	V	699	GLU	CA-C	5.32	1.59	1.52
23	W	630	SER	CA-C	5.32	1.59	1.52
23	W	85	GLU	CA-C	5.31	1.59	1.52
23	W	263	LEU	N-CA	5.31	1.52	1.46
24	O	97	ASP	N-CA	5.30	1.52	1.46
23	W	713	GLY	CA-C	5.30	1.58	1.52
28	X	65	DG	P-O5'	-5.30	1.49	1.60
23	W	518	ARG	CZ-NH2	-5.29	1.26	1.33
22	V	692	LYS	CA-C	5.29	1.59	1.52
22	V	618	PRO	CA-CB	5.29	1.62	1.53
23	W	229	ALA	N-CA	5.28	1.52	1.46
22	V	636	GLU	N-CA	5.27	1.52	1.46
23	W	412	LYS	N-CA	5.27	1.53	1.46
23	W	66	GLU	N-CA	5.26	1.53	1.46
22	V	332	ARG	NE-CZ	-5.26	1.27	1.33
23	W	72	TYR	CA-C	5.26	1.59	1.52
23	W	154	HIS	CA-CB	5.26	1.62	1.53
23	W	548	THR	N-CA	5.26	1.52	1.46
24	O	217	GLY	N-CA	5.25	1.52	1.45
22	V	607	ILE	C-O	-5.25	1.18	1.24
23	W	426	PRO	CA-CB	-5.25	1.47	1.53
22	V	303	ASN	C-N	5.24	1.37	1.33
23	W	257	ASP	CA-C	5.23	1.59	1.52
23	W	491	CYS	CA-C	5.23	1.58	1.53
23	W	310	LEU	CA-CB	5.22	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	693	LEU	CA-C	5.22	1.60	1.53
23	W	341	LYS	CA-CB	5.22	1.61	1.53
23	W	510	THR	CA-C	-5.22	1.45	1.52
22	V	410	TYR	N-CA	5.21	1.52	1.46
22	V	398	ASP	N-CA	5.21	1.52	1.45
23	W	122	THR	CA-C	5.21	1.58	1.52
22	V	623	LEU	C-O	-5.20	1.18	1.24
22	V	386	ASP	N-CA	5.19	1.51	1.46
22	V	316	LEU	CA-CB	5.19	1.61	1.53
23	W	675	GLY	N-CA	5.19	1.52	1.45
23	W	210	HIS	CE1-NE2	5.18	1.37	1.32
22	V	420	SER	N-CA	5.18	1.52	1.46
23	W	95	GLU	CA-C	5.18	1.58	1.52
24	O	197	SER	N-CA	-5.18	1.39	1.46
23	W	482	THR	N-CA	5.17	1.52	1.46
22	V	561	PHE	C-N	5.17	1.40	1.33
22	V	367	SER	N-CA	-5.16	1.39	1.46
23	W	567	LEU	N-CA	-5.16	1.40	1.45
22	V	598	HIS	CB-CG	5.16	1.57	1.50
23	W	418	ILE	N-CA	5.16	1.52	1.46
23	W	658	ARG	CZ-NH2	-5.15	1.26	1.33
23	W	398	THR	CB-OG1	-5.15	1.35	1.43
24	O	61	LEU	N-CA	5.15	1.52	1.46
1	A	475	ARG	CG-CD	5.14	1.67	1.52
23	W	303	ALA	CA-C	5.14	1.60	1.52
23	W	452	GLN	CA-CB	5.14	1.61	1.53
22	V	408	SER	CA-C	-5.13	1.46	1.52
24	O	80	ARG	CA-CB	5.12	1.61	1.53
23	W	168	VAL	N-CA	5.12	1.52	1.46
23	W	328	HIS	ND1-CE1	5.12	1.37	1.32
23	W	501	GLN	CA-C	5.12	1.59	1.52
23	W	96	LYS	N-CA	5.12	1.52	1.46
23	W	75	ARG	CZ-NH2	-5.12	1.26	1.33
22	V	521	GLU	CA-CB	5.11	1.61	1.53
2	B	811	TYR	CA-C	-5.10	1.46	1.52
23	W	679	PHE	CA-CB	5.10	1.62	1.53
24	O	140	HIS	ND1-CE1	5.10	1.37	1.32
22	V	338	ILE	CA-C	5.09	1.58	1.52
22	V	617	LEU	N-CA	5.08	1.51	1.45
23	W	104	PHE	CG-CD1	5.08	1.49	1.38
22	V	333	ALA	CA-C	-5.08	1.45	1.52
23	W	651	PHE	N-CA	-5.08	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	626	VAL	N-CA	5.08	1.52	1.46
23	W	20	GLU	C-N	-5.08	1.27	1.33
23	W	417	ILE	CA-C	-5.08	1.46	1.52
24	0	195	ARG	CZ-NH1	-5.07	1.25	1.32
23	W	286	ARG	CZ-NH1	-5.07	1.25	1.32
23	W	30	ARG	N-CA	5.06	1.52	1.46
23	W	699	GLU	N-CA	5.06	1.52	1.46
23	W	61	ARG	CA-C	5.05	1.59	1.52
23	W	672	THR	N-CA	5.04	1.52	1.46
22	V	420	SER	CA-C	-5.04	1.46	1.52
2	B	1046	THR	CA-CB	5.03	1.62	1.53
23	W	629	GLN	N-CA	-5.03	1.39	1.46
22	V	532	LEU	CA-CB	5.03	1.61	1.53
23	W	531	VAL	C-O	-5.03	1.18	1.24
23	W	322	SER	N-CA	5.02	1.52	1.46
23	W	131	ASP	C-N	-5.01	1.27	1.33
22	V	411	SER	CA-C	5.01	1.58	1.52
24	0	105	GLY	C-N	5.01	1.39	1.33
23	W	335	ARG	CA-C	-5.00	1.46	1.52

All (1030) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	84	HIS	C-N-CD	-14.70	64.75	125.00
3	C	6	GLN	C-N-CD	-14.42	65.87	125.00
29	Y	35	DG	O5'-C5'-C4'	13.55	131.13	110.80
2	B	80	GLU	C-N-CD	-13.12	71.22	125.00
16	P	206	GLU	C-N-CD	-13.01	71.67	125.00
18	R	194	ARG	C-N-CD	-12.98	71.78	125.00
22	V	427	MET	N-CA-C	12.85	138.18	110.80
1	A	261	ARG	C-N-CD	-12.72	72.84	125.00
24	0	77	LYS	C-N-CD	-12.69	72.99	125.00
28	X	56	DA	O3'-P-O5'	-12.47	85.29	104.00
27	3	71	TYR	C-N-CD	-12.21	74.94	125.00
1	A	545	VAL	N-CA-C	12.18	123.04	110.62
3	C	138	ASP	C-N-CD	-12.00	75.81	125.00
23	W	175	TYR	N-CA-C	11.93	127.78	110.24
23	W	26	ARG	NE-CZ-NH2	11.60	129.64	119.20
22	V	520	ARG	O-C-N	11.49	135.33	122.11
22	V	520	ARG	CA-C-N	-11.39	101.10	120.58
22	V	520	ARG	C-N-CA	-11.39	101.10	120.58
22	V	550	PHE	CA-CB-CG	11.12	124.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	358	ARG	NE-CZ-NH2	11.11	129.20	119.20
26	2	236	PHE	CA-CB-CG	-11.06	102.74	113.80
23	W	335	ARG	NE-CZ-NH1	-10.97	110.53	121.50
22	V	270	PHE	CA-CB-CG	10.61	124.41	113.80
23	W	167	GLU	CA-C-N	10.50	128.73	120.33
23	W	167	GLU	C-N-CA	10.50	128.73	120.33
5	E	64	HIS	N-CA-C	10.13	132.38	110.80
23	W	287	ARG	NE-CZ-NH2	9.91	128.12	119.20
29	Y	34	DC	O3'-P-O5'	9.85	118.78	104.00
23	W	26	ARG	NH1-CZ-NH2	-9.79	106.58	119.30
23	W	117	ILE	N-CA-C	9.77	119.72	110.53
22	V	586	GLN	OE1-CD-NE2	-9.76	112.84	122.60
25	1	44	PHE	CA-CB-CG	-9.64	104.16	113.80
22	V	638	GLN	OE1-CD-NE2	-9.63	112.97	122.60
21	U	257	GLN	CA-C-N	-9.58	104.13	122.53
21	U	257	GLN	C-N-CA	-9.58	104.13	122.53
22	V	388	GLN	OE1-CD-NE2	-9.56	113.04	122.60
22	V	634	ARG	NE-CZ-NH2	9.49	127.74	119.20
23	W	147	GLN	OE1-CD-NE2	-9.43	113.17	122.60
22	V	621	ASN	CA-CB-CG	9.40	122.00	112.60
23	W	645	GLN	OE1-CD-NE2	-9.38	113.22	122.60
22	V	377	GLN	OE1-CD-NE2	-9.30	113.30	122.60
29	Y	35	DG	C5'-C4'-C3'	9.28	128.81	114.90
3	C	42	VAL	CA-C-N	-9.22	111.28	120.31
3	C	42	VAL	C-N-CA	-9.22	111.28	120.31
13	M	43	ASP	N-CA-C	-9.17	91.26	110.80
23	W	335	ARG	NE-CZ-NH2	9.12	127.41	119.20
27	3	231	PHE	CA-CB-CG	-9.06	104.74	113.80
26	2	61	PHE	CB-CA-C	-8.97	97.04	110.95
22	V	334	ARG	CD-NE-CZ	8.92	136.88	124.40
23	W	530	VAL	N-CA-CB	8.91	120.72	110.65
22	V	668	GLN	OE1-CD-NE2	-8.89	113.71	122.60
23	W	112	ARG	CA-C-N	8.89	132.19	120.28
23	W	112	ARG	C-N-CA	8.89	132.19	120.28
23	W	270	VAL	CA-C-O	8.85	131.85	120.78
22	V	665	GLN	OE1-CD-NE2	-8.80	113.80	122.60
29	Y	20	DA	O4'-C1'-N9	8.73	121.50	108.40
25	1	34	ILE	CA-C-N	-8.71	111.80	123.12
25	1	34	ILE	C-N-CA	-8.71	111.80	123.12
23	W	76	THR	CA-CB-OG1	8.69	122.64	109.60
26	2	268	PHE	CA-CB-CG	-8.67	105.13	113.80
13	M	94	ASP	N-CA-C	-8.67	92.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	332	PHE	CA-CB-CG	8.66	122.46	113.80
18	R	140	LYS	CA-C-N	-8.57	109.13	119.84
18	R	140	LYS	C-N-CA	-8.57	109.13	119.84
13	M	10	LEU	C-N-CD	-8.57	89.86	125.00
5	E	52	ARG	C-N-CD	-8.56	89.90	125.00
25	1	47	ALA	CB-CA-C	-8.54	106.72	116.54
1	A	475	ARG	NE-CZ-NH1	-8.53	112.97	121.50
20	T	181	GLN	N-CA-C	8.47	120.20	110.97
23	W	343	ARG	NE-CZ-NH2	8.46	126.81	119.20
23	W	193	PHE	CA-CB-CG	8.44	122.23	113.80
23	W	263	LEU	N-CA-CB	-8.42	97.74	110.12
23	W	469	LYS	CA-C-N	8.40	131.32	120.56
23	W	469	LYS	C-N-CA	8.40	131.32	120.56
2	B	141	GLN	N-CA-C	-8.40	92.91	110.80
22	V	484	ILE	N-CA-C	8.40	119.03	111.81
7	G	97	LEU	N-CA-C	8.38	122.56	108.90
9	I	58	ILE	N-CA-C	-8.37	99.84	111.89
29	Y	34	DC	C6-N1-C1'	8.37	132.25	119.70
1	A	932	ARG	CA-C-N	-8.28	106.89	120.72
1	A	932	ARG	C-N-CA	-8.28	106.89	120.72
1	A	666	ARG	CG-CD-NE	8.26	130.17	112.00
23	W	157	PHE	CA-CB-CG	8.23	122.03	113.80
23	W	77	VAL	N-CA-CB	-8.22	105.32	110.50
2	B	62	ALA	CA-C-N	-8.21	111.93	120.38
2	B	62	ALA	C-N-CA	-8.21	111.93	120.38
29	Y	34	DC	C2-N1-C1'	-8.19	107.42	119.70
17	Q	102	VAL	N-CA-C	8.14	126.27	109.34
23	W	521	GLY	CA-C-N	8.12	131.00	120.44
23	W	521	GLY	C-N-CA	8.12	131.00	120.44
22	V	392	PHE	CA-CB-CG	8.10	121.90	113.80
26	2	47	GLU	N-CA-C	8.07	119.99	111.03
23	W	106	GLY	CA-C-O	-8.05	114.56	121.57
1	A	692	SER	N-CA-C	8.05	123.10	113.28
22	V	433	GLN	N-CA-C	8.02	121.64	112.57
13	M	121	ILE	N-CA-C	8.01	118.11	110.42
23	W	667	ALA	N-CA-C	7.99	119.61	111.07
23	W	700	HIS	CB-CG-CD2	-7.97	120.84	131.20
22	V	333	ALA	N-CA-C	7.94	121.91	111.75
9	I	15	ARG	N-CA-C	-7.92	93.92	110.80
1	A	1314	THR	N-CA-C	-7.91	103.20	113.17
23	W	395	SER	CA-C-O	-7.90	110.68	118.34
28	X	77	DC	O4'-C1'-N1	7.89	120.24	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	GLN	N-CA-C	7.88	127.22	109.81
22	V	394	SER	N-CA-C	7.87	121.97	112.38
23	W	345	ARG	N-CA-C	7.86	122.21	112.47
10	J	63	ALA	CA-C-N	7.85	129.66	119.84
10	J	63	ALA	C-N-CA	7.85	129.66	119.84
2	B	76	GLY	N-CA-C	7.83	124.27	110.95
23	W	16	TYR	N-CA-C	7.83	118.32	108.45
1	A	521	VAL	CB-CA-C	-7.82	106.06	114.35
26	2	160	LEU	N-CA-C	-7.80	102.78	111.28
23	W	696	TRP	N-CA-C	7.79	120.81	110.53
13	M	39	LEU	N-CA-C	7.78	119.59	110.41
26	2	162	PHE	CA-CB-CG	-7.70	106.10	113.80
1	A	475	ARG	CD-NE-CZ	7.70	135.18	124.40
22	V	710	GLN	CA-C-N	7.68	130.42	120.44
22	V	710	GLN	C-N-CA	7.68	130.42	120.44
20	T	177	ARG	N-CA-C	7.67	121.47	112.72
23	W	499	ASN	OD1-CG-ND2	-7.67	114.93	122.60
9	I	84	HIS	CA-C-N	7.67	129.42	119.84
9	I	84	HIS	C-N-CA	7.67	129.42	119.84
22	V	640	LEU	O-C-N	7.67	130.29	122.08
23	W	724	MET	CA-C-N	7.66	130.55	120.28
23	W	724	MET	C-N-CA	7.66	130.55	120.28
23	W	497	ARG	CD-NE-CZ	7.65	135.11	124.40
23	W	700	HIS	ND1-CG-CD2	7.64	113.74	106.10
23	W	304	HIS	CB-CG-CD2	-7.63	121.28	131.20
24	0	237	SER	CA-C-N	7.59	128.20	120.38
24	0	237	SER	C-N-CA	7.59	128.20	120.38
22	V	422	GLU	CA-C-O	7.59	128.82	119.11
10	J	63	ALA	O-C-N	7.58	128.21	120.70
23	W	295	ALA	N-CA-C	7.58	119.32	111.14
23	W	329	PHE	CA-CB-CG	7.57	121.37	113.80
2	B	81	PRO	N-CA-C	7.56	119.93	110.70
27	3	182	PHE	CA-CB-CG	-7.56	106.24	113.80
23	W	509	GLU	N-CA-C	7.54	122.15	112.34
22	V	428	GLU	N-CA-C	7.52	120.80	107.80
23	W	250	ASN	OD1-CG-ND2	-7.51	115.09	122.60
22	V	355	CYS	CA-C-N	7.49	130.63	120.44
22	V	355	CYS	C-N-CA	7.49	130.63	120.44
23	W	165	GLY	CA-C-N	7.49	130.93	120.29
23	W	165	GLY	C-N-CA	7.49	130.93	120.29
27	3	127	GLN	N-CA-C	-7.48	103.20	111.36
26	2	35	TYR	CA-CB-CG	-7.47	100.45	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	41	GLU	O-C-N	7.43	131.67	123.27
1	A	475	ARG	CG-CD-NE	-7.43	95.66	112.00
24	0	98	GLN	OE1-CD-NE2	-7.42	115.18	122.60
24	0	206	ARG	NH1-CZ-NH2	-7.41	109.66	119.30
4	D	127	LEU	N-CA-C	-7.41	103.20	111.28
22	V	669	GLU	CA-C-N	7.39	131.54	120.31
22	V	669	GLU	C-N-CA	7.39	131.54	120.31
24	0	123	ASN	CA-C-N	7.38	127.40	119.28
24	0	123	ASN	C-N-CA	7.38	127.40	119.28
24	0	92	VAL	O-C-N	7.38	129.14	121.91
23	W	302	ASP	CA-C-O	7.36	126.81	119.08
16	P	162	VAL	CA-C-N	-7.35	110.65	119.84
16	P	162	VAL	C-N-CA	-7.35	110.65	119.84
26	2	245	LEU	N-CA-C	-7.35	101.37	110.41
23	W	487	ARG	N-CA-C	7.35	120.16	111.71
27	3	16	ASP	CA-C-N	7.33	132.96	120.72
27	3	16	ASP	C-N-CA	7.33	132.96	120.72
23	W	654	PHE	CA-C-N	7.33	130.09	120.28
23	W	654	PHE	C-N-CA	7.33	130.09	120.28
24	0	195	ARG	NE-CZ-NH1	7.31	128.81	121.50
2	B	288	ILE	N-CA-C	7.30	117.91	110.82
14	N	327	GLU	N-CA-C	-7.27	104.94	113.88
23	W	683	ARG	NE-CZ-NH2	7.27	125.74	119.20
23	W	288	LEU	O-C-N	-7.25	114.49	122.03
22	V	486	PRO	CA-C-N	7.23	132.76	121.99
22	V	486	PRO	C-N-CA	7.23	132.76	121.99
22	V	580	ILE	CA-C-O	7.22	128.01	120.36
29	Y	27	DC	C6-N1-C1'	7.18	130.48	119.70
23	W	690	ARG	NE-CZ-NH2	7.17	125.66	119.20
26	2	89	LEU	N-CA-C	-7.14	103.58	111.36
23	W	323	ILE	CA-C-N	7.14	129.84	120.28
23	W	323	ILE	C-N-CA	7.14	129.84	120.28
23	W	24	TYR	N-CA-C	7.10	121.17	112.23
2	B	492	ASP	N-CA-C	7.07	124.47	113.72
22	V	598	HIS	CB-CG-CD2	-7.07	122.01	131.20
26	2	193	PRO	N-CA-C	7.06	119.32	110.70
7	G	96	GLY	N-CA-C	7.06	122.52	111.08
23	W	419	GLU	C-N-CD	-7.04	96.14	125.00
22	V	267	THR	CA-C-O	-7.04	112.01	120.32
22	V	393	THR	O-C-N	-7.04	113.89	122.68
23	W	653	THR	CA-C-N	7.04	129.71	120.28
23	W	653	THR	C-N-CA	7.04	129.71	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	225	SER	N-CA-C	-7.03	103.55	111.14
23	W	232	VAL	CA-CB-CG1	7.02	122.33	110.40
29	Y	27	DC	C2-N1-C1'	-7.02	109.17	119.70
2	B	58	ILE	N-CA-C	7.00	117.76	110.62
23	W	340	VAL	CA-C-N	6.99	129.65	120.28
23	W	340	VAL	C-N-CA	6.99	129.65	120.28
28	X	76	DC	C4'-C3'-O3'	-6.99	99.51	110.00
5	E	126	ILE	N-CA-C	6.98	119.60	108.85
28	X	72	DC	N1-C1'-C2'	6.96	123.94	113.50
1	A	910	LYS	CA-C-N	6.96	128.54	119.84
1	A	910	LYS	C-N-CA	6.96	128.54	119.84
1	A	622	SER	N-CA-C	-6.96	94.44	109.81
23	W	715	GLN	OE1-CD-NE2	-6.95	115.65	122.60
14	N	319	ASP	N-CA-C	6.95	121.13	112.24
9	I	120	GLY	N-CA-C	-6.94	106.23	115.40
23	W	562	GLN	OE1-CD-NE2	-6.94	115.66	122.60
22	V	558	ILE	N-CA-CB	-6.92	101.41	111.52
23	W	328	HIS	CB-CG-CD2	-6.91	122.22	131.20
24	0	147	ASN	OD1-CG-ND2	-6.89	115.71	122.60
23	W	462	SER	CA-C-N	6.89	126.57	119.82
23	W	462	SER	C-N-CA	6.89	126.57	119.82
23	W	186	ARG	NE-CZ-NH1	6.88	128.38	121.50
23	W	98	GLU	CA-C-N	6.87	130.19	122.15
23	W	98	GLU	C-N-CA	6.87	130.19	122.15
22	V	715	LYS	N-CA-C	6.86	118.76	111.28
23	W	343	ARG	NE-CZ-NH1	-6.85	114.65	121.50
25	1	45	VAL	CA-C-N	-6.85	113.54	122.51
25	1	45	VAL	C-N-CA	-6.85	113.54	122.51
22	V	274	GLN	O-C-N	-6.84	116.68	123.46
23	W	97	GLN	OE1-CD-NE2	-6.84	115.76	122.60
22	V	641	GLY	N-CA-C	6.83	120.93	112.73
1	A	475	ARG	CB-CA-C	6.83	120.60	110.62
26	2	193	PRO	CA-N-CD	-6.83	102.43	112.00
23	W	66	GLU	CA-C-N	6.83	134.26	121.97
23	W	66	GLU	C-N-CA	6.83	134.26	121.97
2	B	487	SER	CA-C-N	6.82	126.74	119.85
2	B	487	SER	C-N-CA	6.82	126.74	119.85
14	N	356	GLY	N-CA-C	6.82	129.34	113.18
2	B	802	ASP	N-CA-C	6.82	118.71	111.28
24	0	145	LEU	N-CA-C	6.81	118.70	111.28
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	ASP	N-CA-C	6.80	125.28	110.80
23	W	595	ILE	CB-CA-C	6.79	122.42	111.29
9	I	84	HIS	N-CA-C	6.78	124.79	109.81
23	W	591	GLY	CA-C-O	-6.78	113.68	121.47
22	V	317	ARG	CA-C-O	-6.77	113.04	120.69
23	W	263	LEU	O-C-N	-6.76	114.95	122.12
23	W	497	ARG	NE-CZ-NH1	6.75	128.25	121.50
22	V	608	SER	O-C-N	-6.75	113.83	122.20
23	W	473	PHE	CA-CB-CG	-6.75	107.06	113.80
22	V	711	GLN	OE1-CD-NE2	-6.74	115.86	122.60
23	W	659	HIS	CA-CB-CG	6.74	120.54	113.80
20	T	211	VAL	N-CA-C	6.74	117.49	110.62
22	V	331	GLY	CA-C-N	6.74	129.31	120.28
22	V	331	GLY	C-N-CA	6.74	129.31	120.28
7	G	46	ILE	N-CA-C	6.74	117.52	110.72
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
11	K	112	LYS	CA-C-N	-6.73	111.88	121.50
11	K	112	LYS	C-N-CA	-6.73	111.88	121.50
23	W	34	ALA	CA-C-N	6.72	132.36	122.82
23	W	34	ALA	C-N-CA	6.72	132.36	122.82
29	Y	34	DC	C5'-C4'-C3'	6.72	124.98	114.90
11	K	41	THR	N-CA-C	6.71	118.25	111.07
23	W	467	TYR	CA-C-N	6.71	126.66	119.28
23	W	467	TYR	C-N-CA	6.71	126.66	119.28
23	W	270	VAL	CA-C-N	6.71	130.50	120.17
23	W	270	VAL	C-N-CA	6.71	130.50	120.17
1	A	1304	ILE	N-CA-C	-6.70	106.60	113.10
2	B	163	LEU	N-CA-C	6.70	121.05	112.34
24	O	236	VAL	CA-CB-CG1	6.69	121.78	110.40
22	V	553	ARG	NE-CZ-NH2	6.68	125.21	119.20
22	V	629	HIS	CB-CG-CD2	-6.67	122.52	131.20
24	O	64	VAL	O-C-N	-6.67	116.06	123.26
23	W	723	GLN	OE1-CD-NE2	-6.66	115.94	122.60
22	V	714	GLN	OE1-CD-NE2	-6.65	115.95	122.60
24	O	92	VAL	CA-C-O	-6.65	114.12	121.17
2	B	598	VAL	N-CA-C	6.65	117.34	110.36
22	V	701	LEU	O-C-N	-6.64	115.46	123.10
23	W	629	GLN	CA-C-O	-6.63	113.73	120.96
22	V	358	ARG	NH1-CZ-NH2	-6.62	110.69	119.30
7	G	124	ASN	CA-C-N	-6.62	113.56	120.38
7	G	124	ASN	C-N-CA	-6.62	113.56	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	80	ILE	N-CA-CB	6.62	119.54	110.54
26	2	272	PHE	CA-CB-CG	-6.62	107.18	113.80
1	A	771	VAL	N-CA-C	6.59	117.34	110.62
22	V	598	HIS	CB-CG-ND1	6.59	132.59	122.70
2	B	1076	GLU	N-CA-C	6.58	118.45	111.28
23	W	187	GLN	OE1-CD-NE2	-6.58	116.03	122.60
24	0	59	ARG	NE-CZ-NH2	6.57	125.11	119.20
26	2	242	PHE	CA-CB-CG	-6.56	107.24	113.80
22	V	624	ILE	N-CA-CB	-6.55	103.12	111.64
22	V	366	ASN	CA-CB-CG	6.55	119.15	112.60
2	B	424	ASP	N-CA-C	-6.53	104.08	111.07
22	V	388	GLN	CG-CD-NE2	6.53	126.20	116.40
23	W	152	LEU	O-C-N	-6.53	113.81	121.32
23	W	540	THR	O-C-N	-6.52	114.25	122.27
20	T	25	LYS	N-CA-C	6.52	118.38	111.28
24	0	58	MET	O-C-N	6.50	131.21	123.27
23	W	33	ASP	N-CA-C	6.49	119.18	111.71
22	V	409	THR	CA-C-N	6.49	131.08	120.63
22	V	409	THR	C-N-CA	6.49	131.08	120.63
23	W	120	GLU	CA-C-N	6.49	128.86	120.56
23	W	120	GLU	C-N-CA	6.49	128.86	120.56
28	X	60	DG	O3'-P-O5'	-6.48	94.27	104.00
22	V	418	LYS	CA-C-O	-6.48	114.23	120.90
2	B	408	PHE	N-CA-C	6.48	118.42	111.36
22	V	467	THR	N-CA-C	6.47	118.69	108.79
23	W	406	LEU	CA-C-O	-6.47	114.21	121.00
23	W	161	PHE	CA-CB-CG	6.47	120.27	113.80
23	W	314	VAL	N-CA-CB	6.46	118.11	110.55
22	V	709	GLN	CA-C-N	6.46	128.94	120.28
22	V	709	GLN	C-N-CA	6.46	128.94	120.28
22	V	434	GLU	N-CA-C	6.46	118.40	111.36
23	W	88	ARG	CA-C-N	6.45	129.45	120.29
23	W	88	ARG	C-N-CA	6.45	129.45	120.29
23	W	166	ARG	CD-NE-CZ	6.45	133.43	124.40
2	B	132	VAL	N-CA-C	6.45	117.19	108.17
28	X	59	DC	C2'-C3'-O3'	6.44	121.16	111.50
22	V	614	SER	N-CA-C	6.43	124.50	110.80
2	B	897	ARG	N-CA-C	-6.42	97.12	110.80
22	V	251	PHE	N-CA-C	6.42	117.92	108.86
22	V	328	PHE	CA-C-N	6.42	134.00	121.41
22	V	328	PHE	C-N-CA	6.42	134.00	121.41
23	W	210	HIS	ND1-CG-CD2	6.42	112.52	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	491	CYS	CA-C-N	6.41	126.78	119.92
23	W	491	CYS	C-N-CA	6.41	126.78	119.92
23	W	258	ARG	CA-C-O	-6.41	113.63	120.42
22	V	643	VAL	CA-CB-CG1	6.40	121.28	110.40
22	V	373	GLN	OE1-CD-NE2	-6.40	116.20	122.60
23	W	416	ILE	CA-C-N	6.40	131.89	123.06
23	W	416	ILE	C-N-CA	6.40	131.89	123.06
23	W	698	GLN	OE1-CD-NE2	-6.39	116.20	122.60
29	Y	36	DA	O5'-C5'-C4'	6.39	120.39	110.80
1	A	645	LEU	N-CA-C	6.38	120.90	113.18
23	W	196	ARG	CA-C-N	6.38	128.83	120.28
23	W	196	ARG	C-N-CA	6.38	128.83	120.28
23	W	552	TRP	N-CA-C	-6.38	104.25	111.14
22	V	454	VAL	CA-C-N	6.37	129.34	120.29
22	V	454	VAL	C-N-CA	6.37	129.34	120.29
22	V	281	GLN	O-C-N	6.37	128.71	122.09
23	W	138	THR	CA-C-O	-6.37	113.80	120.55
23	W	416	ILE	O-C-N	-6.36	115.70	122.95
26	2	238	PHE	CA-CB-CG	-6.36	107.44	113.80
23	W	662	GLN	OE1-CD-NE2	-6.36	116.24	122.60
27	3	218	PRO	N-CA-C	-6.35	99.19	111.69
23	W	83	VAL	CA-C-N	6.34	128.55	120.56
23	W	83	VAL	C-N-CA	6.34	128.55	120.56
23	W	511	ARG	NE-CZ-NH2	6.33	124.90	119.20
24	0	224	ASP	N-CA-CB	-6.32	101.57	111.56
22	V	449	LYS	N-CA-C	6.32	118.17	111.28
23	W	242	VAL	CA-C-O	-6.32	114.15	120.85
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	257	ASP	CA-CB-CG	-6.30	106.30	112.60
22	V	480	LEU	CA-C-N	6.30	128.72	120.28
22	V	480	LEU	C-N-CA	6.30	128.72	120.28
22	V	391	ARG	NE-CZ-NH1	-6.29	115.21	121.50
24	0	111	SER	CA-C-N	6.29	132.92	123.05
24	0	111	SER	C-N-CA	6.29	132.92	123.05
13	M	51	GLU	N-CA-C	6.28	118.13	111.28
24	0	105	GLY	CA-C-O	-6.28	116.11	121.57
23	W	70	LEU	CA-C-O	-6.26	113.66	120.36
1	A	133	SER	N-CA-C	6.25	124.12	110.80
22	V	545	GLN	N-CA-C	6.25	118.10	111.28
2	B	978	ILE	N-CA-C	-6.24	103.55	112.35
22	V	689	VAL	O-C-N	-6.24	116.63	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	238	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	A	225	PHE	N-CA-C	6.23	118.08	111.28
27	3	181	ILE	CB-CA-C	-6.23	103.99	111.97
23	W	286	ARG	NE-CZ-NH2	6.23	124.81	119.20
22	V	341	PRO	CB-CA-C	-6.23	103.42	111.39
23	W	113	LYS	CA-C-O	-6.23	113.95	120.55
23	W	447	VAL	O-C-N	6.22	127.91	121.87
1	A	614	ASP	CA-C-N	-6.22	109.66	121.54
1	A	614	ASP	C-N-CA	-6.22	109.66	121.54
24	0	123	ASN	OD1-CG-ND2	-6.21	116.39	122.60
23	W	461	LEU	CA-C-N	6.21	128.78	120.58
23	W	461	LEU	C-N-CA	6.21	128.78	120.58
3	C	225	LYS	CA-C-N	-6.21	113.55	119.76
3	C	225	LYS	C-N-CA	-6.21	113.55	119.76
23	W	272	ARG	NH1-CZ-NH2	-6.21	111.23	119.30
22	V	524	ALA	N-CA-C	6.20	118.04	111.28
23	W	50	VAL	CA-CB-CG1	6.20	120.94	110.40
23	W	345	ARG	CD-NE-CZ	6.20	133.09	124.40
23	W	662	GLN	CG-CD-NE2	6.20	125.70	116.40
23	W	63	TYR	CA-C-N	6.19	126.09	119.28
23	W	63	TYR	C-N-CA	6.19	126.09	119.28
24	0	206	ARG	NE-CZ-NH1	6.18	127.68	121.50
23	W	125	ARG	CD-NE-CZ	6.18	133.06	124.40
2	B	95	LYS	CA-C-N	6.18	126.54	119.93
2	B	95	LYS	C-N-CA	6.18	126.54	119.93
22	V	341	PRO	N-CA-CB	6.18	108.51	103.32
24	0	62	TYR	CA-C-O	6.17	126.96	120.54
26	2	229	ASP	CA-CB-CG	-6.17	106.44	112.60
23	W	592	ARG	NH1-CZ-NH2	-6.16	111.29	119.30
23	W	314	VAL	N-CA-C	6.16	116.33	110.42
22	V	330	ASN	CA-C-O	-6.15	113.42	120.24
23	W	312	ASP	N-CA-C	6.15	117.78	111.14
29	Y	29	DC	N1-C1'-C2'	6.14	122.72	113.50
23	W	463	PRO	N-CA-CB	6.14	109.35	103.52
1	A	540	ASP	N-CA-C	6.14	117.97	111.28
22	V	367	SER	CA-C-N	6.13	129.00	120.29
22	V	367	SER	C-N-CA	6.13	129.00	120.29
22	V	474	ASP	CA-C-N	6.13	133.26	121.54
22	V	474	ASP	C-N-CA	6.13	133.26	121.54
28	X	75	DG	C4-N9-C1'	-6.13	117.80	127.00
22	V	337	VAL	CA-C-N	6.13	131.51	122.99
22	V	337	VAL	C-N-CA	6.13	131.51	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	0	140	HIS	CB-CG-CD2	-6.12	123.25	131.20
29	Y	25	DT	P-O5'-C5'	6.12	129.18	120.00
23	W	301	THR	CA-C-N	6.10	130.42	120.23
23	W	301	THR	C-N-CA	6.10	130.42	120.23
11	K	82	SER	CA-C-N	6.10	125.78	119.56
11	K	82	SER	C-N-CA	6.10	125.78	119.56
24	0	184	ASP	CA-CB-CG	6.10	118.70	112.60
3	C	117	SER	N-CA-C	6.08	118.71	111.71
23	W	332	PHE	O-C-N	-6.08	115.68	122.12
22	V	337	VAL	CA-C-O	-6.07	115.62	121.63
22	V	529	LYS	O-C-N	-6.07	115.28	122.20
2	B	871	VAL	N-CA-C	6.07	115.08	106.53
23	W	210	HIS	CB-CG-CD2	-6.07	123.31	131.20
3	C	199	LYS	CA-C-N	6.06	125.74	119.56
3	C	199	LYS	C-N-CA	6.06	125.74	119.56
23	W	585	GLN	O-C-N	6.05	130.10	122.23
22	V	278	GLU	CA-C-O	-6.05	112.62	120.25
22	V	713	LEU	CA-C-O	-6.04	114.44	120.90
8	H	113	SER	N-CA-C	6.04	118.36	108.52
23	W	183	LEU	CA-C-N	6.03	126.64	120.00
23	W	183	LEU	C-N-CA	6.03	126.64	120.00
22	V	379	LYS	N-CA-C	6.03	119.47	111.75
17	Q	173	ALA	N-CA-C	6.02	117.64	111.14
23	W	569	ILE	N-CA-CB	-6.02	105.21	112.07
26	2	79	PHE	CA-CB-CG	-6.02	107.78	113.80
22	V	404	SER	CB-CA-C	6.02	122.39	110.42
22	V	410	TYR	CA-C-N	6.02	129.67	120.82
22	V	410	TYR	C-N-CA	6.02	129.67	120.82
23	W	30	ARG	CD-NE-CZ	6.02	132.82	124.40
9	I	73	SER	N-CA-C	6.02	120.16	112.34
23	W	164	HIS	CB-CG-CD2	-6.01	123.39	131.20
14	N	362	GLY	CA-C-N	-6.00	112.36	122.92
14	N	362	GLY	C-N-CA	-6.00	112.36	122.92
22	V	651	VAL	CA-C-O	-6.00	113.28	120.78
23	W	122	THR	CA-C-N	6.00	127.34	119.84
23	W	122	THR	C-N-CA	6.00	127.34	119.84
26	2	171	VAL	CB-CA-C	-5.99	104.30	111.97
5	E	132	GLN	N-CA-C	5.99	118.58	111.33
22	V	603	ASN	CA-CB-CG	5.99	118.58	112.60
2	B	156	LEU	N-CA-C	5.98	119.01	110.10
22	V	709	GLN	OE1-CD-NE2	-5.98	116.62	122.60
22	V	611	GLY	O-C-N	5.97	127.93	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1425	GLY	CA-C-N	5.97	125.68	119.05
1	A	1425	GLY	C-N-CA	5.97	125.68	119.05
23	W	298	ALA	N-CA-C	-5.97	98.09	110.80
2	B	80	GLU	N-CA-C	5.96	122.98	109.81
23	W	621	PHE	CA-CB-CG	-5.96	107.84	113.80
26	2	203	PHE	CA-CB-CG	-5.96	107.84	113.80
1	A	1035	GLU	N-CA-C	5.96	117.85	111.36
22	V	607	ILE	CA-CB-CG1	5.95	120.52	110.40
23	W	590	ASN	N-CA-C	5.95	119.79	110.32
18	R	226	ASP	CA-CB-CG	5.95	118.55	112.60
23	W	416	ILE	CA-C-O	5.95	127.43	120.71
22	V	307	ASN	CA-CB-CG	5.95	118.55	112.60
22	V	459	GLN	CA-C-N	5.95	132.90	121.54
22	V	459	GLN	C-N-CA	5.95	132.90	121.54
23	W	592	ARG	NE-CZ-NH1	5.94	127.44	121.50
24	O	158	HIS	CB-CG-CD2	-5.94	123.48	131.20
9	I	85	PRO	N-CA-C	5.94	124.70	112.47
23	W	470	ILE	CB-CG1-CD1	-5.94	101.33	113.80
23	W	606	GLU	O-C-N	-5.94	115.28	122.22
28	X	63	DC	C6-N1-C1'	5.94	128.60	119.70
22	V	561	PHE	O-C-N	-5.93	116.56	123.27
23	W	623	VAL	N-CA-C	-5.93	103.53	108.63
22	V	403	CYS	N-CA-CB	-5.93	102.04	110.46
24	O	235	HIS	CB-CG-CD2	-5.92	123.50	131.20
23	W	442	LEU	CA-C-N	5.92	128.70	120.29
23	W	442	LEU	C-N-CA	5.92	128.70	120.29
23	W	161	PHE	O-C-N	-5.91	115.94	122.09
23	W	480	THR	CA-CB-OG1	5.91	118.47	109.60
1	A	728	THR	CA-C-N	5.91	127.23	119.84
1	A	728	THR	C-N-CA	5.91	127.23	119.84
22	V	633	ARG	NE-CZ-NH2	-5.91	113.88	119.20
23	W	20	GLU	CA-C-O	-5.91	114.29	120.55
24	O	130	SER	N-CA-C	5.90	117.80	111.36
29	Y	25	DT	O5'-C5'-C4'	5.90	119.66	110.80
29	Y	21	DC	O4'-C1'-N1	5.90	117.25	108.40
22	V	527	THR	CA-C-O	-5.90	115.27	121.99
23	W	207	TYR	CA-C-O	-5.90	115.11	121.36
24	O	203	ALA	N-CA-C	5.90	119.09	108.48
3	C	1	MET	CA-C-N	5.89	127.20	119.84
3	C	1	MET	C-N-CA	5.89	127.20	119.84
23	W	650	ASP	CA-C-O	-5.89	114.64	120.70
25	1	34	ILE	N-CA-C	5.88	116.07	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	ASN	N-CA-C	5.87	118.46	111.71
21	U	257	GLN	N-CA-C	5.87	122.03	113.40
23	W	280	ARG	CA-C-O	-5.87	114.20	120.42
1	A	636	ILE	N-CA-C	5.87	116.51	110.82
23	W	92	ASN	OD1-CG-ND2	-5.87	116.73	122.60
23	W	152	LEU	CA-C-N	5.86	125.80	119.76
23	W	152	LEU	C-N-CA	5.86	125.80	119.76
23	W	716	VAL	N-CA-CB	5.86	119.37	110.58
2	B	719	SER	CA-C-N	-5.86	113.58	119.56
2	B	719	SER	C-N-CA	-5.86	113.58	119.56
22	V	485	GLY	CA-C-N	5.86	126.19	119.92
22	V	485	GLY	C-N-CA	5.86	126.19	119.92
24	O	190	LYS	N-CA-C	-5.86	104.98	111.36
28	X	75	DG	C8-N9-C1'	5.85	135.78	127.00
2	B	248	LYS	O-C-N	5.85	129.25	122.17
23	W	312	ASP	N-CA-CB	-5.85	101.59	110.07
26	2	175	LEU	N-CA-CB	5.85	119.23	110.22
23	W	289	VAL	N-CA-C	5.84	116.57	110.62
2	B	399	LEU	N-CA-C	5.83	117.31	111.07
22	V	276	MET	CA-C-O	-5.83	114.73	121.26
22	V	369	VAL	CA-CB-CG1	5.83	120.31	110.40
22	V	674	THR	CA-C-N	5.83	128.02	120.44
22	V	674	THR	C-N-CA	5.83	128.02	120.44
24	O	74	GLN	OE1-CD-NE2	-5.83	116.77	122.60
23	W	685	ALA	N-CA-C	5.82	118.38	111.33
22	V	281	GLN	N-CA-C	5.82	118.09	111.11
23	W	37	HIS	N-CA-C	5.82	117.69	108.79
27	3	153	ASP	N-CA-C	-5.82	104.94	111.28
22	V	335	SER	N-CA-C	5.82	117.91	109.07
2	B	497	LYS	CA-C-N	-5.81	110.88	120.88
2	B	497	LYS	C-N-CA	-5.81	110.88	120.88
6	F	126	THR	N-CA-C	-5.81	107.43	114.75
1	A	476	ILE	N-CA-C	5.81	117.14	108.54
23	W	213	LEU	N-CA-C	5.81	118.39	111.71
24	O	56	GLY	CA-C-N	5.80	131.74	122.10
24	O	56	GLY	C-N-CA	5.80	131.74	122.10
27	3	64	ILE	CB-CA-C	-5.80	104.54	111.97
23	W	92	ASN	CB-CG-ND2	5.80	125.10	116.40
23	W	722	ARG	CD-NE-CZ	5.80	132.51	124.40
23	W	683	ARG	CD-NE-CZ	5.79	132.51	124.40
5	E	63	ALA	CA-C-N	5.79	132.60	121.54
5	E	63	ALA	C-N-CA	5.79	132.60	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	594	GLN	O-C-N	-5.79	115.84	122.09
22	V	461	HIS	CB-CG-CD2	-5.78	123.68	131.20
28	X	63	DC	C2-N1-C1'	-5.78	111.03	119.70
29	Y	35	DG	O3'-P-O5'	5.78	112.67	104.00
22	V	497	GLN	OE1-CD-NE2	-5.78	116.82	122.60
23	W	672	THR	N-CA-C	5.77	119.95	113.02
23	W	548	THR	CA-C-O	-5.77	114.76	120.82
18	R	145	VAL	N-CA-C	-5.77	107.66	113.20
24	0	92	VAL	CB-CA-C	-5.77	104.59	111.97
1	A	785	ILE	N-CA-C	5.77	116.81	111.45
2	B	37	LYS	N-CA-C	-5.76	102.92	110.53
14	N	324	GLU	N-CA-C	5.76	120.38	111.56
23	W	272	ARG	NE-CZ-NH1	5.76	127.26	121.50
23	W	112	ARG	NE-CZ-NH1	5.75	127.25	121.50
23	W	206	VAL	CA-CB-CG1	5.75	120.18	110.40
17	Q	68	GLY	N-CA-C	5.75	120.13	112.77
22	V	416	THR	CB-CA-C	-5.75	99.64	109.65
23	W	154	HIS	CB-CG-ND1	5.75	131.32	122.70
22	V	332	ARG	NE-CZ-NH1	5.74	127.24	121.50
23	W	415	THR	CA-C-O	5.74	127.60	120.54
23	W	702	THR	N-CA-C	5.74	119.90	113.01
22	V	532	LEU	N-CA-C	5.74	118.47	111.82
25	1	48	GLU	N-CA-C	-5.74	98.58	110.80
26	2	403	PHE	CA-C-N	5.74	132.76	122.09
26	2	403	PHE	C-N-CA	5.74	132.76	122.09
23	W	218	ALA	N-CA-C	5.73	117.53	111.28
24	0	160	PRO	CA-C-N	5.73	132.65	121.41
24	0	160	PRO	C-N-CA	5.73	132.65	121.41
23	W	586	GLU	N-CA-C	5.73	117.20	111.07
2	B	759	VAL	CB-CA-C	-5.73	103.29	111.31
23	W	239	ILE	N-CA-C	5.73	116.46	110.62
22	V	527	THR	N-CA-C	5.72	117.45	110.41
22	V	520	ARG	NE-CZ-NH2	5.72	124.35	119.20
22	V	393	THR	N-CA-C	5.72	115.57	108.19
22	V	479	ASP	N-CA-C	5.72	118.45	111.82
22	V	412	MET	O-C-N	-5.71	115.12	122.21
26	2	444	THR	CA-CB-OG1	5.71	118.17	109.60
1	A	619	LYS	N-CA-C	-5.71	99.22	108.41
22	V	338	ILE	CA-C-O	-5.71	114.31	120.36
22	V	488	LEU	N-CA-C	5.71	117.58	111.36
22	V	656	ASN	CA-CB-CG	5.71	118.31	112.60
23	W	593	GLY	CA-C-N	5.70	132.79	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	593	GLY	C-N-CA	5.70	132.79	122.02
29	Y	34	DC	O5'-C5'-C4'	5.70	119.35	110.80
23	W	447	VAL	CA-C-O	-5.70	115.03	120.95
23	W	669	ARG	NE-CZ-NH1	5.70	127.19	121.50
23	W	651	PHE	CA-CB-CG	5.69	119.49	113.80
22	V	551	HIS	CA-CB-CG	-5.69	108.11	113.80
23	W	109	LEU	CA-C-N	5.69	133.45	121.91
23	W	109	LEU	C-N-CA	5.69	133.45	121.91
22	V	307	ASN	N-CA-CB	-5.68	102.17	111.66
22	V	579	TYR	N-CA-C	5.68	118.47	109.50
22	V	295	TYR	N-CA-C	5.67	118.02	110.53
22	V	665	GLN	CG-CD-NE2	5.67	124.91	116.40
23	W	16	TYR	CA-C-N	5.67	129.94	122.51
23	W	16	TYR	C-N-CA	5.67	129.94	122.51
23	W	177	LEU	N-CA-C	5.67	117.14	111.07
22	V	636	GLU	N-CA-C	-5.67	105.01	111.07
23	W	44	SER	CA-C-O	5.66	126.34	119.49
23	W	103	PRO	CB-CA-C	5.66	120.89	111.56
23	W	216	LYS	CA-C-O	-5.66	114.55	120.55
2	B	44	LEU	N-CA-C	5.66	117.25	111.14
13	M	34	CYS	CA-C-N	5.66	125.77	119.32
13	M	34	CYS	C-N-CA	5.66	125.77	119.32
29	Y	21	DC	O3'-P-O5'	5.66	112.48	104.00
22	V	354	ALA	N-CA-C	5.65	117.44	111.28
23	W	207	TYR	CA-CB-CG	5.65	124.07	113.90
5	E	63	ALA	O-C-N	5.65	130.58	123.12
22	V	702	ALA	N-CA-CB	-5.65	102.57	110.25
23	W	215	PRO	CA-C-N	5.65	127.85	120.28
23	W	215	PRO	C-N-CA	5.65	127.85	120.28
22	V	506	GLN	OE1-CD-NE2	-5.65	116.95	122.60
23	W	193	PHE	N-CA-C	5.65	117.44	111.28
23	W	434	HIS	CB-CG-CD2	-5.65	123.86	131.20
23	W	104	PHE	CA-CB-CG	5.64	119.44	113.80
23	W	421	PHE	CA-C-N	-5.64	114.11	122.35
23	W	421	PHE	C-N-CA	-5.64	114.11	122.35
2	B	1065	GLY	CA-C-N	5.64	125.59	119.78
2	B	1065	GLY	C-N-CA	5.64	125.59	119.78
23	W	339	TYR	CA-C-N	5.64	128.43	120.42
23	W	339	TYR	C-N-CA	5.64	128.43	120.42
23	W	697	ILE	N-CA-C	5.64	121.08	109.34
22	V	567	ALA	CA-C-N	5.64	128.15	120.54
22	V	567	ALA	C-N-CA	5.64	128.15	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	677	GLN	N-CA-C	5.64	117.10	111.07
23	W	590	ASN	CA-C-N	5.64	129.16	121.83
23	W	590	ASN	C-N-CA	5.64	129.16	121.83
22	V	375	LYS	CA-C-N	5.63	127.76	120.44
22	V	375	LYS	C-N-CA	5.63	127.76	120.44
2	B	80	GLU	CA-C-N	5.63	126.18	120.38
2	B	80	GLU	C-N-CA	5.63	126.18	120.38
9	I	14	ILE	N-CA-C	5.63	117.10	108.71
22	V	526	LYS	CA-C-N	5.62	131.63	121.06
22	V	526	LYS	C-N-CA	5.62	131.63	121.06
22	V	477	ILE	CA-CB-CG1	5.62	119.96	110.40
23	W	270	VAL	O-C-N	-5.62	115.55	122.57
23	W	414	PHE	CA-CB-CG	5.62	119.42	113.80
26	2	61	PHE	N-CA-CB	5.62	118.13	109.98
27	3	120	THR	CA-C-N	5.62	127.81	120.28
27	3	120	THR	C-N-CA	5.62	127.81	120.28
23	W	220	LEU	O-C-N	-5.61	115.75	122.15
29	Y	30	DG	O4'-C1'-N9	5.61	116.82	108.40
22	V	355	CYS	O-C-N	-5.61	116.18	122.12
22	V	439	ILE	CB-CG1-CD1	5.60	125.57	113.80
23	W	305	LEU	CA-C-N	5.60	127.79	120.28
23	W	305	LEU	C-N-CA	5.60	127.79	120.28
22	V	444	HIS	CA-C-N	5.60	128.55	120.38
22	V	444	HIS	C-N-CA	5.60	128.55	120.38
24	0	113	ARG	N-CA-C	5.60	117.92	109.41
23	W	265	THR	CA-C-N	5.59	129.55	120.60
23	W	265	THR	C-N-CA	5.59	129.55	120.60
1	A	418	TYR	N-CA-C	5.59	117.68	109.24
1	A	890	ARG	N-CA-C	-5.59	100.21	108.99
23	W	306	ALA	CA-C-O	-5.59	114.63	120.55
23	W	154	HIS	CA-CB-CG	-5.58	108.22	113.80
1	A	525	ILE	N-CA-C	5.58	115.77	110.53
23	W	606	GLU	CA-C-O	5.57	126.40	120.10
24	0	178	ASP	O-C-N	-5.57	116.34	121.30
23	W	703	ASP	CA-C-N	5.57	132.18	121.54
23	W	703	ASP	C-N-CA	5.57	132.18	121.54
23	W	197	TYR	CA-C-O	5.57	126.46	120.55
26	2	262	LEU	CB-CA-C	-5.57	102.14	110.88
1	A	75	ALA	CB-CA-C	-5.57	110.14	116.54
23	W	685	ALA	CA-C-O	5.57	126.64	120.63
1	A	1443	ALA	N-CA-C	5.56	117.02	111.07
24	0	99	ASN	N-CA-C	5.56	119.92	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	PRO	CA-C-N	5.56	125.56	119.89
1	A	256	PRO	C-N-CA	5.56	125.56	119.89
23	W	53	LEU	CA-C-O	-5.56	114.66	120.55
1	A	1376	LYS	N-CA-C	5.55	117.14	111.14
7	G	107	PHE	N-CA-C	5.55	118.01	109.07
22	V	429	TRP	CA-C-N	5.55	133.19	122.53
22	V	429	TRP	C-N-CA	5.55	133.19	122.53
23	W	68	THR	CA-C-O	-5.55	115.77	121.87
20	T	234	GLU	CG-CD-OE2	-5.54	105.66	118.40
22	V	405	VAL	CB-CA-C	5.54	120.37	111.29
2	B	711	ILE	CA-C-N	5.53	126.00	120.14
2	B	711	ILE	C-N-CA	5.53	126.00	120.14
22	V	567	ALA	O-C-N	5.53	128.45	122.15
24	0	79	ASN	CA-C-N	-5.53	112.88	120.28
24	0	79	ASN	C-N-CA	-5.53	112.88	120.28
24	0	227	HIS	CA-CB-CG	5.52	119.32	113.80
26	2	182	ALA	N-CA-C	-5.52	102.84	110.35
2	B	1024	GLY	N-CA-C	5.52	121.43	114.25
22	V	268	VAL	CA-C-N	5.52	129.08	120.75
22	V	268	VAL	C-N-CA	5.52	129.08	120.75
2	B	962	THR	CA-C-N	5.51	125.51	119.89
2	B	962	THR	C-N-CA	5.51	125.51	119.89
23	W	251	LEU	CB-CA-C	5.51	119.45	109.37
24	0	98	GLN	CA-C-O	5.51	126.26	120.42
23	W	468	PRO	CA-N-CD	-5.50	104.29	112.00
22	V	675	LYS	N-CA-C	5.50	116.96	111.07
22	V	572	ALA	N-CA-C	5.49	117.27	111.28
23	W	454	VAL	CA-C-N	5.49	131.11	122.33
23	W	454	VAL	C-N-CA	5.49	131.11	122.33
22	V	457	ILE	N-CA-CB	-5.48	102.19	111.23
23	W	439	ASP	CA-C-O	5.48	127.18	120.60
24	0	75	ASP	N-CA-C	5.48	117.25	111.28
24	0	194	ILE	CA-C-O	5.48	127.09	120.74
24	0	226	SER	N-CA-CB	-5.47	102.08	110.12
24	0	123	ASN	O-C-N	-5.47	114.88	121.12
26	2	267	GLU	CA-C-N	-5.47	115.73	122.84
26	2	267	GLU	C-N-CA	-5.47	115.73	122.84
1	A	539	GLN	CB-CA-C	-5.46	110.26	116.54
1	A	464	LEU	N-CA-C	5.46	117.31	111.36
22	V	514	MET	CB-CA-C	5.46	118.88	110.14
25	1	51	ASN	CA-CB-CG	-5.46	107.14	112.60
23	W	489	CYS	CA-C-N	5.46	130.47	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	489	CYS	C-N-CA	5.46	130.47	122.39
22	V	662	LEU	N-CA-CB	-5.46	101.54	110.43
20	T	234	GLU	CA-C-O	-5.45	114.73	121.11
23	W	686	ARG	CA-C-N	5.45	126.95	120.14
23	W	686	ARG	C-N-CA	5.45	126.95	120.14
2	B	983	GLU	CA-C-N	5.45	127.52	120.44
2	B	983	GLU	C-N-CA	5.45	127.52	120.44
23	W	726	GLN	OE1-CD-NE2	-5.45	117.15	122.60
22	V	637	ALA	N-CA-C	5.44	118.13	111.82
23	W	57	MET	CA-C-N	5.44	129.31	120.60
23	W	57	MET	C-N-CA	5.44	129.31	120.60
23	W	334	ARG	N-CA-CB	-5.44	102.12	110.01
23	W	197	TYR	O-C-N	-5.44	116.35	122.12
2	B	753	TYR	CA-C-N	-5.44	114.02	120.11
2	B	753	TYR	C-N-CA	-5.44	114.02	120.11
22	V	433	GLN	OE1-CD-NE2	-5.44	117.16	122.60
22	V	542	ARG	NE-CZ-NH2	5.44	124.09	119.20
17	Q	66	LEU	N-CA-C	5.43	117.20	111.28
23	W	75	ARG	NE-CZ-NH1	5.43	126.93	121.50
28	X	73	DG	C2'-C3'-O3'	5.43	119.64	111.50
1	A	540	ASP	CB-CA-C	-5.43	101.78	110.79
22	V	265	THR	CA-C-O	-5.43	115.21	121.07
24	O	186	ILE	N-CA-C	5.42	116.15	110.62
1	A	1386	ILE	N-CA-C	5.42	116.15	110.62
23	W	487	ARG	NH1-CZ-NH2	-5.42	112.25	119.30
26	2	45	PHE	CA-CB-CG	-5.42	108.38	113.80
2	B	1163	MET	N-CA-C	-5.42	105.53	111.82
23	W	76	THR	N-CA-C	5.42	117.31	109.07
22	V	427	MET	CA-C-N	-5.42	114.58	122.44
22	V	427	MET	C-N-CA	-5.42	114.58	122.44
2	B	248	LYS	CA-C-N	5.41	131.88	121.54
2	B	248	LYS	C-N-CA	5.41	131.88	121.54
22	V	360	ARG	CD-NE-CZ	5.41	131.97	124.40
9	I	35	LEU	N-CA-C	-5.41	102.47	110.48
23	W	645	GLN	CA-C-N	5.41	131.70	121.97
23	W	645	GLN	C-N-CA	5.41	131.70	121.97
24	O	142	GLU	O-C-N	5.41	125.77	121.55
1	A	1115	LYS	N-CA-C	-5.41	99.28	110.80
23	W	601	ARG	NE-CZ-NH2	-5.41	114.33	119.20
29	Y	30	DG	C4-N9-C1'	-5.41	118.89	127.00
26	2	98	THR	CA-C-N	5.40	128.06	120.28
26	2	98	THR	C-N-CA	5.40	128.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	455	ILE	N-CA-C	5.40	115.67	108.27
26	2	35	TYR	CB-CA-C	5.40	121.04	110.67
20	T	233	TRP	N-CA-C	5.40	118.38	109.85
28	X	75	DG	C2'-C3'-O3'	5.40	119.60	111.50
24	0	236	VAL	CB-CA-C	-5.39	104.86	112.14
2	B	882	SER	N-CA-C	-5.39	103.59	111.30
22	V	339	VAL	CA-C-O	5.39	126.05	120.39
5	E	63	ALA	N-CA-C	5.38	117.44	108.02
24	0	134	ALA	CA-C-O	5.38	126.13	120.42
23	W	156	ARG	CD-NE-CZ	5.38	131.94	124.40
23	W	463	PRO	CA-C-N	5.38	131.82	121.54
23	W	463	PRO	C-N-CA	5.38	131.82	121.54
22	V	576	ASN	N-CA-CB	-5.38	103.83	111.84
6	F	84	GLU	CB-CA-C	-5.38	110.36	116.54
1	A	683	GLU	N-CA-C	5.37	116.94	111.14
22	V	253	GLU	CA-C-N	5.37	131.81	121.54
22	V	253	GLU	C-N-CA	5.37	131.81	121.54
29	Y	34	DC	C5'-C4'-O4'	-5.37	101.35	109.40
1	A	898	GLY	N-CA-C	5.36	120.57	114.67
22	V	252	TYR	N-CA-C	5.36	117.70	109.07
22	V	677	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	136	GLN	CA-C-N	5.36	125.17	119.28
1	A	136	GLN	C-N-CA	5.36	125.17	119.28
22	V	252	TYR	O-C-N	-5.35	116.97	123.29
25	1	33	PHE	CA-CB-CG	-5.35	108.45	113.80
20	T	124	TYR	N-CA-C	5.35	122.19	110.80
1	A	480	SER	N-CA-C	5.34	122.18	110.80
23	W	600	ALA	CA-C-N	5.34	127.98	120.28
23	W	600	ALA	C-N-CA	5.34	127.98	120.28
23	W	148	HIS	N-CA-C	5.34	122.18	110.80
24	0	90	TYR	CA-C-N	5.34	127.44	120.28
24	0	90	TYR	C-N-CA	5.34	127.44	120.28
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	118	HIS	CB-CG-CD2	-5.34	124.26	131.20
23	W	313	GLU	N-CA-C	5.33	116.77	111.07
1	A	565	MET	N-CA-C	5.33	117.08	111.28
22	V	361	CYS	N-CA-CB	-5.32	101.57	110.83
22	V	381	TRP	CZ3-CH2-CZ2	-5.32	114.58	121.50
22	V	564	ASN	CA-C-N	5.32	127.75	120.46
22	V	564	ASN	C-N-CA	5.32	127.75	120.46
1	A	1405	MET	N-CA-C	5.31	117.98	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	555	ASN	N-CA-C	5.31	118.77	111.54
2	B	986	GLN	CA-C-N	5.31	125.84	120.00
2	B	986	GLN	C-N-CA	5.31	125.84	120.00
23	W	141	TYR	N-CA-C	5.31	117.07	111.28
23	W	560	ASN	CA-CB-CG	-5.31	107.29	112.60
23	W	669	ARG	NH1-CZ-NH2	-5.31	112.39	119.30
23	W	621	PHE	O-C-N	5.31	129.39	122.38
24	O	131	LEU	O-C-N	-5.31	115.74	122.27
13	M	15	CYS	CA-C-N	5.31	124.49	118.97
13	M	15	CYS	C-N-CA	5.31	124.49	118.97
23	W	435	PHE	CA-C-N	5.31	128.38	120.95
23	W	435	PHE	C-N-CA	5.31	128.38	120.95
28	X	73	DG	C1'-O4'-C4'	-5.30	101.74	109.70
22	V	317	ARG	O-C-N	5.30	127.37	121.43
22	V	575	LEU	CA-C-N	5.30	129.65	122.07
22	V	575	LEU	C-N-CA	5.30	129.65	122.07
23	W	202	ALA	N-CA-C	5.30	118.19	109.76
23	W	253	ARG	N-CA-C	5.30	117.06	111.28
5	E	200	ALA	N-CA-C	-5.30	105.59	111.36
7	G	14	HIS	CA-C-N	5.30	126.46	119.84
7	G	14	HIS	C-N-CA	5.30	126.46	119.84
3	C	260	GLN	CB-CA-C	-5.29	101.85	110.85
2	B	590	LEU	N-CA-C	5.29	117.13	111.36
2	B	953	ASP	N-CA-C	5.29	117.13	111.36
3	C	267	ILE	N-CA-C	-5.29	107.56	112.43
23	W	562	GLN	CB-CG-CD	5.29	121.60	112.60
24	O	237	SER	N-CA-C	5.29	116.08	109.57
23	W	711	ASP	CA-CB-CG	-5.29	107.31	112.60
22	V	366	ASN	N-CA-C	5.29	119.45	112.89
22	V	576	ASN	CA-C-O	5.29	127.67	121.54
24	O	99	ASN	OD1-CG-ND2	-5.29	117.31	122.60
22	V	272	VAL	O-C-N	5.29	127.00	121.87
22	V	634	ARG	NE-CZ-NH1	-5.29	116.21	121.50
24	O	178	ASP	CA-C-N	5.28	124.79	119.19
24	O	178	ASP	C-N-CA	5.28	124.79	119.19
22	V	332	ARG	NH1-CZ-NH2	-5.28	112.43	119.30
24	O	170	ILE	CA-CB-CG1	5.28	119.37	110.40
29	Y	27	DC	C1'-O4'-C4'	-5.28	101.79	109.70
23	W	46	THR	CA-CB-OG1	5.27	117.51	109.60
23	W	450	ARG	N-CA-C	5.27	122.03	110.80
22	V	469	THR	CA-C-N	5.27	131.61	121.54
22	V	469	THR	C-N-CA	5.27	131.61	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	37	HIS	CA-C-N	5.27	127.77	120.92
23	W	37	HIS	C-N-CA	5.27	127.77	120.92
23	W	457	THR	N-CA-CB	-5.27	103.39	111.56
23	W	50	VAL	O-C-N	5.27	127.25	121.83
29	Y	28	DT	C2'-C3'-O3'	5.27	119.40	111.50
24	0	59	ARG	NH1-CZ-NH2	-5.26	112.46	119.30
23	W	169	PRO	N-CA-CB	5.26	109.07	103.39
22	V	332	ARG	CA-CB-CG	5.26	124.62	114.10
2	B	162	LEU	N-CA-C	5.26	118.48	111.75
1	A	322	LEU	CA-C-N	5.25	126.41	119.84
1	A	322	LEU	C-N-CA	5.25	126.41	119.84
22	V	562	ALA	CA-C-N	5.25	131.57	121.54
22	V	562	ALA	C-N-CA	5.25	131.57	121.54
23	W	102	LEU	CA-C-N	5.25	126.41	119.84
23	W	102	LEU	C-N-CA	5.25	126.41	119.84
23	W	319	VAL	CA-C-N	5.25	126.40	119.84
23	W	319	VAL	C-N-CA	5.25	126.40	119.84
2	B	880	LEU	N-CA-C	5.25	117.05	110.91
22	V	282	LYS	CG-CD-CE	5.25	123.36	111.30
23	W	516	VAL	N-CA-C	5.24	115.97	110.62
28	X	73	DG	P-O3'-C3'	5.24	128.07	120.20
23	W	454	VAL	N-CA-CB	-5.24	105.84	112.60
3	C	240	ARG	CA-C-N	5.24	124.69	119.24
3	C	240	ARG	C-N-CA	5.24	124.69	119.24
22	V	315	VAL	CA-C-O	-5.24	114.89	120.39
23	W	564	ASN	OD1-CG-ND2	-5.24	117.36	122.60
29	Y	33	DT	C4'-C3'-O3'	5.23	117.85	110.00
22	V	341	PRO	N-CA-C	5.23	119.43	111.11
22	V	574	ARG	O-C-N	-5.23	116.19	122.15
23	W	87	LEU	CB-CA-C	5.23	119.74	110.85
22	V	552	GLU	N-CA-C	5.23	117.72	111.71
23	W	24	TYR	CA-C-N	5.23	127.24	120.44
23	W	24	TYR	C-N-CA	5.23	127.24	120.44
22	V	545	GLN	CA-C-N	5.23	127.28	120.28
22	V	545	GLN	C-N-CA	5.23	127.28	120.28
26	2	60	LEU	CB-CA-C	-5.23	102.67	110.88
23	W	455	ILE	CA-C-O	-5.23	115.05	120.64
5	E	69	THR	N-CA-C	-5.22	106.59	113.17
23	W	128	LYS	CA-C-N	5.22	128.13	120.71
23	W	128	LYS	C-N-CA	5.22	128.13	120.71
22	V	704	SER	N-CA-C	5.22	119.52	113.20
25	1	3	ASN	CA-C-N	-5.22	115.20	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	3	ASN	C-N-CA	-5.22	115.20	122.71
27	3	50	PHE	CA-CB-CG	-5.22	108.58	113.80
1	A	1470	CYS	N-CA-C	5.21	118.90	112.54
22	V	297	PHE	N-CA-C	5.21	116.99	109.07
22	V	699	GLU	N-CA-C	5.21	116.72	108.96
24	0	73	ASP	CA-CB-CG	5.21	117.81	112.60
22	V	525	ILE	CA-C-O	-5.21	114.56	120.65
3	C	221	ASP	CA-C-N	5.21	125.66	120.04
3	C	221	ASP	C-N-CA	5.21	125.66	120.04
3	C	61	ASP	N-CA-C	5.21	116.64	111.07
23	W	284	GLU	N-CA-CB	5.21	117.56	110.01
26	2	261	PHE	CB-CA-C	-5.21	102.71	110.88
6	F	54	THR	CA-C-N	5.20	125.28	119.87
6	F	54	THR	C-N-CA	5.20	125.28	119.87
7	G	108	ILE	N-CA-C	5.20	115.07	107.37
22	V	678	ARG	CA-C-O	-5.20	115.04	120.55
23	W	199	ILE	O-C-N	-5.20	116.83	121.87
9	I	98	GLN	N-CA-C	5.20	117.39	110.53
26	2	402	ARG	N-CA-C	5.20	117.57	110.24
22	V	285	ILE	CA-CB-CG2	5.19	119.33	110.50
23	W	96	LYS	N-CA-C	5.19	121.86	110.80
24	0	179	PRO	CA-C-O	-5.19	111.71	119.34
23	W	534	GLY	O-C-N	-5.19	118.94	122.62
23	W	494	ILE	O-C-N	-5.19	117.29	123.05
27	3	169	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	220	ARG	N-CA-C	-5.18	105.55	111.14
2	B	646	ARG	N-CA-C	5.18	118.70	112.38
23	W	154	HIS	CG-CD2-NE2	5.18	112.38	107.20
1	A	1192	TRP	N-CA-CB	5.17	118.19	110.22
22	V	341	PRO	CA-C-N	5.17	129.84	122.08
22	V	341	PRO	C-N-CA	5.17	129.84	122.08
23	W	153	PRO	CB-CA-C	5.17	118.14	111.46
21	U	256	THR	N-CA-C	-5.17	107.99	114.56
22	V	708	GLU	O-C-N	5.17	127.60	122.12
23	W	87	LEU	CA-C-N	5.17	127.20	120.28
23	W	87	LEU	C-N-CA	5.17	127.20	120.28
23	W	143	ARG	CA-CB-CG	-5.16	103.78	114.10
20	T	210	VAL	N-CA-C	5.16	116.62	111.00
22	V	639	ARG	NE-CZ-NH2	5.16	123.84	119.20
29	Y	33	DT	O3'-P-O5'	5.16	111.73	104.00
22	V	305	ASP	CA-C-N	5.15	131.25	121.97
22	V	305	ASP	C-N-CA	5.15	131.25	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	283	ARG	NE-CZ-NH2	-5.15	114.56	119.20
22	V	564	ASN	CB-CA-C	5.15	118.56	109.80
1	A	13	CYS	CA-C-N	5.15	125.13	120.03
1	A	13	CYS	C-N-CA	5.15	125.13	120.03
1	A	621	ILE	N-CA-C	5.15	120.05	109.34
2	B	855	ALA	CA-C-N	5.15	125.44	119.93
2	B	855	ALA	C-N-CA	5.15	125.44	119.93
24	O	65	VAL	CA-CB-CG1	5.15	119.15	110.40
22	V	344	ALA	N-CA-CB	-5.14	101.36	111.60
23	W	152	LEU	N-CA-C	5.14	121.18	109.81
28	X	60	DG	C2'-C3'-O3'	5.14	119.22	111.50
11	K	9	SER	N-CA-C	5.14	119.04	112.87
22	V	426	VAL	CA-C-N	5.14	131.36	121.54
22	V	426	VAL	C-N-CA	5.14	131.36	121.54
23	W	170	LEU	O-C-N	-5.14	115.91	120.48
9	I	105	GLU	N-CA-C	5.14	121.74	110.80
23	W	260	GLN	CA-C-N	5.14	125.68	119.98
23	W	260	GLN	C-N-CA	5.14	125.68	119.98
23	W	71	ILE	N-CA-C	5.14	115.88	108.48
2	B	106	SER	N-CA-C	5.13	114.20	108.25
3	C	212	ASP	N-CA-C	-5.13	106.70	113.17
23	W	69	LYS	CG-CD-CE	5.13	123.11	111.30
2	B	972	ILE	N-CA-C	5.13	119.96	108.88
22	V	399	LYS	CA-C-N	5.13	124.74	119.56
22	V	399	LYS	C-N-CA	5.13	124.74	119.56
23	W	205	VAL	CA-C-N	5.13	130.18	123.11
23	W	205	VAL	C-N-CA	5.13	130.18	123.11
23	W	511	ARG	CA-C-N	5.13	131.34	122.32
23	W	511	ARG	C-N-CA	5.13	131.34	122.32
22	V	357	VAL	N-CA-CB	5.12	117.51	110.54
22	V	397	LYS	CA-CB-CG	5.12	124.34	114.10
22	V	580	ILE	O-C-N	-5.12	117.67	123.20
29	Y	27	DC	C4'-C3'-O3'	-5.12	102.32	110.00
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
2	B	1044	GLY	CA-C-N	-5.12	114.72	120.14
2	B	1044	GLY	C-N-CA	-5.12	114.72	120.14
23	W	707	ASN	OD1-CG-ND2	-5.12	117.48	122.60
14	N	346	LYS	CB-CA-C	-5.12	110.69	116.63
22	V	680	LEU	N-CA-C	5.12	116.86	111.28
23	W	641	ARG	CD-NE-CZ	5.11	131.55	124.40
23	W	434	HIS	CA-C-N	5.11	131.75	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	434	HIS	C-N-CA	5.11	131.75	123.37
2	B	294	ASP	CA-C-N	5.11	124.90	119.28
2	B	294	ASP	C-N-CA	5.11	124.90	119.28
1	A	1192	TRP	CA-CB-CG	5.10	123.30	113.60
2	B	984	CYS	N-CA-C	5.10	116.53	111.07
26	2	128	ALA	CA-C-N	-5.10	115.57	123.17
26	2	128	ALA	C-N-CA	-5.10	115.57	123.17
23	W	195	ALA	O-C-N	5.10	127.32	122.07
22	V	577	LYS	CA-C-O	-5.10	115.45	120.19
22	V	419	ARG	CD-NE-CZ	5.10	131.54	124.40
23	W	660	ALA	CA-C-N	5.10	127.62	120.28
23	W	660	ALA	C-N-CA	5.10	127.62	120.28
24	0	234	HIS	CA-CB-CG	5.10	118.90	113.80
26	2	48	LEU	N-CA-C	5.10	121.07	109.81
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
23	W	693	LEU	CB-CA-C	5.09	116.87	109.08
22	V	465	GLY	CA-C-O	-5.09	115.95	120.94
22	V	452	ARG	CA-CB-CG	5.09	124.27	114.10
23	W	483	MET	N-CA-CB	-5.08	102.69	110.42
23	W	538	PHE	O-C-N	5.08	129.06	123.16
23	W	23	SER	CB-CA-C	-5.08	102.90	110.88
23	W	205	VAL	CA-CB-CG1	5.08	119.04	110.40
24	0	80	ARG	CD-NE-CZ	5.08	131.51	124.40
2	B	1112	ASP	CA-C-N	-5.08	113.49	119.84
2	B	1112	ASP	C-N-CA	-5.08	113.49	119.84
1	A	263	ALA	N-CA-C	-5.08	99.99	110.80
22	V	634	ARG	N-CA-C	5.08	117.71	111.82
24	0	233	THR	CA-CB-OG1	5.08	117.22	109.60
23	W	31	THR	CA-CB-CG2	5.07	119.12	110.50
24	0	124	PRO	CA-C-N	5.07	127.07	120.28
24	0	124	PRO	C-N-CA	5.07	127.07	120.28
24	0	212	ALA	CA-C-N	5.07	127.34	120.44
24	0	212	ALA	C-N-CA	5.07	127.34	120.44
21	U	250	MET	N-CA-C	5.07	117.20	111.02
23	W	98	GLU	O-C-N	-5.07	115.85	122.59
23	W	64	PRO	CA-N-CD	-5.07	104.91	112.00
1	A	669	TYR	N-CA-C	5.06	116.48	111.07
27	3	9	ASN	CA-CB-CG	-5.06	107.54	112.60
2	B	643	LEU	N-CA-C	5.06	116.80	111.28
2	B	1160	GLN	N-CA-C	5.06	116.88	111.36
22	V	363	VAL	CA-C-N	-5.06	116.02	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	363	VAL	C-N-CA	-5.06	116.02	123.00
22	V	366	ASN	OD1-CG-ND2	5.06	127.66	122.60
2	B	223	SER	N-CA-C	5.06	116.76	108.52
22	V	466	LEU	N-CA-CB	-5.05	102.06	110.80
13	M	273	GLU	N-CA-C	5.05	116.47	111.07
2	B	1072	ARG	N-CA-C	5.05	118.40	111.54
22	V	543	ALA	N-CA-C	5.05	116.78	111.28
25	1	62	ASP	CA-CB-CG	-5.05	107.55	112.60
23	W	519	ASN	CA-CB-CG	5.04	117.64	112.60
23	W	672	THR	CA-C-N	5.04	130.65	122.53
23	W	672	THR	C-N-CA	5.04	130.65	122.53
22	V	316	LEU	CB-CA-C	-5.04	101.53	111.60
22	V	487	LYS	CA-C-N	5.04	127.44	120.29
22	V	487	LYS	C-N-CA	5.04	127.44	120.29
23	W	43	PRO	CA-C-N	5.04	128.66	120.60
23	W	43	PRO	C-N-CA	5.04	128.66	120.60
24	0	207	VAL	CA-C-N	5.03	127.44	120.29
24	0	207	VAL	C-N-CA	5.03	127.44	120.29
1	A	152	ASN	N-CA-C	5.03	116.33	109.18
23	W	459	GLY	O-C-N	5.03	129.24	122.70
20	T	234	GLU	CG-CD-OE1	5.03	129.96	118.40
23	W	687	GLY	CA-C-N	5.03	127.43	120.29
23	W	687	GLY	C-N-CA	5.03	127.43	120.29
20	T	178	ALA	N-CA-C	-5.03	100.09	110.80
24	0	106	ILE	CA-C-N	5.03	130.68	122.69
24	0	106	ILE	C-N-CA	5.03	130.68	122.69
2	B	704	LEU	N-CA-C	5.02	117.80	109.46
1	A	368	THR	CA-C-N	-5.02	114.82	120.14
1	A	368	THR	C-N-CA	-5.02	114.82	120.14
26	2	249	TYR	CA-C-N	-5.02	114.62	122.05
26	2	249	TYR	C-N-CA	-5.02	114.62	122.05
11	K	21	ILE	N-CA-C	5.02	115.08	107.80
23	W	718	LYS	CA-C-N	5.02	127.01	120.28
23	W	718	LYS	C-N-CA	5.02	127.01	120.28
22	V	311	LYS	CA-C-O	-5.01	113.29	120.16
23	W	468	PRO	N-CA-CB	5.01	108.80	103.39
23	W	699	GLU	CB-CA-C	5.01	118.32	109.80
20	T	81	HIS	CA-C-N	-5.01	114.79	119.85
20	T	81	HIS	C-N-CA	-5.01	114.79	119.85
28	X	70	DG	C2'-C3'-O3'	-5.01	103.98	111.50
26	2	244	THR	N-CA-C	-5.01	105.71	111.07
2	B	164	ASN	N-CA-C	5.01	117.47	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	638	GLU	CA-C-O	-5.01	115.56	120.82
23	W	414	PHE	CA-C-O	-5.00	115.78	121.68
23	W	720	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	0	143	PRO	Mainchain
25	1	17	LYS	Mainchain
26	2	389	ASP	Mainchain,Sidechain
26	2	399	ASP	Sidechain
26	2	403	PHE	Peptide,Mainchain
26	2	406	GLY	Peptide
26	2	409	TYR	Sidechain
26	2	425	ALA	Mainchain
1	A	475	ARG	Sidechain
2	B	234	THR	Peptide
5	E	126	ILE	Peptide
8	H	111	ARG	Peptide
14	N	324	GLU	Peptide
14	N	355	ASP	Peptide
14	N	371	ILE	Peptide
18	R	146	ARG	Peptide
18	R	213	ASP	Sidechain
18	R	214	GLU	Peptide
18	R	215	GLU	Mainchain
18	R	230	GLU	Mainchain
18	R	235	GLU	Sidechain
19	S	148	PRO	Peptide
20	T	123	ASN	Peptide
22	V	247	ASP	Mainchain
22	V	378	PHE	Sidechain
22	V	417	THR	Peptide
22	V	489	TYR	Sidechain
22	V	503	ALA	Peptide
22	V	519	TYR	Sidechain
22	V	530	ARG	Sidechain
22	V	674	THR	Mainchain
23	W	104	PHE	Sidechain
23	W	197	TYR	Sidechain
23	W	206	VAL	Mainchain

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11617	570	0
2	B	9317	0	9312	427	0
3	C	2213	0	2155	80	0
4	D	1062	0	1042	8	0
5	E	1723	0	1745	105	0
6	F	689	0	715	18	0
7	G	1351	0	1358	32	0
8	H	1205	0	1167	54	0
9	I	1013	0	936	76	0
10	J	533	0	556	49	0
11	K	937	0	959	23	0
12	L	388	0	396	14	0
13	M	2391	0	2411	150	0
14	N	930	0	888	32	0
15	O	806	0	818	23	0
16	P	1462	0	1549	68	0
17	Q	1484	0	1499	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	1357	0	1381	154	0
19	S	1138	0	1103	26	0
20	T	1788	0	1819	116	0
21	U	1343	0	1341	67	0
22	V	3855	0	3871	199	0
23	W	5348	0	5372	148	0
24	O	1479	0	1524	39	0
25	1	491	0	507	248	0
26	2	2196	0	2206	578	0
27	3	1526	0	1561	456	0
28	X	1591	0	865	30	0
29	Y	1561	0	865	59	0
30	A	1	0	0	0	0
30	B	1	0	0	0	0
31	A	2	0	0	0	0
31	B	2	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	Q	1	0	0	0	0
31	U	1	0	0	0	0
All	All	62705	0	61538	3294	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 27.

All (3294) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:59:VAL:HG12	27:3:71:TYR:CD1	1.22	1.73
23:W:421:PHE:CE1	23:W:423:ASP:CB	1.83	1.62
22:V:516:PRO:CG	25:1:15:ALA:HB3	1.20	1.61
1:A:1250:ASP:CB	21:U:227:GLU:HG2	1.26	1.60
27:3:59:VAL:CG1	27:3:71:TYR:HD1	1.12	1.59
17:Q:180:PHE:CZ	18:R:211:SER:HB2	1.39	1.58
22:V:531:ILE:HA	22:V:534:TYR:CE2	1.39	1.58
1:A:926:ASN:HD21	1:A:932:ARG:CG	1.12	1.57
23:W:421:PHE:HE1	23:W:423:ASP:CB	1.12	1.56
24:O:54:ARG:HG3	27:3:182:PHE:CE1	1.42	1.55
22:V:315:VAL:HG13	23:W:500:ASP:CB	1.21	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:421:PHE:CE1	23:W:423:ASP:HB2	1.04	1.53
1:A:271:ARG:CD	13:M:73:PRO:HG2	1.37	1.52
1:A:1250:ASP:HB3	21:U:227:GLU:CG	1.10	1.52
22:V:516:PRO:HG3	25:1:15:ALA:CB	1.11	1.52
1:A:927:GLU:HB3	1:A:931:ARG:CG	1.05	1.52
17:Q:180:PHE:CZ	18:R:211:SER:CB	1.91	1.51
23:W:421:PHE:CD1	23:W:423:ASP:HB2	1.41	1.51
1:A:266:MET:CG	1:A:272:ASN:ND2	1.73	1.49
22:V:315:VAL:CG1	23:W:500:ASP:HB2	1.01	1.48
26:2:117:ASN:ND2	27:3:108:ASN:CB	1.76	1.47
1:A:927:GLU:CB	1:A:931:ARG:HG3	1.44	1.46
10:J:62:TYR:C	10:J:64:PRO:HD2	1.36	1.46
26:2:117:ASN:HD21	27:3:108:ASN:CB	1.27	1.45
5:E:51:GLY:O	5:E:52:ARG:CG	1.64	1.45
26:2:117:ASN:CG	27:3:108:ASN:HB2	1.39	1.44
22:V:321:GLU:HB3	23:W:499:ASN:CG	1.38	1.44
2:B:90:GLN:NE2	20:T:141:LEU:HD23	1.30	1.43
22:V:321:GLU:HB3	23:W:499:ASN:ND2	1.25	1.42
26:2:30:VAL:CG2	27:3:25:GLN:HB2	1.49	1.41
22:V:516:PRO:CG	22:V:706:LYS:HZ3	1.30	1.41
1:A:926:ASN:ND2	1:A:932:ARG:CG	1.81	1.40
3:C:5:ASN:O	3:C:7:PRO:CD	1.69	1.38
13:M:47:ASP:O	13:M:49:GLY:N	1.57	1.38
24:0:54:ARG:CG	27:3:182:PHE:HE1	1.35	1.38
17:Q:105:TYR:CE1	18:R:231:GLU:CD	2.02	1.37
1:A:926:ASN:ND2	1:A:932:ARG:HG3	1.32	1.37
2:B:90:GLN:HE21	20:T:141:LEU:CD2	1.38	1.36
17:Q:180:PHE:HZ	18:R:211:SER:CB	1.27	1.36
26:2:31:LEU:HD21	27:3:33:THR:N	1.36	1.36
1:A:1319:LYS:HG2	1:A:1333:GLU:CD	1.51	1.36
1:A:1319:LYS:CG	1:A:1333:GLU:CD	2.00	1.34
2:B:90:GLN:HE22	20:T:141:LEU:CA	1.39	1.34
26:2:28:PRO:N	27:3:25:GLN:CA	1.89	1.33
2:B:80:GLU:CB	2:B:135:GLU:CB	2.06	1.33
26:2:30:VAL:HG23	27:3:25:GLN:CB	1.58	1.33
26:2:117:ASN:OD1	27:3:108:ASN:ND2	1.57	1.33
17:Q:105:TYR:CE1	17:Q:109:HIS:NE2	1.95	1.33
26:2:118:LEU:CD2	27:3:39:ASP:OD1	1.75	1.32
1:A:271:ARG:HD2	13:M:73:PRO:CG	1.57	1.32
1:A:927:GLU:HB3	1:A:931:ARG:CD	1.59	1.32
5:E:52:ARG:HB3	5:E:53:PRO:CD	1.59	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:118:LEU:HD22	27:3:39:ASP:OD1	1.16	1.31
1:A:927:GLU:CB	1:A:931:ARG:CG	2.00	1.31
22:V:325:ARG:NH2	23:W:499:ASN:HB3	1.02	1.31
25:1:1:MET:O	26:2:413:LEU:HG	1.28	1.31
13:M:178:LYS:O	20:T:154:LYS:HB3	1.28	1.31
22:V:523:VAL:HG11	25:1:20:LEU:CD2	1.59	1.31
2:B:79:GLU:O	2:B:80:GLU:HG3	1.12	1.30
1:A:266:MET:HG2	1:A:272:ASN:ND2	1.27	1.29
17:Q:180:PHE:CE2	18:R:211:SER:HB2	1.67	1.29
5:E:64:HIS:CD2	5:E:69:THR:H	1.51	1.29
22:V:321:GLU:HB3	23:W:499:ASN:OD1	1.30	1.29
2:B:80:GLU:HB2	2:B:135:GLU:CB	1.59	1.28
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.54	1.28
24:0:97:ASP:O	27:3:208:ASP:HB3	1.12	1.28
24:0:165:ARG:NH1	24:0:192:ALA:O	1.67	1.28
26:2:118:LEU:HD21	27:3:39:ASP:O	1.23	1.28
5:E:47:LYS:HB2	5:E:48:PRO:CD	1.61	1.27
1:A:271:ARG:CD	13:M:73:PRO:CG	2.09	1.27
13:M:11:PRO:O	13:M:12:ARG:HG2	1.20	1.27
22:V:321:GLU:CB	23:W:499:ASN:HD21	1.45	1.27
2:B:80:GLU:OE1	2:B:135:GLU:HB3	1.20	1.26
1:A:1319:LYS:HD3	1:A:1333:GLU:OE2	1.36	1.26
22:V:325:ARG:NH2	23:W:499:ASN:CB	1.97	1.25
1:A:266:MET:CG	1:A:272:ASN:HD22	1.34	1.25
2:B:90:GLN:NE2	20:T:141:LEU:CD2	1.95	1.25
13:M:94:ASP:OD2	13:M:97:GLY:O	1.52	1.25
2:B:91:ILE:CG2	20:T:141:LEU:HD12	1.65	1.25
17:Q:102:VAL:CG1	17:Q:103:VAL:H	1.38	1.25
26:2:28:PRO:N	27:3:25:GLN:HA	0.95	1.25
17:Q:113:ARG:NH2	18:R:218:LYS:HE2	1.52	1.24
1:A:204:HIS:O	1:A:205:VAL:O	1.55	1.24
3:C:5:ASN:C	3:C:7:PRO:HD3	1.45	1.24
1:A:199:TYR:OH	13:M:93:PHE:CE2	1.84	1.23
22:V:321:GLU:OE2	23:W:500:ASP:CB	1.85	1.23
1:A:927:GLU:CB	1:A:931:ARG:HD2	1.69	1.23
17:Q:29:GLU:CD	18:R:194:ARG:HH21	1.45	1.23
22:V:674:THR:HG23	26:2:392:ARG:NH2	1.53	1.23
22:V:321:GLU:CB	23:W:499:ASN:OD1	1.88	1.22
17:Q:105:TYR:HE1	18:R:231:GLU:CG	1.51	1.22
23:W:59:TYR:CZ	23:W:62:ALA:CB	2.22	1.22
22:V:531:ILE:CG2	22:V:534:TYR:OH	1.88	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:58:ALA:N	27:3:71:TYR:OH	1.73	1.22
8:H:107:GLU:O	8:H:108:ALA:O	1.58	1.21
9:I:14:ILE:HG13	9:I:16:PHE:CE2	1.77	1.20
18:R:190:LEU:CD1	18:R:205:ASP:OD2	1.90	1.20
22:V:516:PRO:CG	25:1:15:ALA:CB	1.90	1.19
25:1:59:GLU:OE2	26:2:402:ARG:NH2	1.75	1.19
17:Q:113:ARG:HH22	18:R:218:LYS:CE	1.53	1.19
1:A:927:GLU:HB2	1:A:931:ARG:HD2	1.21	1.19
22:V:531:ILE:HG23	22:V:534:TYR:CZ	1.78	1.19
23:W:209:TYR:OH	23:W:233:PHE:HA	1.39	1.19
5:E:52:ARG:CB	5:E:53:PRO:HD2	1.71	1.18
22:V:531:ILE:CA	22:V:534:TYR:CE2	2.25	1.18
8:H:85:ALA:O	8:H:87:GLN:OE1	1.58	1.18
2:B:80:GLU:HB3	2:B:135:GLU:CG	1.73	1.18
5:E:64:HIS:NE2	5:E:69:THR:OG1	1.74	1.18
23:W:59:TYR:CZ	23:W:62:ALA:HB1	1.77	1.18
27:3:66:GLU:HA	27:3:132:LEU:HD12	1.22	1.17
22:V:325:ARG:HH22	23:W:499:ASN:CB	1.55	1.17
22:V:516:PRO:HB3	25:1:15:ALA:HB1	1.24	1.17
2:B:79:GLU:O	2:B:80:GLU:CG	1.93	1.16
10:J:63:ALA:N	10:J:64:PRO:CD	2.06	1.16
27:3:59:VAL:N	27:3:71:TYR:CE1	2.12	1.16
2:B:133:ILE:HD13	2:B:139:GLN:HB3	1.18	1.16
25:1:28:ALA:HB1	25:1:31:LYS:HD2	1.27	1.16
26:2:117:ASN:ND2	27:3:108:ASN:HB2	0.85	1.16
27:3:59:VAL:CG1	27:3:71:TYR:CD1	1.97	1.16
25:1:2:VAL:CG1	26:2:456:LYS:HG2	1.74	1.16
2:B:90:GLN:NE2	20:T:141:LEU:HA	1.59	1.15
2:B:80:GLU:O	2:B:135:GLU:HG3	1.45	1.15
1:A:133:SER:O	1:A:135:GLY:N	1.77	1.15
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.42	1.15
1:A:927:GLU:CB	1:A:931:ARG:CD	2.19	1.15
1:A:1114:ALA:C	1:A:1116:ASN:H	1.43	1.15
1:A:1319:LYS:CD	1:A:1333:GLU:OE2	1.94	1.15
22:V:321:GLU:CB	23:W:499:ASN:ND2	2.05	1.15
5:E:54:ARG:CB	5:E:78:GLU:OE1	1.95	1.15
5:E:64:HIS:CD2	5:E:69:THR:N	2.13	1.15
2:B:861:SER:O	2:B:896:LEU:CD2	1.94	1.14
25:1:2:VAL:HG13	26:2:422:LEU:HD11	1.20	1.14
17:Q:109:HIS:ND1	18:R:224:THR:OG1	1.80	1.14
26:2:28:PRO:HA	27:3:33:THR:HB	1.14	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:GLU:OE1	2:B:135:GLU:O	1.66	1.14
23:W:419:GLU:HB3	23:W:420:PRO:CD	1.76	1.14
25:1:1:MET:CG	26:2:413:LEU:HB3	1.76	1.14
2:B:90:GLN:NE2	20:T:141:LEU:CG	2.10	1.14
23:W:421:PHE:HE1	23:W:423:ASP:HB3	1.12	1.14
17:Q:180:PHE:CE2	18:R:211:SER:CB	2.26	1.13
26:2:211:GLN:HG3	26:2:257:SER:HB3	1.29	1.13
27:3:57:LEU:C	27:3:71:TYR:OH	1.92	1.13
13:M:179:GLU:HA	20:T:154:LYS:HG2	1.25	1.13
2:B:80:GLU:CB	2:B:135:GLU:HB2	1.68	1.12
2:B:91:ILE:HG23	20:T:141:LEU:HD12	1.16	1.12
25:1:13:ASP:CG	25:1:14:PRO:HD2	1.74	1.12
2:B:90:GLN:HE22	20:T:141:LEU:CB	1.61	1.12
24:0:54:ARG:CG	27:3:182:PHE:CE1	2.17	1.12
3:C:137:ASN:HB2	3:C:145:GLN:HE22	1.13	1.12
5:E:55:ARG:O	5:E:76:PHE:O	1.67	1.12
23:W:59:TYR:CE2	23:W:62:ALA:CB	2.32	1.12
20:T:141:LEU:O	20:T:143:GLN:OE1	1.66	1.11
25:1:9:LEU:HD13	25:1:48:GLU:HA	1.32	1.11
27:3:59:VAL:HG13	27:3:70:LEU:HB2	1.27	1.11
27:3:57:LEU:O	27:3:71:TYR:HE2	1.30	1.11
10:J:62:TYR:C	10:J:64:PRO:CD	2.22	1.11
22:V:315:VAL:CG1	23:W:500:ASP:CB	1.94	1.11
25:1:5:LEU:CD2	26:2:408:LEU:HD13	1.80	1.11
26:2:42:LEU:HD21	26:2:55:TRP:HB2	1.21	1.11
1:A:266:MET:HG3	1:A:272:ASN:ND2	1.51	1.10
1:A:611:ASP:OD2	1:A:627:LYS:HE3	1.51	1.10
1:A:1319:LYS:HG2	1:A:1333:GLU:CG	1.80	1.10
5:E:51:GLY:O	5:E:52:ARG:HG3	0.95	1.10
23:W:419:GLU:CB	23:W:420:PRO:HD2	1.78	1.10
26:2:160:LEU:HD23	26:2:206:LEU:HD21	1.25	1.10
26:2:163:MET:HE2	26:2:206:LEU:HD12	1.30	1.10
1:A:326:PRO:HB3	13:M:87:GLY:CA	1.81	1.10
25:1:18:GLN:HB2	25:1:44:PHE:CE2	1.86	1.10
1:A:271:ARG:HG2	13:M:73:PRO:HG3	1.33	1.09
22:V:516:PRO:CB	25:1:15:ALA:HB1	1.81	1.09
26:2:171:VAL:HG22	26:2:213:TRP:HA	1.27	1.09
9:I:14:ILE:HG13	9:I:16:PHE:CZ	1.86	1.09
21:U:230:SER:O	21:U:231:ASP:HB2	1.50	1.09
22:V:531:ILE:HG23	22:V:534:TYR:OH	0.92	1.09
25:1:2:VAL:HG11	26:2:456:LYS:CG	1.81	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:192:GLU:HG3	26:2:193:PRO:HD2	1.33	1.09
27:3:49:LEU:HB3	27:3:101:TYR:HB3	1.15	1.09
5:E:64:HIS:NE2	5:E:69:THR:N	1.99	1.09
22:V:519:TYR:CE2	25:1:20:LEU:HG	1.87	1.09
1:A:1250:ASP:HB3	21:U:227:GLU:HG3	1.35	1.09
13:M:94:ASP:O	13:M:97:GLY:N	1.84	1.09
25:1:5:LEU:HD11	26:2:408:LEU:HB3	1.17	1.09
17:Q:29:GLU:OE2	18:R:194:ARG:NH2	1.84	1.08
22:V:321:GLU:OE2	23:W:500:ASP:HB3	0.91	1.08
2:B:225:LEU:HD11	2:B:228:SER:CB	1.81	1.08
27:3:137:LEU:HB3	27:3:180:VAL:HG11	1.34	1.08
2:B:80:GLU:OE1	2:B:135:GLU:CB	2.01	1.08
25:1:5:LEU:HD21	26:2:408:LEU:CD1	1.82	1.08
26:2:30:VAL:H	27:3:25:GLN:CB	1.67	1.07
26:2:30:VAL:H	27:3:25:GLN:HB3	1.00	1.07
2:B:80:GLU:HB3	2:B:135:GLU:CB	1.81	1.07
26:2:159:VAL:HG13	26:2:161:HIS:H	1.16	1.07
27:3:59:VAL:HB	27:3:71:TYR:CE1	1.89	1.07
22:V:516:PRO:HG2	22:V:706:LYS:HZ3	0.97	1.07
2:B:882:SER:O	2:B:887:TYR:CD1	2.06	1.07
22:V:516:PRO:HG2	22:V:706:LYS:NZ	1.70	1.07
25:1:2:VAL:HG11	26:2:456:LYS:HG2	1.09	1.07
5:E:52:ARG:HB3	5:E:53:PRO:HD3	1.30	1.06
24:0:54:ARG:HB2	27:3:209:ILE:HG23	1.35	1.06
13:M:10:LEU:N	13:M:11:PRO:HD2	1.66	1.06
17:Q:102:VAL:HG13	17:Q:103:VAL:N	1.37	1.06
13:M:11:PRO:O	13:M:12:ARG:CG	2.03	1.06
2:B:80:GLU:HB3	2:B:135:GLU:HG3	1.25	1.06
23:W:424:ARG:O	23:W:425:THR:HG23	1.52	1.06
2:B:225:LEU:HD11	2:B:228:SER:HB2	1.38	1.06
24:0:97:ASP:O	27:3:208:ASP:CB	2.02	1.06
5:E:54:ARG:HB2	5:E:78:GLU:OE1	1.51	1.05
17:Q:51:LEU:HD11	18:R:163:LEU:HD11	1.10	1.05
17:Q:180:PHE:CZ	18:R:211:SER:HB3	1.84	1.05
27:3:22:TRP:O	27:3:25:GLN:HG3	1.56	1.05
9:I:62:VAL:O	9:I:64:GLU:N	1.89	1.05
17:Q:108:ASP:O	18:R:234:GLU:OE2	1.72	1.05
25:1:1:MET:CB	26:2:413:LEU:HB3	1.87	1.05
22:V:674:THR:HG23	26:2:392:ARG:CZ	1.85	1.04
27:3:57:LEU:O	27:3:71:TYR:CE2	2.10	1.04
13:M:178:LYS:O	20:T:154:LYS:CB	2.04	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:105:TYR:CE1	18:R:231:GLU:CG	2.34	1.04
17:Q:180:PHE:HZ	18:R:211:SER:CA	1.68	1.04
25:1:5:LEU:HD12	26:2:409:TYR:O	1.56	1.04
22:V:516:PRO:CG	22:V:706:LYS:NZ	2.18	1.04
1:A:326:PRO:HB3	13:M:87:GLY:HA2	1.38	1.04
1:A:926:ASN:HD22	1:A:932:ARG:HG3	1.22	1.03
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.10	1.03
26:2:234:LEU:HD21	26:2:237:LEU:HD12	1.36	1.03
17:Q:51:LEU:CD1	18:R:163:LEU:HD11	1.87	1.03
22:V:516:PRO:CB	25:1:15:ALA:CB	2.36	1.03
26:2:81:LYS:HE3	26:2:93:LEU:HD21	1.40	1.03
1:A:212:LYS:O	1:A:213:LYS:HB3	1.55	1.02
1:A:326:PRO:CB	13:M:87:GLY:HA2	1.88	1.02
3:C:5:ASN:O	3:C:7:PRO:HD3	0.86	1.02
24:0:54:ARG:CD	27:3:182:PHE:HE1	1.72	1.02
25:1:4:VAL:HG12	26:2:411:GLN:O	1.55	1.02
1:A:927:GLU:CA	1:A:931:ARG:HG3	1.89	1.02
2:B:90:GLN:NE2	20:T:141:LEU:CB	2.22	1.02
5:E:52:ARG:HB3	5:E:53:PRO:HD2	1.26	1.02
16:P:206:GLU:HG3	16:P:236:LYS:NZ	1.75	1.02
24:0:54:ARG:NE	27:3:182:PHE:CE1	2.26	1.02
16:P:206:GLU:HG3	16:P:236:LYS:HZ2	1.20	1.02
2:B:90:GLN:HE22	20:T:141:LEU:HA	0.90	1.02
3:C:212:ASP:O	3:C:214:ASP:N	1.93	1.02
25:1:34:ILE:HG12	25:1:50:VAL:HG11	1.39	1.02
16:P:297:LYS:CB	16:P:298:PRO:CD	2.36	1.01
22:V:528:LYS:HE2	29:Y:25:DT:C5'	1.88	1.01
26:2:117:ASN:CG	27:3:108:ASN:CB	2.20	1.01
27:3:196:LEU:HD21	27:3:223:LEU:HD23	1.42	1.01
2:B:1066:PRO:HB3	13:M:46:ILE:HD13	1.38	1.01
29:Y:36:DA:C4	29:Y:37:DG:N7	2.29	1.01
1:A:266:MET:HG2	1:A:272:ASN:HD21	1.24	1.01
2:B:861:SER:O	2:B:896:LEU:HD23	1.57	1.01
3:C:212:ASP:C	3:C:214:ASP:H	1.69	1.01
22:V:523:VAL:HG11	25:1:20:LEU:HD21	1.02	1.01
26:2:199:ALA:HB3	26:2:202:GLN:HE22	1.22	1.01
27:3:59:VAL:CB	27:3:71:TYR:CE1	2.43	1.01
1:A:265:VAL:O	1:A:272:ASN:ND2	1.91	1.00
1:A:1113:SER:O	1:A:1114:ALA:CB	2.04	1.00
23:W:59:TYR:CE2	23:W:62:ALA:HB3	1.95	1.00
24:0:77:LYS:O	24:0:79:ASN:N	1.93	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:895:PHE:O	2:B:897:ARG:NH1	1.94	1.00
22:V:315:VAL:HG11	23:W:500:ASP:HB2	1.42	1.00
22:V:515:SER:HB3	22:V:539:ASN:HD21	1.27	1.00
1:A:927:GLU:HB3	1:A:931:ARG:HG2	1.42	1.00
5:E:52:ARG:CB	5:E:53:PRO:CD	2.27	1.00
10:J:63:ALA:N	10:J:64:PRO:HD2	1.74	1.00
17:Q:23:ARG:NH2	18:R:209:GLN:H	1.59	1.00
22:V:613:THR:O	22:V:614:SER:HB2	1.59	1.00
27:3:58:ALA:CA	27:3:71:TYR:CZ	2.44	1.00
27:3:148:ASN:HB2	27:3:157:MET:HE2	1.42	1.00
23:W:419:GLU:HB3	23:W:420:PRO:HD2	1.02	0.99
2:B:92:TYR:HB3	20:T:145:LEU:HB2	1.41	0.99
10:J:64:PRO:C	10:J:66:GLU:H	1.66	0.99
1:A:265:VAL:C	1:A:272:ASN:HD21	1.71	0.99
5:E:47:LYS:CB	5:E:48:PRO:HD2	1.91	0.99
1:A:1113:SER:O	1:A:1114:ALA:HB2	1.56	0.99
1:A:622:SER:O	1:A:624:GLY:N	1.95	0.99
5:E:47:LYS:HB2	5:E:48:PRO:HD2	1.00	0.99
1:A:326:PRO:CA	13:M:87:GLY:HA2	1.92	0.99
25:1:1:MET:HE1	26:2:440:LEU:HD13	1.44	0.98
1:A:197:GLU:OE2	13:M:93:PHE:CE2	2.16	0.98
2:B:225:LEU:CD1	2:B:228:SER:HB2	1.92	0.98
23:W:209:TYR:OH	23:W:233:PHE:CA	2.10	0.98
2:B:878:ASP:O	2:B:879:GLU:O	1.81	0.98
26:2:196:ILE:HD11	26:2:210:ALA:HB2	1.45	0.98
1:A:271:ARG:CG	13:M:73:PRO:HG3	1.94	0.98
22:V:523:VAL:CG1	25:1:20:LEU:HD21	1.94	0.98
26:2:118:LEU:CD2	27:3:39:ASP:O	2.12	0.98
8:H:85:ALA:C	8:H:87:GLN:OE1	2.06	0.97
16:P:206:GLU:CG	16:P:236:LYS:HZ2	1.76	0.97
17:Q:109:HIS:CG	18:R:224:THR:OG1	2.17	0.97
27:3:173:GLN:HA	27:3:176:ASN:HD21	1.28	0.97
23:W:584:TYR:CD1	23:W:594:ALA:HB2	1.99	0.97
1:A:133:SER:C	1:A:135:GLY:H	1.72	0.97
5:E:55:ARG:N	5:E:78:GLU:OE2	1.96	0.97
1:A:47:THR:O	1:A:48:GLU:O	1.82	0.97
20:T:153:TYR:CZ	20:T:155:PRO:HB3	2.00	0.97
1:A:265:VAL:O	1:A:272:ASN:OD1	1.82	0.97
26:2:176:ALA:HB1	26:2:178:LEU:HD13	1.47	0.97
26:2:100:LEU:HD11	26:2:119:ARG:HG3	1.46	0.97
27:3:165:LYS:HD2	27:3:195:VAL:HG22	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ALA:HB2	20:T:201:ASP:HB3	1.46	0.97
8:H:66:GLU:O	8:H:67:ASP:HB2	1.62	0.96
5:E:47:LYS:HE2	5:E:52:ARG:HB2	1.45	0.96
22:V:531:ILE:HG23	22:V:534:TYR:HH	1.29	0.96
27:3:59:VAL:CB	27:3:71:TYR:CD1	2.47	0.96
17:Q:105:TYR:O	17:Q:109:HIS:CD2	2.19	0.96
23:W:298:ALA:HA	23:W:421:PHE:CE2	2.01	0.96
2:B:80:GLU:CD	2:B:135:GLU:HB3	1.89	0.96
2:B:91:ILE:HG23	20:T:141:LEU:CD1	1.95	0.96
1:A:1319:LYS:CG	1:A:1333:GLU:OE2	2.06	0.96
2:B:133:ILE:HA	2:B:139:GLN:HA	1.48	0.96
3:C:7:PRO:HG2	11:K:97:GLU:OE2	1.65	0.96
1:A:926:ASN:HD21	1:A:932:ARG:HG2	0.82	0.96
1:A:1319:LYS:CD	1:A:1356:ARG:HH12	1.79	0.96
20:T:177:ARG:C	20:T:179:ASP:H	1.74	0.95
29:Y:36:DA:C6	29:Y:37:DG:C6	2.53	0.95
2:B:861:SER:O	2:B:896:LEU:HD22	1.66	0.95
23:W:59:TYR:CE1	23:W:62:ALA:HB1	2.02	0.95
5:E:54:ARG:HB3	5:E:78:GLU:OE1	1.67	0.95
21:U:251:ALA:O	21:U:253:THR:N	1.97	0.95
27:3:133:LEU:HD23	27:3:177:PHE:CD1	2.01	0.95
1:A:495:ASP:O	1:A:497:ASP:N	1.98	0.95
1:A:1319:LYS:HG2	1:A:1333:GLU:OE2	1.63	0.95
25:1:13:ASP:OD2	25:1:17:LYS:HB3	1.65	0.95
25:1:18:GLN:HB2	25:1:44:PHE:HE2	1.26	0.95
26:2:28:PRO:HA	27:3:33:THR:CB	1.95	0.95
26:2:211:GLN:HA	26:2:261:PHE:CZ	2.02	0.95
27:3:59:VAL:HB	27:3:71:TYR:HE1	1.25	0.95
22:V:321:GLU:CA	23:W:499:ASN:HD21	1.78	0.95
25:1:2:VAL:CG1	26:2:422:LEU:HD11	1.96	0.95
2:B:133:ILE:O	2:B:134:LYS:O	1.83	0.95
5:E:64:HIS:NE2	5:E:69:THR:CA	2.29	0.95
26:2:118:LEU:HD11	27:3:43:VAL:CG2	1.95	0.95
22:V:531:ILE:HA	22:V:534:TYR:CD2	2.01	0.94
23:W:209:TYR:HH	23:W:233:PHE:HA	1.31	0.94
10:J:63:ALA:N	10:J:64:PRO:HD3	1.79	0.94
22:V:516:PRO:HA	25:1:15:ALA:O	1.65	0.94
25:1:1:MET:HB3	26:2:413:LEU:CG	1.98	0.94
13:M:39:LEU:O	13:M:40:VAL:O	1.84	0.94
21:U:256:THR:OG1	21:U:272:THR:HG22	1.66	0.94
21:U:231:ASP:O	21:U:232:GLU:CG	2.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:696:TRP:CD1	23:W:697:ILE:HG12	2.02	0.94
26:2:117:ASN:N	27:3:104:LEU:HD21	1.83	0.94
5:E:64:HIS:CE1	5:E:69:THR:OG1	2.19	0.94
1:A:265:VAL:O	1:A:272:ASN:CG	2.10	0.94
22:V:528:LYS:HE2	29:Y:25:DT:H5'	1.46	0.94
2:B:78:VAL:O	2:B:79:GLU:HB2	1.66	0.94
1:A:206:ASN:O	1:A:208:ASP:N	2.00	0.94
18:R:190:LEU:HD11	18:R:205:ASP:OD2	1.65	0.94
26:2:35:TYR:CE1	26:2:62:LEU:HG	2.02	0.94
2:B:76:GLY:O	2:B:77:GLU:HB2	1.67	0.94
22:V:325:ARG:HH21	23:W:499:ASN:HB3	1.20	0.94
25:1:9:LEU:HD22	25:1:51:ASN:HD22	1.33	0.94
22:V:515:SER:CB	22:V:539:ASN:HD21	1.80	0.93
1:A:1310:HIS:HB3	21:U:252:LYS:HD3	1.48	0.93
2:B:80:GLU:O	2:B:135:GLU:CG	2.16	0.93
16:P:297:LYS:HA	16:P:297:LYS:CE	1.96	0.93
22:V:631:GLY:O	22:V:632:SER:CB	2.14	0.93
27:3:187:GLN:HG3	27:3:189:ILE:HG12	1.51	0.93
5:E:64:HIS:HD2	5:E:68:PRO:HA	1.33	0.93
17:Q:105:TYR:CD1	18:R:231:GLU:OE2	2.21	0.93
17:Q:105:TYR:CD1	18:R:231:GLU:CD	2.46	0.93
8:H:64:LEU:HB3	8:H:84:ARG:HD3	1.48	0.93
26:2:30:VAL:N	27:3:25:GLN:HB3	1.82	0.93
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.51	0.93
26:2:177:GLN:HA	26:2:220:LEU:CD2	1.99	0.93
27:3:133:LEU:HD13	27:3:133:LEU:H	1.33	0.93
26:2:118:LEU:HD23	27:3:42:MET:HB2	1.50	0.93
1:A:1114:ALA:C	1:A:1116:ASN:N	2.18	0.92
9:I:105:GLU:O	9:I:106:ASP:HB2	1.69	0.92
15:O:3:TYR:O	15:O:5:LEU:N	2.01	0.92
18:R:162:GLY:O	18:R:164:GLY:N	2.01	0.92
3:C:7:PRO:CG	11:K:97:GLU:OE2	2.17	0.92
27:3:11:LEU:HD22	27:3:160:ARG:HG2	1.51	0.92
22:V:523:VAL:CG1	25:1:20:LEU:CD2	2.45	0.92
27:3:190:LEU:HA	27:3:210:THR:HG22	1.50	0.92
2:B:80:GLU:CB	2:B:135:GLU:HB3	1.94	0.92
27:3:165:LYS:HE3	27:3:200:SER:CB	2.00	0.92
17:Q:113:ARG:HH22	18:R:218:LYS:HE3	1.34	0.92
22:V:531:ILE:HA	22:V:534:TYR:HE2	1.10	0.92
8:H:85:ALA:CA	8:H:87:GLN:OE1	2.18	0.91
9:I:85:PRO:O	9:I:86:CYS:C	2.12	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:230:SER:O	21:U:231:ASP:CB	2.18	0.91
25:1:8:VAL:HG11	25:1:45:VAL:CG1	1.99	0.91
2:B:92:TYR:CG	20:T:145:LEU:HD13	2.03	0.91
20:T:153:TYR:OH	20:T:155:PRO:HB3	1.69	0.91
24:0:97:ASP:OD1	27:3:208:ASP:OD1	1.88	0.91
26:2:118:LEU:HD22	27:3:39:ASP:CG	1.94	0.91
1:A:551:ARG:CD	1:A:625:ASP:OD2	2.17	0.91
16:P:297:LYS:HA	16:P:297:LYS:HE2	1.49	0.91
18:R:162:GLY:C	18:R:164:GLY:H	1.79	0.91
1:A:926:ASN:ND2	1:A:932:ARG:HG2	1.59	0.91
2:B:225:LEU:CD1	2:B:228:SER:CB	2.49	0.91
2:B:721:ARG:HG3	2:B:977:THR:HG22	1.52	0.91
2:B:90:GLN:HE21	20:T:141:LEU:HD23	0.87	0.91
26:2:81:LYS:CE	26:2:93:LEU:HD21	2.00	0.91
27:3:58:ALA:C	27:3:71:TYR:CZ	2.49	0.91
27:3:137:LEU:CB	27:3:180:VAL:HG11	2.01	0.91
1:A:1319:LYS:HG2	1:A:1333:GLU:HG2	1.53	0.90
22:V:516:PRO:CD	22:V:706:LYS:HZ3	1.84	0.90
24:0:54:ARG:HG3	27:3:182:PHE:CZ	2.05	0.90
5:E:55:ARG:HG2	5:E:76:PHE:HB3	1.51	0.90
23:W:59:TYR:CE1	23:W:62:ALA:CB	2.53	0.90
26:2:81:LYS:HD2	26:2:89:LEU:HD21	1.52	0.90
25:1:1:MET:HB3	26:2:413:LEU:HB3	1.52	0.90
26:2:159:VAL:HG22	26:2:160:LEU:HD12	1.51	0.90
24:0:98:GLN:OE1	27:3:209:ILE:HA	1.70	0.90
1:A:926:ASN:OD1	1:A:931:ARG:HB3	1.72	0.89
22:V:315:VAL:HG13	23:W:500:ASP:CA	2.03	0.89
3:C:137:ASN:CB	3:C:145:GLN:HE22	1.84	0.89
1:A:1319:LYS:HD3	1:A:1356:ARG:HH12	1.35	0.89
25:1:47:ALA:CB	25:1:50:VAL:HB	2.03	0.89
1:A:1250:ASP:CB	21:U:227:GLU:CG	2.06	0.89
25:1:8:VAL:HG11	25:1:45:VAL:HG13	1.55	0.89
27:3:165:LYS:HG3	27:3:203:LEU:HD12	1.52	0.89
1:A:608:THR:C	1:A:610:PRO:HD2	1.98	0.89
26:2:160:LEU:HB3	26:2:206:LEU:HD11	1.53	0.89
1:A:212:LYS:O	1:A:213:LYS:CB	2.19	0.89
1:A:199:TYR:OH	13:M:93:PHE:HE2	1.26	0.89
27:3:177:PHE:CE2	27:3:181:ILE:HD11	2.08	0.88
1:A:199:TYR:CZ	13:M:93:PHE:CZ	2.60	0.88
1:A:1319:LYS:HG3	1:A:1333:GLU:CD	1.96	0.88
23:W:696:TRP:CD1	23:W:697:ILE:CG1	2.57	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:4:VAL:HG11	26:2:412:PHE:HD2	1.36	0.88
27:3:70:LEU:HD13	27:3:115:ILE:HD11	1.55	0.88
26:2:160:LEU:CA	26:2:206:LEU:HD11	2.04	0.88
2:B:225:LEU:HD11	2:B:228:SER:HB3	1.56	0.88
26:2:117:ASN:CB	27:3:42:MET:CE	2.51	0.88
5:E:64:HIS:CE1	5:E:69:THR:HG1	1.91	0.88
26:2:243:SER:CB	26:2:258:LEU:HD22	2.04	0.88
17:Q:113:ARG:NH2	18:R:218:LYS:CE	2.23	0.87
26:2:163:MET:SD	26:2:196:ILE:HG21	2.14	0.87
25:1:28:ALA:CB	25:1:31:LYS:HD2	2.04	0.87
26:2:118:LEU:HD11	27:3:43:VAL:HG22	1.56	0.87
27:3:177:PHE:CD2	27:3:181:ILE:HD11	2.08	0.87
10:J:62:TYR:O	10:J:64:PRO:HD2	1.75	0.87
5:E:48:PRO:O	5:E:49:SER:HB2	1.72	0.87
23:W:584:TYR:CE2	23:W:614:TYR:HB2	2.10	0.87
1:A:153:ILE:O	1:A:154:CYS:O	1.93	0.87
16:P:162:VAL:HG23	16:P:164:GLN:NE2	1.88	0.87
26:2:160:LEU:CD2	26:2:206:LEU:HD21	2.04	0.87
26:2:160:LEU:CB	26:2:206:LEU:HD11	2.04	0.87
27:3:59:VAL:CG1	27:3:70:LEU:HB2	2.03	0.87
23:W:37:HIS:CE1	23:W:454:VAL:HG13	2.09	0.87
26:2:45:PHE:HB2	26:2:51:LEU:HD13	1.56	0.87
26:2:117:ASN:OD1	27:3:108:ASN:CB	2.23	0.87
26:2:218:GLN:HB3	26:2:264:HIS:CD2	2.08	0.87
27:3:165:LYS:HE3	27:3:200:SER:HB2	1.56	0.87
1:A:153:ILE:O	1:A:154:CYS:C	2.18	0.87
1:A:355:MET:SD	2:B:1091:ARG:NH1	2.48	0.87
23:W:430:ASN:HB3	23:W:431:PRO:HD2	1.54	0.87
2:B:91:ILE:CG2	20:T:141:LEU:CD1	2.52	0.87
27:3:71:TYR:CD2	27:3:72:PRO:HD2	2.08	0.87
13:M:86:LYS:HA	13:M:86:LYS:CE	2.05	0.87
13:M:182:ALA:HB2	20:T:154:LYS:HG3	1.56	0.87
2:B:80:GLU:CB	2:B:135:GLU:HG3	2.05	0.86
2:B:90:GLN:HE21	20:T:141:LEU:CG	1.80	0.86
26:2:48:LEU:HB3	26:2:49:PRO:HD3	1.57	0.86
17:Q:24:GLY:CA	18:R:210:PHE:CE2	2.58	0.86
23:W:421:PHE:CD1	23:W:423:ASP:CB	2.31	0.86
1:A:204:HIS:O	1:A:205:VAL:C	2.18	0.86
13:M:44:ARG:HE	13:M:46:ILE:CG2	1.88	0.86
15:O:3:TYR:HB3	15:O:98:CYS:SG	2.15	0.86
25:1:1:MET:HB3	26:2:413:LEU:CB	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:138:PRO:HG3	26:2:189:GLU:HG3	1.57	0.86
26:2:224:GLN:HB2	26:2:268:PHE:CZ	2.09	0.86
27:3:14:VAL:HG21	27:3:163:VAL:HG22	1.57	0.86
27:3:64:ILE:HG13	27:3:123:ASP:HB3	1.57	0.86
1:A:271:ARG:CG	13:M:73:PRO:CG	2.52	0.86
23:W:59:TYR:CG	23:W:62:ALA:HB2	2.11	0.86
25:1:1:MET:O	26:2:413:LEU:CG	2.21	0.86
26:2:30:VAL:HG23	27:3:25:GLN:HB2	0.86	0.86
26:2:117:ASN:OD1	27:3:108:ASN:CG	2.18	0.86
27:3:178:MET:HE2	27:3:202:LEU:CD1	2.05	0.86
2:B:133:ILE:HD13	2:B:139:GLN:CB	2.03	0.86
5:E:51:GLY:C	5:E:52:ARG:HG3	2.01	0.86
20:T:177:ARG:NH1	20:T:209:PRO:O	2.07	0.86
26:2:218:GLN:HB3	26:2:264:HIS:HD2	1.38	0.86
26:2:171:VAL:HG22	26:2:213:TRP:CA	2.06	0.86
27:3:58:ALA:C	27:3:71:TYR:CE1	2.53	0.86
15:O:3:TYR:C	15:O:5:LEU:H	1.83	0.86
17:Q:105:TYR:HE1	18:R:231:GLU:HG3	1.40	0.86
25:1:2:VAL:HG13	26:2:422:LEU:CD1	2.03	0.86
17:Q:105:TYR:CD1	17:Q:109:HIS:NE2	2.32	0.86
27:3:69:PHE:CZ	27:3:139:LYS:HB3	2.10	0.86
26:2:81:LYS:CD	26:2:89:LEU:HD21	2.06	0.85
1:A:271:ARG:NE	13:M:73:PRO:HG2	1.91	0.85
22:V:316:LEU:HB2	22:V:321:GLU:HG3	1.58	0.85
23:W:696:TRP:NE1	23:W:697:ILE:HG12	1.90	0.85
25:1:1:MET:SD	26:2:415:GLN:O	2.34	0.85
26:2:31:LEU:CD2	27:3:33:THR:N	2.32	0.85
27:3:100:LYS:HB3	27:3:103:LEU:HD13	1.58	0.85
1:A:923:ASP:O	1:A:932:ARG:NH1	2.09	0.85
2:B:1066:PRO:CB	13:M:46:ILE:HD13	2.05	0.85
9:I:15:ARG:O	9:I:16:PHE:O	1.93	0.85
21:U:231:ASP:O	21:U:232:GLU:HG2	1.75	0.85
26:2:211:GLN:HG3	26:2:257:SER:CB	2.05	0.85
27:3:160:ARG:HB3	27:3:190:LEU:HD21	1.57	0.85
13:M:107:MET:HG2	29:Y:63:DG:H22	1.41	0.85
22:V:631:GLY:O	22:V:632:SER:HB2	1.76	0.85
26:2:118:LEU:CD2	27:3:42:MET:HB2	2.06	0.85
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.57	0.85
26:2:31:LEU:N	27:3:25:GLN:O	2.08	0.85
22:V:612:ASP:C	22:V:614:SER:H	1.83	0.85
26:2:81:LYS:CD	26:2:93:LEU:HD21	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:59:VAL:HG12	27:3:71:TYR:CG	2.07	0.85
27:3:190:LEU:HA	27:3:210:THR:CG2	2.05	0.85
23:W:59:TYR:CD2	23:W:62:ALA:HB2	2.12	0.85
1:A:324:GLY:HA2	13:M:90:ALA:HB3	1.57	0.85
2:B:751:LEU:HD12	2:B:808:SER:HB3	1.56	0.85
16:P:206:GLU:CG	16:P:236:LYS:NZ	2.36	0.85
26:2:221:GLN:HG2	26:2:268:PHE:CZ	2.11	0.85
5:E:64:HIS:CD2	5:E:70:ASP:H	1.95	0.85
16:P:297:LYS:HB3	16:P:298:PRO:HD2	1.59	0.84
27:3:124:ILE:HD13	27:3:125:LYS:N	1.91	0.84
1:A:930:LEU:O	1:A:931:ARG:O	1.94	0.84
2:B:179:LEU:HD11	2:B:771:GLU:HG2	1.59	0.84
23:W:298:ALA:HA	23:W:421:PHE:CD2	2.12	0.84
26:2:159:VAL:HG22	26:2:160:LEU:H	1.41	0.84
1:A:271:ARG:NE	13:M:73:PRO:CG	2.40	0.84
1:A:477:LEU:HD11	1:A:483:ARG:HD3	1.58	0.84
27:3:49:LEU:HB3	27:3:101:TYR:CB	2.05	0.84
8:H:85:ALA:HA	8:H:87:GLN:OE1	1.78	0.84
25:1:2:VAL:CG1	26:2:422:LEU:CD1	2.55	0.84
27:3:49:LEU:CB	27:3:101:TYR:HB3	2.05	0.84
5:E:62:VAL:CG2	5:E:72:MET:HB3	2.07	0.84
26:2:78:GLU:O	26:2:81:LYS:HG2	1.77	0.84
1:A:1313:GLN:HE22	1:A:1318:LYS:HE2	1.41	0.84
17:Q:109:HIS:HA	18:R:234:GLU:OE1	1.76	0.84
26:2:176:ALA:CB	26:2:178:LEU:HD13	2.07	0.84
27:3:178:MET:HE2	27:3:202:LEU:HD12	1.57	0.84
16:P:162:VAL:O	16:P:163:PRO:C	2.20	0.84
26:2:177:GLN:HA	26:2:220:LEU:HD21	1.56	0.84
27:3:58:ALA:HA	27:3:71:TYR:CE2	2.12	0.84
26:2:221:GLN:NE2	26:2:230:LEU:HB2	1.93	0.84
17:Q:109:HIS:CG	18:R:224:THR:CB	2.61	0.84
26:2:159:VAL:HG22	26:2:160:LEU:CD1	2.08	0.84
26:2:229:ASP:O	26:2:233:ILE:HG12	1.78	0.84
2:B:91:ILE:HG22	20:T:141:LEU:HD12	1.56	0.83
26:2:118:LEU:CD2	27:3:39:ASP:HA	2.07	0.83
27:3:184:ALA:HA	27:3:187:GLN:HG2	1.57	0.83
1:A:927:GLU:HB3	1:A:931:ARG:HG3	0.84	0.83
26:2:160:LEU:HD23	26:2:206:LEU:CD2	2.07	0.83
17:Q:23:ARG:CZ	18:R:209:GLN:H	1.91	0.83
26:2:118:LEU:HD12	26:2:119:ARG:N	1.92	0.83
1:A:609:HIS:N	1:A:610:PRO:CD	2.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:516:PRO:CG	25:1:15:ALA:HB1	1.95	0.83
22:V:516:PRO:HG3	25:1:15:ALA:HB2	1.57	0.83
25:1:52:VAL:HG23	25:1:53:LEU:HD12	1.59	0.83
26:2:57:MET:HA	26:2:60:LEU:CD1	2.09	0.83
2:B:80:GLU:HB2	2:B:135:GLU:HB2	0.86	0.83
13:M:94:ASP:O	13:M:97:GLY:CA	2.27	0.83
26:2:167:PRO:O	26:2:171:VAL:HG23	1.76	0.83
13:M:94:ASP:HB2	13:M:99:SER:H	1.44	0.83
26:2:30:VAL:CB	27:3:25:GLN:HB2	2.07	0.83
26:2:160:LEU:O	26:2:164:VAL:HG23	1.79	0.83
27:3:196:LEU:HD21	27:3:223:LEU:CD2	2.09	0.83
22:V:703:PHE:HZ	22:V:712:LEU:HD22	1.44	0.83
1:A:326:PRO:HB3	13:M:86:LYS:O	1.78	0.82
18:R:195:PRO:HB2	18:R:199:LYS:CD	2.09	0.82
22:V:315:VAL:HG12	23:W:500:ASP:HB2	1.54	0.82
25:1:9:LEU:HB2	25:1:51:ASN:HD21	1.43	0.82
26:2:28:PRO:CA	27:3:25:GLN:HA	2.08	0.82
26:2:259:LEU:HD12	26:2:260:ASN:N	1.94	0.82
27:3:57:LEU:HD23	27:3:58:ALA:N	1.91	0.82
13:M:92:SER:O	13:M:93:PHE:O	1.96	0.82
26:2:86:SER:HB3	26:2:140:LYS:HE2	1.60	0.82
1:A:271:ARG:HG2	13:M:73:PRO:CG	2.10	0.82
2:B:79:GLU:C	2:B:80:GLU:HG3	2.04	0.82
2:B:1117:HIS:HB2	2:B:1127:ILE:HD13	1.61	0.82
25:1:47:ALA:HB2	25:1:50:VAL:HB	1.61	0.82
1:A:999:ARG:HE	8:H:99:ILE:HD12	1.43	0.82
17:Q:29:GLU:CD	18:R:194:ARG:NH2	2.31	0.82
5:E:55:ARG:HG2	5:E:76:PHE:CB	2.10	0.82
27:3:12:VAL:HG21	27:3:161:ILE:HG12	1.61	0.82
22:V:321:GLU:HB2	23:W:499:ASN:OD1	1.78	0.82
22:V:523:VAL:HG21	25:1:20:LEU:HG	1.61	0.82
26:2:100:LEU:HG	26:2:119:ARG:HE	1.45	0.82
26:2:221:GLN:OE1	26:2:224:GLN:HA	1.80	0.82
25:1:52:VAL:CG2	25:1:53:LEU:HD12	2.09	0.82
1:A:1251:ASN:ND2	21:U:227:GLU:HB3	1.95	0.82
1:A:1251:ASN:HA	21:U:234:LYS:HE3	1.61	0.82
26:2:174:ASP:OD1	26:2:179:LEU:HD12	1.80	0.82
26:2:174:ASP:O	26:2:220:LEU:HD23	1.79	0.81
3:C:135:ARG:O	3:C:136:ASP:HB3	1.79	0.81
25:1:59:GLU:OE1	26:2:402:ARG:NH1	2.13	0.81
17:Q:24:GLY:CA	18:R:210:PHE:HE2	1.92	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:175:LEU:HB3	26:2:216:MET:SD	2.20	0.81
27:3:12:VAL:CG2	27:3:161:ILE:HG12	2.11	0.81
1:A:1313:GLN:NE2	1:A:1318:LYS:HB2	1.95	0.81
2:B:133:ILE:HG23	2:B:139:GLN:HG2	1.63	0.81
2:B:223:SER:O	2:B:224:CYS:HB3	1.79	0.81
13:M:179:GLU:CA	20:T:154:LYS:HG2	2.09	0.81
20:T:177:ARG:O	20:T:179:ASP:N	2.14	0.81
22:V:612:ASP:OD2	22:V:635:GLN:OE1	1.98	0.81
26:2:177:GLN:CD	26:2:220:LEU:HD22	2.06	0.81
1:A:595:ILE:HG21	1:A:675:VAL:HG21	1.62	0.81
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.12	0.81
13:M:47:ASP:C	13:M:49:GLY:N	2.39	0.81
18:R:195:PRO:HB2	18:R:199:LYS:HD2	1.63	0.81
23:W:59:TYR:CD1	23:W:62:ALA:HB2	2.16	0.81
5:E:64:HIS:NE2	5:E:69:THR:CB	2.42	0.81
25:1:50:VAL:HG12	25:1:54:GLN:HG2	1.62	0.81
1:A:199:TYR:OH	13:M:93:PHE:CZ	2.33	0.80
16:P:206:GLU:C	16:P:208:ARG:H	1.89	0.80
26:2:37:HIS:HB3	26:2:38:PRO:HD3	1.61	0.80
25:1:34:ILE:HG22	25:1:46:ILE:HD11	1.63	0.80
27:3:216:LYS:H	27:3:216:LYS:HD2	1.43	0.80
26:2:256:ASP:O	26:2:259:LEU:HG	1.82	0.80
27:3:144:ILE:CD1	27:3:147:MET:HE3	2.11	0.80
1:A:1319:LYS:CD	1:A:1356:ARG:NH1	2.43	0.80
8:H:100:GLU:HG3	8:H:101:GLY:H	1.45	0.80
17:Q:108:ASP:C	18:R:234:GLU:OE2	2.25	0.80
22:V:516:PRO:HA	25:1:15:ALA:C	2.04	0.80
26:2:30:VAL:HG23	27:3:25:GLN:OE1	1.81	0.80
26:2:117:ASN:HB3	27:3:42:MET:HE3	1.62	0.80
17:Q:24:GLY:C	18:R:210:PHE:HE2	1.89	0.80
17:Q:105:TYR:CE1	17:Q:109:HIS:CE1	2.70	0.80
22:V:516:PRO:CB	22:V:706:LYS:HZ3	1.94	0.80
25:1:9:LEU:CD1	25:1:48:GLU:HA	2.09	0.80
1:A:1022:ILE:H	1:A:1034:GLN:HE22	1.29	0.80
1:A:1251:ASN:CG	21:U:227:GLU:HB3	2.07	0.80
2:B:290:TYR:HB3	2:B:562:ALA:HB1	1.62	0.80
26:2:30:VAL:CG2	27:3:25:GLN:OE1	2.29	0.80
26:2:42:LEU:HD12	26:2:59:MET:CE	2.11	0.80
26:2:251:VAL:HG11	26:2:254:MET:HG3	1.62	0.80
27:3:214:TYR:O	27:3:215:LEU:HD23	1.82	0.80
1:A:326:PRO:HB3	13:M:86:LYS:C	2.07	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:144:ALA:HA	23:W:148:HIS:C	2.06	0.80
26:2:35:TYR:CD1	26:2:62:LEU:HG	2.16	0.80
27:3:11:LEU:CD2	27:3:160:ARG:HG2	2.12	0.80
27:3:121:LYS:O	27:3:124:ILE:HB	1.81	0.80
1:A:1123:ARG:NH2	1:A:1381:GLU:OE1	2.14	0.80
22:V:674:THR:CG2	26:2:392:ARG:CZ	2.59	0.80
26:2:93:LEU:HA	26:2:96:TRP:CD1	2.17	0.80
2:B:631:GLN:HB3	2:B:685:LYS:HE2	1.64	0.80
17:Q:109:HIS:CB	18:R:224:THR:HB	2.11	0.80
26:2:224:GLN:HB2	26:2:268:PHE:CE2	2.17	0.79
27:3:165:LYS:HE2	27:3:167:ALA:O	1.81	0.79
29:Y:36:DA:C4	29:Y:37:DG:C5	2.70	0.79
2:B:27:TRP:CE2	2:B:762:ARG:HG2	2.18	0.79
2:B:1068:GLN:O	2:B:1072:ARG:N	2.15	0.79
26:2:117:ASN:CG	27:3:42:MET:CE	2.55	0.79
1:A:199:TYR:CZ	13:M:93:PHE:CE2	2.70	0.79
5:E:62:VAL:HG23	5:E:72:MET:HB3	1.61	0.79
27:3:64:ILE:HG23	27:3:128:HIS:CD2	2.17	0.79
1:A:427:ILE:HG12	13:M:38:GLY:O	1.82	0.79
2:B:882:SER:O	2:B:887:TYR:CE1	2.35	0.79
8:H:107:GLU:O	8:H:108:ALA:C	2.26	0.79
21:U:251:ALA:C	21:U:253:THR:H	1.90	0.79
25:1:1:MET:CB	26:2:413:LEU:CB	2.60	0.79
27:3:57:LEU:C	27:3:71:TYR:CZ	2.60	0.79
27:3:14:VAL:CG2	27:3:163:VAL:HG22	2.13	0.79
4:D:54:GLU:OE2	7:G:28:GLN:NE2	2.15	0.79
9:I:85:PRO:O	9:I:86:CYS:O	2.00	0.79
20:T:177:ARG:C	20:T:179:ASP:N	2.37	0.79
25:1:13:ASP:OD2	25:1:17:LYS:CB	2.30	0.79
9:I:14:ILE:HG12	9:I:16:PHE:CG	2.18	0.79
13:M:179:GLU:HG2	20:T:154:LYS:HE3	1.65	0.79
14:N:332:GLU:HG2	15:O:92:LYS:HB3	1.63	0.79
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.13	0.79
17:Q:102:VAL:CG1	17:Q:103:VAL:N	2.12	0.79
26:2:205:LEU:O	26:2:209:PRO:HD2	1.81	0.79
17:Q:70:LYS:NZ	18:R:226:ASP:O	2.16	0.79
17:Q:111:ARG:NH1	17:Q:188:TYR:OH	2.16	0.79
27:3:222:SER:O	27:3:225:GLN:HG2	1.83	0.79
2:B:92:TYR:CD2	20:T:145:LEU:HD13	2.18	0.79
25:1:1:MET:HA	26:2:414:SER:H	1.46	0.79
26:2:52:ALA:O	26:2:56:VAL:HG13	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:57:LYS:O	9:I:59:THR:HG23	1.83	0.79
2:B:483:ARG:HH11	2:B:526:LEU:HB2	1.48	0.78
17:Q:180:PHE:CE2	18:R:211:SER:HB3	2.09	0.78
23:W:421:PHE:CE1	23:W:423:ASP:CG	2.60	0.78
27:3:151:VAL:HG12	27:3:155:GLN:O	1.84	0.78
1:A:1319:LYS:HD3	1:A:1356:ARG:NH1	1.97	0.78
17:Q:105:TYR:CE1	18:R:231:GLU:HG3	2.14	0.78
20:T:142:SER:O	20:T:144:GLN:N	2.15	0.78
20:T:145:LEU:O	20:T:147:LYS:N	2.14	0.78
27:3:58:ALA:HA	27:3:71:TYR:CZ	2.18	0.78
1:A:609:HIS:N	1:A:610:PRO:HD2	1.99	0.78
25:1:34:ILE:CG2	25:1:46:ILE:HD11	2.13	0.78
25:1:38:ILE:HA	25:1:44:PHE:HD1	1.48	0.78
26:2:77:LYS:HD3	26:2:78:GLU:N	1.97	0.78
26:2:181:GLN:OE1	26:2:229:ASP:HB2	1.83	0.78
26:2:203:PHE:CD2	26:2:205:LEU:HD23	2.18	0.78
1:A:45:GLU:OE1	1:A:48:GLU:HG3	1.84	0.78
1:A:45:GLU:OE1	1:A:48:GLU:CG	2.32	0.78
2:B:803:ARG:NH2	2:B:951:GLN:OE1	2.16	0.78
3:C:5:ASN:C	3:C:7:PRO:CD	2.39	0.78
9:I:14:ILE:HG13	9:I:16:PHE:CD2	2.18	0.78
26:2:118:LEU:CD1	27:3:39:ASP:OD1	2.31	0.78
26:2:118:LEU:CG	27:3:39:ASP:OD1	2.32	0.78
2:B:714:PRO:HD2	2:B:1001:PRO:HB3	1.64	0.78
17:Q:23:ARG:CZ	18:R:209:GLN:N	2.46	0.78
17:Q:109:HIS:CE1	18:R:224:THR:OG1	2.37	0.78
22:V:523:VAL:CB	25:1:20:LEU:HD23	2.14	0.78
22:V:703:PHE:CZ	22:V:712:LEU:HD22	2.18	0.78
23:W:419:GLU:CB	23:W:420:PRO:CD	2.46	0.78
25:1:1:MET:HB3	26:2:413:LEU:HD23	1.65	0.78
26:2:207:ASP:O	26:2:211:GLN:HG2	1.84	0.78
26:2:234:LEU:O	26:2:234:LEU:HD23	1.83	0.78
21:U:231:ASP:O	21:U:232:GLU:HG3	1.81	0.78
26:2:190:PRO:O	26:2:194:PRO:HD2	1.83	0.78
26:2:211:GLN:CG	26:2:257:SER:HB3	2.13	0.78
5:E:64:HIS:CD2	5:E:70:ASP:N	2.52	0.78
23:W:424:ARG:O	23:W:425:THR:CG2	2.32	0.78
26:2:34:LEU:O	26:2:38:PRO:HD2	1.84	0.78
26:2:196:ILE:CD1	26:2:210:ALA:HB2	2.13	0.78
26:2:53:LYS:O	26:2:56:VAL:HG22	1.84	0.78
26:2:159:VAL:HG13	26:2:161:HIS:N	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:189:GLU:HB2	26:2:190:PRO:HD3	1.66	0.78
27:3:147:MET:O	27:3:151:VAL:HG23	1.84	0.78
2:B:225:LEU:O	2:B:227:ASN:N	2.15	0.78
8:H:85:ALA:O	8:H:87:GLN:CD	2.26	0.78
17:Q:23:ARG:HH12	18:R:209:GLN:HB2	1.47	0.78
5:E:61:LEU:HD13	5:E:73:PHE:HD1	1.49	0.77
25:1:13:ASP:OD1	25:1:14:PRO:HD2	1.83	0.77
26:2:221:GLN:HE22	26:2:230:LEU:HB2	1.47	0.77
27:3:59:VAL:HG11	27:3:71:TYR:HD1	1.41	0.77
2:B:133:ILE:CD1	2:B:139:GLN:HB3	2.07	0.77
7:G:111:HIS:NE2	17:Q:124:ARG:O	2.18	0.77
24:0:54:ARG:NE	27:3:182:PHE:HE1	1.73	0.77
25:1:1:MET:HG3	26:2:415:GLN:O	1.85	0.77
25:1:10:ILE:CG2	26:2:407:VAL:HG21	2.15	0.77
26:2:30:VAL:HG23	27:3:25:GLN:CG	2.15	0.77
14:N:316:SER:OG	16:P:235:ARG:NH1	2.17	0.77
17:Q:109:HIS:CG	18:R:224:THR:HB	2.19	0.77
10:J:64:PRO:C	10:J:66:GLU:N	2.34	0.77
27:3:185:GLN:HA	27:3:185:GLN:HE21	1.48	0.77
2:B:735:VAL:HG22	2:B:750:VAL:HG13	1.67	0.77
22:V:516:PRO:CD	25:1:15:ALA:HB3	2.11	0.77
26:2:117:ASN:CG	27:3:42:MET:HE2	2.09	0.77
26:2:163:MET:CE	26:2:206:LEU:HD12	2.14	0.77
27:3:185:GLN:NE2	27:3:210:THR:HA	2.00	0.77
1:A:608:THR:CB	1:A:610:PRO:HD2	2.14	0.77
21:U:231:ASP:C	21:U:232:GLU:HG2	2.09	0.77
22:V:516:PRO:CB	22:V:706:LYS:NZ	2.48	0.77
25:1:38:ILE:HG22	25:1:44:PHE:CD1	2.19	0.77
25:1:1:MET:HE3	26:2:415:GLN:C	2.10	0.77
25:1:25:GLU:CD	25:1:35:ILE:HG12	2.09	0.77
26:2:179:LEU:HB3	26:2:184:LEU:HD11	1.65	0.77
26:2:208:THR:HG23	26:2:209:PRO:HD3	1.66	0.77
26:2:211:GLN:HA	26:2:261:PHE:HZ	1.49	0.77
26:2:42:LEU:HD21	26:2:55:TRP:CB	2.10	0.77
1:A:199:TYR:CZ	13:M:93:PHE:HZ	2.01	0.76
1:A:648:SER:O	1:A:651:SER:OG	2.02	0.76
1:A:927:GLU:C	1:A:931:ARG:HG3	2.09	0.76
1:A:1114:ALA:O	1:A:1116:ASN:N	2.13	0.76
18:R:190:LEU:HD12	18:R:205:ASP:OD2	1.86	0.76
26:2:44:VAL:HG13	26:2:45:PHE:CD1	2.20	0.76
27:3:59:VAL:CA	27:3:71:TYR:CE1	2.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:147:MET:HE1	27:3:157:MET:SD	2.25	0.76
22:V:674:THR:CG2	26:2:392:ARG:NH2	2.43	0.76
25:1:1:MET:CE	26:2:440:LEU:HD13	2.16	0.76
5:E:40:PHE:CE2	5:E:46:ASP:OD2	2.38	0.76
24:0:54:ARG:HB2	27:3:209:ILE:CG2	2.14	0.76
1:A:199:TYR:CE1	13:M:93:PHE:CZ	2.73	0.76
1:A:271:ARG:CD	13:M:73:PRO:HG3	2.07	0.76
2:B:761:THR:H	2:B:764:MET:HE3	1.51	0.76
26:2:117:ASN:HD21	27:3:108:ASN:HB3	1.47	0.76
26:2:208:THR:HG23	26:2:209:PRO:CD	2.16	0.76
27:3:172:LEU:HD13	27:3:172:LEU:O	1.86	0.76
1:A:331:LYS:NZ	29:Y:63:DG:O6	2.19	0.76
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.17	0.76
2:B:896:LEU:HD21	2:B:901:THR:HG21	1.65	0.76
27:3:190:LEU:HD23	27:3:190:LEU:H	1.51	0.76
27:3:14:VAL:CG2	27:3:163:VAL:HA	2.16	0.76
2:B:490:GLY:O	2:B:491:ARG:CB	2.33	0.76
17:Q:39:ARG:NH2	18:R:159:ASP:OD2	2.18	0.76
22:V:444:HIS:O	22:V:447:PRO:HD2	1.85	0.76
22:V:528:LYS:HE2	29:Y:25:DT:H5"	1.65	0.76
27:3:58:ALA:N	27:3:71:TYR:CZ	2.51	0.76
1:A:927:GLU:HG2	1:A:931:ARG:HH11	1.50	0.75
14:N:320:VAL:HG11	16:P:236:LYS:HG2	1.68	0.75
22:V:523:VAL:HG11	25:1:20:LEU:HD23	1.64	0.75
22:V:534:TYR:CE1	22:V:535:THR:OG1	2.39	0.75
26:2:86:SER:HB3	26:2:140:LYS:CE	2.16	0.75
26:2:218:GLN:NE2	26:2:265:LEU:HA	2.00	0.75
1:A:131:ALA:O	1:A:133:SER:N	2.18	0.75
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.17	0.75
9:I:14:ILE:CG1	9:I:16:PHE:CD2	2.70	0.75
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.21	0.75
25:1:1:MET:HB3	26:2:413:LEU:CD2	2.15	0.75
25:1:38:ILE:H	25:1:38:ILE:HD13	1.50	0.75
26:2:118:LEU:HD22	27:3:39:ASP:HA	1.65	0.75
27:3:57:LEU:C	27:3:71:TYR:CE2	2.63	0.75
17:Q:105:TYR:HE1	18:R:231:GLU:CB	2.00	0.75
25:1:1:MET:SD	26:2:413:LEU:HB3	2.25	0.75
1:A:206:ASN:C	1:A:208:ASP:H	1.94	0.75
17:Q:105:TYR:O	17:Q:109:HIS:HD2	1.69	0.75
25:1:2:VAL:CG1	26:2:456:LYS:CG	2.53	0.75
1:A:375:ILE:HB	1:A:666:ARG:HD2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:127:LYS:N	26:2:178:LEU:HD23	2.01	0.75
26:2:234:LEU:CD2	26:2:237:LEU:HD12	2.14	0.75
2:B:462:ALA:HB2	28:X:40:DT:H5"	1.67	0.75
11:K:39:ASP:OD1	11:K:39:ASP:N	2.18	0.75
25:1:24:ASP:OD2	25:1:57:VAL:HG11	1.85	0.75
26:2:163:MET:HE2	26:2:206:LEU:CD1	2.15	0.75
26:2:243:SER:HB3	26:2:258:LEU:HD22	1.69	0.75
27:3:8:LEU:HD23	27:3:54:SER:HB3	1.68	0.75
27:3:11:LEU:HD22	27:3:160:ARG:CG	2.16	0.75
1:A:611:ASP:OD2	1:A:627:LYS:CE	2.34	0.75
9:I:62:VAL:O	9:I:63:ASP:C	2.30	0.75
22:V:611:GLY:HA2	22:V:615:PHE:HB3	1.68	0.75
2:B:529:MET:HE2	2:B:623:ARG:HB2	1.68	0.75
26:2:180:SER:O	26:2:184:LEU:HG	1.87	0.75
27:3:148:ASN:CB	27:3:157:MET:HE2	2.17	0.75
2:B:80:GLU:CB	2:B:135:GLU:CG	2.48	0.75
1:A:326:PRO:HA	13:M:87:GLY:HA2	1.67	0.74
2:B:490:GLY:O	2:B:491:ARG:HB2	1.86	0.74
17:Q:52:LEU:HB3	17:Q:54:PHE:HD1	1.50	0.74
22:V:321:GLU:OE1	23:W:499:ASN:OD1	2.05	0.74
26:2:100:LEU:CD1	26:2:119:ARG:HG3	2.16	0.74
27:3:38:ILE:O	27:3:41:VAL:HG12	1.87	0.74
22:V:523:VAL:HG21	25:1:20:LEU:CD2	2.17	0.74
2:B:80:GLU:OE1	2:B:135:GLU:C	2.30	0.74
9:I:14:ILE:CG1	9:I:16:PHE:CE2	2.66	0.74
16:P:206:GLU:CB	16:P:236:LYS:HZ2	2.01	0.74
25:1:1:MET:HB2	26:2:418:PHE:CB	2.18	0.74
26:2:196:ILE:HD11	26:2:210:ALA:CB	2.17	0.74
17:Q:51:LEU:HD11	18:R:163:LEU:CD1	2.05	0.74
23:W:608:ILE:HG23	23:W:614:TYR:CE2	2.22	0.74
27:3:133:LEU:HD23	27:3:177:PHE:HD1	1.50	0.74
13:M:91:ALA:O	13:M:92:SER:CB	2.35	0.74
26:2:53:LYS:HE3	26:2:95:ILE:HD11	1.67	0.74
23:W:430:ASN:HB3	23:W:431:PRO:CD	2.16	0.74
26:2:35:TYR:CD2	26:2:62:LEU:HB3	2.22	0.74
26:2:51:LEU:HD23	26:2:51:LEU:O	1.87	0.74
1:A:326:PRO:CB	13:M:87:GLY:CA	2.56	0.74
26:2:132:ASP:O	26:2:135:GLN:HG2	1.88	0.74
26:2:160:LEU:HA	26:2:206:LEU:HD11	1.70	0.74
1:A:1250:ASP:CG	21:U:227:GLU:HG2	2.10	0.73
2:B:56:GLN:OE1	20:T:141:LEU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:23:ARG:NE	18:R:207:SER:O	2.20	0.73
22:V:522:TYR:HE2	25:1:62:ASP:CG	1.96	0.73
1:A:1177:TYR:H	9:I:51:SER:HB3	1.53	0.73
2:B:988:LYS:NZ	2:B:1026:GLU:OE2	2.17	0.73
14:N:341:LYS:HB3	14:N:352:HIS:HB2	1.68	0.73
1:A:117:LEU:N	1:A:232:GLU:OE2	2.19	0.73
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	1.70	0.73
3:C:212:ASP:C	3:C:214:ASP:N	2.38	0.73
13:M:39:LEU:O	13:M:40:VAL:C	2.31	0.73
27:3:141:LEU:O	27:3:144:ILE:HG22	1.89	0.73
17:Q:100:VAL:O	17:Q:102:VAL:N	2.20	0.73
22:V:523:VAL:CG1	25:1:20:LEU:HD23	2.19	0.73
25:1:34:ILE:HD13	25:1:54:GLN:OE1	1.88	0.73
26:2:251:VAL:HG11	26:2:254:MET:CG	2.18	0.73
27:3:214:TYR:HE2	27:3:216:LYS:HE2	1.53	0.73
22:V:612:ASP:C	22:V:614:SER:N	2.46	0.73
25:1:34:ILE:HG12	25:1:50:VAL:CG1	2.18	0.73
1:A:197:GLU:OE2	13:M:93:PHE:CD2	2.41	0.73
22:V:516:PRO:HG2	22:V:706:LYS:CE	2.18	0.73
22:V:667:THR:HA	25:1:62:ASP:OD1	1.89	0.73
25:1:1:MET:HG2	26:2:413:LEU:C	2.14	0.73
26:2:118:LEU:HD21	27:3:39:ASP:C	2.12	0.73
1:A:1319:LYS:HD2	1:A:1356:ARG:HH12	1.53	0.73
2:B:914:GLU:OE1	2:B:914:GLU:N	2.21	0.73
3:C:274:ILE:HD12	11:K:84:GLN:HB3	1.69	0.73
25:1:9:LEU:HD22	25:1:51:ASN:ND2	2.04	0.73
26:2:172:SER:HA	26:2:175:LEU:CD2	2.19	0.73
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.71	0.73
18:R:194:ARG:O	18:R:196:ASP:O	2.06	0.73
27:3:226:TYR:HA	27:3:230:VAL:HG23	1.71	0.73
5:E:47:LYS:CE	5:E:52:ARG:HB2	2.18	0.73
25:1:1:MET:C	26:2:413:LEU:HG	2.12	0.73
8:H:146:LYS:HE2	8:H:147:LYS:HG3	1.71	0.72
17:Q:102:VAL:HG13	17:Q:103:VAL:H	0.60	0.72
25:1:1:MET:HG3	26:2:418:PHE:HB2	1.69	0.72
25:1:5:LEU:HD21	26:2:408:LEU:HD13	0.87	0.72
26:2:237:LEU:O	26:2:240:LEU:HD13	1.88	0.72
27:3:111:ILE:HG13	27:3:112:VAL:N	2.02	0.72
27:3:144:ILE:HG12	27:3:147:MET:HE3	1.71	0.72
23:W:59:TYR:CD2	23:W:62:ALA:CB	2.71	0.72
26:2:41:CYS:O	26:2:44:VAL:HG12	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:60:LEU:HD11	26:2:95:ILE:HB	1.71	0.72
26:2:218:GLN:HE22	26:2:265:LEU:HA	1.54	0.72
26:2:243:SER:HB2	26:2:258:LEU:HD22	1.71	0.72
5:E:54:ARG:HB2	5:E:78:GLU:CD	2.15	0.72
22:V:504:LYS:HB3	22:V:654:GLU:O	1.89	0.72
26:2:117:ASN:HB3	27:3:42:MET:CE	2.18	0.72
27:3:12:VAL:HG23	27:3:161:ILE:HG23	1.70	0.72
29:Y:36:DA:C4	29:Y:37:DG:C8	2.78	0.72
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.71	0.72
3:C:40:ALA:HB1	3:C:171:LYS:HB3	1.70	0.72
10:J:64:PRO:O	10:J:66:GLU:N	2.21	0.72
16:P:162:VAL:O	16:P:164:GLN:NE2	2.21	0.72
17:Q:23:ARG:NH1	18:R:209:GLN:HB2	2.03	0.72
26:2:175:LEU:HD22	26:2:216:MET:SD	2.29	0.72
26:2:199:ALA:HB3	26:2:202:GLN:NE2	2.02	0.72
3:C:240:ARG:NH1	3:C:242:GLU:OE2	2.23	0.72
20:T:154:LYS:HD2	20:T:154:LYS:H	1.52	0.72
8:H:66:GLU:O	8:H:67:ASP:CB	2.38	0.72
26:2:117:ASN:ND2	27:3:42:MET:HE1	2.04	0.72
1:A:622:SER:C	1:A:624:GLY:H	1.96	0.72
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.69	0.72
16:P:167:ASN:ND2	29:Y:79:DT:O2	2.22	0.72
27:3:69:PHE:CE1	27:3:139:LYS:HD2	2.25	0.72
27:3:222:SER:HB2	27:3:226:TYR:HE2	1.54	0.72
22:V:315:VAL:HG12	23:W:500:ASP:CB	2.17	0.72
23:W:73:CYS:HB2	23:W:209:TYR:CZ	2.24	0.72
26:2:118:LEU:HD22	27:3:39:ASP:CA	2.19	0.72
24:0:76:LEU:O	24:0:77:LYS:O	2.08	0.72
25:1:2:VAL:HG12	26:2:422:LEU:HD13	1.72	0.72
2:B:874:PRO:O	2:B:877:GLU:OE1	2.08	0.72
26:2:117:ASN:HB2	27:3:104:LEU:HD11	1.71	0.72
27:3:217:VAL:HG13	27:3:226:TYR:CZ	2.25	0.72
26:2:134:SER:O	26:2:138:PRO:HD2	1.89	0.71
27:3:59:VAL:CB	27:3:71:TYR:HE1	1.93	0.71
27:3:66:GLU:CA	27:3:132:LEU:HD12	2.13	0.71
5:E:1:MET:HE3	5:E:3:ASP:HB3	1.71	0.71
23:W:584:TYR:HD1	23:W:594:ALA:HB2	1.52	0.71
26:2:35:TYR:CG	26:2:62:LEU:HD12	2.25	0.71
26:2:192:GLU:HG3	26:2:193:PRO:CD	2.18	0.71
17:Q:110:MET:SD	18:R:222:SER:HB2	2.30	0.71
17:Q:180:PHE:HZ	18:R:211:SER:HA	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:519:TYR:HE2	25:1:20:LEU:HG	1.53	0.71
22:V:689:VAL:HB	26:2:391:ILE:HD11	1.69	0.71
26:2:171:VAL:HG12	26:2:216:MET:SD	2.30	0.71
23:W:696:TRP:CD1	23:W:697:ILE:HG13	2.25	0.71
23:W:209:TYR:OH	23:W:234:ASP:N	2.23	0.71
25:1:1:MET:HG2	26:2:413:LEU:HB3	1.71	0.71
25:1:1:MET:HE2	26:2:413:LEU:O	1.90	0.71
25:1:28:ALA:HB3	25:1:31:LYS:HB2	1.71	0.71
27:3:165:LYS:HG3	27:3:203:LEU:CD1	2.20	0.71
1:A:960:ARG:NH2	1:A:961:GLU:OE2	2.24	0.71
3:C:135:ARG:O	3:C:136:ASP:CB	2.38	0.71
26:2:42:LEU:HD12	26:2:59:MET:HE1	1.71	0.71
22:V:648:LYS:O	22:V:650:MET:N	2.24	0.71
23:W:73:CYS:C	23:W:209:TYR:CE2	2.69	0.71
2:B:1085:ARG:NH2	29:Y:53:DG:OP2	2.24	0.71
18:R:190:LEU:CD1	18:R:205:ASP:CG	2.64	0.71
21:U:229:ALA:HB1	21:U:234:LYS:HB3	1.72	0.71
25:1:18:GLN:CB	25:1:44:PHE:HE2	2.00	0.71
26:2:118:LEU:CD2	27:3:39:ASP:CA	2.68	0.71
27:3:18:ASN:CG	27:3:20:ILE:HD13	2.15	0.71
3:C:67:ARG:HH12	10:J:2:ILE:HG13	1.55	0.71
5:E:10:LEU:HD21	5:E:55:ARG:HH21	1.55	0.71
13:M:94:ASP:CG	13:M:97:GLY:O	2.34	0.71
22:V:523:VAL:HG21	25:1:20:LEU:CG	2.21	0.71
1:A:1112:VAL:HB	21:U:252:LYS:O	1.90	0.70
26:2:86:SER:CB	26:2:140:LYS:HE2	2.20	0.70
4:D:90:LYS:HE2	4:D:130:ILE:HD11	1.72	0.70
5:E:51:GLY:O	5:E:52:ARG:HG2	1.84	0.70
13:M:44:ARG:HE	13:M:46:ILE:HG22	1.53	0.70
23:W:589:GLU:O	23:W:594:ALA:HB1	1.91	0.70
25:1:29:LEU:HD23	25:1:30:GLY:N	2.06	0.70
26:2:126:GLY:C	26:2:178:LEU:HD23	2.16	0.70
3:C:137:ASN:HB2	3:C:145:GLN:NE2	1.99	0.70
27:3:177:PHE:CZ	27:3:203:LEU:HD23	2.27	0.70
2:B:777:ASN:O	10:J:47:ARG:NH1	2.24	0.70
2:B:874:PRO:O	2:B:876:ASN:N	2.24	0.70
5:E:48:PRO:O	5:E:49:SER:CB	2.39	0.70
22:V:515:SER:HB3	22:V:539:ASN:ND2	2.05	0.70
1:A:199:TYR:CE1	13:M:93:PHE:HZ	2.08	0.70
5:E:51:GLY:C	5:E:52:ARG:CG	2.62	0.70
26:2:218:GLN:OE1	26:2:265:LEU:HA	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:51:MET:HE3	27:3:52:ASN:ND2	2.07	0.70
27:3:59:VAL:N	27:3:71:TYR:CD1	2.59	0.70
2:B:76:GLY:O	2:B:77:GLU:CB	2.40	0.70
5:E:52:ARG:CB	5:E:53:PRO:HD3	2.11	0.70
22:V:528:LYS:CE	29:Y:25:DT:H5"	2.21	0.70
23:W:209:TYR:HE1	23:W:233:PHE:CD1	2.09	0.70
25:1:2:VAL:HG12	26:2:456:LYS:HE2	1.74	0.70
26:2:218:GLN:CD	26:2:265:LEU:HA	2.17	0.70
24:0:54:ARG:NE	27:3:182:PHE:CD1	2.60	0.70
1:A:1192:TRP:HE3	1:A:1192:TRP:H	1.40	0.70
27:3:133:LEU:HD22	27:3:134:ALA:H	1.56	0.70
28:X:65:DG:C2	29:Y:30:DG:C2	2.80	0.70
1:A:79:THR:HG23	13:M:43:ASP:OD1	1.92	0.69
9:I:14:ILE:HG12	9:I:16:PHE:CD1	2.26	0.69
22:V:519:TYR:CE2	25:1:20:LEU:CG	2.72	0.69
25:1:8:VAL:HG11	25:1:45:VAL:HG12	1.74	0.69
27:3:162:LEU:HA	27:3:192:ASP:OD1	1.92	0.69
2:B:48:ASP:OD1	2:B:159:THR:OG1	2.09	0.69
26:2:163:MET:O	26:2:167:PRO:HD2	1.91	0.69
26:2:189:GLU:HA	26:2:192:GLU:HG2	1.72	0.69
2:B:52:GLN:HE22	20:T:142:SER:HB2	1.55	0.69
2:B:69:ALA:HB2	2:B:423:ILE:HB	1.73	0.69
17:Q:105:TYR:CZ	17:Q:109:HIS:NE2	2.53	0.69
22:V:516:PRO:HB2	22:V:706:LYS:NZ	2.07	0.69
23:W:59:TYR:CE1	23:W:62:ALA:HB2	2.27	0.69
22:V:612:ASP:CG	22:V:635:GLN:CD	2.59	0.69
22:V:674:THR:OG1	26:2:392:ARG:NE	2.26	0.69
23:W:298:ALA:HA	23:W:421:PHE:HE2	1.55	0.69
26:2:185:MET:SD	26:2:232:GLU:HB2	2.32	0.69
27:3:69:PHE:CZ	27:3:139:LYS:HD2	2.27	0.69
5:E:10:LEU:HD21	5:E:55:ARG:HE	1.56	0.69
9:I:61:GLU:O	9:I:63:ASP:N	2.25	0.69
16:P:206:GLU:O	16:P:208:ARG:N	2.25	0.69
25:1:1:MET:CG	26:2:415:GLN:O	2.41	0.69
2:B:74:ALA:CB	20:T:201:ASP:HB3	2.22	0.69
2:B:295:PRO:HB2	9:I:11:PHE:HD2	1.58	0.69
8:H:106:THR:C	8:H:108:ALA:H	2.00	0.69
17:Q:180:PHE:HE2	18:R:211:SER:CB	2.00	0.69
26:2:118:LEU:HD11	27:3:43:VAL:HG23	1.75	0.69
27:3:144:ILE:CG1	27:3:147:MET:HE3	2.23	0.69
26:2:140:LYS:HD3	26:2:162:PHE:HE1	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:163:MET:CE	26:2:206:LEU:HB3	2.23	0.69
26:2:199:ALA:CB	26:2:202:GLN:HE22	2.02	0.69
1:A:1313:GLN:HE22	1:A:1318:LYS:CE	2.05	0.69
2:B:133:ILE:C	2:B:134:LYS:O	2.34	0.69
2:B:313:GLU:OE2	19:S:153:ARG:NH2	2.26	0.69
5:E:10:LEU:CD2	5:E:55:ARG:HE	2.05	0.69
25:1:4:VAL:CG1	26:2:411:GLN:O	2.38	0.69
25:1:53:LEU:HD12	25:1:53:LEU:H	1.57	0.69
26:2:130:SER:O	26:2:133:THR:HG22	1.92	0.69
22:V:612:ASP:O	22:V:614:SER:N	2.26	0.69
26:2:81:LYS:HD2	26:2:89:LEU:CD2	2.20	0.69
28:X:65:DG:C2	29:Y:30:DG:N2	2.60	0.69
1:A:1313:GLN:NE2	1:A:1318:LYS:HE2	2.08	0.69
13:M:47:ASP:O	13:M:49:GLY:CA	2.40	0.69
17:Q:102:VAL:HG22	17:Q:103:VAL:HG13	1.75	0.69
26:2:81:LYS:HE3	26:2:93:LEU:CD2	2.20	0.69
1:A:551:ARG:NH1	1:A:625:ASP:OD2	2.26	0.68
24:0:54:ARG:CD	27:3:182:PHE:CE1	2.60	0.68
25:1:55:GLU:OE2	26:2:402:ARG:HG3	1.93	0.68
26:2:48:LEU:CB	26:2:49:PRO:HD3	2.19	0.68
26:2:211:GLN:HA	26:2:261:PHE:CE1	2.28	0.68
1:A:272:ASN:ND2	1:A:272:ASN:O	2.26	0.68
2:B:323:SER:OG	2:B:335:ARG:NH1	2.27	0.68
5:E:64:HIS:NE2	5:E:69:THR:C	2.50	0.68
27:3:215:LEU:HD12	27:3:230:VAL:CG1	2.23	0.68
1:A:266:MET:HG2	1:A:272:ASN:HD22	1.02	0.68
2:B:78:VAL:O	2:B:79:GLU:CB	2.41	0.68
26:2:181:GLN:HG3	26:2:229:ASP:CG	2.18	0.68
1:A:49:GLY:O	1:A:52:PRO:HD2	1.92	0.68
22:V:531:ILE:CG2	22:V:534:TYR:CZ	2.64	0.68
26:2:251:VAL:HG12	26:2:254:MET:H	1.58	0.68
27:3:114:GLU:O	27:3:118:LEU:HD23	1.92	0.68
26:2:176:ALA:HB1	26:2:178:LEU:CD1	2.23	0.68
1:A:540:ASP:HB2	2:B:790:GLN:NE2	2.09	0.68
13:M:44:ARG:NE	13:M:46:ILE:CG2	2.57	0.68
14:N:324:GLU:HA	16:P:188:ARG:HH12	1.58	0.68
20:T:177:ARG:NH2	20:T:212:TYR:HB2	2.09	0.68
22:V:321:GLU:CB	23:W:499:ASN:CG	2.32	0.68
22:V:415:HIS:HA	22:V:421:TRP:CD1	2.29	0.68
25:1:10:ILE:HG21	26:2:407:VAL:HG21	1.76	0.68
27:3:18:ASN:CG	27:3:64:ILE:HD11	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:HD2	13:M:73:PRO:HG2	0.70	0.68
1:A:632:ASN:HA	1:A:992:LYS:HD2	1.74	0.68
17:Q:102:VAL:HG13	17:Q:103:VAL:HG22	1.76	0.68
1:A:197:GLU:OE1	1:A:308:LYS:NZ	2.26	0.68
25:1:13:ASP:CG	25:1:14:PRO:CD	2.61	0.68
25:1:39:ASP:OD1	25:1:43:VAL:HB	1.94	0.68
1:A:207:GLU:O	1:A:209:SER:N	2.28	0.67
1:A:1180:ASN:HB3	9:I:33:ARG:HH22	1.59	0.67
1:A:1319:LYS:HD2	1:A:1356:ARG:NH1	2.07	0.67
2:B:13:ASP:OD1	2:B:636:LYS:NZ	2.27	0.67
2:B:225:LEU:C	2:B:227:ASN:H	2.01	0.67
2:B:839:GLY:HA3	2:B:891:ASP:HB3	1.76	0.67
13:M:91:ALA:O	13:M:92:SER:HB2	1.94	0.67
17:Q:52:LEU:HB3	17:Q:54:PHE:CD1	2.28	0.67
18:R:195:PRO:O	18:R:199:LYS:HD2	1.93	0.67
26:2:170:ALA:HB1	26:2:213:TRP:CZ3	2.29	0.67
26:2:211:GLN:HB3	26:2:261:PHE:HE1	1.59	0.67
17:Q:51:LEU:CD1	18:R:163:LEU:CD1	2.70	0.67
26:2:117:ASN:CB	27:3:42:MET:HE3	2.22	0.67
26:2:172:SER:O	26:2:175:LEU:HD23	1.95	0.67
27:3:187:GLN:HG3	27:3:189:ILE:CG1	2.24	0.67
1:A:111:CYS:SG	1:A:114:CYS:HB3	2.33	0.67
8:H:65:TYR:CE2	8:H:70:LEU:HB3	2.30	0.67
1:A:608:THR:OG1	1:A:610:PRO:HD2	1.94	0.67
2:B:591:ARG:NH2	2:B:601:VAL:O	2.27	0.67
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.25	0.67
25:1:19:PHE:O	25:1:23:LEU:HG	1.95	0.67
27:3:130:GLU:HB2	27:3:173:GLN:NE2	2.09	0.67
27:3:159:SER:OG	27:3:189:ILE:HD12	1.94	0.67
1:A:266:MET:HG3	1:A:272:ASN:CG	2.18	0.67
1:A:326:PRO:HB3	13:M:87:GLY:N	2.09	0.67
27:3:187:GLN:CG	27:3:189:ILE:HG12	2.24	0.67
26:2:56:VAL:O	26:2:60:LEU:HG	1.94	0.67
26:2:118:LEU:HD13	27:3:39:ASP:OD1	1.93	0.67
26:2:181:GLN:CD	26:2:229:ASP:HB2	2.19	0.67
27:3:22:TRP:O	27:3:25:GLN:CG	2.40	0.67
27:3:111:ILE:O	27:3:115:ILE:HD13	1.94	0.67
1:A:460:ARG:NH2	1:A:493:ASN:HB2	2.10	0.67
2:B:331:THR:HB	2:B:334:LYS:HB2	1.75	0.67
2:B:861:SER:C	2:B:896:LEU:HD23	2.19	0.67
22:V:667:THR:HA	25:1:62:ASP:CG	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:56:VAL:HG11	26:2:91:SER:HB2	1.77	0.67
1:A:1313:GLN:NE2	1:A:1316:ASN:OD1	2.25	0.67
22:V:516:PRO:CD	22:V:706:LYS:NZ	2.54	0.67
2:B:90:GLN:NE2	20:T:141:LEU:HG	2.06	0.67
25:1:1:MET:HE3	26:2:415:GLN:CA	2.24	0.67
1:A:551:ARG:CZ	1:A:625:ASP:OD2	2.43	0.66
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.76	0.66
15:O:3:TYR:HD1	15:O:98:CYS:HG	1.40	0.66
27:3:217:VAL:HG13	27:3:226:TYR:CE2	2.30	0.66
16:P:203:ARG:HH21	16:P:203:ARG:HG3	1.59	0.66
17:Q:102:VAL:CG1	17:Q:103:VAL:HG22	2.25	0.66
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.76	0.66
22:V:415:HIS:CD2	22:V:416:THR:HG23	2.31	0.66
22:V:516:PRO:HB3	25:1:15:ALA:CB	2.05	0.66
25:1:59:GLU:OE2	26:2:402:ARG:CZ	2.41	0.66
1:A:460:ARG:HH21	1:A:493:ASN:HB2	1.61	0.66
2:B:216:ALA:HB2	2:B:241:ALA:HB2	1.77	0.66
9:I:84:HIS:CG	9:I:85:PRO:CD	2.68	0.66
22:V:355:CYS:HG	22:V:381:TRP:CD1	2.13	0.66
21:U:153:ARG:NH2	21:U:166:GLU:OE2	2.28	0.66
26:2:160:LEU:HD12	26:2:160:LEU:H	1.60	0.66
28:X:45:DC:H42	29:Y:48:DC:H42	1.41	0.66
1:A:271:ARG:HE	13:M:73:PRO:CD	2.09	0.66
1:A:326:PRO:CB	13:M:86:LYS:O	2.43	0.66
26:2:117:ASN:HD21	27:3:108:ASN:CA	2.05	0.66
26:2:218:GLN:CG	26:2:268:PHE:HB3	2.26	0.66
27:3:207:CYS:SG	27:3:214:TYR:HB2	2.34	0.66
29:Y:36:DA:C5	29:Y:37:DG:C5	2.83	0.66
25:1:8:VAL:HG12	25:1:9:LEU:N	2.10	0.66
1:A:522:PRO:HA	1:A:666:ARG:HH21	1.59	0.66
17:Q:24:GLY:CA	18:R:210:PHE:CD2	2.79	0.66
27:3:146:ARG:O	27:3:149:LYS:HG2	1.96	0.66
8:H:106:THR:O	8:H:108:ALA:N	2.29	0.66
18:R:142:LYS:NZ	18:R:172:GLU:OE2	2.26	0.66
25:1:35:ILE:HG22	25:1:46:ILE:HD12	1.78	0.66
27:3:45:GLY:O	27:3:49:LEU:HD23	1.96	0.66
5:E:64:HIS:HD2	5:E:68:PRO:CA	2.06	0.66
18:R:194:ARG:C	18:R:196:ASP:H	2.02	0.66
22:V:631:GLY:O	22:V:632:SER:HB3	1.96	0.66
26:2:171:VAL:HG13	26:2:216:MET:CB	2.26	0.66
2:B:1066:PRO:HB3	13:M:46:ILE:CD1	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:422:PHE:O	2:B:426:GLY:N	2.29	0.65
17:Q:57:LYS:NZ	28:X:28:DG:OP1	2.29	0.65
20:T:145:LEU:O	20:T:145:LEU:HG	1.96	0.65
2:B:73:HIS:O	2:B:75:SER:N	2.28	0.65
22:V:426:VAL:HG13	22:V:427:MET:H	1.61	0.65
25:1:10:ILE:HG22	26:2:407:VAL:HG21	1.79	0.65
27:3:106:SER:O	27:3:110:VAL:HG23	1.97	0.65
27:3:137:LEU:HB3	27:3:180:VAL:CG1	2.20	0.65
1:A:271:ARG:HE	13:M:73:PRO:CG	2.09	0.65
5:E:47:LYS:CB	5:E:48:PRO:CD	2.42	0.65
9:I:14:ILE:CG1	9:I:16:PHE:CZ	2.74	0.65
22:V:612:ASP:CG	22:V:635:GLN:OE1	2.39	0.65
25:1:1:MET:SD	26:2:419:GLU:HB2	2.37	0.65
25:1:34:ILE:CG1	25:1:50:VAL:HG11	2.21	0.65
26:2:270:LEU:HD23	26:2:273:GLN:HE21	1.62	0.65
5:E:64:HIS:CD2	5:E:68:PRO:HA	2.24	0.65
9:I:84:HIS:H	9:I:84:HIS:CD2	2.12	0.65
23:W:421:PHE:HB3	23:W:431:PRO:HG3	1.77	0.65
23:W:696:TRP:HD1	23:W:697:ILE:HG13	1.61	0.65
1:A:51:ARG:H	1:A:52:PRO:HD2	1.61	0.65
2:B:490:GLY:O	2:B:491:ARG:CG	2.44	0.65
2:B:1040:GLN:H	2:B:1040:GLN:CD	2.05	0.65
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.77	0.65
18:R:195:PRO:CB	18:R:199:LYS:HD2	2.26	0.65
18:R:225:VAL:HG12	18:R:227:SER:H	1.61	0.65
26:2:189:GLU:HA	26:2:192:GLU:CG	2.26	0.65
26:2:236:PHE:CZ	26:2:262:LEU:HD22	2.32	0.65
27:3:184:ALA:CA	27:3:187:GLN:HG2	2.25	0.65
26:2:57:MET:HA	26:2:60:LEU:HD11	1.76	0.65
3:C:132:SER:HB3	3:C:147:ASP:HB2	1.78	0.65
13:M:178:LYS:NZ	13:M:279:GLY:O	2.27	0.65
23:W:298:ALA:CA	23:W:421:PHE:CE2	2.80	0.65
2:B:312:GLN:OE1	19:S:153:ARG:NH1	2.29	0.65
9:I:61:GLU:C	9:I:63:ASP:H	2.04	0.65
18:R:138:ALA:C	18:R:140:LYS:H	2.05	0.65
26:2:173:GLN:CD	26:2:179:LEU:HD21	2.21	0.65
22:V:516:PRO:CA	25:1:15:ALA:O	2.44	0.65
26:2:117:ASN:ND2	27:3:42:MET:CE	2.60	0.65
29:Y:36:DA:C2	29:Y:37:DG:C4	2.84	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:OE1	1:A:48:GLU:N	2.30	0.65
2:B:873:LEU:HB3	2:B:874:PRO:CD	2.24	0.65
1:A:210:GLN:O	1:A:211:GLU:CB	2.45	0.64
26:2:45:PHE:HB2	26:2:51:LEU:CD1	2.26	0.64
27:3:17:ALA:CB	27:3:63:HIS:HD2	2.10	0.64
27:3:58:ALA:CA	27:3:71:TYR:OH	2.39	0.64
16:P:206:GLU:C	16:P:208:ARG:N	2.56	0.64
17:Q:180:PHE:CZ	18:R:211:SER:CA	2.60	0.64
21:U:227:GLU:O	21:U:228:MET:O	2.15	0.64
22:V:366:ASN:HD21	22:V:613:THR:HG22	1.62	0.64
1:A:212:LYS:HB3	1:A:212:LYS:NZ	2.12	0.64
1:A:385:ALA:HA	1:A:450:MET:HE3	1.79	0.64
15:O:3:TYR:C	15:O:5:LEU:N	2.51	0.64
23:W:423:ASP:C	23:W:425:THR:H	2.05	0.64
26:2:211:GLN:CB	26:2:261:PHE:HE1	2.11	0.64
26:2:266:ARG:O	26:2:270:LEU:HB2	1.97	0.64
27:3:130:GLU:HB2	27:3:173:GLN:HE22	1.61	0.64
2:B:98:HIS:HB2	2:B:108:MET:HE2	1.79	0.64
20:T:146:ASP:O	20:T:147:LYS:HB3	1.97	0.64
23:W:581:LEU:HD21	23:W:608:ILE:HG21	1.78	0.64
25:1:35:ILE:HG22	25:1:46:ILE:CD1	2.27	0.64
27:3:192:ASP:HB2	27:3:231:PHE:CE1	2.32	0.64
2:B:225:LEU:HD13	2:B:228:SER:HB2	1.77	0.64
17:Q:24:GLY:HA2	18:R:210:PHE:CD2	2.33	0.64
23:W:59:TYR:CZ	23:W:62:ALA:HB2	2.29	0.64
26:2:28:PRO:CA	27:3:25:GLN:C	2.70	0.64
27:3:64:ILE:HB	27:3:123:ASP:OD2	1.98	0.64
7:G:97:LEU:HB3	7:G:108:ILE:HB	1.78	0.64
26:2:202:GLN:HE21	26:2:202:GLN:H	1.44	0.64
27:3:14:VAL:HG22	27:3:163:VAL:HA	1.78	0.64
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.63	0.64
2:B:883:THR:O	2:B:884:ASN:C	2.41	0.64
9:I:14:ILE:HG13	9:I:16:PHE:CE1	2.33	0.64
20:T:141:LEU:C	20:T:141:LEU:HD22	2.23	0.64
26:2:42:LEU:CD2	26:2:55:TRP:HB2	2.13	0.64
26:2:159:VAL:HG11	26:2:161:HIS:HD2	1.62	0.64
1:A:22:GLN:HE22	1:A:1448:SER:HB2	1.63	0.64
1:A:622:SER:C	1:A:624:GLY:N	2.53	0.64
5:E:64:HIS:HD2	5:E:69:THR:N	1.93	0.64
23:W:584:TYR:CZ	23:W:614:TYR:HB2	2.31	0.64
26:2:220:LEU:O	26:2:220:LEU:HD13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:ARG:NH2	1:A:1415:THR:OG1	2.30	0.64
1:A:1027:ASP:OD1	5:E:162:ARG:NH1	2.31	0.64
27:3:70:LEU:HD13	27:3:115:ILE:CD1	2.28	0.64
1:A:1298:LEU:O	1:A:1300:GLY:N	2.31	0.64
3:C:84:TYR:CZ	3:C:167:LYS:HE3	2.32	0.64
9:I:14:ILE:CG1	9:I:16:PHE:CG	2.80	0.64
17:Q:109:HIS:HB3	18:R:224:THR:HB	1.78	0.64
18:R:194:ARG:C	18:R:196:ASP:N	2.56	0.64
25:1:38:ILE:HB	25:1:44:PHE:HE1	1.63	0.64
25:1:59:GLU:CD	26:2:402:ARG:NH1	2.56	0.64
26:2:160:LEU:HB3	26:2:206:LEU:CD1	2.27	0.64
1:A:264:VAL:O	1:A:266:MET:N	2.31	0.63
18:R:190:LEU:HD11	18:R:205:ASP:HB2	1.80	0.63
22:V:517:GLU:HB2	22:V:713:LEU:HD22	1.80	0.63
26:2:117:ASN:ND2	27:3:108:ASN:CA	2.57	0.63
26:2:177:GLN:OE1	26:2:220:LEU:HD22	1.98	0.63
1:A:1196:TYR:OH	1:A:1247:PHE:O	2.11	0.63
2:B:80:GLU:CG	2:B:135:GLU:HB3	2.28	0.63
9:I:84:HIS:CG	9:I:85:PRO:HD3	1.91	0.63
13:M:94:ASP:HB2	13:M:99:SER:N	2.11	0.63
13:M:182:ALA:CB	20:T:154:LYS:HG3	2.29	0.63
27:3:149:LYS:HG3	27:3:150:GLU:N	2.12	0.63
1:A:926:ASN:OD1	1:A:931:ARG:HD3	1.98	0.63
2:B:595:ASP:OD1	20:T:129:ARG:NH1	2.30	0.63
13:M:44:ARG:HE	13:M:46:ILE:HG23	1.63	0.63
25:1:13:ASP:OD1	25:1:14:PRO:CD	2.46	0.63
25:1:35:ILE:HA	25:1:46:ILE:HG13	1.80	0.63
27:3:131:THR:O	27:3:133:LEU:HD13	1.97	0.63
2:B:53:MET:SD	20:T:140:ARG:HD2	2.37	0.63
2:B:92:TYR:HB3	20:T:145:LEU:CB	2.22	0.63
13:M:11:PRO:O	13:M:12:ARG:CB	2.46	0.63
24:0:77:LYS:H	24:0:77:LYS:HD2	1.63	0.63
26:2:44:VAL:HG13	26:2:45:PHE:HD1	1.59	0.63
27:3:144:ILE:HD13	27:3:147:MET:HE3	1.80	0.63
29:Y:56:DG:H2''	29:Y:57:DA:H5'	1.80	0.63
3:C:78:ILE:HD11	3:C:81:LYS:HE3	1.80	0.63
10:J:62:TYR:HB3	10:J:64:PRO:CD	2.28	0.63
20:T:177:ARG:HH22	20:T:212:TYR:HB2	1.62	0.63
26:2:35:TYR:CZ	26:2:62:LEU:HG	2.34	0.63
27:3:17:ALA:HB1	27:3:63:HIS:HD2	1.63	0.63
27:3:160:ARG:NH2	27:3:190:LEU:HD12	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ASP:CG	1:A:626:THR:HG1	2.06	0.63
16:P:162:VAL:HG23	16:P:164:GLN:HE21	1.62	0.63
26:2:60:LEU:HD11	26:2:95:ILE:CB	2.29	0.63
26:2:140:LYS:HG2	26:2:162:PHE:CE1	2.33	0.63
27:3:64:ILE:CG1	27:3:123:ASP:HB3	2.29	0.63
1:A:930:LEU:O	1:A:931:ARG:C	2.42	0.63
1:A:1112:VAL:HG12	1:A:1311:LEU:HD21	1.81	0.63
2:B:309:PHE:CE2	9:I:40:ARG:HD2	2.33	0.63
2:B:1120:ASN:HB3	2:B:1145:GLN:HB3	1.81	0.63
25:1:18:GLN:NE2	25:1:44:PHE:HZ	1.97	0.63
26:2:100:LEU:HG	26:2:119:ARG:NE	2.13	0.63
2:B:225:LEU:CD1	2:B:228:SER:HB3	2.23	0.63
11:K:56:VAL:HA	11:K:77:THR:HG22	1.81	0.63
18:R:190:LEU:CD1	18:R:205:ASP:HB2	2.29	0.63
26:2:117:ASN:CG	27:3:108:ASN:ND2	2.50	0.63
26:2:258:LEU:HG	26:2:262:LEU:CD2	2.28	0.63
27:3:134:ALA:HB2	27:3:176:ASN:OD1	1.99	0.63
27:3:214:TYR:CE2	27:3:216:LYS:HE2	2.32	0.63
1:A:927:GLU:CG	1:A:931:ARG:HH11	2.11	0.63
10:J:3:ILE:HD12	10:J:15:GLY:HA2	1.81	0.63
13:M:10:LEU:O	13:M:12:ARG:N	2.32	0.63
1:A:425:ASP:CG	13:M:39:LEU:HD11	2.24	0.62
1:A:927:GLU:H	1:A:931:ARG:CD	2.12	0.62
1:A:1179:PRO:HG2	9:I:33:ARG:HG3	1.79	0.62
5:E:55:ARG:H	5:E:78:GLU:CD	2.04	0.62
14:N:344:ARG:NH2	29:Y:79:DT:OP2	2.30	0.62
26:2:89:LEU:HD23	26:2:89:LEU:O	1.99	0.62
26:2:123:LEU:O	26:2:123:LEU:HD23	1.99	0.62
27:3:24:LYS:HE2	27:3:220:MET:SD	2.38	0.62
27:3:70:LEU:CD1	27:3:115:ILE:HD11	2.27	0.62
1:A:244:ARG:HG2	1:A:245:PRO:HD2	1.81	0.62
1:A:339:LEU:HD11	2:B:1161:GLU:HG2	1.81	0.62
1:A:609:HIS:O	1:A:610:PRO:O	2.16	0.62
2:B:958:CYS:SG	2:B:959:GLU:N	2.72	0.62
9:I:58:ILE:C	9:I:60:HIS:H	2.07	0.62
17:Q:35:ASP:OD1	18:R:161:ARG:NH2	2.33	0.62
17:Q:36:ILE:O	17:Q:41:SER:OG	2.16	0.62
20:T:202:LEU:HD12	20:T:205:ILE:HD11	1.81	0.62
21:U:252:LYS:HA	21:U:252:LYS:CE	2.28	0.62
26:2:173:GLN:HG2	26:2:179:LEU:HG	1.80	0.62
3:C:5:ASN:O	3:C:7:PRO:CG	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:23:ASP:O	8:H:25:VAL:N	2.32	0.62
9:I:89:CYS:HB3	9:I:119:CYS:SG	2.39	0.62
13:M:108:SER:HB3	13:M:112:ARG:HH11	1.64	0.62
26:2:118:LEU:CD2	27:3:39:ASP:C	2.72	0.62
2:B:133:ILE:HG23	2:B:139:GLN:CG	2.29	0.62
8:H:88:PHE:HD2	8:H:144:LEU:HB3	1.65	0.62
23:W:584:TYR:CG	23:W:594:ALA:HB2	2.34	0.62
25:1:2:VAL:HG12	26:2:422:LEU:CD1	2.27	0.62
25:1:8:VAL:O	26:2:407:VAL:HG12	1.99	0.62
26:2:93:LEU:HA	26:2:96:TRP:HD1	1.64	0.62
27:3:59:VAL:HB	27:3:71:TYR:CD1	2.25	0.62
4:D:70:ARG:NH1	7:G:140:ASP:OD1	2.31	0.62
14:N:321:SER:OG	16:P:243:LYS:NZ	2.26	0.62
20:T:236:LYS:NZ	20:T:238:GLU:O	2.33	0.62
23:W:209:TYR:OH	23:W:233:PHE:C	2.42	0.62
25:1:38:ILE:HB	25:1:44:PHE:CE1	2.34	0.62
25:1:50:VAL:HA	25:1:53:LEU:HD13	1.82	0.62
26:2:197:THR:HG21	26:2:239:GLN:CD	2.24	0.62
1:A:896:LEU:HD23	1:A:1080:ILE:HD12	1.82	0.62
1:A:927:GLU:CB	1:A:931:ARG:HH11	2.13	0.62
23:W:298:ALA:CA	23:W:421:PHE:HE2	2.12	0.62
26:2:189:GLU:O	26:2:193:PRO:HD2	2.00	0.62
27:3:184:ALA:HA	27:3:187:GLN:CG	2.28	0.62
18:R:144:ASN:ND2	18:R:173:GLU:OE2	2.28	0.62
26:2:28:PRO:CA	27:3:25:GLN:CA	2.73	0.62
26:2:218:GLN:HG2	26:2:268:PHE:HB3	1.82	0.62
27:3:165:LYS:O	27:3:165:LYS:HD3	1.98	0.62
1:A:950:ASN:OD1	1:A:954:ARG:NH1	2.33	0.62
1:A:1375:ARG:NH1	1:A:1379:GLU:OE1	2.32	0.62
6:F:65:VAL:HG13	6:F:104:ILE:HD11	1.80	0.62
18:R:194:ARG:O	18:R:199:LYS:HB2	2.00	0.62
25:1:17:LYS:O	25:1:20:LEU:HB3	2.00	0.62
26:2:30:VAL:HG23	27:3:25:GLN:CD	2.23	0.62
27:3:9:ASN:O	27:3:56:LYS:HD3	1.99	0.62
27:3:46:ASN:CG	27:3:104:LEU:HD22	2.24	0.62
1:A:603:ILE:HD11	1:A:988:TRP:CE2	2.35	0.62
13:M:10:LEU:C	13:M:12:ARG:H	2.07	0.62
25:1:1:MET:HB2	26:2:418:PHE:HB3	1.81	0.62
25:1:1:MET:HG2	26:2:414:SER:N	2.15	0.62
25:1:47:ALA:HB1	25:1:50:VAL:HB	1.81	0.62
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:952:GLU:OE1	2:B:952:GLU:N	2.25	0.61
1:A:611:ASP:CG	1:A:626:THR:OG1	2.44	0.61
1:A:1251:ASN:ND2	21:U:227:GLU:O	2.33	0.61
8:H:105:SER:HB2	8:H:108:ALA:HB2	1.81	0.61
27:3:133:LEU:HD22	27:3:134:ALA:N	2.14	0.61
29:Y:36:DA:C2	29:Y:37:DG:C5	2.88	0.61
1:A:779:ILE:O	1:A:783:GLN:HG3	2.00	0.61
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.82	0.61
3:C:67:ARG:HH21	3:C:148:ILE:HD11	1.65	0.61
5:E:64:HIS:CE1	5:E:70:ASP:O	2.54	0.61
22:V:316:LEU:HB2	22:V:321:GLU:CG	2.29	0.61
26:2:46:ARG:CD	26:2:85:GLU:HB2	2.30	0.61
26:2:117:ASN:CG	27:3:108:ASN:CG	2.65	0.61
1:A:890:ARG:CZ	1:A:1023:VAL:HB	2.30	0.61
2:B:552:ASN:OD1	2:B:553:LEU:N	2.33	0.61
12:L:28:ILE:O	12:L:28:ILE:HG22	2.00	0.61
14:N:333:ASN:OD1	14:N:361:ASN:N	2.26	0.61
23:W:37:HIS:CE1	23:W:454:VAL:CG1	2.82	0.61
23:W:423:ASP:O	23:W:425:THR:N	2.33	0.61
23:W:584:TYR:HB2	23:W:594:ALA:HB2	1.81	0.61
26:2:60:LEU:CD1	26:2:95:ILE:HB	2.31	0.61
27:3:190:LEU:H	27:3:190:LEU:CD2	2.12	0.61
1:A:1313:GLN:HE22	1:A:1318:LYS:CD	2.14	0.61
2:B:924:ARG:NH1	3:C:60:HIS:HB2	2.16	0.61
17:Q:54:PHE:HD2	18:R:194:ARG:HD2	1.65	0.61
26:2:203:PHE:HD2	26:2:205:LEU:HD23	1.64	0.61
29:Y:36:DA:C6	29:Y:37:DG:O6	2.54	0.61
29:Y:36:DA:C5	29:Y:37:DG:C6	2.88	0.61
1:A:77:ASN:ND2	13:M:43:ASP:CG	2.59	0.61
26:2:29:GLY:N	27:3:25:GLN:HB3	2.15	0.61
5:E:62:VAL:HG21	5:E:72:MET:HB3	1.82	0.61
5:E:64:HIS:NE2	5:E:70:ASP:N	2.49	0.61
8:H:64:LEU:HB3	8:H:84:ARG:CD	2.28	0.61
9:I:14:ILE:CG1	9:I:16:PHE:CE1	2.84	0.61
14:N:22:ILE:HD11	14:N:43:LYS:HB2	1.82	0.61
17:Q:54:PHE:CD2	18:R:194:ARG:CD	2.83	0.61
26:2:251:VAL:CG1	26:2:254:MET:HG3	2.30	0.61
27:3:18:ASN:O	27:3:21:TRP:HD1	1.84	0.61
27:3:100:LYS:HG3	27:3:101:TYR:N	2.16	0.61
1:A:1102:MET:HB2	1:A:1389:ASP:OD1	2.00	0.61
2:B:80:GLU:OE1	2:B:135:GLU:CA	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:761:THR:H	2:B:764:MET:CE	2.13	0.61
10:J:63:ALA:O	10:J:65:LEU:N	2.26	0.61
23:W:59:TYR:OH	23:W:63:TYR:CE2	2.52	0.61
23:W:432:ILE:HG12	23:W:434:HIS:CE1	2.36	0.61
24:0:77:LYS:C	24:0:79:ASN:N	2.56	0.61
25:1:9:LEU:CB	25:1:51:ASN:HD21	2.14	0.61
26:2:236:PHE:CE2	26:2:262:LEU:HD13	2.36	0.61
22:V:368:ALA:O	22:V:371:VAL:HG22	2.00	0.61
22:V:520:ARG:HG3	25:1:23:LEU:HD11	1.83	0.61
27:3:8:LEU:HA	27:3:54:SER:HB3	1.83	0.61
1:A:93:PRO:HB3	1:A:251:THR:HG22	1.82	0.61
7:G:78:ARG:NH1	7:G:79:PRO:O	2.33	0.61
19:S:111:LYS:HE3	19:S:149:LEU:HD21	1.82	0.61
1:A:267:GLN:H	13:M:49:GLY:HA2	1.66	0.60
2:B:875:GLU:OE1	2:B:875:GLU:HA	2.01	0.60
13:M:182:ALA:HB2	20:T:154:LYS:CG	2.26	0.60
25:1:1:MET:HA	26:2:414:SER:N	2.15	0.60
26:2:56:VAL:HG11	26:2:91:SER:CB	2.31	0.60
2:B:52:GLN:NE2	20:T:142:SER:HB2	2.15	0.60
27:3:143:TYR:O	27:3:146:ARG:HG2	2.01	0.60
2:B:133:ILE:O	2:B:133:ILE:HG22	2.00	0.60
19:S:115:LYS:NZ	19:S:117:GLY:O	2.32	0.60
22:V:593:LEU:HD11	22:V:615:PHE:CZ	2.36	0.60
1:A:927:GLU:O	1:A:931:ARG:HB2	2.00	0.60
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.84	0.60
18:R:190:LEU:HD11	18:R:205:ASP:CB	2.31	0.60
21:U:251:ALA:C	21:U:253:THR:N	2.51	0.60
25:1:1:MET:HA	26:2:413:LEU:HA	1.83	0.60
26:2:30:VAL:HG12	26:2:34:LEU:HD23	1.82	0.60
16:P:298:PRO:O	16:P:300:ILE:HG12	2.00	0.60
18:R:190:LEU:HD11	18:R:205:ASP:CG	2.25	0.60
24:0:55:LEU:HD12	27:3:178:MET:CE	2.31	0.60
25:1:10:ILE:C	25:1:10:ILE:HD13	2.26	0.60
26:2:42:LEU:HD12	26:2:59:MET:HE3	1.83	0.60
5:E:51:GLY:O	5:E:52:ARG:CB	2.37	0.60
18:R:224:THR:O	18:R:225:VAL:C	2.44	0.60
27:3:71:TYR:CG	27:3:72:PRO:HD2	2.17	0.60
27:3:222:SER:HB2	27:3:226:TYR:CE2	2.37	0.60
1:A:364:ARG:HE	1:A:500:GLU:CD	2.10	0.60
1:A:720:ALA:HB1	9:I:108:MET:HG2	1.84	0.60
1:A:1319:LYS:CG	1:A:1333:GLU:HG2	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:TYR:HD1	5:E:65:ASN:H	1.49	0.60
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.84	0.60
22:V:534:TYR:CD1	22:V:535:THR:N	2.70	0.60
24:O:54:ARG:C	27:3:209:ILE:HD11	2.25	0.60
11:K:62:LYS:HE2	11:K:72:ILE:HD11	1.83	0.60
23:W:175:TYR:HD1	23:W:175:TYR:H	1.46	0.60
26:2:83:GLN:OE1	26:2:83:GLN:HA	2.01	0.60
27:3:42:MET:HE2	27:3:108:ASN:CG	2.27	0.60
1:A:1250:ASP:OD2	21:U:227:GLU:HB2	2.00	0.60
2:B:90:GLN:NE2	20:T:141:LEU:CA	2.25	0.60
3:C:117:SER:HB3	3:C:130:VAL:HG21	1.83	0.60
5:E:71:GLN:HE21	5:E:99:ILE:HA	1.66	0.60
26:2:159:VAL:HG13	26:2:160:LEU:N	2.17	0.60
27:3:173:GLN:CA	27:3:176:ASN:HD21	2.10	0.60
1:A:425:ASP:HB3	13:M:39:LEU:CD1	2.32	0.60
1:A:621:ILE:HG22	1:A:621:ILE:O	2.02	0.60
2:B:78:VAL:O	2:B:78:VAL:HG12	2.01	0.60
5:E:55:ARG:N	5:E:78:GLU:CD	2.59	0.60
16:P:162:VAL:HG23	16:P:162:VAL:O	2.02	0.60
23:W:421:PHE:CB	23:W:431:PRO:HG3	2.32	0.60
17:Q:54:PHE:CD2	18:R:194:ARG:HD2	2.36	0.59
23:W:584:TYR:HB2	23:W:594:ALA:CB	2.32	0.59
26:2:164:VAL:HG13	26:2:209:PRO:HG2	1.83	0.59
26:2:259:LEU:HD12	26:2:259:LEU:C	2.27	0.59
25:1:53:LEU:HD12	25:1:53:LEU:N	2.18	0.59
26:2:171:VAL:HG13	26:2:216:MET:HB2	1.83	0.59
27:3:14:VAL:HG23	27:3:163:VAL:HA	1.84	0.59
27:3:196:LEU:CD2	27:3:223:LEU:HD23	2.25	0.59
27:3:213:LEU:HD23	27:3:230:VAL:HG12	1.84	0.59
1:A:153:ILE:O	1:A:153:ILE:HG22	2.03	0.59
1:A:621:ILE:O	1:A:623:PRO:N	2.35	0.59
13:M:44:ARG:NE	13:M:46:ILE:HG22	2.16	0.59
26:2:196:ILE:HA	26:2:202:GLN:OE1	2.02	0.59
26:2:206:LEU:HD22	26:2:206:LEU:N	2.17	0.59
2:B:228:SER:O	2:B:405:ARG:NH1	2.36	0.59
2:B:838:GLN:HB3	2:B:890:ARG:HA	1.84	0.59
3:C:56:SER:HG	3:C:158:GLU:H	1.46	0.59
5:E:45:GLY:C	5:E:47:LYS:H	2.11	0.59
18:R:162:GLY:C	18:R:164:GLY:N	2.46	0.59
22:V:612:ASP:OD2	22:V:639:ARG:NH1	2.35	0.59
28:X:51:DC:H2"	28:X:52:DG:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:CE2	1:A:218:PRO:HG3	2.37	0.59
17:Q:117:ASP:OD1	17:Q:174:ARG:NH1	2.35	0.59
25:1:18:GLN:HB2	25:1:44:PHE:CZ	2.37	0.59
27:3:110:VAL:O	27:3:114:GLU:HG2	2.02	0.59
1:A:841:MET:HE1	2:B:503:ASN:CG	2.27	0.59
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.83	0.59
2:B:297:MET:SD	2:B:373:LEU:HD22	2.42	0.59
27:3:160:ARG:HB3	27:3:190:LEU:CD2	2.32	0.59
1:A:857:THR:HG21	1:A:1100:THR:HA	1.84	0.59
2:B:490:GLY:O	2:B:491:ARG:HG2	2.02	0.59
22:V:703:PHE:CZ	22:V:712:LEU:CD2	2.86	0.59
25:1:29:LEU:HD23	25:1:29:LEU:C	2.27	0.59
27:3:215:LEU:CD1	27:3:230:VAL:HG13	2.32	0.59
1:A:478:PRO:HB2	1:A:479:TRP:CE3	2.38	0.59
1:A:1021:VAL:HA	1:A:1034:GLN:NE2	2.18	0.59
2:B:133:ILE:O	2:B:134:LYS:C	2.45	0.59
18:R:195:PRO:O	18:R:196:ASP:CB	2.50	0.59
26:2:202:GLN:NE2	26:2:202:GLN:H	2.00	0.59
26:2:215:PHE:CD2	26:2:264:HIS:HB2	2.37	0.59
27:3:131:THR:HG23	27:3:133:LEU:CD1	2.32	0.59
1:A:800:PHE:CZ	1:A:815:TYR:HE1	2.21	0.59
2:B:883:THR:O	2:B:885:ARG:N	2.36	0.59
13:M:44:ARG:NE	13:M:46:ILE:HG23	2.17	0.59
25:1:34:ILE:O	25:1:46:ILE:HG13	2.03	0.59
25:1:38:ILE:H	25:1:38:ILE:CD1	2.16	0.59
26:2:203:PHE:CE2	26:2:205:LEU:HD23	2.38	0.59
27:3:174:TYR:CE1	27:3:178:MET:HE3	2.37	0.59
1:A:1416:ARG:HB3	1:A:1433:GLU:OE1	2.03	0.58
2:B:289:ILE:O	2:B:291:ASP:N	2.35	0.58
5:E:160:LEU:HD21	5:E:167:GLU:HG3	1.84	0.58
17:Q:28:ILE:HG21	18:R:190:LEU:HD13	1.85	0.58
21:U:132:ARG:N	21:U:167:GLU:OE2	2.36	0.58
23:W:37:HIS:ND1	23:W:454:VAL:HG13	2.16	0.58
23:W:209:TYR:CE1	23:W:233:PHE:CD1	2.90	0.58
26:2:44:VAL:HG13	26:2:45:PHE:N	2.17	0.58
26:2:160:LEU:HD12	26:2:160:LEU:N	2.18	0.58
1:A:69:GLY:HA2	1:A:77:ASN:HA	1.85	0.58
1:A:1192:TRP:O	1:A:1196:TYR:N	2.34	0.58
2:B:685:LYS:HA	2:B:688:ALA:HB3	1.86	0.58
22:V:520:ARG:HD3	25:1:19:PHE:HB3	1.85	0.58
25:1:1:MET:HB3	26:2:413:LEU:HG	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:2:VAL:HB	26:2:456:LYS:HD3	1.85	0.58
25:1:34:ILE:HG22	25:1:46:ILE:CD1	2.32	0.58
26:2:217:LEU:HD23	26:2:233:ILE:CD1	2.32	0.58
27:3:169:ASP:CG	27:3:202:LEU:HD23	2.28	0.58
1:A:930:LEU:C	1:A:931:ARG:O	2.45	0.58
21:U:252:LYS:O	21:U:253:THR:CB	2.51	0.58
27:3:169:ASP:CB	27:3:202:LEU:HD23	2.33	0.58
1:A:551:ARG:NE	1:A:625:ASP:OD2	2.36	0.58
1:A:799:PRO:O	1:A:806:THR:HG22	2.03	0.58
1:A:1251:ASN:OD1	21:U:197:ASN:ND2	2.36	0.58
6:F:62:ARG:NH1	6:F:127:ASP:O	2.27	0.58
23:W:73:CYS:CB	23:W:209:TYR:CZ	2.86	0.58
26:2:30:VAL:HG22	27:3:25:GLN:OE1	2.03	0.58
26:2:62:LEU:HD13	26:2:62:LEU:C	2.28	0.58
27:3:131:THR:CG2	27:3:133:LEU:HD12	2.33	0.58
27:3:190:LEU:HD23	27:3:190:LEU:N	2.18	0.58
1:A:298:ALA:HB1	1:A:303:ILE:HD11	1.85	0.58
25:1:2:VAL:CG1	26:2:456:LYS:CD	2.82	0.58
26:2:177:GLN:HE22	26:2:220:LEU:HA	1.68	0.58
26:2:220:LEU:HD13	26:2:220:LEU:C	2.29	0.58
1:A:35:SER:OG	1:A:37:THR:HG22	2.04	0.58
1:A:643:LYS:HD3	21:U:301:CYS:SG	2.43	0.58
5:E:10:LEU:HD21	5:E:55:ARG:NH2	2.18	0.58
25:1:18:GLN:CD	25:1:44:PHE:HZ	2.11	0.58
1:A:521:VAL:C	1:A:666:ARG:HH21	2.11	0.58
3:C:148:ILE:HG12	10:J:5:VAL:HG22	1.86	0.58
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.85	0.58
23:W:419:GLU:O	23:W:420:PRO:O	2.20	0.58
26:2:35:TYR:CB	26:2:62:LEU:HD12	2.33	0.58
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.85	0.58
1:A:417:LYS:HG2	1:A:449:HIS:CE1	2.39	0.58
7:G:31:PHE:HE1	7:G:48:VAL:HB	1.68	0.58
21:U:226:GLU:HG3	21:U:238:LYS:NZ	2.18	0.58
28:X:48:DG:H2''	28:X:49:DA:H5''	1.84	0.58
3:C:137:ASN:CB	3:C:145:GLN:NE2	2.63	0.58
20:T:4:ARG:NE	20:T:102:ASP:OD2	2.35	0.58
21:U:226:GLU:HG3	21:U:238:LYS:HZ1	1.67	0.58
22:V:613:THR:O	22:V:614:SER:CB	2.36	0.58
26:2:236:PHE:CZ	26:2:258:LEU:HD11	2.39	0.58
29:Y:36:DA:N9	29:Y:37:DG:N7	2.50	0.58
1:A:353:ASN:HD21	2:B:1071:ASN:HD21	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ILE:HD11	1:A:669:TYR:HB3	1.85	0.58
2:B:1129:ASN:HA	2:B:1135:TYR:HD1	1.69	0.58
25:1:8:VAL:HG12	25:1:9:LEU:H	1.69	0.58
26:2:118:LEU:HD12	26:2:118:LEU:C	2.28	0.58
27:3:215:LEU:HD12	27:3:230:VAL:HG13	1.85	0.58
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.34	0.57
2:B:73:HIS:C	2:B:75:SER:H	2.12	0.57
2:B:471:ASN:OD1	2:B:472:ARG:N	2.37	0.57
13:M:86:LYS:HA	13:M:86:LYS:HE2	1.83	0.57
1:A:522:PRO:CA	1:A:666:ARG:HH21	2.17	0.57
1:A:631:GLU:HG3	1:A:988:TRP:HH2	1.69	0.57
1:A:927:GLU:HG2	1:A:931:ARG:NH1	2.18	0.57
13:M:10:LEU:N	13:M:11:PRO:CD	2.53	0.57
23:W:209:TYR:HH	23:W:233:PHE:CA	2.09	0.57
26:2:82:ALA:HA	26:2:89:LEU:HD11	1.85	0.57
1:A:565:MET:HE2	11:K:61:TYR:HA	1.85	0.57
2:B:91:ILE:HG22	20:T:141:LEU:CD1	2.29	0.57
2:B:1016:SER:HB3	2:B:1022:LEU:HB3	1.86	0.57
9:I:14:ILE:CG1	9:I:16:PHE:CD1	2.87	0.57
27:3:16:ASP:O	27:3:21:TRP:NE1	2.27	0.57
27:3:172:LEU:HD13	27:3:172:LEU:C	2.29	0.57
1:A:210:GLN:O	1:A:211:GLU:HB2	2.03	0.57
2:B:724:TYR:HB3	2:B:728:MET:HE3	1.85	0.57
8:H:95:LYS:HB3	8:H:139:SER:HA	1.85	0.57
17:Q:102:VAL:HG13	17:Q:103:VAL:CA	2.32	0.57
22:V:321:GLU:HA	23:W:499:ASN:HD21	1.65	0.57
27:3:44:LEU:HD13	27:3:44:LEU:C	2.30	0.57
1:A:480:SER:HB3	2:B:1059:ILE:HD12	1.86	0.57
1:A:948:ILE:HG23	1:A:1007:ILE:HD11	1.85	0.57
2:B:800:ALA:O	2:B:805:PHE:HB3	2.05	0.57
13:M:47:ASP:O	13:M:48:VAL:C	2.38	0.57
18:R:190:LEU:HD13	18:R:205:ASP:OD2	1.97	0.57
23:W:584:TYR:CB	23:W:594:ALA:HB2	2.33	0.57
27:3:216:LYS:H	27:3:216:LYS:CD	2.13	0.57
1:A:133:SER:C	1:A:135:GLY:N	2.40	0.57
10:J:9:THR:OG1	10:J:47:ARG:NH2	2.35	0.57
18:R:190:LEU:HD12	18:R:205:ASP:CG	2.29	0.57
20:T:142:SER:C	20:T:144:GLN:H	2.12	0.57
21:U:252:LYS:HA	21:U:252:LYS:HE3	1.86	0.57
24:O:109:THR:HB	24:O:144:SER:H	1.67	0.57
27:3:14:VAL:HG23	27:3:163:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:187:GLN:NE2	27:3:189:ILE:HG13	2.20	0.57
1:A:114:CYS:HB2	1:A:184:CYS:SG	2.44	0.57
1:A:800:PHE:HZ	1:A:815:TYR:HE1	1.53	0.57
1:A:922:PHE:CE2	1:A:932:ARG:NH1	2.73	0.57
2:B:496:ALA:HB3	2:B:498:PRO:HD2	1.87	0.57
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.86	0.57
9:I:62:VAL:HG23	9:I:64:GLU:HG2	1.86	0.57
15:O:3:TYR:CD1	15:O:98:CYS:SG	2.93	0.57
17:Q:24:GLY:HA3	18:R:210:PHE:CD2	2.38	0.57
18:R:144:ASN:OD1	18:R:145:VAL:N	2.36	0.57
29:Y:18:DG:C2	29:Y:19:DC:C2	2.93	0.57
1:A:931:ARG:O	1:A:933:THR:N	2.37	0.57
2:B:468:GLN:OE1	2:B:481:HIS:NE2	2.38	0.57
2:B:720:PRO:O	2:B:724:TYR:HD2	1.88	0.57
2:B:755:GLN:HB2	2:B:777:ASN:ND2	2.19	0.57
2:B:1022:LEU:HD12	2:B:1023:ARG:HG3	1.87	0.57
20:T:129:ARG:HA	20:T:132:ILE:HD12	1.87	0.57
24:O:77:LYS:HD2	24:O:77:LYS:N	2.19	0.57
26:2:30:VAL:N	27:3:25:GLN:CB	2.52	0.57
26:2:185:MET:HB2	26:2:229:ASP:OD1	2.04	0.57
2:B:834:ARG:O	2:B:885:ARG:NH1	2.38	0.57
13:M:94:ASP:O	13:M:97:GLY:C	2.48	0.57
17:Q:16:ARG:HD2	17:Q:19:LYS:HB2	1.86	0.57
21:U:291:CYS:SG	21:U:293:GLU:HB2	2.45	0.57
22:V:514:MET:SD	22:V:537:ASN:ND2	2.78	0.57
28:X:14:DA:H2"	28:X:15:DA:C8	2.40	0.57
1:A:47:THR:C	1:A:48:GLU:O	2.46	0.56
1:A:129:ILE:O	1:A:132:LYS:HB2	2.05	0.56
2:B:80:GLU:HB3	2:B:135:GLU:HB3	1.71	0.56
2:B:326:ALA:HB2	2:B:338:TYR:CE2	2.40	0.56
2:B:875:GLU:O	2:B:876:ASN:HB2	2.04	0.56
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.86	0.56
3:C:117:SER:OG	3:C:147:ASP:OD2	2.16	0.56
26:2:117:ASN:HB2	27:3:104:LEU:CD1	2.35	0.56
27:3:210:THR:HG22	27:3:210:THR:O	2.04	0.56
27:3:223:LEU:HD11	27:3:227:LEU:HD11	1.87	0.56
29:Y:36:DA:C5	29:Y:37:DG:N7	2.73	0.56
1:A:364:ARG:NH2	1:A:500:GLU:OE1	2.37	0.56
1:A:614:ASP:O	1:A:615:SER:OG	2.20	0.56
27:3:19:PRO:HG2	27:3:123:ASP:O	2.05	0.56
27:3:195:VAL:HG21	27:3:214:TYR:OH	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:LYS:N	28:X:47:DC:OP1	2.37	0.56
1:A:1319:LYS:CG	1:A:1333:GLU:CG	2.60	0.56
1:A:1319:LYS:CD	1:A:1333:GLU:CD	2.57	0.56
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.39	0.56
17:Q:42:CYS:O	17:Q:95:ASN:ND2	2.38	0.56
20:T:146:ASP:O	20:T:147:LYS:CB	2.53	0.56
22:V:519:TYR:HD2	25:1:20:LEU:HB2	1.71	0.56
25:1:1:MET:CB	26:2:418:PHE:HB2	2.35	0.56
25:1:52:VAL:HG22	25:1:53:LEU:HD12	1.87	0.56
26:2:60:LEU:HD11	26:2:95:ILE:CG2	2.35	0.56
26:2:117:ASN:HD22	27:3:42:MET:HE1	1.70	0.56
27:3:21:TRP:O	27:3:24:LYS:HB2	2.05	0.56
27:3:57:LEU:HD23	27:3:58:ALA:C	2.31	0.56
27:3:178:MET:SD	27:3:181:ILE:HD12	2.46	0.56
2:B:704:LEU:HD22	2:B:708:ALA:CB	2.36	0.56
18:R:99:LEU:HD12	18:R:124:LEU:HD12	1.86	0.56
26:2:47:GLU:HG3	26:2:48:LEU:N	2.20	0.56
26:2:130:SER:HB2	26:2:173:GLN:OE1	2.06	0.56
27:3:42:MET:SD	27:3:111:ILE:HD13	2.46	0.56
27:3:223:LEU:O	27:3:223:LEU:HD13	2.05	0.56
2:B:882:SER:O	2:B:887:TYR:CG	2.57	0.56
8:H:106:THR:C	8:H:108:ALA:N	2.63	0.56
27:3:144:ILE:HG12	27:3:147:MET:CE	2.34	0.56
27:3:165:LYS:HZ1	27:3:200:SER:H	1.54	0.56
2:B:45:ASP:HB3	2:B:534:VAL:HG11	1.87	0.56
2:B:74:ALA:HB2	20:T:201:ASP:CB	2.29	0.56
3:C:130:VAL:O	3:C:134:ASN:ND2	2.39	0.56
17:Q:29:GLU:OE1	18:R:194:ARG:NH2	2.32	0.56
22:V:319:TYR:CE2	22:V:320:GLN:HG3	2.41	0.56
22:V:519:TYR:CD2	25:1:20:LEU:HB2	2.41	0.56
25:1:1:MET:HB2	26:2:418:PHE:HB2	1.88	0.56
26:2:160:LEU:H	26:2:160:LEU:CD1	2.18	0.56
19:S:110:PHE:HD1	19:S:148:PRO:HA	1.70	0.56
27:3:58:ALA:CA	27:3:71:TYR:CE2	2.82	0.56
1:A:464:LEU:HD21	1:A:1100:THR:HG21	1.88	0.56
1:A:631:GLU:HG3	1:A:988:TRP:CH2	2.40	0.56
1:A:939:VAL:HA	1:A:942:VAL:HG22	1.87	0.56
2:B:728:MET:HE2	2:B:942:LYS:HE2	1.88	0.56
9:I:75:ASP:HB3	9:I:78:LEU:HD12	1.86	0.56
13:M:290:ARG:NH1	28:X:5:DG:OP1	2.39	0.56
19:S:49:ARG:NH1	19:S:96:GLN:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:HD22	13:M:43:ASP:CG	2.14	0.56
1:A:108:ARG:NH1	1:A:145:TYR:OH	2.36	0.56
1:A:521:VAL:O	1:A:666:ARG:NH2	2.38	0.56
1:A:1085:GLU:OE2	6:F:59:LYS:HE2	2.05	0.56
16:P:206:GLU:HG3	16:P:236:LYS:HZ3	1.67	0.56
25:1:31:LYS:O	25:1:32:LYS:HB2	2.06	0.56
25:1:36:GLN:HB3	25:1:45:VAL:HG12	1.88	0.56
26:2:206:LEU:HD22	26:2:206:LEU:H	1.71	0.56
1:A:678:ASN:O	1:A:681:LEU:HB3	2.06	0.56
1:A:1223:ASP:OD2	1:A:1224:ARG:NH1	2.38	0.56
3:C:142:TYR:O	3:C:144:GLU:N	2.39	0.56
7:G:93:ASN:OD1	7:G:94:LYS:N	2.38	0.56
26:2:423:ALA:HA	26:2:426:ARG:HE	1.70	0.56
1:A:1113:SER:O	1:A:1114:ALA:HB3	2.03	0.55
27:3:21:TRP:CD2	27:3:34:LEU:HD23	2.42	0.55
27:3:165:LYS:HD3	27:3:165:LYS:C	2.31	0.55
1:A:606:HIS:HB2	1:A:627:LYS:HA	1.87	0.55
1:A:930:LEU:HD21	8:H:107:GLU:OE1	2.06	0.55
1:A:1103:THR:HG23	1:A:1106:THR:H	1.71	0.55
2:B:329:GLY:H	2:B:335:ARG:HH21	1.54	0.55
2:B:747:LEU:HD21	2:B:810:PHE:HE1	1.71	0.55
26:2:181:GLN:HA	26:2:181:GLN:HE21	1.70	0.55
29:Y:36:DA:N3	29:Y:37:DG:C8	2.75	0.55
1:A:121:SER:HA	1:A:126:ILE:HG21	1.87	0.55
2:B:92:TYR:HE1	20:T:143:GLN:HE21	1.54	0.55
9:I:57:LYS:C	9:I:59:THR:N	2.63	0.55
17:Q:109:HIS:HE1	18:R:231:GLU:CB	2.19	0.55
27:3:44:LEU:HD13	27:3:44:LEU:O	2.06	0.55
1:A:266:MET:CG	1:A:272:ASN:HD21	1.90	0.55
1:A:1319:LYS:HG3	1:A:1333:GLU:OE1	2.07	0.55
2:B:35:ASP:OD2	2:B:646:ARG:NH1	2.37	0.55
15:O:64:THR:HG21	16:P:188:ARG:HD2	1.89	0.55
17:Q:109:HIS:CG	18:R:224:THR:HG1	2.15	0.55
18:R:84:TYR:OH	18:R:88:ARG:NH1	2.38	0.55
22:V:531:ILE:CB	22:V:534:TYR:CE2	2.89	0.55
25:1:1:MET:CG	26:2:418:PHE:HB2	2.35	0.55
1:A:138:LYS:HB2	1:A:1445:HIS:CE1	2.41	0.55
13:M:44:ARG:HG3	13:M:46:ILE:HG23	1.89	0.55
20:T:228:ILE:O	20:T:230:LYS:N	2.38	0.55
22:V:504:LYS:HD2	22:V:654:GLU:O	2.07	0.55
1:A:685:HIS:HB3	2:B:784:SER:OG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:85:PRO:C	9:I:86:CYS:O	2.49	0.55
19:S:172:ASN:OD1	19:S:173:HIS:N	2.38	0.55
25:1:34:ILE:HG23	25:1:50:VAL:HG11	1.89	0.55
27:3:133:LEU:H	27:3:133:LEU:CD1	2.10	0.55
1:A:279:LYS:HB2	1:A:336:LEU:HD21	1.88	0.55
1:A:428:ASP:OD1	1:A:430:ARG:N	2.37	0.55
1:A:875:TYR:O	6:F:53:THR:HG22	2.06	0.55
1:A:1313:GLN:CD	1:A:1318:LYS:HB2	2.32	0.55
2:B:901:THR:OG1	2:B:902:GLY:N	2.31	0.55
5:E:10:LEU:HD21	5:E:55:ARG:NE	2.21	0.55
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.42	0.55
10:J:10:CYS:SG	10:J:11:GLY:N	2.79	0.55
13:M:94:ASP:O	13:M:97:GLY:O	2.25	0.55
17:Q:24:GLY:HA2	18:R:210:PHE:CE2	2.40	0.55
21:U:256:THR:HG1	21:U:272:THR:HG22	1.69	0.55
25:1:52:VAL:HG23	25:1:53:LEU:N	2.21	0.55
1:A:611:ASP:O	1:A:612:ASP:HB2	2.06	0.55
1:A:1299:GLN:HG2	1:A:1300:GLY:N	2.21	0.55
1:A:1316:ASN:HA	21:U:292:ASN:O	2.07	0.55
2:B:240:LEU:O	2:B:253:GLY:HA2	2.07	0.55
22:V:531:ILE:CA	22:V:534:TYR:HE2	1.90	0.55
2:B:35:ASP:CG	2:B:646:ARG:HH12	2.15	0.55
5:E:185:ILE:HG13	5:E:189:GLN:OE1	2.07	0.55
7:G:107:PHE:CZ	17:Q:127:PHE:HZ	2.24	0.55
1:A:230:ASP:OD1	1:A:244:ARG:NH1	2.40	0.55
10:J:3:ILE:HD13	10:J:18:TRP:CB	2.37	0.55
12:L:19:CYS:SG	12:L:20:GLY:N	2.80	0.55
13:M:178:LYS:C	20:T:154:LYS:CB	2.77	0.55
14:N:323:GLU:HG3	14:N:325:GLY:HA3	1.89	0.55
18:R:93:ASP:O	18:R:140:LYS:NZ	2.35	0.55
26:2:53:LYS:CE	26:2:95:ILE:HD11	2.36	0.55
26:2:208:THR:O	26:2:212:LEU:HG	2.07	0.55
27:3:223:LEU:HD13	27:3:227:LEU:HG	1.88	0.55
1:A:133:SER:O	1:A:134:LYS:C	2.45	0.54
2:B:116:ARG:HH12	12:L:42:ARG:HH11	1.53	0.54
2:B:704:LEU:HD22	2:B:708:ALA:HB1	1.89	0.54
5:E:15:LYS:NZ	5:E:33:LEU:O	2.40	0.54
22:V:251:PHE:O	22:V:257:LYS:HA	2.06	0.54
22:V:516:PRO:HD2	22:V:706:LYS:NZ	2.22	0.54
26:2:123:LEU:CD2	26:2:178:LEU:HD11	2.37	0.54
26:2:123:LEU:HD21	26:2:178:LEU:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:177:GLN:NE2	26:2:220:LEU:HA	2.22	0.54
1:A:355:MET:HE3	1:A:1431:SER:HB2	1.88	0.54
1:A:1307:VAL:HG11	1:A:1339:ASP:OD2	2.06	0.54
19:S:47:LEU:HD23	20:T:104:LEU:HD13	1.89	0.54
26:2:159:VAL:HG22	26:2:160:LEU:N	2.16	0.54
22:V:523:VAL:HG21	25:1:20:LEU:HD23	1.88	0.54
26:2:37:HIS:HB3	26:2:38:PRO:CD	2.35	0.54
26:2:211:GLN:HB3	26:2:261:PHE:CE1	2.40	0.54
27:3:64:ILE:HG23	27:3:128:HIS:CG	2.42	0.54
27:3:100:LYS:O	27:3:103:LEU:HB2	2.08	0.54
17:Q:109:HIS:HB3	18:R:224:THR:CB	2.38	0.54
17:Q:110:MET:HE1	18:R:222:SER:OG	2.08	0.54
22:V:325:ARG:HH22	23:W:499:ASN:HB3	0.72	0.54
23:W:608:ILE:O	23:W:614:TYR:OH	2.21	0.54
25:1:3:ASN:CB	26:2:412:PHE:O	2.54	0.54
29:Y:48:DC:H2"	29:Y:49:DG:C8	2.41	0.54
1:A:516:GLN:HG3	1:A:520:MET:HE2	1.90	0.54
1:A:549:THR:HG21	1:A:640:LEU:HG	1.90	0.54
1:A:597:PRO:O	1:A:599:HIS:N	2.40	0.54
22:V:638:GLN:O	22:V:642:ARG:HG2	2.08	0.54
25:1:34:ILE:HG21	25:1:54:GLN:CD	2.32	0.54
26:2:199:ALA:HB1	26:2:201:PHE:CD2	2.43	0.54
1:A:924:TYR:OH	1:A:949:GLN:HA	2.08	0.54
2:B:80:GLU:C	2:B:135:GLU:HG3	2.29	0.54
5:E:52:ARG:HB2	5:E:53:PRO:HD2	1.80	0.54
16:P:161:ILE:O	16:P:161:ILE:HG23	2.07	0.54
26:2:28:PRO:CA	27:3:33:THR:HB	2.10	0.54
2:B:92:TYR:HE2	2:B:146:LYS:NZ	2.06	0.54
3:C:9:VAL:HG11	11:K:105:PHE:HA	1.89	0.54
5:E:54:ARG:HG2	5:E:54:ARG:HH11	1.72	0.54
19:S:126:ILE:O	19:S:137:ALA:HA	2.08	0.54
20:T:141:LEU:O	20:T:143:GLN:N	2.38	0.54
22:V:531:ILE:C	22:V:534:TYR:CE2	2.85	0.54
1:A:294:GLU:HA	1:A:298:ALA:HB2	1.88	0.54
1:A:1341:VAL:O	1:A:1343:LEU:N	2.38	0.54
26:2:214:TYR:CD2	26:2:261:PHE:CD2	2.95	0.54
1:A:1123:ARG:NH1	1:A:1126:GLU:OE1	2.39	0.54
2:B:649:ASN:OD1	2:B:650:ASN:N	2.41	0.54
2:B:991:ALA:HB1	10:J:43:TYR:HB2	1.90	0.54
13:M:290:ARG:HH12	28:X:5:DG:P	2.31	0.54
22:V:534:TYR:CD1	22:V:534:TYR:C	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:667:THR:HA	25:1:62:ASP:OD2	2.07	0.54
23:W:428:ILE:HA	23:W:430:ASN:ND2	2.23	0.54
25:1:1:MET:CE	26:2:415:GLN:C	2.80	0.54
27:3:223:LEU:HD13	27:3:223:LEU:C	2.33	0.54
2:B:27:TRP:CD2	2:B:762:ARG:HG2	2.43	0.54
2:B:489:ILE:HG13	2:B:490:GLY:H	1.73	0.54
3:C:262:GLN:HG3	11:K:18:LYS:HG2	1.90	0.54
5:E:177:ASP:OD1	5:E:178:PRO:HD2	2.08	0.54
24:0:54:ARG:CB	27:3:209:ILE:HG23	2.25	0.54
26:2:81:LYS:HG3	26:2:82:ALA:N	2.21	0.54
26:2:86:SER:O	26:2:90:LEU:HD13	2.08	0.54
2:B:739:ASN:HB3	10:J:62:TYR:CZ	2.44	0.53
3:C:7:PRO:HG3	11:K:97:GLU:OE2	2.04	0.53
9:I:14:ILE:HA	9:I:16:PHE:CE1	2.43	0.53
23:W:423:ASP:C	23:W:425:THR:N	2.64	0.53
25:1:25:GLU:HG2	25:1:32:LYS:HA	1.89	0.53
27:3:106:SER:O	27:3:109:GLU:HG3	2.08	0.53
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.90	0.53
2:B:91:ILE:N	20:T:141:LEU:HG	2.23	0.53
3:C:58:VAL:HG21	10:J:59:LEU:HB3	1.90	0.53
17:Q:14:LEU:HD21	17:Q:102:VAL:HG21	1.90	0.53
17:Q:105:TYR:CE1	18:R:231:GLU:OE1	2.59	0.53
20:T:26:TYR:HE2	20:T:124:TYR:HH	1.54	0.53
22:V:520:ARG:NE	22:V:521:GLU:OE2	2.30	0.53
26:2:222:THR:HG23	26:2:222:THR:O	2.07	0.53
1:A:137:PRO:HB2	1:A:1445:HIS:NE2	2.23	0.53
5:E:47:LYS:HB2	5:E:48:PRO:HD3	1.77	0.53
10:J:62:TYR:CA	10:J:64:PRO:HD2	2.30	0.53
13:M:44:ARG:HH11	13:M:46:ILE:HG22	1.72	0.53
25:1:4:VAL:HG11	26:2:412:PHE:CD2	2.29	0.53
1:A:522:PRO:HA	1:A:666:ARG:NH2	2.24	0.53
1:A:1111:GLY:HA2	21:U:254:GLY:HA2	1.90	0.53
26:2:141:HIS:HA	26:2:162:PHE:CE2	2.43	0.53
26:2:160:LEU:CG	26:2:206:LEU:HD21	2.39	0.53
27:3:191:ILE:N	27:3:210:THR:HG21	2.24	0.53
1:A:460:ARG:NE	1:A:492:TYR:O	2.32	0.53
1:A:603:ILE:HD11	1:A:988:TRP:NE1	2.23	0.53
2:B:853:LEU:HD12	12:L:46:LYS:HE3	1.91	0.53
2:B:1152:PRO:HG2	2:B:1155:CYS:HB2	1.89	0.53
26:2:31:LEU:HG	27:3:25:GLN:O	2.09	0.53
26:2:211:GLN:HE21	26:2:257:SER:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:ILE:HG21	2:B:298:MET:HE1	1.91	0.53
13:M:225:PRO:HG2	13:M:228:VAL:HG23	1.90	0.53
17:Q:105:TYR:HE1	18:R:231:GLU:HB2	1.73	0.53
18:R:140:LYS:HB3	18:R:141:PRO:HD3	1.89	0.53
19:S:103:ASN:HB2	19:S:107:GLY:HA3	1.89	0.53
20:T:12:ALA:HB2	20:T:106:LEU:HD23	1.91	0.53
27:3:15:VAL:HG23	27:3:15:VAL:O	2.08	0.53
27:3:58:ALA:C	27:3:71:TYR:OH	2.51	0.53
17:Q:105:TYR:CE1	18:R:231:GLU:HB2	2.43	0.53
18:R:151:LEU:HD13	18:R:154:LEU:HD13	1.89	0.53
26:2:30:VAL:O	26:2:34:LEU:HD23	2.09	0.53
26:2:159:VAL:CG1	26:2:161:HIS:H	2.06	0.53
27:3:21:TRP:CG	27:3:34:LEU:HD23	2.44	0.53
1:A:542:LEU:HD23	1:A:774:ALA:HA	1.91	0.53
5:E:112:PRO:HA	5:E:115:LYS:HE2	1.91	0.53
7:G:94:LYS:HG3	7:G:95:VAL:HG23	1.90	0.53
18:R:78:LEU:HD11	18:R:124:LEU:HD21	1.89	0.53
21:U:227:GLU:O	21:U:228:MET:C	2.52	0.53
26:2:138:PRO:O	26:2:139:ASP:HB2	2.08	0.53
26:2:241:SER:O	26:2:245:LEU:HD23	2.09	0.53
27:3:160:ARG:NH2	27:3:192:ASP:HB3	2.23	0.53
27:3:204:GLN:HG2	27:3:214:TYR:CZ	2.44	0.53
1:A:1248:ASN:HD21	1:A:1255:LEU:HA	1.74	0.53
8:H:17:PRO:C	8:H:19:GLY:H	2.17	0.53
9:I:15:ARG:O	9:I:15:ARG:HG3	2.08	0.53
27:3:105:THR:HG23	27:3:106:SER:N	2.23	0.53
2:B:1029:TYR:HA	2:B:1036:LYS:HA	1.91	0.53
3:C:56:SER:OG	3:C:158:GLU:N	2.27	0.53
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:870:SER:HB2	1:A:882:SER:HB3	1.90	0.52
2:B:92:TYR:CB	20:T:145:LEU:HD13	2.38	0.52
17:Q:109:HIS:HE1	18:R:231:GLU:HA	1.73	0.52
22:V:325:ARG:HH21	23:W:499:ASN:CB	1.95	0.52
28:X:65:DG:N3	29:Y:30:DG:N2	2.57	0.52
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.43	0.52
26:2:221:GLN:CD	26:2:230:LEU:HB2	2.34	0.52
1:A:47:THR:O	1:A:48:GLU:C	2.52	0.52
1:A:535:MET:O	1:A:669:TYR:OH	2.25	0.52
2:B:329:GLY:H	2:B:335:ARG:NH2	2.07	0.52
22:V:523:VAL:CG2	25:1:20:LEU:CD2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:611:GLY:HA2	22:V:615:PHE:CB	2.37	0.52
25:1:59:GLU:CD	26:2:402:ARG:HH12	2.14	0.52
29:Y:36:DA:N1	29:Y:37:DG:C6	2.76	0.52
2:B:367:TYR:OH	2:B:371:ARG:NH1	2.42	0.52
25:1:8:VAL:CG1	25:1:45:VAL:HG13	2.35	0.52
26:2:138:PRO:HG3	26:2:189:GLU:CG	2.35	0.52
26:2:192:GLU:CG	26:2:193:PRO:HD2	2.23	0.52
1:A:389:THR:HB	1:A:417:LYS:HD3	1.90	0.52
2:B:157:ARG:N	2:B:161:CYS:SG	2.71	0.52
2:B:927:ARG:HG3	2:B:1054:MET:HE2	1.92	0.52
5:E:29:THR:HG22	5:E:31:ASP:H	1.75	0.52
16:P:203:ARG:HG3	16:P:203:ARG:NH2	2.25	0.52
22:V:531:ILE:O	22:V:534:TYR:CZ	2.62	0.52
27:3:133:LEU:HD13	27:3:133:LEU:N	2.14	0.52
27:3:222:SER:HB3	27:3:225:GLN:HG2	1.92	0.52
2:B:160:TYR:HE1	20:T:144:GLN:HG2	1.74	0.52
2:B:182:GLY:HA2	2:B:184:TYR:CE1	2.45	0.52
2:B:873:LEU:CB	2:B:874:PRO:HD3	2.35	0.52
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.75	0.52
8:H:92:MET:HE2	8:H:143:LEU:HD22	1.91	0.52
13:M:10:LEU:C	13:M:12:ARG:N	2.68	0.52
14:N:359:ASN:ND2	14:N:364:ASP:OD1	2.43	0.52
22:V:523:VAL:CG2	25:1:20:LEU:HD23	2.39	0.52
22:V:531:ILE:O	22:V:534:TYR:CE2	2.63	0.52
22:V:689:VAL:CB	26:2:391:ILE:HD11	2.39	0.52
25:1:35:ILE:O	25:1:35:ILE:HG13	2.08	0.52
29:Y:36:DA:N3	29:Y:37:DG:C5	2.78	0.52
2:B:45:ASP:OD2	2:B:531:TYR:OH	2.25	0.52
2:B:195:ILE:HD11	2:B:481:HIS:HE2	1.73	0.52
27:3:10:LEU:HD21	27:3:143:TYR:CD2	2.45	0.52
27:3:18:ASN:O	27:3:21:TRP:CD1	2.63	0.52
27:3:70:LEU:HD22	27:3:114:GLU:HB3	1.91	0.52
29:Y:36:DA:C6	29:Y:37:DG:C5	2.97	0.52
1:A:11:SER:O	1:A:13:CYS:N	2.43	0.52
1:A:208:ASP:OD1	1:A:209:SER:N	2.41	0.52
1:A:219:GLU:O	1:A:222:HIS:HB3	2.08	0.52
9:I:15:ARG:C	9:I:16:PHE:O	2.53	0.52
9:I:105:GLU:O	9:I:106:ASP:CB	2.41	0.52
17:Q:23:ARG:CD	18:R:207:SER:O	2.57	0.52
17:Q:69:ASP:O	17:Q:70:LYS:HB2	2.10	0.52
25:1:4:VAL:HG12	26:2:411:GLN:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:ASN:OD1	21:U:227:GLU:HB3	2.09	0.52
2:B:289:ILE:HD13	2:B:297:MET:SD	2.50	0.52
2:B:952:GLU:HG3	3:C:39:ILE:HG23	1.91	0.52
26:2:193:PRO:HB2	26:2:194:PRO:HD3	1.92	0.52
27:3:10:LEU:HD22	27:3:147:MET:HG2	1.92	0.52
27:3:42:MET:CG	27:3:111:ILE:HD11	2.40	0.52
28:X:40:DT:H2"	28:X:41:DT:H5"	1.92	0.52
1:A:602:CYS:HB2	1:A:655:ILE:HD12	1.91	0.52
1:A:800:PHE:HZ	1:A:815:TYR:CE1	2.28	0.52
1:A:1162:GLU:HA	1:A:1304:ILE:HD11	1.92	0.52
2:B:483:ARG:NH1	2:B:526:LEU:HB2	2.20	0.52
2:B:939:HIS:NE2	2:B:980:HIS:HA	2.24	0.52
16:P:297:LYS:C	16:P:299:ARG:H	2.17	0.52
18:R:194:ARG:O	18:R:196:ASP:N	2.43	0.52
21:U:290:VAL:HG22	21:U:297:ARG:HG2	1.90	0.52
22:V:593:LEU:HD11	22:V:615:PHE:HZ	1.75	0.52
26:2:257:SER:O	26:2:261:PHE:HD1	1.93	0.52
27:3:226:TYR:O	27:3:230:VAL:HB	2.10	0.52
29:Y:30:DG:N3	29:Y:31:DG:C5	2.78	0.52
1:A:220:ARG:O	1:A:221:VAL:C	2.52	0.51
1:A:261:ARG:O	1:A:263:ALA:N	2.42	0.51
2:B:92:TYR:CD1	20:T:141:LEU:HD21	2.44	0.51
2:B:151:LYS:N	2:B:441:SER:OG	2.39	0.51
2:B:628:VAL:HG22	2:B:694:THR:C	2.35	0.51
24:0:77:LYS:HG2	24:0:225:GLU:OE2	2.09	0.51
25:1:2:VAL:HG12	26:2:456:LYS:HG2	1.79	0.51
27:3:14:VAL:HG23	27:3:14:VAL:O	2.09	0.51
27:3:64:ILE:HG21	27:3:128:HIS:CB	2.40	0.51
27:3:141:LEU:HG	27:3:187:GLN:HE22	1.75	0.51
1:A:1036:ASN:C	1:A:1036:ASN:HD22	2.18	0.51
26:2:160:LEU:HB3	26:2:206:LEU:HD21	1.93	0.51
1:A:489:THR:OG1	1:A:494:ALA:O	2.28	0.51
17:Q:108:ASP:OD1	17:Q:111:ARG:NH2	2.19	0.51
23:W:584:TYR:HB2	23:W:591:GLY:HA3	1.92	0.51
1:A:1479:LYS:HD3	6:F:103:PRO:HA	1.93	0.51
2:B:738:THR:HG22	2:B:772:LEU:HD21	1.93	0.51
2:B:866:ILE:HG13	2:B:867:ILE:N	2.25	0.51
14:N:353:LEU:HB2	14:N:370:ALA:HB3	1.91	0.51
23:W:209:TYR:HH	23:W:234:ASP:H	1.57	0.51
27:3:121:LYS:HD3	27:3:121:LYS:N	2.25	0.51
1:A:430:ARG:NH2	13:M:26:ASP:OD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ILE:HD13	2:B:985:LEU:HD22	1.93	0.51
18:R:190:LEU:CD1	18:R:205:ASP:CB	2.88	0.51
26:2:179:LEU:CB	26:2:184:LEU:HD11	2.40	0.51
27:3:131:THR:HG23	27:3:133:LEU:HD12	1.92	0.51
27:3:165:LYS:HE3	27:3:200:SER:OG	2.09	0.51
1:A:743:ARG:HD2	21:U:257:GLN:HG2	1.92	0.51
19:S:29:MET:HE2	19:S:146:PHE:HE2	1.75	0.51
22:V:523:VAL:HB	25:1:20:LEU:HD23	1.93	0.51
25:1:21:LEU:O	25:1:24:ASP:HB3	2.10	0.51
26:2:46:ARG:HD3	26:2:85:GLU:HB2	1.93	0.51
26:2:215:PHE:CE2	26:2:264:HIS:HB2	2.46	0.51
1:A:1172:ASN:OD1	1:A:1173:THR:N	2.43	0.51
2:B:1124:ILE:HD12	2:B:1124:ILE:H	1.76	0.51
3:C:154:ARG:N	3:C:157:GLN:OE1	2.38	0.51
5:E:192:LYS:HE3	5:E:194:ILE:HD11	1.93	0.51
7:G:10:GLU:HB3	7:G:67:LEU:HD11	1.92	0.51
23:W:581:LEU:C	23:W:581:LEU:HD13	2.36	0.51
26:2:207:ASP:OD2	26:2:254:MET:HE2	2.10	0.51
2:B:733:MET:HE1	2:B:1054:MET:HE3	1.92	0.51
2:B:1117:HIS:O	2:B:1127:ILE:HG12	2.11	0.51
7:G:151:ARG:HB2	7:G:158:PHE:CE1	2.46	0.51
18:R:193:ASN:HB3	18:R:197:LYS:HA	1.92	0.51
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.75	0.51
23:W:209:TYR:CZ	23:W:233:PHE:HA	2.40	0.51
26:2:236:PHE:CE2	26:2:262:LEU:CD1	2.94	0.51
26:2:236:PHE:CE1	26:2:261:PHE:CB	2.94	0.51
1:A:476:ILE:HD12	1:A:476:ILE:N	2.25	0.51
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.93	0.51
1:A:980:PRO:HB2	1:A:981:CYS:SG	2.51	0.51
2:B:906:GLN:HG2	12:L:45:TYR:HE1	1.75	0.51
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.93	0.51
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.91	0.51
10:J:62:TYR:CB	10:J:64:PRO:CD	2.88	0.51
16:P:269:ARG:HB3	16:P:335:PHE:HB3	1.92	0.51
17:Q:35:ASP:CG	18:R:161:ARG:HH22	2.18	0.51
26:2:51:LEU:CD2	26:2:55:TRP:CD1	2.94	0.51
26:2:236:PHE:CZ	26:2:262:LEU:CD2	2.94	0.51
27:3:12:VAL:HG12	27:3:58:ALA:HB3	1.92	0.51
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.51	0.50
8:H:10:PHE:CE2	8:H:39:LEU:HD13	2.46	0.50
17:Q:54:PHE:HD2	18:R:194:ARG:CD	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:55:LEU:HD12	27:3:178:MET:HE3	1.93	0.50
26:2:57:MET:HA	26:2:60:LEU:CG	2.41	0.50
29:Y:36:DA:H2"	29:Y:37:DG:H8	1.76	0.50
2:B:116:ARG:NH1	12:L:42:ARG:HH11	2.08	0.50
2:B:499:ARG:HH11	2:B:520:VAL:HG22	1.76	0.50
3:C:267:ILE:HG21	3:C:274:ILE:HD13	1.93	0.50
26:2:231:VAL:O	26:2:234:LEU:HB3	2.11	0.50
10:J:28:GLU:HG2	10:J:30:THR:HG22	1.93	0.50
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.46	0.50
17:Q:180:PHE:CZ	18:R:211:SER:HA	2.38	0.50
26:2:199:ALA:HB1	26:2:201:PHE:CE2	2.47	0.50
27:3:100:LYS:HB3	27:3:103:LEU:CD1	2.38	0.50
27:3:187:GLN:O	27:3:188:ASN:HB2	2.12	0.50
1:A:85:PHE:HD1	1:A:257:PRO:HD3	1.76	0.50
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.94	0.50
13:M:52:TRP:CD1	13:M:67:VAL:HG22	2.47	0.50
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.77	0.50
13:M:178:LYS:NZ	29:Y:86:DC:OP1	2.45	0.50
15:O:66:ARG:HB3	15:O:73:THR:HB	1.92	0.50
16:P:297:LYS:HE2	16:P:297:LYS:CA	2.33	0.50
18:R:177:ASN:HD22	18:R:177:ASN:C	2.19	0.50
20:T:139:VAL:C	20:T:141:LEU:H	2.18	0.50
22:V:519:TYR:HE2	25:1:20:LEU:CG	2.19	0.50
26:2:140:LYS:CG	26:2:162:PHE:CE1	2.94	0.50
26:2:214:TYR:CB	26:2:261:PHE:CE2	2.95	0.50
1:A:138:LYS:NZ	1:A:1441:GLU:OE2	2.45	0.50
9:I:84:HIS:ND1	9:I:85:PRO:HD3	2.23	0.50
13:M:17:ASN:OD1	13:M:18:HIS:N	2.44	0.50
21:U:215:ILE:HG23	21:U:219:LEU:HD23	1.92	0.50
21:U:252:LYS:O	21:U:253:THR:HB	2.11	0.50
22:V:516:PRO:HG2	22:V:706:LYS:HE2	1.92	0.50
22:V:520:ARG:CG	25:1:23:LEU:HD11	2.42	0.50
26:2:35:TYR:CD1	26:2:35:TYR:N	2.79	0.50
1:A:126:ILE:HD13	1:A:129:ILE:HD12	1.93	0.50
1:A:463:THR:HG22	1:A:468:SER:HB3	1.94	0.50
1:A:873:VAL:HB	1:A:1083:PRO:HA	1.94	0.50
1:A:1408:ARG:NH2	1:A:1421:ARG:O	2.45	0.50
2:B:160:TYR:CE1	20:T:144:GLN:HG2	2.46	0.50
2:B:351:VAL:HG11	2:B:361:LYS:HA	1.94	0.50
2:B:746:THR:HG22	2:B:812:ARG:NH1	2.27	0.50
2:B:1125:MET:H	2:B:1163:MET:HE1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:86:LYS:HA	13:M:86:LYS:NZ	2.27	0.50
26:2:57:MET:HA	26:2:60:LEU:HG	1.93	0.50
26:2:93:LEU:CD2	26:2:96:TRP:HE1	2.25	0.50
26:2:223:ALA:O	26:2:224:GLN:HB3	2.12	0.50
27:3:64:ILE:CG2	27:3:128:HIS:HB3	2.42	0.50
27:3:178:MET:HE2	27:3:202:LEU:HD13	1.92	0.50
1:A:199:TYR:CE1	13:M:93:PHE:CE2	2.98	0.50
2:B:939:HIS:CD2	2:B:980:HIS:HA	2.47	0.50
5:E:111:THR:HG21	28:X:58:DT:OP1	2.12	0.50
26:2:30:VAL:CG1	26:2:34:LEU:HD23	2.40	0.50
27:3:60:ILE:HG22	27:3:61:ALA:N	2.26	0.50
27:3:216:LYS:O	27:3:216:LYS:HG2	2.11	0.50
26:2:51:LEU:HD23	26:2:51:LEU:C	2.37	0.50
27:3:108:ASN:O	27:3:111:ILE:HG12	2.12	0.50
27:3:202:LEU:HD22	27:3:202:LEU:N	2.27	0.50
1:A:595:ILE:C	1:A:595:ILE:HD12	2.37	0.50
1:A:1181:PRO:C	1:A:1183:SER:H	2.18	0.50
2:B:387:HIS:CD2	2:B:504:THR:HG21	2.46	0.50
2:B:714:PRO:O	2:B:717:ASN:HB2	2.11	0.50
8:H:17:PRO:O	8:H:19:GLY:N	2.45	0.50
13:M:57:ASN:ND2	29:Y:54:DA:OP2	2.44	0.50
16:P:311:VAL:HG11	29:Y:81:DA:C2	2.47	0.50
17:Q:58:GLN:OE1	18:R:194:ARG:NH1	2.45	0.50
23:W:73:CYS:O	23:W:209:TYR:CE2	2.65	0.50
23:W:116:CYS:SG	23:W:191:PRO:HD2	2.51	0.50
23:W:430:ASN:CB	23:W:431:PRO:CD	2.86	0.50
24:0:54:ARG:CB	27:3:209:ILE:CG2	2.87	0.50
26:2:77:LYS:CD	26:2:78:GLU:HG3	2.41	0.50
26:2:181:GLN:HE21	26:2:181:GLN:CA	2.23	0.50
26:2:181:GLN:HE22	26:2:220:LEU:HD12	1.76	0.50
27:3:107:ALA:O	27:3:111:ILE:HG23	2.11	0.50
1:A:691:ASP:HB3	1:A:766:PHE:HB2	1.94	0.49
2:B:563:ASP:OD1	2:B:610:ARG:NH1	2.45	0.49
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.76	0.49
2:B:1069:ILE:HG12	13:M:48:VAL:CG1	2.42	0.49
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.45	0.49
17:Q:18:ALA:O	17:Q:22:ILE:HG12	2.12	0.49
18:R:93:ASP:HB3	18:R:95:HIS:CE1	2.47	0.49
20:T:139:VAL:HG12	20:T:141:LEU:N	2.27	0.49
20:T:141:LEU:HD23	20:T:143:GLN:NE2	2.27	0.49
23:W:494:ILE:HD11	23:W:680:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:1:MET:HE1	26:2:440:LEU:CD1	2.31	0.49
25:1:1:MET:HA	26:2:413:LEU:CA	2.42	0.49
26:2:100:LEU:CG	26:2:119:ARG:HE	2.22	0.49
26:2:199:ALA:CB	26:2:201:PHE:CE2	2.95	0.49
27:3:137:LEU:CD1	27:3:177:PHE:CE1	2.95	0.49
28:X:14:DA:N6	29:Y:80:DT:O4	2.43	0.49
28:X:62:DG:N2	29:Y:33:DT:O2	2.45	0.49
1:A:281:ALA:O	1:A:285:LYS:HG3	2.11	0.49
1:A:375:ILE:HG21	1:A:666:ARG:NH1	2.27	0.49
1:A:460:ARG:HB2	1:A:501:MET:SD	2.52	0.49
2:B:968:ASN:CG	2:B:969:PRO:HD2	2.37	0.49
7:G:44:PHE:CD2	7:G:103:PRO:HG2	2.47	0.49
13:M:86:LYS:CE	13:M:86:LYS:CA	2.86	0.49
19:S:125:TYR:CD1	19:S:139:PRO:HA	2.47	0.49
22:V:667:THR:CA	25:1:62:ASP:OD1	2.59	0.49
26:2:208:THR:HG23	26:2:209:PRO:HD2	1.91	0.49
27:3:10:LEU:CD2	27:3:143:TYR:HE2	2.25	0.49
27:3:12:VAL:HG23	27:3:12:VAL:O	2.10	0.49
27:3:12:VAL:HG22	27:3:161:ILE:HA	1.94	0.49
27:3:216:LYS:HD2	27:3:216:LYS:N	2.22	0.49
27:3:217:VAL:CG1	27:3:226:TYR:CE2	2.95	0.49
28:X:47:DC:H42	29:Y:47:DG:H22	1.59	0.49
1:A:817:PRO:HG2	1:A:818:GLU:OE1	2.12	0.49
2:B:380:ARG:HE	2:B:609:GLU:CD	2.19	0.49
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.95	0.49
14:N:312:GLU:HB3	14:N:313:PRO:HD3	1.95	0.49
23:W:325:THR:HG22	23:W:329:PHE:CE2	2.47	0.49
25:1:45:VAL:CG2	26:2:409:TYR:CE2	2.95	0.49
26:2:188:THR:HG23	26:2:189:GLU:N	2.27	0.49
26:2:426:ARG:HD2	26:2:444:THR:CG2	2.43	0.49
27:3:215:LEU:HD12	27:3:230:VAL:CG2	2.42	0.49
1:A:1192:TRP:HE1	1:A:1248:ASN:HB3	1.77	0.49
2:B:101:ARG:O	13:M:175:ARG:NH2	2.45	0.49
2:B:628:VAL:HG12	2:B:633:LEU:HD23	1.94	0.49
5:E:54:ARG:HG2	5:E:54:ARG:NH1	2.26	0.49
17:Q:102:VAL:HG13	17:Q:103:VAL:CG2	2.41	0.49
26:2:28:PRO:N	27:3:25:GLN:CB	2.71	0.49
26:2:81:LYS:CE	26:2:89:LEU:HD21	2.42	0.49
26:2:89:LEU:HD23	26:2:93:LEU:HG	1.94	0.49
26:2:245:LEU:HD22	26:2:245:LEU:N	2.27	0.49
27:3:10:LEU:CD2	27:3:143:TYR:CE2	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:53:ARG:HA	27:3:101:TYR:HE1	1.78	0.49
27:3:59:VAL:HG13	27:3:59:VAL:O	2.12	0.49
27:3:220:MET:N	27:3:221:PRO:HD2	2.28	0.49
1:A:85:PHE:CD1	1:A:257:PRO:HD3	2.48	0.49
1:A:138:LYS:HB2	1:A:1445:HIS:HE1	1.76	0.49
1:A:520:MET:HG3	1:A:522:PRO:HD2	1.93	0.49
1:A:929:ALA:C	1:A:931:ARG:H	2.20	0.49
2:B:509:VAL:HG11	2:B:524:LYS:HB3	1.95	0.49
2:B:905:ASP:OD1	2:B:924:ARG:NH1	2.46	0.49
13:M:92:SER:O	13:M:93:PHE:C	2.56	0.49
1:A:606:HIS:O	1:A:608:THR:N	2.45	0.49
1:A:927:GLU:H	1:A:931:ARG:HD3	1.76	0.49
2:B:191:GLU:OE2	2:B:472:ARG:NH1	2.46	0.49
5:E:62:VAL:CG2	5:E:72:MET:O	2.60	0.49
18:R:213:ASP:HB2	18:R:215:GLU:HA	1.93	0.49
24:0:55:LEU:N	27:3:209:ILE:HD11	2.28	0.49
26:2:35:TYR:CD1	26:2:62:LEU:CD1	2.95	0.49
26:2:42:LEU:HD22	26:2:52:ALA:HA	1.95	0.49
26:2:236:PHE:CZ	26:2:258:LEU:CD1	2.95	0.49
27:3:12:VAL:CG2	27:3:161:ILE:HA	2.42	0.49
27:3:166:ALA:O	27:3:198:SER:HB2	2.13	0.49
27:3:174:TYR:HD1	27:3:202:LEU:HD11	1.78	0.49
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.48	0.49
1:A:924:TYR:CE1	1:A:949:GLN:HG2	2.47	0.49
16:P:311:VAL:HG11	29:Y:81:DA:H2	1.78	0.49
25:1:2:VAL:HG23	25:1:2:VAL:O	2.11	0.49
27:3:100:LYS:HG3	27:3:101:TYR:H	1.74	0.49
27:3:195:VAL:HG23	27:3:214:TYR:CE1	2.48	0.49
1:A:361:PHE:HD1	1:A:388:MET:HE3	1.78	0.49
1:A:641:CYS:SG	1:A:643:LYS:N	2.86	0.49
1:A:1213:ARG:NH2	1:A:1215:GLU:OE2	2.46	0.49
2:B:803:ARG:HH12	2:B:951:GLN:HE22	1.59	0.49
20:T:177:ARG:HE	20:T:208:GLN:HB2	1.77	0.49
24:0:54:ARG:CG	27:3:182:PHE:CZ	2.80	0.49
26:2:203:PHE:CE2	26:2:205:LEU:CD2	2.96	0.49
1:A:375:ILE:HG13	1:A:666:ARG:HH11	1.77	0.49
1:A:927:GLU:O	1:A:931:ARG:HG3	2.13	0.49
2:B:309:PHE:HE2	9:I:25:TYR:HE2	1.59	0.49
2:B:474:THR:HG23	2:B:477:SER:H	1.78	0.49
2:B:733:MET:HE3	2:B:1051:LEU:O	2.12	0.49
14:N:332:GLU:CD	15:O:92:LYS:HD3	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:596:LEU:HG	23:W:597:LEU:N	2.27	0.49
26:2:176:ALA:O	26:2:177:GLN:HB2	2.12	0.49
27:3:42:MET:HE2	27:3:108:ASN:CB	2.42	0.49
1:A:924:TYR:CZ	1:A:949:GLN:HA	2.48	0.49
26:2:90:LEU:CD2	26:2:140:LYS:HD3	2.42	0.49
26:2:133:THR:HG23	26:2:134:SER:N	2.28	0.49
26:2:170:ALA:CB	26:2:213:TRP:CZ3	2.95	0.49
27:3:160:ARG:HE	27:3:190:LEU:HG	1.78	0.49
28:X:65:DG:N2	29:Y:30:DG:C2	2.81	0.49
1:A:546:ARG:HB3	1:A:640:LEU:O	2.13	0.48
1:A:1392:TYR:OH	1:A:1394:ASN:HA	2.12	0.48
2:B:68:GLN:OE1	2:B:81:PRO:HB2	2.13	0.48
2:B:513:GLU:HG3	2:B:726:SER:HB3	1.94	0.48
8:H:37:MET:HG2	8:H:127:GLY:HA3	1.95	0.48
25:1:45:VAL:HG21	26:2:409:TYR:CE2	2.48	0.48
26:2:77:LYS:HD3	26:2:78:GLU:HG3	1.94	0.48
26:2:166:SER:HB3	26:2:167:PRO:CD	2.43	0.48
27:3:177:PHE:CZ	27:3:203:LEU:CD2	2.95	0.48
1:A:484:LEU:N	1:A:484:LEU:HD23	2.28	0.48
2:B:73:HIS:C	2:B:75:SER:N	2.71	0.48
2:B:838:GLN:O	2:B:891:ASP:N	2.40	0.48
16:P:242:GLN:HG3	16:P:248:ALA:HB3	1.94	0.48
26:2:159:VAL:N	26:2:162:PHE:HB3	2.28	0.48
26:2:189:GLU:CA	26:2:192:GLU:HG2	2.41	0.48
26:2:198:SER:OG	26:2:238:PHE:HE2	1.96	0.48
2:B:414:GLU:HG2	2:B:436:LYS:HD3	1.95	0.48
9:I:62:VAL:O	9:I:64:GLU:CA	2.61	0.48
20:T:37:ARG:HH22	20:T:62:LEU:HB2	1.78	0.48
22:V:516:PRO:CA	25:1:15:ALA:C	2.83	0.48
23:W:624:PRO:O	23:W:656:ALA:HB1	2.12	0.48
24:0:209:THR:HA	24:0:219:TYR:CD1	2.48	0.48
26:2:28:PRO:N	27:3:25:GLN:C	2.65	0.48
26:2:35:TYR:CE2	26:2:62:LEU:CB	2.96	0.48
1:A:1427:LEU:HD23	1:A:1456:GLU:HB3	1.94	0.48
2:B:20:ASP:OD1	2:B:21:LEU:N	2.45	0.48
3:C:67:ARG:HH22	10:J:2:ILE:HG13	1.77	0.48
3:C:242:GLU:OE1	3:C:242:GLU:N	2.46	0.48
17:Q:28:ILE:HG21	18:R:205:ASP:OD2	2.13	0.48
17:Q:36:ILE:HD13	17:Q:52:LEU:HD21	1.96	0.48
19:S:118:VAL:HG13	19:S:120:GLU:HG3	1.95	0.48
22:V:516:PRO:HB2	22:V:706:LYS:HZ1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:37:HIS:NE2	23:W:454:VAL:CG1	2.76	0.48
1:A:621:ILE:O	1:A:623:PRO:HD3	2.14	0.48
1:A:689:ILE:O	1:A:692:SER:OG	2.29	0.48
2:B:81:PRO:O	2:B:82:PRO:C	2.55	0.48
3:C:68:LEU:O	3:C:71:ILE:HG12	2.13	0.48
7:G:91:GLN:HG2	17:Q:145:PHE:CE1	2.47	0.48
11:K:61:TYR:HA	11:K:72:ILE:O	2.14	0.48
13:M:79:ASP:OD1	13:M:79:ASP:N	2.46	0.48
20:T:160:GLN:HA	20:T:163:ILE:HD12	1.94	0.48
25:1:34:ILE:HG22	25:1:46:ILE:CG1	2.44	0.48
26:2:211:GLN:HE21	26:2:257:SER:HB3	1.78	0.48
26:2:251:VAL:HG11	26:2:254:MET:SD	2.53	0.48
1:A:45:GLU:OE1	1:A:48:GLU:HG2	2.12	0.48
1:A:1188:GLU:O	1:A:1192:TRP:HZ3	1.97	0.48
1:A:1410:HIS:N	5:E:174:GLN:HE22	2.12	0.48
2:B:200:MET:HE1	2:B:220:GLU:OE2	2.14	0.48
2:B:1022:LEU:CD1	2:B:1023:ARG:HG3	2.44	0.48
3:C:44:ILE:HD11	3:C:238:SER:HB2	1.94	0.48
7:G:114:PRO:HB2	7:G:116:GLU:HG2	1.95	0.48
9:I:39:CYS:HB3	9:I:42:CYS:SG	2.53	0.48
13:M:297:PRO:HG3	13:M:310:VAL:HG11	1.93	0.48
17:Q:28:ILE:CG2	18:R:205:ASP:OD2	2.62	0.48
22:V:315:VAL:CG1	23:W:500:ASP:HB3	2.26	0.48
22:V:522:TYR:CE2	25:1:62:ASP:CG	2.69	0.48
24:0:55:LEU:HD12	27:3:178:MET:HE1	1.95	0.48
25:1:38:ILE:CG2	25:1:44:PHE:CE1	2.96	0.48
26:2:60:LEU:CD1	26:2:95:ILE:CG2	2.91	0.48
1:A:206:ASN:C	1:A:208:ASP:N	2.61	0.48
1:A:924:TYR:HH	1:A:949:GLN:HA	1.78	0.48
2:B:100:GLU:O	2:B:103:GLY:N	2.39	0.48
2:B:874:PRO:C	2:B:876:ASN:H	2.17	0.48
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.95	0.48
5:E:11:TRP:O	5:E:15:LYS:HG2	2.14	0.48
8:H:111:ARG:HB3	8:H:127:GLY:O	2.13	0.48
22:V:514:MET:SD	22:V:537:ASN:CG	2.97	0.48
22:V:523:VAL:CB	25:1:20:LEU:CD2	2.85	0.48
26:2:178:LEU:HD12	26:2:178:LEU:N	2.28	0.48
27:3:21:TRP:HA	27:3:24:LYS:CG	2.43	0.48
1:A:809:HIS:CE1	2:B:697:GLU:OE2	2.66	0.48
1:A:1036:ASN:ND2	1:A:1037:ALA:N	2.62	0.48
2:B:841:ARG:HD2	2:B:895:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:GLU:HG3	12:L:27:GLU:O	2.13	0.48
13:M:60:ALA:O	13:M:62:LYS:N	2.45	0.48
17:Q:100:VAL:C	17:Q:102:VAL:N	2.72	0.48
21:U:290:VAL:HG13	21:U:297:ARG:HG2	1.96	0.48
22:V:612:ASP:OD2	22:V:635:GLN:CD	2.56	0.48
23:W:285:TYR:CE1	23:W:403:PHE:CZ	3.01	0.48
26:2:28:PRO:C	27:3:25:GLN:O	2.57	0.48
1:A:362:SER:HB3	2:B:1084:LEU:HD12	1.95	0.48
1:A:1155:LYS:HD3	21:U:249:GLN:OE1	2.13	0.48
22:V:504:LYS:CB	22:V:654:GLU:O	2.58	0.48
23:W:608:ILE:HG23	23:W:614:TYR:CZ	2.48	0.48
25:1:43:VAL:HG12	25:1:44:PHE:N	2.27	0.48
26:2:100:LEU:HD11	26:2:119:ARG:CG	2.31	0.48
27:3:165:LYS:NZ	27:3:200:SER:H	2.12	0.48
28:X:41:DT:H1'	28:X:42:DT:H3'	1.95	0.48
2:B:911:LEU:HD13	2:B:915:GLY:HA2	1.96	0.48
13:M:235:ILE:HD11	13:M:300:PHE:CE1	2.49	0.48
22:V:634:ARG:HG2	22:V:679:PHE:CZ	2.48	0.48
23:W:263:LEU:C	23:W:263:LEU:HD23	2.39	0.48
25:1:22:TYR:CD1	25:1:22:TYR:C	2.92	0.48
25:1:53:LEU:H	25:1:53:LEU:CD1	2.26	0.48
26:2:35:TYR:CD1	26:2:62:LEU:CG	2.92	0.48
26:2:211:GLN:CA	26:2:261:PHE:CE1	2.95	0.48
27:3:124:ILE:O	27:3:127:GLN:HB2	2.14	0.48
29:Y:22:DG:H2'	29:Y:23:DT:C6	2.48	0.48
7:G:98:PHE:CZ	17:Q:152:PHE:HE1	2.31	0.47
13:M:205:SER:OG	16:P:278:GLN:NE2	2.43	0.47
17:Q:23:ARG:NH2	18:R:209:GLN:N	2.43	0.47
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.79	0.47
23:W:28:LEU:HD13	23:W:28:LEU:C	2.38	0.47
25:1:18:GLN:OE1	25:1:19:PHE:CD1	2.67	0.47
26:2:28:PRO:O	27:3:25:GLN:O	2.32	0.47
26:2:89:LEU:CD2	26:2:93:LEU:HG	2.44	0.47
26:2:171:VAL:CG2	26:2:213:TRP:HA	2.19	0.47
26:2:236:PHE:CD1	26:2:261:PHE:HB3	2.49	0.47
27:3:160:ARG:HB2	27:3:190:LEU:HG	1.96	0.47
1:A:532:ARG:HB3	1:A:649:ALA:HB2	1.96	0.47
1:A:999:ARG:HE	8:H:99:ILE:CD1	2.22	0.47
1:A:1186:VAL:HG12	1:A:1188:GLU:HG2	1.96	0.47
2:B:101:ARG:HB3	13:M:131:PRO:HG2	1.96	0.47
2:B:274:ARG:HE	2:B:308:ALA:HB1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:LEU:HD13	7:G:75:ILE:HD11	1.95	0.47
10:J:7:CYS:SG	10:J:48:MET:HE3	2.54	0.47
17:Q:109:HIS:CB	18:R:224:THR:CB	2.84	0.47
18:R:138:ALA:C	18:R:140:LYS:N	2.70	0.47
18:R:153:ARG:O	18:R:157:GLN:N	2.46	0.47
22:V:615:PHE:CD1	22:V:615:PHE:C	2.91	0.47
24:0:165:ARG:HB2	24:0:193:LYS:O	2.14	0.47
25:1:3:ASN:HB2	26:2:412:PHE:O	2.13	0.47
25:1:38:ILE:HG22	25:1:44:PHE:CE1	2.48	0.47
25:1:57:VAL:CG2	25:1:61:MET:HE3	2.44	0.47
26:2:203:PHE:CD2	26:2:204:LEU:N	2.82	0.47
27:3:216:LYS:O	27:3:218:PRO:HD3	2.14	0.47
13:M:86:LYS:HE2	13:M:86:LYS:CA	2.43	0.47
19:S:25:LYS:HD3	19:S:141:HIS:CD2	2.49	0.47
20:T:154:LYS:HD2	20:T:154:LYS:N	2.26	0.47
26:2:163:MET:HE1	26:2:206:LEU:HB3	1.94	0.47
26:2:218:GLN:HG2	26:2:268:PHE:CB	2.44	0.47
26:2:236:PHE:HE2	26:2:262:LEU:CD1	2.27	0.47
1:A:220:ARG:HD2	1:A:223:GLU:OE1	2.14	0.47
1:A:246:GLU:HG2	1:A:247:TRP:CD1	2.50	0.47
1:A:621:ILE:O	1:A:623:PRO:CD	2.63	0.47
1:A:766:PHE:CE1	1:A:781:ILE:HG12	2.49	0.47
2:B:91:ILE:H	20:T:141:LEU:HG	1.79	0.47
2:B:202:THR:O	2:B:204:THR:N	2.47	0.47
3:C:61:ASP:OD2	12:L:48:ARG:NH1	2.48	0.47
8:H:128:ASP:N	8:H:128:ASP:OD1	2.46	0.47
13:M:169:ARG:HH11	13:M:206:VAL:HG21	1.79	0.47
13:M:178:LYS:O	20:T:154:LYS:CG	2.62	0.47
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.96	0.47
20:T:141:LEU:CD2	20:T:141:LEU:C	2.88	0.47
20:T:177:ARG:CZ	20:T:212:TYR:HB2	2.44	0.47
22:V:315:VAL:CG1	23:W:500:ASP:CG	2.80	0.47
22:V:361:CYS:HB3	22:V:405:VAL:HG21	1.96	0.47
26:2:93:LEU:CA	26:2:96:TRP:CD1	2.94	0.47
26:2:211:GLN:CB	26:2:261:PHE:CE1	2.95	0.47
27:3:10:LEU:CD1	27:3:56:LYS:HG2	2.44	0.47
27:3:226:TYR:CA	27:3:230:VAL:HG23	2.42	0.47
2:B:529:MET:HE2	2:B:623:ARG:CB	2.42	0.47
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.79	0.47
7:G:110:ARG:HA	7:G:113:ILE:HD12	1.97	0.47
8:H:56:PHE:HA	8:H:148:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:195:PHE:CZ	13:M:199:LEU:HD11	2.49	0.47
22:V:321:GLU:OE2	23:W:500:ASP:CA	2.59	0.47
22:V:370:SER:O	22:V:374:TRP:HD1	1.96	0.47
26:2:138:PRO:HD3	26:2:189:GLU:CD	2.40	0.47
26:2:205:LEU:HD22	26:2:205:LEU:N	2.30	0.47
1:A:90:LEU:O	1:A:291:ARG:NH2	2.47	0.47
1:A:490:THR:HG23	21:U:282:ASP:HB3	1.96	0.47
3:C:171:LYS:HE3	11:K:10:PHE:HB3	1.96	0.47
7:G:146:LYS:NZ	7:G:165:ASP:OD2	2.36	0.47
8:H:81:ARG:C	8:H:83:SER:H	2.22	0.47
13:M:44:ARG:NH1	13:M:46:ILE:HG22	2.29	0.47
13:M:235:ILE:HD11	13:M:300:PHE:HE1	1.79	0.47
19:S:174:PHE:O	19:S:178:GLN:HG2	2.14	0.47
26:2:117:ASN:CB	27:3:42:MET:HE1	2.42	0.47
27:3:10:LEU:HA	27:3:56:LYS:HG2	1.96	0.47
27:3:124:ILE:HD13	27:3:124:ILE:C	2.38	0.47
1:A:297:GLY:HA3	17:Q:57:LYS:HG3	1.96	0.47
1:A:351:ARG:HG3	2:B:1088:GLU:OE2	2.15	0.47
1:A:777:SER:OG	1:A:779:ILE:HG22	2.15	0.47
1:A:1128:ILE:HD11	1:A:1401:LEU:HD21	1.97	0.47
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.39	0.47
2:B:26:CYS:SG	2:B:27:TRP:N	2.87	0.47
2:B:754:PRO:HB2	2:B:773:PRO:CG	2.45	0.47
3:C:143:VAL:HG23	3:C:144:GLU:H	1.80	0.47
5:E:55:ARG:HG2	5:E:76:PHE:HB2	1.94	0.47
13:M:99:SER:HG	28:X:34:DA:H61	1.62	0.47
15:O:64:THR:OG1	15:O:75:VAL:HB	2.15	0.47
21:U:292:ASN:O	21:U:294:CYS:N	2.47	0.47
25:1:50:VAL:CG1	25:1:54:GLN:HG2	2.41	0.47
26:2:46:ARG:CD	26:2:85:GLU:CB	2.93	0.47
26:2:201:PHE:CD1	26:2:202:GLN:N	2.83	0.47
29:Y:36:DA:C1'	29:Y:37:DG:C8	2.97	0.47
1:A:1408:ARG:HD2	1:A:1422:GLN:HE22	1.80	0.47
2:B:613:ARG:HD3	2:B:615:TYR:CE2	2.50	0.47
3:C:67:ARG:NH1	10:J:2:ILE:HG13	2.28	0.47
8:H:66:GLU:O	8:H:66:GLU:HG2	2.13	0.47
13:M:39:LEU:C	13:M:40:VAL:O	2.56	0.47
17:Q:105:TYR:CE1	18:R:231:GLU:CB	2.86	0.47
23:W:73:CYS:HB3	23:W:209:TYR:CG	2.49	0.47
23:W:143:ARG:HG2	23:W:143:ARG:HH11	1.80	0.47
23:W:657:MET:O	23:W:660:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:9:LEU:N	25:1:9:LEU:HD12	2.30	0.47
25:1:38:ILE:CB	25:1:44:PHE:CE1	2.98	0.47
27:3:70:LEU:HD22	27:3:114:GLU:CB	2.44	0.47
27:3:131:THR:HG23	27:3:133:LEU:HD13	1.95	0.47
27:3:137:LEU:HD11	27:3:177:PHE:CE1	2.50	0.47
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.74	0.47
1:A:1013:VAL:HG11	1:A:1046:ARG:HG2	1.97	0.47
2:B:119:THR:HG23	2:B:187:ILE:HA	1.97	0.47
2:B:1062:ARG:HH11	2:B:1082:GLY:HA2	1.80	0.47
5:E:21:CYS:SG	5:E:62:VAL:HG11	2.55	0.47
15:O:66:ARG:N	15:O:73:THR:O	2.48	0.47
17:Q:110:MET:SD	18:R:222:SER:CB	3.02	0.47
21:U:226:GLU:CG	21:U:238:LYS:NZ	2.78	0.47
22:V:689:VAL:CG2	26:2:391:ILE:CD1	2.93	0.47
25:1:22:TYR:O	25:1:25:GLU:HB3	2.15	0.47
26:2:51:LEU:HD21	26:2:55:TRP:CD1	2.50	0.47
26:2:85:GLU:O	26:2:89:LEU:HB2	2.15	0.47
27:3:64:ILE:HG21	27:3:128:HIS:HB3	1.97	0.47
27:3:177:PHE:O	27:3:181:ILE:HG13	2.15	0.47
1:A:1250:ASP:HB3	21:U:227:GLU:HG2	0.47	0.47
1:A:1274:GLU:O	1:A:1276:VAL:N	2.48	0.47
1:A:1408:ARG:HD2	1:A:1422:GLN:NE2	2.30	0.47
2:B:873:LEU:CB	2:B:874:PRO:CD	2.90	0.47
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.96	0.47
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.50	0.47
22:V:593:LEU:HD21	22:V:615:PHE:HZ	1.78	0.47
25:1:38:ILE:O	25:1:38:ILE:HG12	2.15	0.47
25:1:53:LEU:O	25:1:57:VAL:HG12	2.15	0.47
26:2:96:TRP:CH2	26:2:97:HIS:CE1	3.03	0.47
27:3:56:LYS:HD3	27:3:56:LYS:N	2.30	0.47
28:X:45:DC:H2'	28:X:46:DG:C8	2.49	0.47
29:Y:30:DG:C4	29:Y:31:DG:C5	3.02	0.47
29:Y:31:DG:H2''	29:Y:32:DC:C6	2.50	0.47
1:A:58:MET:HE3	1:A:258:LEU:HD21	1.96	0.46
1:A:199:TYR:CZ	13:M:93:PHE:HE2	2.23	0.46
8:H:7:GLU:OE2	8:H:57:ARG:NH2	2.48	0.46
9:I:93:GLU:O	9:I:115:THR:HG22	2.15	0.46
16:P:298:PRO:O	16:P:299:ARG:C	2.57	0.46
23:W:73:CYS:HB2	23:W:209:TYR:CE1	2.50	0.46
24:0:77:LYS:C	24:0:79:ASN:H	2.03	0.46
26:2:240:LEU:HD12	26:2:240:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:12:VAL:CG2	27:3:161:ILE:HG23	2.43	0.46
1:A:561:MET:HG2	11:K:58:PHE:CD1	2.50	0.46
1:A:592:PHE:CZ	1:A:595:ILE:HD11	2.50	0.46
2:B:195:ILE:HG21	2:B:486:ASN:HB2	1.97	0.46
2:B:1115:GLN:OE1	2:B:1115:GLN:N	2.47	0.46
5:E:55:ARG:HB3	5:E:76:PHE:O	2.16	0.46
20:T:94:THR:HG22	20:T:109:ILE:HA	1.97	0.46
22:V:366:ASN:ND2	22:V:613:THR:HG22	2.30	0.46
23:W:73:CYS:CB	23:W:209:TYR:CE1	2.99	0.46
23:W:73:CYS:HB3	23:W:209:TYR:CD1	2.51	0.46
26:2:28:PRO:HA	27:3:25:GLN:C	2.40	0.46
28:X:39:DT:H2'	28:X:40:DT:C6	2.49	0.46
1:A:111:CYS:SG	1:A:114:CYS:CB	3.02	0.46
1:A:1036:ASN:C	1:A:1036:ASN:ND2	2.73	0.46
2:B:91:ILE:HG22	20:T:141:LEU:CG	2.45	0.46
2:B:187:ILE:HD11	2:B:448:LEU:HD23	1.98	0.46
2:B:854:ILE:O	2:B:907:VAL:HG21	2.15	0.46
2:B:936:ALA:HB2	2:B:942:LYS:HA	1.97	0.46
2:B:992:ASN:O	10:J:46:ARG:NH2	2.48	0.46
3:C:149:LEU:HD21	3:C:152:LYS:HE3	1.97	0.46
15:O:50:GLN:O	15:O:53:ARG:NH1	2.47	0.46
17:Q:172:ASP:O	17:Q:176:LEU:N	2.39	0.46
19:S:125:TYR:HD1	19:S:139:PRO:HA	1.81	0.46
26:2:30:VAL:HB	27:3:25:GLN:O	2.16	0.46
27:3:165:LYS:HZ1	27:3:200:SER:N	2.12	0.46
27:3:196:LEU:HB3	27:3:220:MET:SD	2.56	0.46
1:A:117:LEU:HD23	1:A:119:VAL:H	1.80	0.46
1:A:495:ASP:HB3	2:B:792:ASP:OD2	2.16	0.46
2:B:212:ASP:N	2:B:212:ASP:OD1	2.46	0.46
2:B:422:PHE:CD1	2:B:422:PHE:C	2.92	0.46
13:M:12:ARG:NH1	13:M:23:LEU:O	2.48	0.46
18:R:78:LEU:HB2	18:R:119:LEU:HD22	1.98	0.46
22:V:321:GLU:CG	23:W:499:ASN:ND2	2.76	0.46
23:W:175:TYR:CD1	23:W:175:TYR:N	2.76	0.46
25:1:40:ASP:HB2	25:1:43:VAL:H	1.81	0.46
26:2:30:VAL:HB	27:3:24:LYS:O	2.15	0.46
1:A:1251:ASN:HD21	21:U:227:GLU:HB3	1.77	0.46
2:B:80:GLU:O	2:B:135:GLU:HG2	2.10	0.46
2:B:651:TYR:HA	2:B:655:ASP:OD2	2.16	0.46
2:B:1069:ILE:HA	2:B:1072:ARG:HE	1.80	0.46
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:109:HIS:HE1	18:R:231:GLU:CA	2.28	0.46
17:Q:113:ARG:HH21	18:R:218:LYS:HE2	1.68	0.46
18:R:195:PRO:HB2	18:R:199:LYS:CB	2.46	0.46
1:A:364:ARG:NE	1:A:500:GLU:CD	2.73	0.46
1:A:908:THR:C	1:A:910:LYS:H	2.23	0.46
5:E:64:HIS:CE1	5:E:69:THR:C	2.94	0.46
6:F:56:TYR:HD1	6:F:124:ILE:HB	1.80	0.46
13:M:289:TYR:HA	13:M:292:ILE:HG12	1.96	0.46
18:R:149:LYS:HD2	18:R:175:LEU:H	1.81	0.46
18:R:195:PRO:HB2	18:R:199:LYS:HD3	1.94	0.46
20:T:179:ASP:O	20:T:181:GLN:N	2.48	0.46
25:1:2:VAL:HG11	26:2:456:LYS:CB	2.44	0.46
26:2:96:TRP:CZ2	26:2:97:HIS:NE2	2.83	0.46
26:2:217:LEU:CD2	26:2:233:ILE:HD11	2.45	0.46
26:2:223:ALA:C	26:2:225:SER:H	2.24	0.46
27:3:10:LEU:N	27:3:56:LYS:HE3	2.31	0.46
27:3:10:LEU:HB2	27:3:56:LYS:HE3	1.97	0.46
1:A:406:VAL:HG21	1:A:440:LEU:HD11	1.97	0.46
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.55	0.46
2:B:225:LEU:C	2:B:227:ASN:N	2.67	0.46
2:B:751:LEU:HD12	2:B:751:LEU:HA	1.81	0.46
2:B:800:ALA:C	2:B:805:PHE:HB3	2.41	0.46
3:C:138:ASP:OD1	3:C:139:PRO:HD2	2.16	0.46
5:E:62:VAL:HG22	5:E:72:MET:O	2.15	0.46
9:I:15:ARG:NH1	9:I:46:GLN:OE1	2.48	0.46
13:M:22:ILE:HG23	13:M:35:PRO:HG2	1.96	0.46
21:U:280:SER:HB2	21:U:284:PRO:HA	1.98	0.46
22:V:444:HIS:O	22:V:447:PRO:CD	2.61	0.46
24:0:77:LYS:HA	24:0:77:LYS:HE3	1.97	0.46
25:1:2:VAL:HG12	26:2:456:LYS:CE	2.44	0.46
25:1:10:ILE:HG12	25:1:43:VAL:CG1	2.45	0.46
26:2:81:LYS:CG	26:2:82:ALA:N	2.79	0.46
1:A:27:SER:O	1:A:31:LEU:N	2.42	0.46
1:A:181:HIS:N	1:A:181:HIS:CD2	2.82	0.46
1:A:890:ARG:NH2	1:A:1023:VAL:HB	2.30	0.46
2:B:739:ASN:HB3	10:J:62:TYR:OH	2.16	0.46
5:E:172:ARG:HD2	5:E:210:GLN:HB3	1.98	0.46
8:H:65:TYR:CD2	8:H:70:LEU:HD23	2.50	0.46
1:A:608:THR:OG1	1:A:610:PRO:CD	2.64	0.46
1:A:1195:VAL:HG12	21:U:192:ARG:HD3	1.98	0.46
3:C:5:ASN:O	3:C:7:PRO:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:262:GLN:O	3:C:266:GLU:HG2	2.16	0.46
5:E:14:ARG:NH1	5:E:58:LEU:O	2.49	0.46
14:N:11:PRO:HA	14:N:14:TYR:HD2	1.81	0.46
22:V:321:GLU:CA	23:W:499:ASN:ND2	2.58	0.46
23:W:37:HIS:CG	23:W:454:VAL:HG13	2.50	0.46
25:1:22:TYR:HD1	25:1:23:LEU:HD23	1.80	0.46
26:2:31:LEU:HG	27:3:25:GLN:C	2.41	0.46
26:2:35:TYR:CD2	26:2:62:LEU:CB	2.95	0.46
26:2:123:LEU:HD23	26:2:123:LEU:C	2.41	0.46
26:2:170:ALA:C	26:2:213:TRP:CZ3	2.94	0.46
27:3:8:LEU:HD23	27:3:54:SER:CB	2.42	0.46
1:A:19:LYS:HD3	2:B:1174:VAL:HG23	1.98	0.46
1:A:691:ASP:OD1	1:A:765:ASN:N	2.48	0.46
1:A:809:HIS:HE1	2:B:697:GLU:OE2	1.98	0.46
1:A:1450:PRO:O	1:A:1452:LYS:HG3	2.15	0.46
3:C:45:ILE:HG22	3:C:73:LEU:HD12	1.98	0.46
3:C:49:TRP:O	3:C:163:ALA:HA	2.16	0.46
6:F:56:TYR:CD1	6:F:124:ILE:HB	2.50	0.46
9:I:61:GLU:C	9:I:63:ASP:N	2.67	0.46
9:I:98:GLN:NE2	9:I:108:MET:SD	2.89	0.46
25:1:38:ILE:CG2	25:1:44:PHE:CD1	2.94	0.46
25:1:57:VAL:HG13	25:1:58:GLY:N	2.31	0.46
26:2:187:SER:OG	26:2:190:PRO:HD2	2.16	0.46
26:2:214:TYR:CE1	26:2:233:ILE:HG23	2.51	0.46
27:3:9:ASN:C	27:3:56:LYS:HE3	2.41	0.46
27:3:64:ILE:CG2	27:3:128:HIS:CB	2.94	0.46
27:3:125:LYS:C	27:3:127:GLN:H	2.24	0.46
1:A:693:ILE:HG21	2:B:1023:ARG:NE	2.31	0.45
3:C:44:ILE:HD11	3:C:238:SER:CB	2.46	0.45
5:E:25:GLY:O	5:E:65:ASN:HA	2.16	0.45
7:G:152:VAL:HG22	7:G:157:ILE:HG13	1.98	0.45
8:H:23:ASP:OD1	8:H:23:ASP:N	2.49	0.45
18:R:138:ALA:O	18:R:140:LYS:N	2.49	0.45
25:1:38:ILE:HA	25:1:44:PHE:CD1	2.37	0.45
26:2:118:LEU:HD21	27:3:39:ASP:OD1	1.95	0.45
27:3:69:PHE:HE1	27:3:139:LYS:HD2	1.77	0.45
27:3:141:LEU:C	27:3:144:ILE:HG22	2.41	0.45
1:A:632:ASN:CA	1:A:992:LYS:HD2	2.43	0.45
2:B:163:LEU:HD12	2:B:163:LEU:N	2.31	0.45
2:B:201:ALA:HB3	2:B:206:TYR:OH	2.16	0.45
2:B:952:GLU:HG3	3:C:39:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:961:ILE:H	2:B:961:ILE:HG13	1.55	0.45
8:H:24:ARG:O	8:H:45:ILE:N	2.49	0.45
8:H:84:ARG:C	8:H:86:ASP:N	2.74	0.45
8:H:100:GLU:HG3	8:H:101:GLY:N	2.25	0.45
10:J:44:CYS:O	10:J:47:ARG:HG3	2.15	0.45
23:W:299:ARG:O	23:W:300:GLU:CD	2.60	0.45
23:W:623:VAL:HG23	23:W:681:ASP:HB2	1.98	0.45
26:2:211:GLN:CD	26:2:261:PHE:CE1	2.94	0.45
26:2:221:GLN:HG2	26:2:268:PHE:HZ	1.75	0.45
27:3:15:VAL:HG12	27:3:164:ILE:HD12	1.97	0.45
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.98	0.45
2:B:403:LEU:O	2:B:407:MET:HG2	2.17	0.45
2:B:487:SER:HA	2:B:488:PRO:HD3	1.67	0.45
5:E:62:VAL:HG23	5:E:72:MET:CB	2.40	0.45
6:F:109:TYR:CD1	6:F:115:TYR:HB3	2.51	0.45
16:P:239:ARG:HD2	16:P:239:ARG:HA	1.57	0.45
26:2:203:PHE:CG	26:2:204:LEU:N	2.84	0.45
26:2:236:PHE:CD1	26:2:239:GLN:CD	2.95	0.45
27:3:190:LEU:HA	27:3:210:THR:HG21	1.91	0.45
27:3:228:LEU:HD23	27:3:228:LEU:C	2.41	0.45
28:X:32:DG:H2''	28:X:33:DA:O5'	2.16	0.45
28:X:67:DG:C2	28:X:68:DC:C2	3.04	0.45
1:A:262:PRO:HD3	1:A:342:ARG:HH12	1.81	0.45
1:A:533:PRO:CG	1:A:654:HIS:HB2	2.46	0.45
5:E:40:PHE:HE2	5:E:46:ASP:OD2	1.93	0.45
5:E:64:HIS:CD2	5:E:67:ASP:O	2.69	0.45
9:I:66:THR:C	9:I:68:ILE:H	2.24	0.45
14:N:354:LYS:HA	14:N:369:LYS:HA	1.99	0.45
16:P:157:GLU:CD	16:P:333:LYS:HD3	2.40	0.45
16:P:206:GLU:HB3	16:P:236:LYS:HZ2	1.81	0.45
20:T:191:PHE:HA	20:T:197:TYR:HE2	1.81	0.45
23:W:299:ARG:HG3	23:W:300:GLU:HG2	1.97	0.45
26:2:90:LEU:HD21	26:2:140:LYS:HD3	1.98	0.45
26:2:117:ASN:HB2	27:3:104:LEU:CG	2.46	0.45
27:3:64:ILE:CG2	27:3:128:HIS:CG	2.99	0.45
29:Y:56:DG:C2'	29:Y:57:DA:H5'	2.46	0.45
1:A:37:THR:O	1:A:39:GLY:N	2.50	0.45
1:A:261:ARG:HB3	1:A:276:LEU:HD22	1.98	0.45
1:A:686:THR:OG1	1:A:687:ILE:N	2.49	0.45
8:H:65:TYR:HE2	8:H:70:LEU:HB3	1.79	0.45
9:I:54:TYR:OH	9:I:56:ASN:ND2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:LYS:HB3	12:L:23:HIS:HE1	1.82	0.45
18:R:77:VAL:HA	18:R:80:LYS:HE3	1.98	0.45
25:1:18:GLN:CD	25:1:44:PHE:CZ	2.92	0.45
25:1:54:GLN:O	25:1:57:VAL:HG12	2.16	0.45
26:2:30:VAL:N	27:3:25:GLN:O	2.50	0.45
27:3:42:MET:CG	27:3:111:ILE:CD1	2.95	0.45
1:A:1112:VAL:HB	21:U:253:THR:HB	1.99	0.45
2:B:285:LEU:O	2:B:289:ILE:HG22	2.16	0.45
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.99	0.45
5:E:64:HIS:C	5:E:65:ASN:O	2.60	0.45
10:J:63:ALA:H	10:J:64:PRO:HD3	1.75	0.45
17:Q:109:HIS:CE1	18:R:231:GLU:HG3	2.52	0.45
20:T:26:TYR:HE2	20:T:124:TYR:OH	2.00	0.45
20:T:142:SER:C	20:T:144:GLN:N	2.73	0.45
20:T:168:LYS:C	20:T:170:LYS:H	2.24	0.45
26:2:30:VAL:CG1	26:2:34:LEU:CD2	2.94	0.45
27:3:160:ARG:HE	27:3:160:ARG:HB2	1.58	0.45
29:Y:71:DA:H2'	29:Y:71:DA:OP2	2.15	0.45
1:A:780:ASN:ND2	2:B:976:MET:SD	2.89	0.45
2:B:698:ILE:O	2:B:699:HIS:HB2	2.17	0.45
2:B:1101:GLN:OE1	6:F:64:ARG:NH1	2.50	0.45
3:C:149:LEU:HD23	10:J:2:ILE:HD13	1.98	0.45
7:G:97:LEU:HD23	7:G:108:ILE:HD12	1.97	0.45
19:S:165:GLU:HA	19:S:168:ASN:HB2	1.97	0.45
22:V:514:MET:HE2	22:V:664:SER:HB3	1.99	0.45
26:2:89:LEU:HD23	26:2:89:LEU:C	2.42	0.45
27:3:219:GLN:OE1	27:3:219:GLN:HA	2.17	0.45
28:X:13:DT:H2''	28:X:14:DA:H8	1.81	0.45
1:A:275:ASP:HA	1:A:278:HIS:HB2	1.99	0.45
1:A:1192:TRP:HA	1:A:1195:VAL:HB	1.98	0.45
1:A:1319:LYS:H	1:A:1356:ARG:HH22	1.64	0.45
2:B:758:LEU:O	2:B:996:ILE:HG23	2.16	0.45
2:B:1040:GLN:CD	2:B:1040:GLN:N	2.71	0.45
3:C:147:ASP:OD2	3:C:148:ILE:HG22	2.17	0.45
14:N:315:ASN:HA	16:P:239:ARG:HH12	1.82	0.45
16:P:206:GLU:CD	16:P:236:LYS:NZ	2.75	0.45
18:R:157:GLN:HG2	18:R:160:GLN:HB3	1.99	0.45
20:T:8:ASP:HB3	20:T:105:SER:HA	1.99	0.45
26:2:84:GLU:OE1	26:2:84:GLU:HA	2.15	0.45
27:3:121:LYS:HD3	27:3:121:LYS:H	1.80	0.45
27:3:148:ASN:ND2	27:3:157:MET:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:H	13:M:49:GLY:CA	2.29	0.45
1:A:546:ARG:HG3	1:A:547:LYS:H	1.81	0.45
1:A:581:LYS:NZ	8:H:86:ASP:O	2.49	0.45
1:A:625:ASP:O	1:A:638:GLY:HA2	2.17	0.45
1:A:1467:GLY:O	1:A:1470:CYS:HB2	2.17	0.45
2:B:243:GLY:N	2:B:252:ILE:HG21	2.32	0.45
3:C:260:GLN:O	3:C:260:GLN:HG3	2.17	0.45
5:E:172:ARG:CD	5:E:210:GLN:HB3	2.47	0.45
8:H:113:SER:OG	8:H:126:GLN:HG2	2.17	0.45
9:I:58:ILE:C	9:I:60:HIS:N	2.73	0.45
23:W:37:HIS:NE2	23:W:454:VAL:HG11	2.32	0.45
27:3:59:VAL:N	27:3:71:TYR:CZ	2.70	0.45
1:A:157:GLY:N	1:A:181:HIS:NE2	2.64	0.45
1:A:608:THR:HB	1:A:610:PRO:HD2	1.97	0.45
1:A:1250:ASP:CA	21:U:227:GLU:HG3	2.47	0.45
17:Q:71:PHE:CE1	17:Q:106:LYS:HE3	2.52	0.45
26:2:28:PRO:C	27:3:25:GLN:C	2.85	0.45
26:2:164:VAL:HG13	26:2:209:PRO:CG	2.45	0.45
27:3:148:ASN:CG	27:3:157:MET:HE2	2.42	0.45
1:A:611:ASP:OD2	1:A:627:LYS:HG3	2.17	0.44
2:B:62:ALA:N	2:B:63:PRO:HD3	2.32	0.44
2:B:298:MET:O	2:B:301:VAL:HG12	2.15	0.44
2:B:514:THR:HG21	2:B:521:GLY:HA2	1.99	0.44
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.98	0.44
9:I:119:CYS:HB3	9:I:121:HIS:H	1.82	0.44
17:Q:24:GLY:O	18:R:210:PHE:HE2	1.99	0.44
18:R:157:GLN:OE1	18:R:162:GLY:HA2	2.17	0.44
24:0:106:ILE:HD11	24:0:127:HIS:HB3	1.99	0.44
26:2:35:TYR:HB2	26:2:62:LEU:HD12	1.98	0.44
1:A:389:THR:HB	1:A:417:LYS:CD	2.48	0.44
1:A:797:ARG:NH2	1:A:820:ARG:HB2	2.33	0.44
2:B:235:ILE:HD11	2:B:347:MET:HG3	1.99	0.44
2:B:1116:VAL:HG11	2:B:1125:MET:SD	2.57	0.44
9:I:14:ILE:HA	9:I:16:PHE:CD1	2.52	0.44
13:M:91:ALA:O	13:M:92:SER:OG	2.36	0.44
13:M:246:PRO:HB2	16:P:306:VAL:HG21	1.99	0.44
14:N:324:GLU:HA	16:P:188:ARG:NH1	2.29	0.44
16:P:171:THR:HG22	16:P:220:VAL:HG22	1.98	0.44
16:P:298:PRO:HB2	16:P:320:GLU:HB3	1.99	0.44
17:Q:24:GLY:C	18:R:210:PHE:CE2	2.80	0.44
19:S:143:TRP:C	19:S:143:TRP:CD1	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:517:GLU:CB	22:V:713:LEU:HD22	2.46	0.44
22:V:647:LYS:O	22:V:648:LYS:O	2.35	0.44
22:V:666:ASP:CB	25:1:17:LYS:HZ3	2.29	0.44
26:2:203:PHE:CD2	26:2:205:LEU:CD2	2.95	0.44
26:2:217:LEU:CD2	26:2:233:ILE:CD1	2.95	0.44
27:3:71:TYR:CG	27:3:71:TYR:O	2.70	0.44
27:3:144:ILE:O	27:3:144:ILE:HD13	2.17	0.44
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.44
1:A:1187:ALA:HB3	9:I:1:MET:HE1	2.00	0.44
2:B:132:VAL:HG12	2:B:134:LYS:HG3	1.99	0.44
2:B:549:SER:OG	2:B:577:HIS:NE2	2.44	0.44
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.99	0.44
6:F:62:ARG:HH12	6:F:127:ASP:C	2.20	0.44
9:I:61:GLU:HG3	9:I:103:ARG:CZ	2.48	0.44
10:J:21:TYR:CG	10:J:49:LEU:HD21	2.52	0.44
16:P:180:LEU:HA	16:P:183:ILE:HD12	1.99	0.44
21:U:225:ALA:HB3	21:U:228:MET:HA	1.99	0.44
26:2:219:TYR:CD1	26:2:219:TYR:C	2.95	0.44
27:3:24:LYS:HE2	27:3:196:LEU:HB3	1.98	0.44
27:3:228:LEU:HD23	27:3:228:LEU:O	2.18	0.44
29:Y:30:DG:H1'	29:Y:31:DG:C8	2.52	0.44
1:A:107:LEU:HD23	1:A:191:ILE:HD13	1.99	0.44
1:A:1050:CYS:HB3	1:A:1053:ARG:HG2	1.98	0.44
2:B:711:ILE:HA	2:B:712:PRO:HD3	1.95	0.44
16:P:165:LEU:HD23	16:P:168:ILE:HD11	1.99	0.44
17:Q:102:VAL:HG11	17:Q:103:VAL:HG22	1.99	0.44
20:T:177:ARG:NH1	20:T:212:TYR:HB2	2.33	0.44
24:0:54:ARG:HA	27:3:209:ILE:HD13	1.06	0.44
26:2:130:SER:HB2	26:2:179:LEU:HD23	1.98	0.44
26:2:189:GLU:HB2	26:2:190:PRO:CD	2.43	0.44
28:X:38:DT:H4'	28:X:39:DT:H4'	1.98	0.44
29:Y:36:DA:N3	29:Y:37:DG:C4	2.86	0.44
2:B:87:LYS:NZ	2:B:89:GLU:OE2	2.51	0.44
2:B:302:LYS:HE2	9:I:23:MET:SD	2.57	0.44
2:B:453:TRP:CG	2:B:463:ARG:HB2	2.53	0.44
2:B:646:ARG:HA	2:B:649:ASN:HB3	1.98	0.44
2:B:803:ARG:HH21	3:C:177:ASN:HD22	1.66	0.44
2:B:898:THR:OG1	2:B:899:SER:N	2.49	0.44
2:B:1066:PRO:HA	13:M:46:ILE:HG21	1.99	0.44
5:E:61:LEU:HD11	5:E:71:GLN:HG3	2.00	0.44
15:O:84:VAL:HG23	15:O:85:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:223:VAL:O	18:R:223:VAL:HG23	2.17	0.44
22:V:370:SER:O	22:V:374:TRP:CD1	2.71	0.44
23:W:37:HIS:CD2	23:W:454:VAL:CG1	3.00	0.44
25:1:11:GLU:HG2	26:2:404:THR:OG1	2.17	0.44
25:1:18:GLN:HG3	25:1:19:PHE:H	1.82	0.44
26:2:123:LEU:CD2	26:2:178:LEU:CD1	2.95	0.44
27:3:60:ILE:HG23	27:3:68:ARG:O	2.17	0.44
3:C:71:ILE:O	3:C:71:ILE:HG13	2.16	0.44
5:E:64:HIS:CD2	5:E:68:PRO:C	2.89	0.44
14:N:349:TRP:HB3	14:N:351:PHE:CE1	2.52	0.44
19:S:45:ALA:HA	19:S:102:VAL:HA	2.00	0.44
25:1:3:ASN:HB3	26:2:412:PHE:O	2.18	0.44
25:1:4:VAL:HG22	25:1:5:LEU:N	2.32	0.44
25:1:59:GLU:CD	26:2:402:ARG:CZ	2.89	0.44
26:2:159:VAL:HG12	26:2:161:HIS:HB2	1.99	0.44
27:3:65:GLN:O	27:3:132:LEU:HD11	2.18	0.44
1:A:262:PRO:O	1:A:263:ALA:HB3	2.18	0.44
1:A:425:ASP:HB3	13:M:39:LEU:HD11	2.00	0.44
1:A:640:LEU:HD13	1:A:645:LEU:HD13	2.00	0.44
1:A:1112:VAL:HG22	1:A:1309:MET:HE3	2.00	0.44
1:A:1372:GLU:CD	5:E:193:ILE:HD13	2.42	0.44
2:B:295:PRO:HB2	9:I:11:PHE:CD2	2.46	0.44
2:B:714:PRO:CD	2:B:1001:PRO:HB3	2.41	0.44
2:B:1028:LEU:HA	2:B:1028:LEU:HD12	1.51	0.44
8:H:130:ASN:O	8:H:134:GLY:N	2.50	0.44
11:K:29:ASN:ND2	11:K:78:THR:O	2.50	0.44
17:Q:128:LYS:N	17:Q:163:GLU:O	2.51	0.44
21:U:224:THR:HG22	21:U:228:MET:HE3	1.99	0.44
25:1:1:MET:SD	26:2:419:GLU:N	2.90	0.44
26:2:218:GLN:HE22	26:2:265:LEU:CA	2.28	0.44
27:3:34:LEU:O	27:3:34:LEU:HD13	2.17	0.44
27:3:160:ARG:CB	27:3:190:LEU:CD2	2.95	0.44
1:A:19:LYS:HD2	2:B:1173:SER:H	1.81	0.44
1:A:51:ARG:NH2	2:B:878:ASP:OD1	2.51	0.44
1:A:203:LYS:HA	1:A:203:LYS:CE	2.46	0.44
1:A:728:THR:HG23	1:A:736:THR:HG23	1.99	0.44
2:B:116:ARG:O	2:B:117:ASN:HB2	2.18	0.44
2:B:872:THR:HG23	2:B:888:THR:O	2.18	0.44
3:C:1:MET:HA	3:C:2:PRO:HD3	1.83	0.44
3:C:149:LEU:HD23	10:J:2:ILE:CD1	2.47	0.44
7:G:98:PHE:CZ	17:Q:145:PHE:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:TYR:HD2	8:H:70:LEU:HD23	1.82	0.44
10:J:21:TYR:HB2	10:J:38:LEU:CD1	2.48	0.44
17:Q:19:LYS:HA	17:Q:22:ILE:HG12	1.98	0.44
22:V:282:LYS:HE3	22:V:482:PHE:CD1	2.53	0.44
23:W:419:GLU:HB2	23:W:432:ILE:HG22	1.98	0.44
25:1:7:GLY:C	25:1:8:VAL:HG23	2.43	0.44
26:2:61:PHE:CE1	26:2:99:GLN:NE2	2.85	0.44
26:2:206:LEU:CD2	26:2:206:LEU:H	2.31	0.44
26:2:214:TYR:HB3	26:2:261:PHE:CE2	2.53	0.44
26:2:258:LEU:HG	26:2:262:LEU:HD21	1.99	0.44
1:A:350:VAL:HG11	1:A:1431:SER:HA	1.99	0.44
1:A:610:PRO:O	1:A:612:ASP:N	2.50	0.44
2:B:646:ARG:O	2:B:646:ARG:HG2	2.16	0.44
4:D:26:PHE:HE2	7:G:78:ARG:HG2	1.82	0.44
9:I:35:LEU:HB3	9:I:48:ALA:HB3	1.99	0.44
24:0:165:ARG:HD3	24:0:194:ILE:HG12	2.00	0.44
25:1:34:ILE:CG2	25:1:50:VAL:HG11	2.48	0.44
26:2:60:LEU:CD1	26:2:95:ILE:CB	2.95	0.44
26:2:117:ASN:ND2	27:3:104:LEU:O	2.51	0.44
27:3:124:ILE:O	27:3:124:ILE:HG23	2.18	0.44
27:3:184:ALA:C	27:3:187:GLN:HG2	2.43	0.44
1:A:368:THR:OG1	1:A:483:ARG:NH1	2.51	0.43
1:A:1249:ASP:HB2	21:U:196:SER:HB2	2.00	0.43
1:A:1484:MET:H	1:A:1484:MET:HG2	1.54	0.43
2:B:319:ASN:OD1	2:B:332:LYS:HG3	2.18	0.43
2:B:1107:LEU:HD23	2:B:1107:LEU:HA	1.80	0.43
3:C:10:ARG:NH2	3:C:24:GLU:OE2	2.36	0.43
4:D:71:PHE:HE1	7:G:142:GLU:HG2	1.83	0.43
10:J:62:TYR:CB	10:J:64:PRO:HD2	2.46	0.43
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.99	0.43
17:Q:23:ARG:NH1	18:R:209:GLN:CB	2.79	0.43
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.83	0.43
20:T:177:ARG:NE	20:T:208:GLN:HB2	2.33	0.43
22:V:405:VAL:HG12	22:V:406:ALA:H	1.82	0.43
22:V:531:ILE:CG1	22:V:534:TYR:HE2	2.31	0.43
24:0:60:HIS:CE1	24:0:159:MET:SD	3.11	0.43
26:2:140:LYS:HD3	26:2:162:PHE:CE1	2.47	0.43
27:3:64:ILE:HB	27:3:123:ASP:CG	2.43	0.43
29:Y:80:DT:H2"	29:Y:81:DA:C8	2.52	0.43
1:A:455:ILE:HD13	1:A:520:MET:HE1	1.99	0.43
1:A:1301:ILE:HG21	1:A:1345:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:VAL:N	2:B:468:GLN:O	2.41	0.43
2:B:453:TRP:HB2	2:B:463:ARG:HB2	2.00	0.43
13:M:10:LEU:HD12	13:M:10:LEU:HA	1.81	0.43
16:P:163:PRO:HA	16:P:262:CYS:HB3	2.01	0.43
20:T:98:GLU:HA	20:T:104:LEU:HD23	2.00	0.43
22:V:415:HIS:HD2	22:V:416:THR:HG23	1.82	0.43
22:V:428:GLU:CD	22:V:461:HIS:H	2.26	0.43
22:V:446:ILE:HD12	22:V:451:PHE:HB3	1.99	0.43
26:2:56:VAL:HG23	26:2:57:MET:N	2.31	0.43
26:2:117:ASN:ND2	27:3:108:ASN:N	2.65	0.43
26:2:166:SER:HB3	26:2:167:PRO:HD3	2.01	0.43
26:2:243:SER:HB3	26:2:258:LEU:CD2	2.45	0.43
27:3:187:GLN:CD	27:3:189:ILE:HG13	2.43	0.43
29:Y:46:DC:H2"	29:Y:47:DG:C8	2.53	0.43
1:A:97:VAL:HG21	1:A:322:LEU:HD21	1.99	0.43
1:A:378:VAL:O	1:A:475:ARG:N	2.51	0.43
1:A:416:ALA:HA	1:A:448:ARG:HA	1.99	0.43
1:A:546:ARG:HG3	1:A:547:LYS:N	2.34	0.43
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.17	0.43
2:B:249:LYS:O	2:B:249:LYS:HG2	2.19	0.43
3:C:52:ILE:HG21	3:C:55:ASN:HB2	2.01	0.43
7:G:158:PHE:CE1	17:Q:139:LEU:HB2	2.53	0.43
27:3:178:MET:O	27:3:182:PHE:HD2	2.01	0.43
27:3:178:MET:HA	27:3:181:ILE:HD12	2.00	0.43
27:3:222:SER:HB3	27:3:225:GLN:CD	2.43	0.43
1:A:527:THR:HG22	1:A:532:ARG:O	2.17	0.43
1:A:608:THR:OG1	1:A:610:PRO:HG2	2.18	0.43
2:B:22:TRP:O	2:B:24:GLU:N	2.51	0.43
2:B:1069:ILE:HG12	13:M:48:VAL:HG11	2.01	0.43
9:I:119:CYS:C	9:I:121:HIS:H	2.24	0.43
10:J:66:GLU:HB3	12:L:23:HIS:CE1	2.54	0.43
17:Q:23:ARG:CZ	18:R:209:GLN:HB2	2.48	0.43
18:R:194:ARG:HD3	18:R:194:ARG:HA	1.44	0.43
19:S:31:PHE:N	20:T:92:THR:O	2.40	0.43
22:V:514:MET:HE3	25:1:16:MET:CE	2.48	0.43
26:2:35:TYR:CD1	26:2:62:LEU:HD12	2.53	0.43
26:2:223:ALA:H	26:2:268:PHE:HE1	1.64	0.43
26:2:270:LEU:HD23	26:2:270:LEU:C	2.43	0.43
27:3:59:VAL:CA	27:3:71:TYR:CD1	2.99	0.43
27:3:174:TYR:HE1	27:3:178:MET:HE3	1.77	0.43
2:B:291:ASP:C	2:B:293:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:GLN:HG2	12:L:45:TYR:CE1	2.51	0.43
3:C:155:LYS:HB3	10:J:65:LEU:HD22	1.99	0.43
5:E:73:PHE:HD2	5:E:90:TYR:OH	2.02	0.43
8:H:75:TYR:HD1	8:H:75:TYR:H	1.65	0.43
21:U:247:GLU:HA	21:U:250:MET:HG2	2.00	0.43
26:2:117:ASN:CA	27:3:104:LEU:HD21	2.47	0.43
27:3:121:LYS:H	27:3:121:LYS:CD	2.32	0.43
1:A:936:GLU:HB2	1:A:939:VAL:HG23	2.00	0.43
2:B:880:LEU:HD13	2:B:880:LEU:HA	1.79	0.43
8:H:34:SER:HB2	8:H:36:LYS:NZ	2.33	0.43
14:N:22:ILE:HG13	14:N:43:LYS:HD2	2.00	0.43
15:O:64:THR:CG2	16:P:188:ARG:HB3	2.47	0.43
17:Q:109:HIS:CE1	18:R:231:GLU:HB2	2.54	0.43
20:T:159:HIS:O	20:T:162:ASN:HB3	2.18	0.43
23:W:416:ILE:HA	23:W:434:HIS:O	2.19	0.43
26:2:87:THR:C	26:2:89:LEU:H	2.27	0.43
26:2:94:ARG:HD2	26:2:95:ILE:CD1	2.47	0.43
26:2:214:TYR:OH	26:2:265:LEU:HD13	2.18	0.43
26:2:224:GLN:N	26:2:268:PHE:HZ	2.16	0.43
26:2:236:PHE:HZ	26:2:258:LEU:HD11	1.83	0.43
1:A:388:MET:HB3	1:A:388:MET:HE2	1.59	0.43
1:A:865:ILE:HD12	1:A:866:LYS:N	2.34	0.43
1:A:931:ARG:C	1:A:933:THR:N	2.77	0.43
1:A:1158:LEU:HD21	1:A:1308:TYR:CE2	2.54	0.43
1:A:1168:LYS:HD3	1:A:1306:LYS:HG2	2.01	0.43
14:N:46:TRP:HZ2	15:O:11:LEU:HD12	1.83	0.43
16:P:237:TYR:O	16:P:240:VAL:HG22	2.19	0.43
19:S:16:VAL:O	20:T:39:GLU:HA	2.19	0.43
26:2:127:LYS:CA	26:2:178:LEU:HD23	2.48	0.43
26:2:159:VAL:HG22	26:2:160:LEU:HD13	1.95	0.43
26:2:201:PHE:CD1	26:2:201:PHE:C	2.96	0.43
26:2:203:PHE:HD2	26:2:205:LEU:H	1.65	0.43
26:2:409:TYR:CD2	26:2:443:VAL:HG22	2.54	0.43
27:3:229:TRP:CD1	27:3:229:TRP:C	2.96	0.43
29:Y:36:DA:N9	29:Y:37:DG:C8	2.87	0.43
1:A:371:PRO:HD2	2:B:788:TYR:CZ	2.54	0.43
1:A:376:ASP:CB	1:A:522:PRO:HD3	2.45	0.43
1:A:477:LEU:HB2	1:A:478:PRO:HD2	2.00	0.43
1:A:510:GLU:HG2	6:F:67:GLY:C	2.44	0.43
1:A:609:HIS:N	1:A:610:PRO:HD3	2.30	0.43
1:A:1412:MET:SD	1:A:1422:GLN:NE2	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:111:ASP:O	11:K:113:GLN:N	2.52	0.43
13:M:106:THR:HA	29:Y:63:DG:H21	1.84	0.43
22:V:519:TYR:HA	22:V:522:TYR:HB3	2.01	0.43
23:W:421:PHE:CD1	23:W:423:ASP:CG	2.92	0.43
26:2:117:ASN:HD21	27:3:108:ASN:N	2.16	0.43
26:2:215:PHE:CE2	26:2:264:HIS:ND1	2.86	0.43
26:2:270:LEU:HA	26:2:273:GLN:HG3	2.00	0.43
29:Y:18:DG:N2	29:Y:19:DC:C2	2.87	0.43
1:A:220:ARG:O	1:A:223:GLU:N	2.52	0.43
1:A:485:ASN:OD1	1:A:486:LEU:N	2.52	0.43
1:A:486:LEU:HD12	1:A:496:PHE:CE2	2.53	0.43
1:A:522:PRO:HG3	1:A:666:ARG:HE	1.84	0.43
1:A:561:MET:SD	11:K:51:LEU:HD21	2.59	0.43
1:A:827:TYR:HH	1:A:839:HIS:HE2	1.66	0.43
1:A:927:GLU:N	1:A:931:ARG:CD	2.80	0.43
1:A:1282:ASP:OD1	1:A:1283:VAL:HG23	2.19	0.43
2:B:42:GLN:HG2	2:B:526:LEU:HD11	2.00	0.43
2:B:51:ILE:HD13	2:B:51:ILE:HA	1.89	0.43
2:B:874:PRO:C	2:B:876:ASN:N	2.77	0.43
2:B:1022:LEU:HD11	2:B:1023:ARG:NH1	2.34	0.43
5:E:18:MET:HE3	5:E:32:GLU:OE2	2.19	0.43
16:P:206:GLU:OE1	16:P:236:LYS:NZ	2.52	0.43
17:Q:109:HIS:HE1	18:R:231:GLU:HB2	1.83	0.43
17:Q:151:THR:HB	17:Q:152:PHE:H	1.74	0.43
22:V:524:ALA:HB2	25:1:23:LEU:HD13	2.01	0.43
23:W:584:TYR:CB	23:W:591:GLY:HA3	2.49	0.43
25:1:13:ASP:OD2	25:1:17:LYS:HB2	2.15	0.43
25:1:25:GLU:OE2	25:1:35:ILE:HG12	2.18	0.43
25:1:50:VAL:HG12	25:1:50:VAL:O	2.18	0.43
26:2:35:TYR:CG	26:2:62:LEU:CD1	2.99	0.43
29:Y:64:DC:N4	29:Y:65:DG:O6	2.51	0.43
1:A:910:LYS:HB3	1:A:963:ARG:HH12	1.84	0.43
1:A:1177:TYR:N	9:I:51:SER:HB3	2.27	0.43
2:B:728:MET:SD	2:B:940:GLY:HA2	2.59	0.43
2:B:1119:CYS:HB3	2:B:1122:CYS:O	2.18	0.43
6:F:64:ARG:HH22	7:G:61:PRO:HB3	1.82	0.43
9:I:57:LYS:HB3	9:I:59:THR:CG2	2.49	0.43
9:I:62:VAL:O	9:I:64:GLU:CB	2.66	0.43
10:J:62:TYR:HB2	10:J:64:PRO:HG2	2.00	0.43
13:M:75:LEU:O	13:M:114:MET:HE3	2.18	0.43
16:P:190:ALA:HB2	16:P:202:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:195:PRO:C	18:R:199:LYS:HD2	2.44	0.43
20:T:165:TYR:O	20:T:169:LYS:HG2	2.18	0.43
25:1:8:VAL:CG1	25:1:9:LEU:N	2.80	0.43
26:2:34:LEU:N	26:2:34:LEU:HD22	2.33	0.43
26:2:118:LEU:HD23	27:3:42:MET:CB	2.35	0.43
1:A:365:THR:HG22	1:A:482:PHE:CE2	2.54	0.42
1:A:483:ARG:NH2	2:B:788:TYR:CE2	2.87	0.42
1:A:868:MET:HE1	1:A:1400:LEU:HG	2.00	0.42
1:A:1029:LEU:H	5:E:162:ARG:NH1	2.17	0.42
1:A:1130:ILE:HD12	1:A:1411:LEU:HD13	2.01	0.42
2:B:92:TYR:HD1	20:T:141:LEU:HD21	1.82	0.42
2:B:229:SER:HA	2:B:405:ARG:HH22	1.84	0.42
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.02	0.42
2:B:1005:ALA:O	2:B:1007:ASN:N	2.52	0.42
10:J:62:TYR:HB3	10:J:64:PRO:HD3	2.00	0.42
13:M:32:MET:O	13:M:40:VAL:HA	2.19	0.42
14:N:28:ILE:HD13	15:O:35:GLN:HG2	2.01	0.42
14:N:46:TRP:CZ2	15:O:11:LEU:HD12	2.54	0.42
22:V:519:TYR:HB3	25:1:16:MET:HG3	2.00	0.42
26:2:236:PHE:CE1	26:2:239:GLN:NE2	2.87	0.42
27:3:184:ALA:O	27:3:187:GLN:HG2	2.19	0.42
29:Y:89:DC:H2"	29:Y:90:DC:C5	2.54	0.42
1:A:613:GLU:HG2	21:U:262:THR:HB	2.01	0.42
1:A:620:HIS:O	1:A:621:ILE:HB	2.19	0.42
1:A:1319:LYS:HD2	1:A:1319:LYS:HA	1.36	0.42
2:B:707:CYS:C	2:B:709:SER:H	2.27	0.42
2:B:1162:LEU:HD23	2:B:1162:LEU:HA	1.68	0.42
5:E:11:TRP:CZ2	5:E:36:THR:HA	2.54	0.42
14:N:32:ASP:HB3	14:N:34:VAL:HG23	2.00	0.42
20:T:121:SER:OG	20:T:122:GLU:N	2.52	0.42
20:T:159:HIS:ND1	20:T:160:GLN:N	2.65	0.42
22:V:514:MET:HB3	25:1:16:MET:SD	2.59	0.42
27:3:141:LEU:HA	27:3:144:ILE:HG22	2.01	0.42
1:A:1050:CYS:SG	1:A:1051:SER:N	2.92	0.42
2:B:17:ILE:HG23	2:B:18:THR:HG23	2.01	0.42
2:B:127:ASP:OD2	2:B:144:HIS:NE2	2.47	0.42
2:B:819:SER:H	2:B:827:GLU:HB2	1.84	0.42
2:B:953:ASP:O	2:B:1031:GLY:HA3	2.19	0.42
9:I:84:HIS:HB2	9:I:85:PRO:HD3	0.86	0.42
13:M:35:PRO:HB2	13:M:36:GLU:OE1	2.19	0.42
22:V:615:PHE:O	22:V:615:PHE:CG	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:4:VAL:CG1	26:2:412:PHE:HD2	2.20	0.42
26:2:57:MET:CA	26:2:60:LEU:HG	2.49	0.42
26:2:171:VAL:CG1	26:2:216:MET:SD	3.06	0.42
27:3:133:LEU:CD2	27:3:134:ALA:N	2.82	0.42
27:3:154:ASN:CG	27:3:155:GLN:H	2.26	0.42
27:3:159:SER:HG	27:3:189:ILE:HD12	1.85	0.42
1:A:197:GLU:HG3	1:A:199:TYR:HE1	1.84	0.42
1:A:265:VAL:HG23	1:A:266:MET:H	1.85	0.42
1:A:359:VAL:HA	2:B:1111:SER:HB3	2.00	0.42
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.54	0.42
1:A:1473:LEU:HB3	7:G:59:ILE:HD12	2.01	0.42
2:B:90:GLN:HE21	20:T:141:LEU:HG	1.72	0.42
2:B:92:TYR:HE1	20:T:143:GLN:NE2	2.15	0.42
2:B:757:PRO:HA	2:B:1047:TYR:CD2	2.54	0.42
3:C:84:TYR:CE1	3:C:167:LYS:HE3	2.55	0.42
9:I:16:PHE:HB3	9:I:22:ASN:O	2.19	0.42
10:J:44:CYS:SG	10:J:45:CYS:N	2.92	0.42
14:N:314:LEU:HD12	16:P:242:GLN:NE2	2.34	0.42
17:Q:30:HIS:CE1	17:Q:62:VAL:HG22	2.54	0.42
26:2:133:THR:CG2	26:2:134:SER:N	2.83	0.42
26:2:230:LEU:C	26:2:230:LEU:HD13	2.44	0.42
27:3:137:LEU:HD12	27:3:177:PHE:CE1	2.54	0.42
27:3:160:ARG:CZ	27:3:190:LEU:CD1	2.97	0.42
1:A:689:ILE:HG13	1:A:690:GLY:N	2.34	0.42
1:A:1413:ALA:O	1:A:1418:GLY:HA3	2.19	0.42
2:B:184:TYR:HE2	2:B:191:GLU:HG2	1.84	0.42
13:M:252:SER:OG	29:Y:85:DG:OP1	2.30	0.42
22:V:689:VAL:CG2	26:2:391:ILE:HD13	2.50	0.42
23:W:73:CYS:CB	23:W:209:TYR:CE2	3.02	0.42
23:W:73:CYS:HB3	23:W:209:TYR:CD2	2.54	0.42
26:2:159:VAL:HG11	26:2:161:HIS:CD2	2.49	0.42
26:2:188:THR:CG2	26:2:189:GLU:N	2.83	0.42
27:3:69:PHE:CZ	27:3:139:LYS:CB	2.95	0.42
27:3:144:ILE:HG13	27:3:159:SER:OG	2.20	0.42
28:X:1:DG:H2"	28:X:2:DA:C8	2.55	0.42
1:A:81:CYS:HA	1:A:82:PRO:HD2	1.89	0.42
1:A:927:GLU:CA	1:A:931:ARG:CG	2.72	0.42
1:A:1410:HIS:HB2	5:E:174:GLN:NE2	2.34	0.42
2:B:422:PHE:CZ	2:B:429:PHE:HB2	2.55	0.42
2:B:871:VAL:HG13	2:B:890:ARG:HB2	2.01	0.42
3:C:27:ASP:OD1	3:C:28:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:LEU:HD13	4:D:114:LEU:HD13	2.02	0.42
5:E:64:HIS:ND1	5:E:70:ASP:O	2.52	0.42
8:H:65:TYR:CD2	8:H:70:LEU:HB3	2.54	0.42
10:J:6:ARG:H	10:J:14:VAL:H	1.65	0.42
13:M:108:SER:HB3	13:M:112:ARG:NH1	2.32	0.42
14:N:333:ASN:HB3	14:N:359:ASN:O	2.20	0.42
16:P:255:ILE:HG21	16:P:258:MET:HE3	2.01	0.42
17:Q:35:ASP:HA	17:Q:38:ILE:HD12	2.01	0.42
20:T:138:PRO:HG2	20:T:140:ARG:NH2	2.35	0.42
27:3:9:ASN:OD1	27:3:158:LYS:HB3	2.19	0.42
27:3:42:MET:SD	27:3:111:ILE:CD1	3.07	0.42
1:A:1176:TYR:HE1	9:I:52:CYS:HB2	1.85	0.42
2:B:251:ALA:O	2:B:254:GLN:NE2	2.53	0.42
2:B:268:PRO:HD2	2:B:271:ILE:HD12	2.02	0.42
2:B:1114:TYR:HE2	2:B:1156:LYS:HD3	1.84	0.42
3:C:7:PRO:HG2	11:K:97:GLU:CD	2.39	0.42
3:C:146:ASP:O	3:C:148:ILE:N	2.49	0.42
7:G:91:GLN:HG2	17:Q:145:PHE:CZ	2.55	0.42
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.34	0.42
12:L:35:ARG:NH1	12:L:42:ARG:HE	2.17	0.42
15:O:3:TYR:CB	15:O:98:CYS:SG	2.97	0.42
16:P:325:PHE:HA	16:P:328:ILE:HG22	2.01	0.42
26:2:172:SER:C	26:2:175:LEU:HD23	2.43	0.42
27:3:71:TYR:HD2	27:3:72:PRO:HD2	1.72	0.42
27:3:100:LYS:HB2	27:3:100:LYS:HE2	1.89	0.42
27:3:100:LYS:CB	27:3:103:LEU:HD13	2.41	0.42
27:3:128:HIS:NE2	27:3:130:GLU:CG	2.82	0.42
27:3:197:ASP:O	27:3:198:SER:HB3	2.20	0.42
28:X:16:DA:H2''	28:X:17:DA:C8	2.55	0.42
1:A:425:ASP:CB	13:M:39:LEU:HD11	2.49	0.42
1:A:1178:ASP:HB3	1:A:1260:ARG:HH22	1.85	0.42
1:A:1473:LEU:HD23	6:F:104:ILE:HD12	2.02	0.42
2:B:132:VAL:CG1	2:B:134:LYS:HG3	2.50	0.42
2:B:707:CYS:SG	2:B:730:LYS:NZ	2.92	0.42
4:D:126:GLU:O	4:D:130:ILE:N	2.43	0.42
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.55	0.42
25:1:1:MET:HE3	26:2:415:GLN:N	2.35	0.42
25:1:18:GLN:CB	25:1:44:PHE:CE2	2.76	0.42
26:2:47:GLU:HG3	26:2:48:LEU:H	1.83	0.42
26:2:140:LYS:CD	26:2:162:PHE:HE1	2.29	0.42
27:3:14:VAL:CG2	27:3:163:VAL:HG13	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:HD2	13:M:73:PRO:CB	2.38	0.42
1:A:621:ILE:C	1:A:623:PRO:N	2.77	0.42
1:A:1432:PHE:HD1	1:A:1433:GLU:HB2	1.84	0.42
2:B:90:GLN:CD	20:T:141:LEU:HA	2.35	0.42
2:B:191:GLU:CD	2:B:743:ARG:HH22	2.28	0.42
2:B:475:PHE:CE2	2:B:479:LEU:HD22	2.55	0.42
2:B:527:ALA:HA	2:B:705:GLY:HA2	2.02	0.42
9:I:28:GLU:HG3	9:I:29:ASP:N	2.34	0.42
11:K:5:PRO:HD2	11:K:8:GLU:OE1	2.19	0.42
13:M:37:CYS:SG	13:M:38:GLY:N	2.88	0.42
16:P:206:GLU:HB3	16:P:207:PRO:HD3	1.74	0.42
21:U:278:THR:HG22	21:U:285:MET:SD	2.60	0.42
22:V:315:VAL:HG13	23:W:500:ASP:HB2	0.42	0.42
23:W:421:PHE:HD1	23:W:423:ASP:CB	2.13	0.42
26:2:77:LYS:HD3	26:2:78:GLU:CG	2.50	0.42
26:2:89:LEU:CD2	26:2:89:LEU:C	2.93	0.42
26:2:123:LEU:CD2	26:2:123:LEU:C	2.93	0.42
27:3:11:LEU:CD1	27:3:48:HIS:NE2	2.82	0.42
27:3:18:ASN:ND2	27:3:64:ILE:HD11	2.35	0.42
1:A:743:ARG:HD2	21:U:257:GLN:CG	2.50	0.42
1:A:1098:PRO:HA	1:A:1101:GLN:OE1	2.20	0.42
2:B:196:ALA:HB3	2:B:485:LEU:HA	2.02	0.42
15:O:79:VAL:HG21	15:O:93:VAL:HG12	2.01	0.42
16:P:162:VAL:CG2	16:P:164:GLN:NE2	2.72	0.42
20:T:145:LEU:C	20:T:147:LYS:N	2.78	0.42
20:T:153:TYR:CD1	20:T:153:TYR:C	2.96	0.42
23:W:25:MET:SD	23:W:58:ALA:HB2	2.59	0.42
26:2:236:PHE:CE1	26:2:261:PHE:HB3	2.54	0.42
27:3:111:ILE:HG13	27:3:112:VAL:H	1.84	0.42
27:3:202:LEU:N	27:3:202:LEU:CD2	2.82	0.42
2:B:38:GLY:H	2:B:41:ARG:HG2	1.85	0.41
2:B:380:ARG:NE	2:B:609:GLU:OE1	2.48	0.41
2:B:711:ILE:HG21	2:B:711:ILE:HD13	1.76	0.41
17:Q:24:GLY:O	18:R:210:PHE:CE2	2.73	0.41
23:W:15:ASP:HA	23:W:100:GLU:OE2	2.20	0.41
23:W:419:GLU:HB3	23:W:420:PRO:HD3	1.84	0.41
26:2:171:VAL:HG13	26:2:216:MET:HB3	1.98	0.41
27:3:105:THR:CG2	27:3:106:SER:N	2.82	0.41
27:3:228:LEU:C	27:3:228:LEU:CD2	2.93	0.41
1:A:16:ARG:NE	2:B:1172:MET:SD	2.92	0.41
1:A:366:VAL:O	1:A:481:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ARG:NH2	1:A:550:LYS:HD2	2.35	0.41
1:A:1313:GLN:HE22	1:A:1318:LYS:HD2	1.82	0.41
2:B:715:ASP:OD1	2:B:715:ASP:N	2.46	0.41
2:B:747:LEU:HD23	2:B:747:LEU:C	2.45	0.41
3:C:1:MET:HB3	3:C:3:TYR:CE2	2.56	0.41
8:H:96:VAL:HB	8:H:137:VAL:O	2.20	0.41
14:N:318:ASP:OD1	16:P:239:ARG:NH2	2.53	0.41
18:R:195:PRO:O	18:R:196:ASP:HB2	2.19	0.41
19:S:177:MET:HE3	19:S:177:MET:HB3	1.83	0.41
22:V:534:TYR:HE1	22:V:535:THR:OG1	1.98	0.41
25:1:1:MET:N	26:2:418:PHE:CB	2.83	0.41
25:1:10:ILE:C	25:1:10:ILE:CD1	2.93	0.41
26:2:176:ALA:HB3	26:2:178:LEU:HD13	1.97	0.41
26:2:204:LEU:HD23	26:2:254:MET:HE3	2.02	0.41
27:3:64:ILE:CB	27:3:123:ASP:HB3	2.50	0.41
27:3:217:VAL:HG12	27:3:218:PRO:O	2.20	0.41
27:3:221:PRO:C	27:3:223:LEU:H	2.27	0.41
1:A:24:GLY:O	2:B:1166:SER:HB3	2.20	0.41
1:A:153:ILE:HG22	1:A:155:GLU:OE2	2.20	0.41
1:A:354:LEU:HD23	1:A:1459:MET:HE3	2.02	0.41
1:A:693:ILE:HG21	2:B:1023:ARG:HE	1.85	0.41
1:A:1479:LYS:NZ	6:F:121:ASP:OD1	2.44	0.41
3:C:259:LEU:HD22	11:K:42:LEU:HD11	2.00	0.41
5:E:45:GLY:C	5:E:47:LYS:N	2.77	0.41
10:J:35:LEU:HD22	10:J:40:LEU:HD22	2.02	0.41
17:Q:154:CYS:SG	17:Q:155:THR:N	2.94	0.41
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.55	0.41
20:T:139:VAL:C	20:T:141:LEU:N	2.77	0.41
20:T:174:LYS:HG2	28:X:20:DG:H4'	2.02	0.41
22:V:423:ALA:HA	22:V:427:MET:SD	2.60	0.41
25:1:31:LYS:C	25:1:33:PHE:H	2.28	0.41
26:2:221:GLN:O	26:2:268:PHE:CE1	2.74	0.41
26:2:270:LEU:C	26:2:270:LEU:CD2	2.94	0.41
27:3:14:VAL:HG22	27:3:162:LEU:O	2.21	0.41
27:3:109:GLU:HG3	27:3:110:VAL:N	2.35	0.41
1:A:592:PHE:CZ	1:A:640:LEU:HD11	2.55	0.41
1:A:595:ILE:HD12	1:A:596:ILE:N	2.36	0.41
1:A:620:HIS:C	1:A:621:ILE:HG12	2.44	0.41
1:A:692:SER:O	1:A:828:LEU:HD22	2.20	0.41
1:A:1043:ILE:HG22	1:A:1046:ARG:HH22	1.86	0.41
1:A:1130:ILE:HD11	1:A:1405:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ILE:O	2:B:85:LEU:HD12	2.20	0.41
2:B:414:GLU:HA	2:B:417:ILE:HG22	2.01	0.41
2:B:771:GLU:OE2	10:J:58:LYS:HE3	2.20	0.41
2:B:1073:GLN:HG2	2:B:1112:ASP:HB2	2.03	0.41
6:F:68:THR:HG21	7:G:59:ILE:HG21	2.02	0.41
9:I:68:ILE:HG23	9:I:122:ARG:HD2	2.00	0.41
16:P:171:THR:HG23	16:P:256:GLN:HG3	2.02	0.41
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.20	0.41
18:R:151:LEU:HB3	18:R:154:LEU:HB3	2.02	0.41
26:2:93:LEU:HD23	26:2:96:TRP:HE1	1.85	0.41
27:3:41:VAL:HG13	27:3:42:MET:N	2.35	0.41
1:A:320:ASN:HB2	1:A:338:SER:HB3	2.03	0.41
1:A:366:VAL:HB	1:A:481:THR:HG22	2.01	0.41
1:A:542:LEU:O	1:A:545:VAL:HG12	2.20	0.41
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.55	0.41
1:A:602:CYS:HB2	1:A:655:ILE:CD1	2.51	0.41
1:A:902:GLU:CD	1:A:982:ASN:HB2	2.46	0.41
2:B:92:TYR:HE2	2:B:146:LYS:HZ2	1.66	0.41
2:B:501:LEU:CD1	2:B:505:LEU:HD22	2.50	0.41
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.55	0.41
3:C:70:LEU:HD23	3:C:70:LEU:HA	1.84	0.41
25:1:1:MET:HG2	26:2:413:LEU:CB	2.47	0.41
26:2:62:LEU:C	26:2:62:LEU:CD1	2.94	0.41
26:2:170:ALA:C	26:2:213:TRP:HZ3	2.27	0.41
29:Y:80:DT:H6	29:Y:80:DT:H2'	1.71	0.41
1:A:478:PRO:O	1:A:479:TRP:HB2	2.20	0.41
1:A:566:PHE:HB3	1:A:674:THR:HG22	2.01	0.41
1:A:576:GLN:HB2	8:H:73:GLY:O	2.20	0.41
2:B:274:ARG:HA	2:B:278:PHE:O	2.20	0.41
2:B:280:SER:HB2	2:B:283:ASP:OD2	2.21	0.41
2:B:962:THR:HA	2:B:963:PRO:HD3	1.80	0.41
5:E:61:LEU:HD12	5:E:72:MET:O	2.21	0.41
9:I:49:ASP:CG	9:I:50:ASN:H	2.28	0.41
9:I:101:SER:OG	9:I:104:ALA:HB2	2.21	0.41
13:M:36:GLU:OE1	13:M:36:GLU:N	2.54	0.41
16:P:283:TYR:CD2	16:P:285:PRO:HD3	2.55	0.41
16:P:295:MET:HG3	16:P:297:LYS:H	1.85	0.41
22:V:518:PHE:CD1	22:V:713:LEU:HD13	2.55	0.41
22:V:612:ASP:OD1	22:V:635:GLN:CG	2.69	0.41
25:1:43:VAL:CG1	25:1:44:PHE:N	2.83	0.41
25:1:52:VAL:CG2	25:1:53:LEU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:175:LEU:CD2	26:2:216:MET:SD	3.07	0.41
26:2:202:GLN:HE21	26:2:202:GLN:N	2.15	0.41
29:Y:77:DT:C6	29:Y:78:DT:H72	2.56	0.41
1:A:153:ILE:HD13	1:A:153:ILE:N	2.36	0.41
1:A:608:THR:OG1	1:A:610:PRO:CG	2.68	0.41
1:A:823:VAL:HG13	1:A:835:GLU:HB3	2.02	0.41
1:A:1179:PRO:HA	1:A:1209:PRO:HA	2.03	0.41
1:A:1250:ASP:CB	21:U:227:GLU:HG3	2.14	0.41
1:A:1251:ASN:OD1	21:U:227:GLU:O	2.37	0.41
2:B:41:ARG:HD2	2:B:41:ARG:HA	1.68	0.41
2:B:237:VAL:HG12	2:B:372:LEU:HD22	2.03	0.41
2:B:810:PHE:N	2:B:925:SER:O	2.43	0.41
2:B:1043:ILE:HG21	2:B:1043:ILE:HD13	1.74	0.41
3:C:4:ALA:HB2	11:K:93:ASP:OD1	2.21	0.41
9:I:11:PHE:CD1	9:I:55:VAL:HG22	2.56	0.41
13:M:45:VAL:HG13	13:M:48:VAL:HG22	2.03	0.41
17:Q:54:PHE:CD2	18:R:194:ARG:HG3	2.56	0.41
21:U:194:ARG:HH12	21:U:223:MET:HE2	1.86	0.41
1:A:114:CYS:C	1:A:116:LYS:H	2.29	0.41
1:A:271:ARG:NE	13:M:73:PRO:CD	2.76	0.41
1:A:537:ILE:HD13	1:A:537:ILE:HA	1.82	0.41
2:B:282:ARG:HH11	9:I:21:ASN:HD21	1.67	0.41
2:B:299:GLU:OE2	2:B:302:LYS:HE3	2.21	0.41
2:B:631:GLN:HE21	2:B:685:LYS:HD2	1.85	0.41
3:C:116:THR:HG21	3:C:146:ASP:HB2	2.03	0.41
14:N:12:LYS:O	14:N:15:ARG:HB2	2.21	0.41
16:P:206:GLU:OE2	16:P:206:GLU:HA	2.20	0.41
20:T:161:TYR:O	20:T:164:GLU:HB3	2.21	0.41
21:U:165:GLU:OE1	21:U:165:GLU:N	2.53	0.41
22:V:390:CYS:SG	22:V:399:LYS:HE3	2.61	0.41
23:W:212:LEU:C	23:W:212:LEU:HD13	2.46	0.41
26:2:206:LEU:CD2	26:2:206:LEU:N	2.84	0.41
26:2:224:GLN:CB	26:2:268:PHE:CZ	2.94	0.41
1:A:271:ARG:HB3	1:A:272:ASN:H	1.52	0.41
1:A:495:ASP:C	1:A:497:ASP:N	2.73	0.41
1:A:505:LEU:HA	1:A:506:PRO:HD2	1.83	0.41
1:A:544:ALA:HB2	1:A:680:LEU:HD22	2.03	0.41
1:A:598:GLY:HA2	1:A:633:GLY:HA3	2.02	0.41
1:A:924:TYR:OH	1:A:952:LEU:HB2	2.21	0.41
1:A:924:TYR:C	1:A:926:ASN:H	2.29	0.41
1:A:929:ALA:C	1:A:931:ARG:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:ARG:HA	1:A:954:ARG:HD3	1.80	0.41
1:A:1024:ASN:OD1	1:A:1025:GLY:N	2.54	0.41
2:B:128:ILE:HG21	2:B:431:LEU:HD21	2.03	0.41
2:B:451:GLY:HA2	2:B:467:SER:HB3	2.02	0.41
2:B:626:LEU:HG	2:B:698:ILE:HG22	2.03	0.41
2:B:674:MET:HE2	2:B:690:CYS:SG	2.60	0.41
2:B:849:ASP:OD1	2:B:850:ASP:N	2.53	0.41
2:B:877:GLU:OE1	2:B:877:GLU:N	2.54	0.41
2:B:1125:MET:HG3	2:B:1163:MET:HE1	2.02	0.41
5:E:11:TRP:HZ2	5:E:36:THR:HA	1.86	0.41
5:E:171:PRO:HB2	5:E:207:ARG:HD2	2.02	0.41
7:G:31:PHE:CE1	7:G:48:VAL:HB	2.52	0.41
8:H:78:THR:HG21	11:K:78:THR:CG2	2.51	0.41
16:P:229:GLN:HA	16:P:232:LEU:HB3	2.03	0.41
18:R:133:ILE:HG13	18:R:136:LYS:HG3	2.02	0.41
18:R:167:LEU:HD22	18:R:200:ILE:HB	2.02	0.41
18:R:195:PRO:CB	18:R:199:LYS:CD	2.86	0.41
22:V:514:MET:HE2	22:V:667:THR:HG21	2.02	0.41
22:V:518:PHE:HB2	25:1:16:MET:SD	2.61	0.41
22:V:519:TYR:CE2	22:V:523:VAL:HG21	2.55	0.41
22:V:531:ILE:HG23	22:V:534:TYR:CE2	2.45	0.41
25:1:14:PRO:HG2	25:1:17:LYS:HB2	2.02	0.41
25:1:52:VAL:O	25:1:56:ARG:HG2	2.21	0.41
26:2:28:PRO:CA	27:3:33:THR:CB	2.84	0.41
26:2:86:SER:HB2	26:2:140:LYS:HE2	2.03	0.41
26:2:236:PHE:HZ	26:2:258:LEU:CD1	2.34	0.41
26:2:236:PHE:CD2	26:2:236:PHE:C	2.94	0.41
27:3:187:GLN:CG	27:3:189:ILE:CG1	2.94	0.41
28:X:44:DT:H2''	28:X:45:DC:C4'	2.51	0.41
1:A:84:HIS:C	1:A:257:PRO:HG3	2.45	0.41
1:A:931:ARG:C	1:A:933:THR:H	2.28	0.41
1:A:1161:LEU:HD11	1:A:1346:VAL:HG22	2.02	0.41
2:B:971:ALA:O	2:B:975:ARG:HD2	2.21	0.41
9:I:62:VAL:O	9:I:64:GLU:HB3	2.21	0.41
9:I:84:HIS:CD2	9:I:84:HIS:N	2.83	0.41
12:L:38:GLU:O	13:M:226:LYS:NZ	2.32	0.41
20:T:155:PRO:O	20:T:156:VAL:HG22	2.21	0.41
20:T:179:ASP:OD1	20:T:183:VAL:HG23	2.21	0.41
25:1:20:LEU:HD13	25:1:20:LEU:C	2.46	0.41
26:2:181:GLN:HA	26:2:181:GLN:NE2	2.34	0.41
27:3:69:PHE:HZ	27:3:139:LYS:HD2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:HH21	13:M:45:VAL:HB	1.85	0.40
1:A:517:GLU:OE1	6:F:62:ARG:NE	2.43	0.40
1:A:1231:ILE:O	1:A:1235:ILE:HG12	2.21	0.40
2:B:613:ARG:HD3	2:B:615:TYR:HE2	1.86	0.40
2:B:617:ASP:O	2:B:620:ARG:NH2	2.50	0.40
2:B:927:ARG:NH2	2:B:1057:ASP:OD1	2.54	0.40
3:C:42:VAL:CB	3:C:178:PRO:HG3	2.44	0.40
5:E:116:GLN:O	5:E:119:VAL:HB	2.21	0.40
9:I:96:PHE:HB3	9:I:112:TYR:CD1	2.55	0.40
17:Q:42:CYS:C	17:Q:95:ASN:HD21	2.29	0.40
20:T:139:VAL:HG12	20:T:141:LEU:H	1.86	0.40
22:V:297:PHE:CG	22:V:298:ARG:N	2.89	0.40
26:2:174:ASP:OD2	26:2:213:TRP:CZ3	2.74	0.40
26:2:251:VAL:CG1	26:2:254:MET:CG	2.95	0.40
27:3:34:LEU:HD13	27:3:34:LEU:C	2.46	0.40
27:3:44:LEU:C	27:3:44:LEU:CD1	2.94	0.40
27:3:222:SER:HB3	27:3:225:GLN:CG	2.51	0.40
1:A:297:GLY:HA3	17:Q:57:LYS:CG	2.50	0.40
1:A:818:GLU:HG2	1:A:819:SER:N	2.36	0.40
1:A:974:ASP:HB2	1:A:1317:LYS:NZ	2.36	0.40
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.51	0.40
1:A:1176:TYR:HB2	1:A:1211:LEU:HD23	2.03	0.40
2:B:23:GLN:CD	2:B:679:PRO:HG2	2.46	0.40
2:B:1163:MET:C	2:B:1165:MET:N	2.79	0.40
5:E:197:SER:HB3	5:E:201:GLY:H	1.85	0.40
8:H:15:ILE:HG13	8:H:52:LEU:HD23	2.04	0.40
12:L:18:ILE:HD11	12:L:47:LYS:HG3	2.02	0.40
13:M:200:LYS:HB3	13:M:200:LYS:HE2	1.75	0.40
16:P:268:ILE:O	16:P:337:LYS:HE3	2.20	0.40
17:Q:136:PHE:HD1	17:Q:140:GLU:OE1	2.03	0.40
20:T:177:ARG:HH22	20:T:212:TYR:CB	2.29	0.40
21:U:247:GLU:OE1	21:U:250:MET:HG3	2.22	0.40
22:V:353:ALA:O	22:V:357:VAL:HG23	2.21	0.40
22:V:520:ARG:HB2	25:1:19:PHE:HB2	2.02	0.40
22:V:593:LEU:HD11	22:V:615:PHE:CE1	2.56	0.40
26:2:34:LEU:CD2	26:2:34:LEU:N	2.84	0.40
26:2:93:LEU:HA	26:2:93:LEU:HD23	1.77	0.40
26:2:93:LEU:O	26:2:96:TRP:CD1	2.74	0.40
26:2:236:PHE:HZ	26:2:262:LEU:CD2	2.35	0.40
27:3:60:ILE:CG2	27:3:61:ALA:N	2.84	0.40
27:3:114:GLU:OE1	27:3:114:GLU:HA	2.21	0.40

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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	0.40
27:3:191:ILE:H	27:3:210:THR:HG21	1.85	0.40
27:3:222:SER:HB3	27:3:225:GLN:OE1	2.21	0.40
1:A:212:LYS:HB3	1:A:212:LYS:HZ3	1.85	0.40
1:A:275:ASP:OD1	1:A:276:LEU:N	2.55	0.40
1:A:713:VAL:HG21	1:A:745:LEU:HD11	2.04	0.40
1:A:927:GLU:HG3	1:A:929:ALA:H	1.86	0.40
2:B:957:THR:HG21	2:B:1026:GLU:OE1	2.22	0.40
2:B:1152:PRO:HG2	2:B:1155:CYS:CB	2.51	0.40
10:J:2:ILE:HD12	10:J:3:ILE:N	2.36	0.40
17:Q:182:GLU:O	17:Q:186:PRO:HD3	2.22	0.40
25:1:7:GLY:C	25:1:8:VAL:CG2	2.94	0.40
25:1:39:ASP:OD2	26:2:434:GLU:OE2	2.39	0.40
26:2:30:VAL:CB	27:3:25:GLN:CB	2.91	0.40
26:2:51:LEU:CD2	26:2:51:LEU:C	2.94	0.40
26:2:93:LEU:CA	26:2:96:TRP:HD1	2.31	0.40
26:2:399:ASP:OD1	26:2:402:ARG:NH1	2.55	0.40
1:A:286:ILE:HD11	1:A:310:LEU:HA	2.04	0.40
1:A:622:SER:O	1:A:623:PRO:C	2.56	0.40
2:B:51:ILE:HD12	2:B:51:ILE:HG23	1.64	0.40
2:B:698:ILE:HD13	2:B:698:ILE:HG21	1.71	0.40
2:B:1068:GLN:HA	13:M:51:GLU:CD	2.46	0.40
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.56	0.40
10:J:8:PHE:CD2	10:J:48:MET:HE1	2.56	0.40
18:R:149:LYS:HD3	18:R:175:LEU:HB2	2.03	0.40
23:W:233:PHE:HB2	23:W:456:ILE:HG22	2.02	0.40
25:1:38:ILE:CB	25:1:44:PHE:CD1	3.04	0.40
27:3:172:LEU:C	27:3:172:LEU:CD1	2.94	0.40
1:A:118:LEU:HD12	1:A:148:CYS:HB3	2.02	0.40
1:A:136:GLN:HG3	1:A:139:LYS:H	1.85	0.40
1:A:601:ASN:CG	1:A:988:TRP:HZ3	2.28	0.40
1:A:823:VAL:HA	1:A:835:GLU:HG2	2.03	0.40
1:A:1471:PHE:HZ	6:F:61:GLU:HA	1.87	0.40
2:B:181:PRO:HD3	2:B:475:PHE:HE1	1.86	0.40
2:B:191:GLU:OE1	2:B:472:ARG:HD2	2.21	0.40
16:P:206:GLU:CB	16:P:236:LYS:NZ	2.76	0.40
17:Q:149:THR:HG23	17:Q:151:THR:H	1.86	0.40
18:R:224:THR:O	18:R:224:THR:HG23	2.20	0.40
20:T:37:ARG:NH2	20:T:62:LEU:HB2	2.36	0.40
23:W:535:ILE:HG12	23:W:617:ALA:HB3	2.04	0.40
26:2:94:ARG:HD2	26:2:95:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:195:CYS:SG	26:2:196:ILE:N	2.95	0.40
27:3:42:MET:HG2	27:3:111:ILE:CD1	2.52	0.40
27:3:222:SER:O	27:3:226:TYR:CD2	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1450/1970 (74%)	1262 (87%)	123 (8%)	65 (4%)	2	17
2	B	1163/1174 (99%)	1011 (87%)	106 (9%)	46 (4%)	2	18
3	C	273/275 (99%)	242 (89%)	21 (8%)	10 (4%)	2	20
4	D	127/142 (89%)	118 (93%)	9 (7%)	0	100	100
5	E	208/210 (99%)	188 (90%)	13 (6%)	7 (3%)	3	21
6	F	84/127 (66%)	78 (93%)	6 (7%)	0	100	100
7	G	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
8	H	148/150 (99%)	119 (80%)	19 (13%)	10 (7%)	1	11
9	I	123/125 (98%)	92 (75%)	18 (15%)	13 (11%)	0	6
10	J	65/67 (97%)	51 (78%)	8 (12%)	6 (9%)	0	8
11	K	115/117 (98%)	110 (96%)	2 (2%)	3 (3%)	4	25
12	L	44/58 (76%)	33 (75%)	9 (20%)	2 (4%)	2	17
13	M	308/316 (98%)	263 (85%)	25 (8%)	20 (6%)	1	12
14	N	109/376 (29%)	100 (92%)	7 (6%)	2 (2%)	6	34
15	O	97/109 (89%)	92 (95%)	4 (4%)	1 (1%)	12	49
16	P	183/339 (54%)	169 (92%)	9 (5%)	5 (3%)	4	25
17	Q	176/439 (40%)	154 (88%)	14 (8%)	8 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	163/291 (56%)	132 (81%)	21 (13%)	10 (6%)	1	13
19	S	134/517 (26%)	123 (92%)	8 (6%)	3 (2%)	5	29
20	T	218/249 (88%)	185 (85%)	20 (9%)	13 (6%)	1	13
21	U	168/301 (56%)	149 (89%)	10 (6%)	9 (5%)	1	15
22	V	473/782 (60%)	400 (85%)	44 (9%)	29 (6%)	1	13
23	W	661/760 (87%)	570 (86%)	68 (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%)	6448 (88%)	610 (8%)	298 (4%)	4	18

All (298) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ALA
1	A	48	GLU
1	A	132	LYS
1	A	134	LYS
1	A	154	CYS
1	A	205	VAL
1	A	208	ASP
1	A	211	GLU
1	A	261	ARG
1	A	262	PRO
1	A	264	VAL
1	A	265	VAL
1	A	295	GLN
1	A	344	LYS
1	A	496	PHE
1	A	598	GLY
1	A	605	THR
1	A	607	SER
1	A	610	PRO
1	A	622	SER
1	A	623	PRO
1	A	911	PRO
1	A	931	ARG

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Mol	Chain	Res	Type
1	A	932	ARG
1	A	1114	ALA
1	A	1117	VAL
1	A	1200	PRO
1	A	1299	GLN
1	A	1342	SER
2	B	61	ASP
2	B	63	PRO
2	B	74	ALA
2	B	77	GLU
2	B	78	VAL
2	B	79	GLU
2	B	81	PRO
2	B	134	LYS
2	B	141	GLN
2	B	203	ASN
2	B	226	GLU
2	B	231	PRO
2	B	249	LYS
2	B	491	ARG
2	B	876	ASN
2	B	879	GLU
2	B	898	THR
2	B	901	THR
2	B	1136	GLU
2	B	1166	SER
3	C	6	GLN
3	C	7	PRO
3	C	136	ASP
3	C	139	PRO
3	C	143	VAL
3	C	213	GLU
5	E	47	LYS
5	E	49	SER
5	E	53	PRO
5	E	64	HIS
5	E	65	ASN
8	H	18	GLU
8	H	65	TYR
8	H	67	ASP
8	H	86	ASP
8	H	107	GLU

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Mol	Chain	Res	Type
8	H	108	ALA
9	I	15	ARG
9	I	16	PHE
9	I	62	VAL
9	I	63	ASP
9	I	85	PRO
9	I	86	CYS
9	I	99	SER
9	I	106	ASP
9	I	118	HIS
10	J	64	PRO
11	K	112	LYS
13	M	11	PRO
13	M	12	ARG
13	M	40	VAL
13	M	42	GLY
13	M	43	ASP
13	M	48	VAL
13	M	92	SER
13	M	93	PHE
13	M	94	ASP
14	N	355	ASP
15	O	4	GLN
16	P	207	PRO
17	Q	25	PHE
17	Q	102	VAL
17	Q	118	GLU
18	R	140	LYS
18	R	195	PRO
18	R	196	ASP
18	R	215	GLU
20	T	124	TYR
20	T	143	GLN
20	T	145	LEU
20	T	146	ASP
21	U	228	MET
21	U	231	ASP
21	U	253	THR
21	U	277	GLN
21	U	293	GLU
22	V	385	ASP
22	V	427	MET

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Mol	Chain	Res	Type
22	V	461	HIS
22	V	491	ALA
22	V	499	ASN
22	V	613	THR
22	V	614	SER
22	V	616	ASP
22	V	632	SER
22	V	648	LYS
22	V	649	GLY
23	W	67	VAL
23	W	420	PRO
23	W	424	ARG
23	W	430	ASN
23	W	504	ILE
23	W	573	ASP
23	W	595	ILE
23	W	630	SER
24	0	77	LYS
24	0	78	PRO
25	1	48	GLU
26	2	49	PRO
27	3	120	THR
1	A	77	ASN
1	A	195	GLY
1	A	207	GLU
1	A	213	LYS
1	A	299	ALA
1	A	452	ASP
1	A	531	ASN
1	A	611	ASP
1	A	929	ALA
1	A	1115	LYS
1	A	1275	VAL
1	A	1315	ASP
2	B	23	GLN
2	B	224	CYS
2	B	428	ASP
2	B	518	HIS
2	B	527	ALA
2	B	549	SER
2	B	561	ILE
2	B	875	GLU

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Mol	Chain	Res	Type
2	B	897	ARG
5	E	48	PRO
8	H	149	ALA
9	I	92	LYS
10	J	2	ILE
16	P	208	ARG
16	P	297	LYS
16	P	299	ARG
17	Q	70	LYS
17	Q	101	ASN
17	Q	125	ALA
18	R	147	ASP
18	R	163	LEU
20	T	147	LYS
20	T	156	VAL
20	T	171	GLU
20	T	180	LYS
20	T	229	HIS
21	U	252	LYS
22	V	254	GLN
22	V	404	SER
22	V	460	ALA
22	V	615	PHE
23	W	124	LEU
23	W	408	SER
23	W	646	ILE
26	2	223	ALA
26	2	231	VAL
1	A	184	CYS
1	A	374	SER
1	A	599	HIS
1	A	894	ASP
1	A	1102	MET
1	A	1103	THR
1	A	1265	ASP
1	A	1435	THR
2	B	513	GLU
2	B	685	LYS
2	B	884	ASN
8	H	24	ARG
10	J	6	ARG
10	J	65	LEU

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Mol	Chain	Res	Type
11	K	69	HIS
11	K	80	ASP
13	M	10	LEU
13	M	56	SER
13	M	61	THR
13	M	86	LYS
13	M	87	GLY
13	M	95	GLU
13	M	306	PHE
17	Q	158	HIS
18	R	149	LYS
18	R	174	ALA
19	S	154	THR
20	T	142	SER
20	T	155	PRO
21	U	279	ARG
21	U	294	CYS
22	V	343	GLY
23	W	147	GLN
23	W	155	CYS
23	W	509	GLU
27	3	198	SER
1	A	300	ALA
1	A	615	SER
2	B	80	GLU
2	B	118	LEU
2	B	839	GLY
2	B	873	LEU
2	B	1006	VAL
12	L	16	ILE
13	M	44	ARG
13	M	89	GLY
13	M	101	TYR
14	N	312	GLU
16	P	163	PRO
17	Q	126	SER
18	R	156	ASP
19	S	151	ARG
20	T	141	LEU
20	T	178	ALA
21	U	233	LEU
22	V	310	LEU

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Mol	Chain	Res	Type
22	V	475	ASP
22	V	502	ILE
22	V	629	HIS
1	A	51	ARG
1	A	65	ILE
1	A	204	HIS
1	A	271	ARG
1	A	485	ASN
1	A	817	PRO
1	A	935	GLN
1	A	1274	GLU
2	B	75	SER
2	B	290	TYR
2	B	460	HIS
2	B	493	GLY
2	B	521	GLY
2	B	1025	ASN
2	B	1129	ASN
3	C	147	ASP
9	I	12	VAL
10	J	30	THR
19	S	160	ALA
22	V	470	LEU
22	V	650	MET
23	W	152	LEU
23	W	551	SER
24	0	79	ASN
26	2	430	VAL
1	A	612	ASP
1	A	650	GLY
1	A	726	GLU
1	A	729	PRO
3	C	74	ILE
8	H	21	LYS
8	H	139	SER
9	I	67	GLN
18	R	139	PHE
22	V	436	GLY
22	V	582	GLY
23	W	36	GLY
23	W	111	SER
23	W	345	ARG

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Mol	Chain	Res	Type
23	W	697	ILE
1	A	687	ILE
22	V	311	LYS
22	V	651	VAL
2	B	253	GLY
3	C	218	ALA
9	I	68	ILE
12	L	20	GLY
22	V	457	ILE
23	W	495	ILE
24	O	216	GLY
1	A	621	ILE
13	M	38	GLY
22	V	405	VAL
23	W	174	ILE
25	1	2	VAL
2	B	136	GLY
3	C	151	VAL
5	E	52	ARG
10	J	5	VAL
22	V	426	VAL
23	W	45	GLY
24	O	56	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1279/1748 (73%)	1230 (96%)	49 (4%)	29	50
2	B	1020/1028 (99%)	987 (97%)	33 (3%)	34	56
3	C	252/252 (100%)	250 (99%)	2 (1%)	73	80
4	D	119/126 (94%)	118 (99%)	1 (1%)	73	80
5	E	192/192 (100%)	184 (96%)	8 (4%)	26	48
6	F	74/111 (67%)	73 (99%)	1 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	152/153 (99%)	150 (99%)	2 (1%)	61	74
8	H	131/131 (100%)	127 (97%)	4 (3%)	35	56
9	I	112/112 (100%)	104 (93%)	8 (7%)	13	35
10	J	56/56 (100%)	54 (96%)	2 (4%)	31	52
11	K	106/106 (100%)	100 (94%)	6 (6%)	18	40
12	L	43/55 (78%)	42 (98%)	1 (2%)	44	64
13	M	263/268 (98%)	256 (97%)	7 (3%)	39	61
14	N	105/324 (32%)	105 (100%)	0	100	100
15	O	90/98 (92%)	90 (100%)	0	100	100
16	P	159/293 (54%)	156 (98%)	3 (2%)	50	67
17	Q	164/373 (44%)	158 (96%)	6 (4%)	30	51
18	R	150/261 (58%)	146 (97%)	4 (3%)	39	61
19	S	121/448 (27%)	118 (98%)	3 (2%)	42	63
20	T	196/218 (90%)	188 (96%)	8 (4%)	27	49
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%)	542 (94%)	35 (6%)	17	38
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%)	6326 (96%)	241 (4%)	31	51

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	48	GLU
1	A	72	GLN
1	A	87	HIS
1	A	117	LEU
1	A	132	LYS
1	A	181	HIS
1	A	203	LYS
1	A	205	VAL

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Mol	Chain	Res	Type
1	A	212	LYS
1	A	220	ARG
1	A	261	ARG
1	A	264	VAL
1	A	271	ARG
1	A	277	THR
1	A	343	LEU
1	A	449	HIS
1	A	463	THR
1	A	477	LEU
1	A	488	VAL
1	A	500	GLU
1	A	508	SER
1	A	546	ARG
1	A	587	THR
1	A	595	ILE
1	A	611	ASP
1	A	619	LYS
1	A	849	ASP
1	A	908	THR
1	A	954	ARG
1	A	981	CYS
1	A	1036	ASN
1	A	1050	CYS
1	A	1066	ASP
1	A	1075	LYS
1	A	1115	LYS
1	A	1139	LEU
1	A	1192	TRP
1	A	1203	ASP
1	A	1282	ASP
1	A	1298	LEU
1	A	1309	MET
1	A	1318	LYS
1	A	1319	LYS
1	A	1337	GLU
1	A	1339	ASP
1	A	1379	GLU
1	A	1420	ASN
1	A	1484	MET
2	B	73	HIS
2	B	79	GLU

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Mol	Chain	Res	Type
2	B	129	THR
2	B	133	ILE
2	B	146	LYS
2	B	156	LEU
2	B	161	CYS
2	B	168	ASP
2	B	225	LEU
2	B	226	GLU
2	B	287	HIS
2	B	302	LYS
2	B	422	PHE
2	B	548	TRP
2	B	591	ARG
2	B	666	ASP
2	B	711	ILE
2	B	737	ILE
2	B	782	ILE
2	B	785	TYR
2	B	790	GLN
2	B	793	SER
2	B	853	LEU
2	B	880	LEU
2	B	896	LEU
2	B	897	ARG
2	B	921	ILE
2	B	941	GLN
2	B	957	THR
2	B	1022	LEU
2	B	1054	MET
2	B	1069	ILE
2	B	1127	ILE
3	C	195	THR
3	C	273	THR
4	D	33	LEU
5	E	46	ASP
5	E	47	LYS
5	E	50	GLU
5	E	55	ARG
5	E	62	VAL
5	E	64	HIS
5	E	69	THR
5	E	127	LEU

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Mol	Chain	Res	Type
6	F	121	ASP
7	G	22	LEU
7	G	128	TYR
8	H	38	ASP
8	H	70	LEU
8	H	84	ARG
8	H	107	GLU
9	I	14	ILE
9	I	15	ARG
9	I	60	HIS
9	I	61	GLU
9	I	62	VAL
9	I	66	THR
9	I	84	HIS
9	I	103	ARG
10	J	36	ASP
10	J	47	ARG
11	K	39	ASP
11	K	48	SER
11	K	63	VAL
11	K	67	LEU
11	K	111	ASP
11	K	112	LYS
12	L	19	CYS
13	M	10	LEU
13	M	14	THR
13	M	47	ASP
13	M	86	LYS
13	M	129	ASN
13	M	133	ASN
13	M	200	LYS
16	P	203	ARG
16	P	239	ARG
16	P	297	LYS
17	Q	102	VAL
17	Q	128	LYS
17	Q	135	THR
17	Q	139	LEU
17	Q	177	LEU
17	Q	202	GLU
18	R	163	LEU
18	R	194	ARG

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Mol	Chain	Res	Type
18	R	205	ASP
18	R	206	LYS
19	S	35	ASP
19	S	166	ARG
19	S	177	MET
20	T	141	LEU
20	T	153	TYR
20	T	154	LYS
20	T	156	VAL
20	T	177	ARG
20	T	185	ASP
20	T	201	ASP
20	T	204	ASP
21	U	226	GLU
21	U	227	GLU
21	U	233	LEU
21	U	252	LYS
21	U	257	GLN
21	U	276	VAL
21	U	292	ASN
21	U	299	LYS
21	U	301	CYS
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	612	ASP
23	W	37	HIS
23	W	64	PRO
23	W	87	LEU

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Mol	Chain	Res	Type
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
23	W	175	TYR
23	W	196	ARG
23	W	263	LEU
23	W	283	ASP
23	W	288	LEU
23	W	299	ARG
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	432	ILE
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

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Mol	Chain	Res	Type
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
26	2	430	VAL
26	2	452	LYS
27	3	24	LYS
27	3	37	CYS
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 (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	96	HIS
1	A	122	ASN
1	A	136	GLN
1	A	267	GLN
1	A	272	ASN
1	A	372	ASN
1	A	493	ASN
1	A	502	ASN
1	A	677	ASN
1	A	700	GLN
1	A	731	ASN
1	A	746	ASN
1	A	764	ASN
1	A	765	ASN
1	A	783	GLN

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Mol	Chain	Res	Type
1	A	1034	GLN
1	A	1036	ASN
1	A	1093	GLN
1	A	1190	GLN
1	A	1313	GLN
1	A	1316	ASN
1	A	1445	HIS
2	B	90	GLN
2	B	175	ASN
2	B	631	GLN
2	B	717	ASN
2	B	725	GLN
2	B	749	HIS
2	B	986	GLN
2	B	1021	HIS
2	B	1071	ASN
2	B	1117	HIS
3	C	6	GLN
3	C	66	HIS
3	C	134	ASN
3	C	173	HIS
3	C	260	GLN
4	D	102	ASN
5	E	22	HIS
5	E	132	GLN
5	E	148	HIS
7	G	9	HIS
7	G	24	ASN
8	H	126	GLN
8	H	133	HIS
9	I	84	HIS
10	J	52	HIS
10	J	61	ASN
11	K	40	HIS
12	L	23	HIS
13	M	129	ASN
16	P	256	GLN
16	P	327	ASN
18	R	95	HIS
18	R	188	GLN
19	S	27	ASN
19	S	53	ASN

Continued on next page...

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Mol	Chain	Res	Type
19	S	141	HIS
19	S	173	HIS
20	T	181	GLN
21	U	205	ASN
21	U	257	GLN
22	V	281	GLN
22	V	286	HIS
22	V	366	ASN
22	V	377	GLN
22	V	415	HIS
22	V	459	GLN
22	V	537	ASN
22	V	539	ASN
22	V	599	ASN
22	V	621	ASN
22	V	665	GLN
22	V	677	GLN
23	W	187	GLN
23	W	316	GLN
23	W	328	HIS
23	W	430	ASN
23	W	434	HIS
24	0	60	HIS
25	1	27	ASN
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	52	ASN
27	3	63	HIS
27	3	148	ASN
27	3	155	GLN
27	3	185	GLN
27	3	187	GLN
27	3	225	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

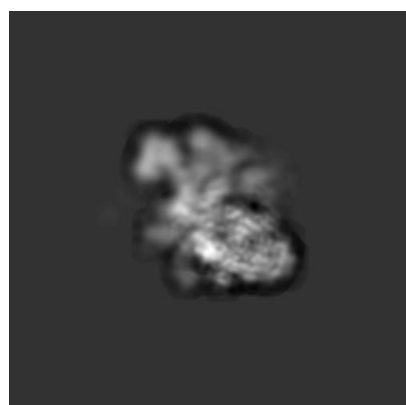
6 Map visualisation [i](#)

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

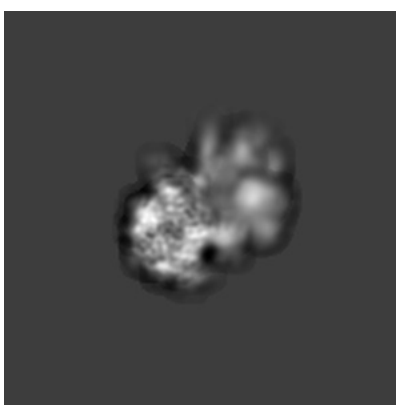
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

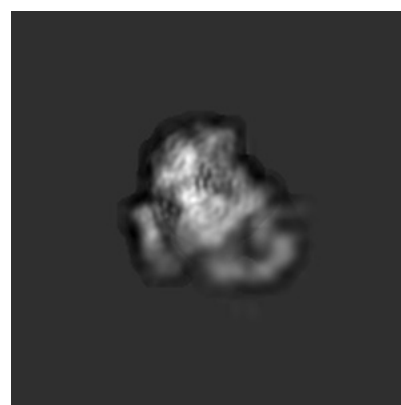
6.1.1 Primary map



X



Y

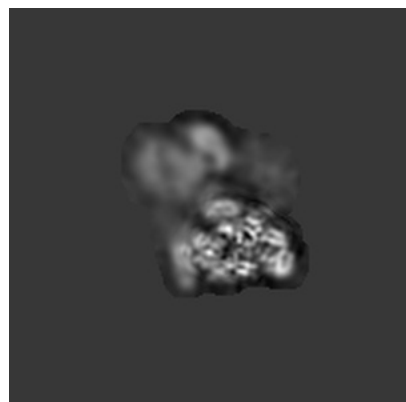


Z

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

6.2 Central slices [i](#)

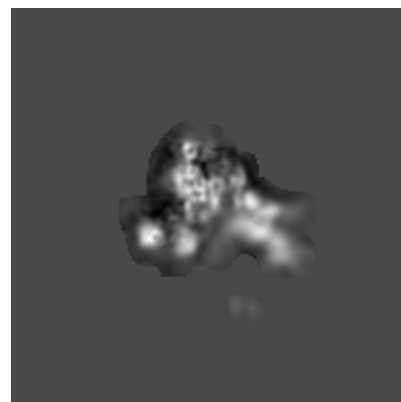
6.2.1 Primary map



X Index: 96



Y Index: 96

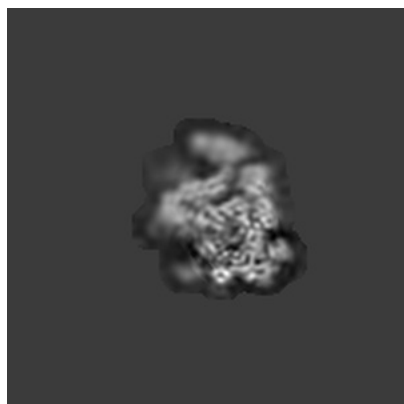


Z Index: 96

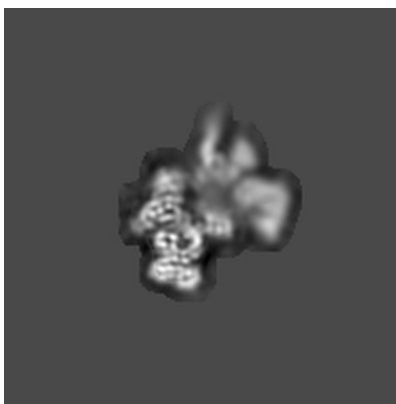
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

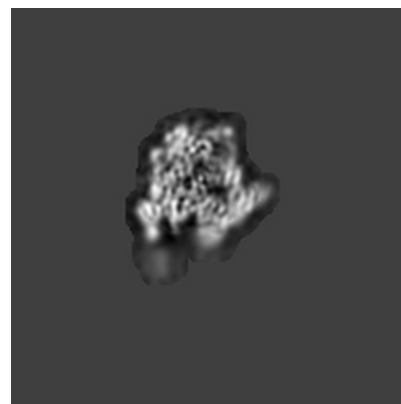
6.3.1 Primary map



X Index: 84



Y Index: 93

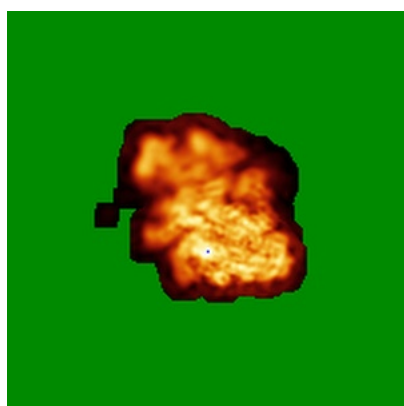


Z Index: 76

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

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

6.4.1 Primary map



X



Y

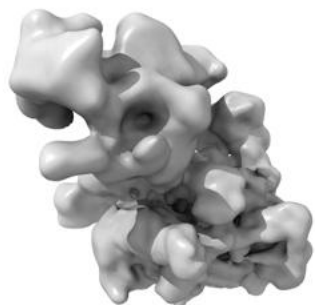


Z

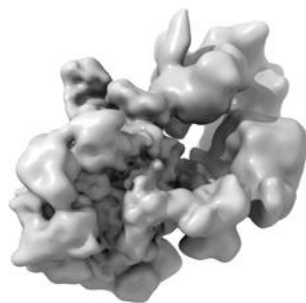
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

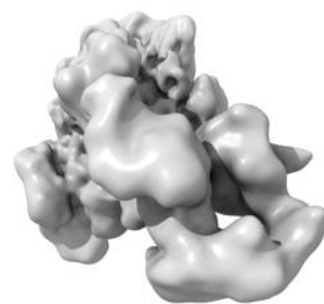
6.5.1 Primary map



X



Y



Z

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

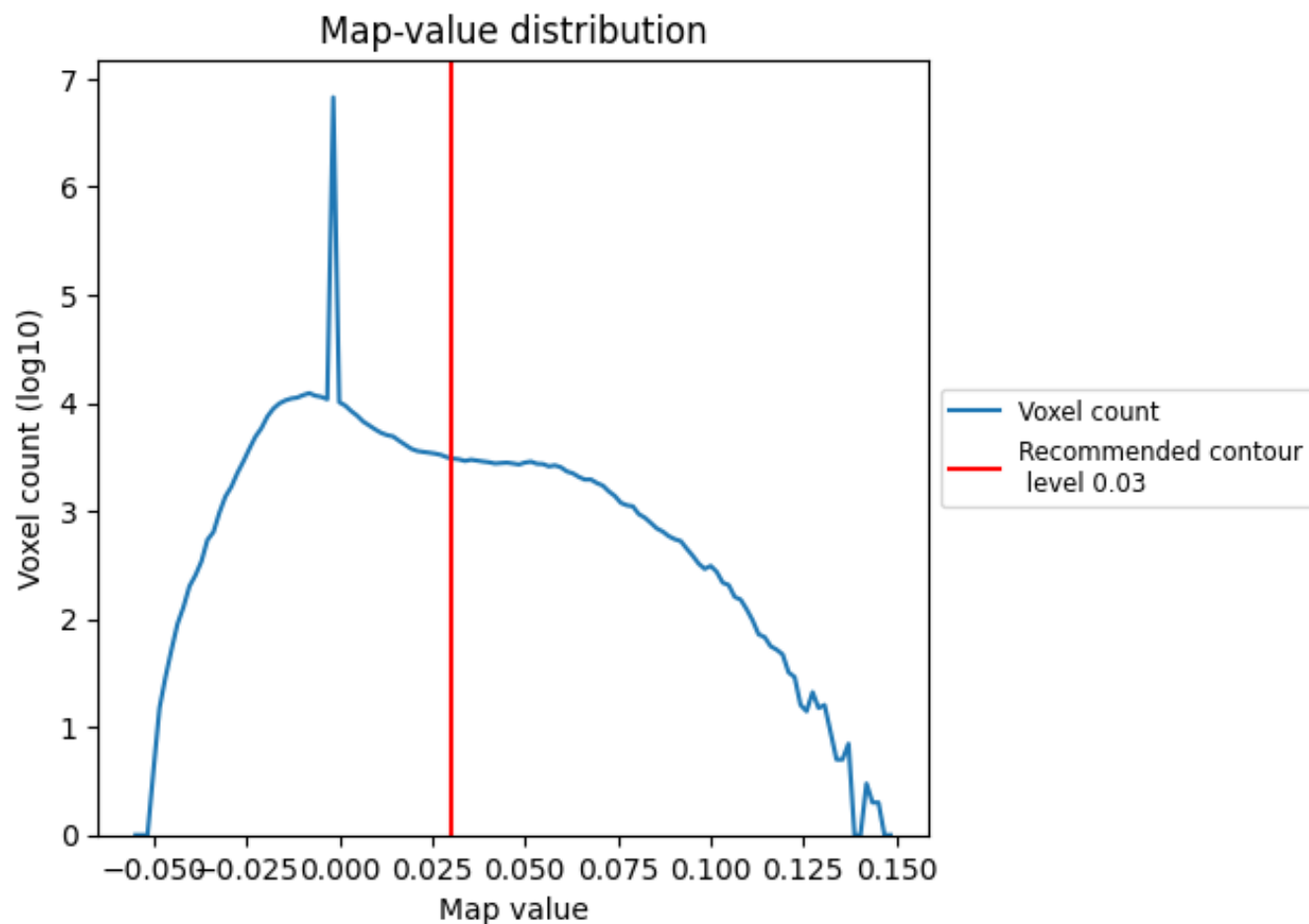
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

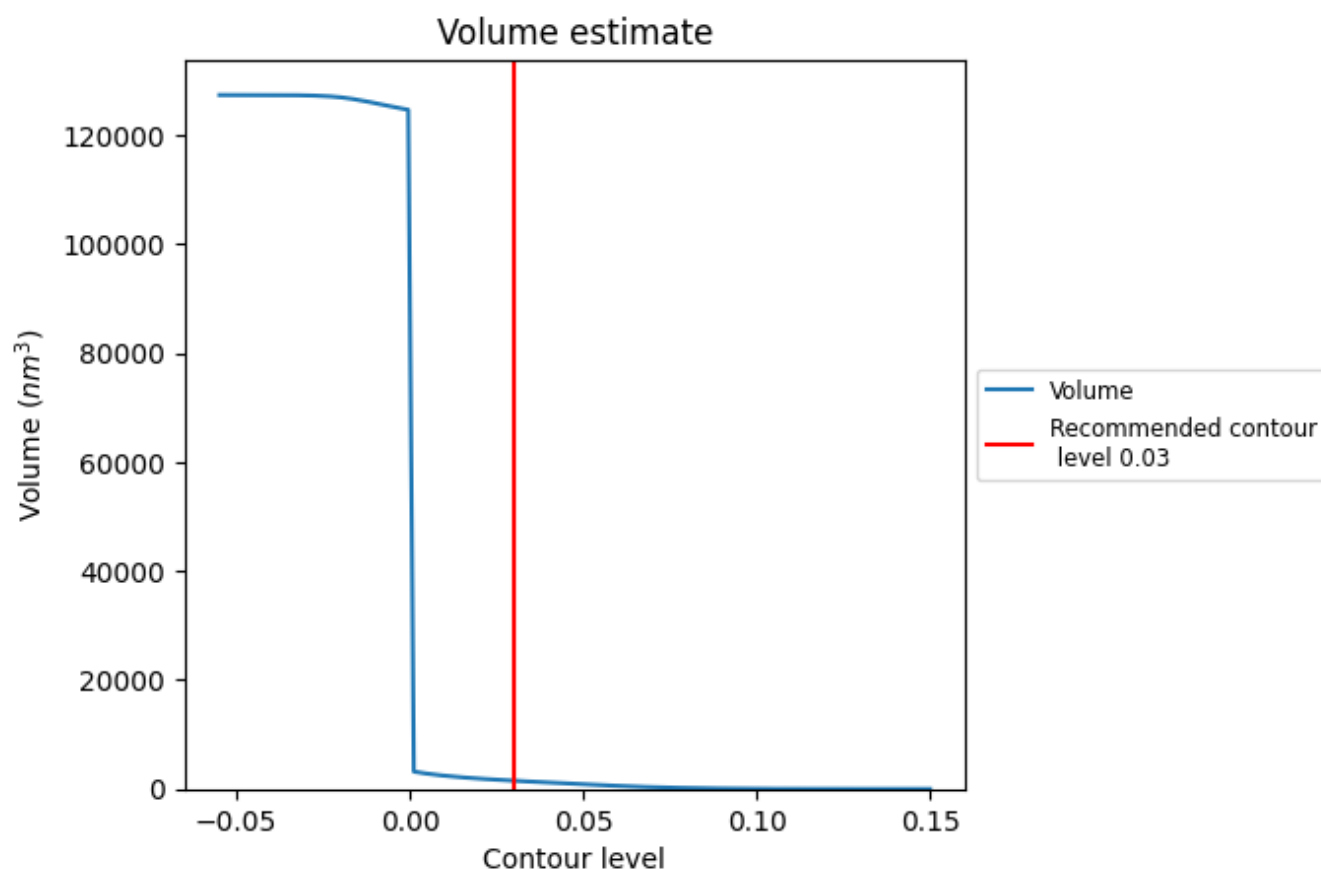
This section contains the results of statistical analysis of the map.

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.

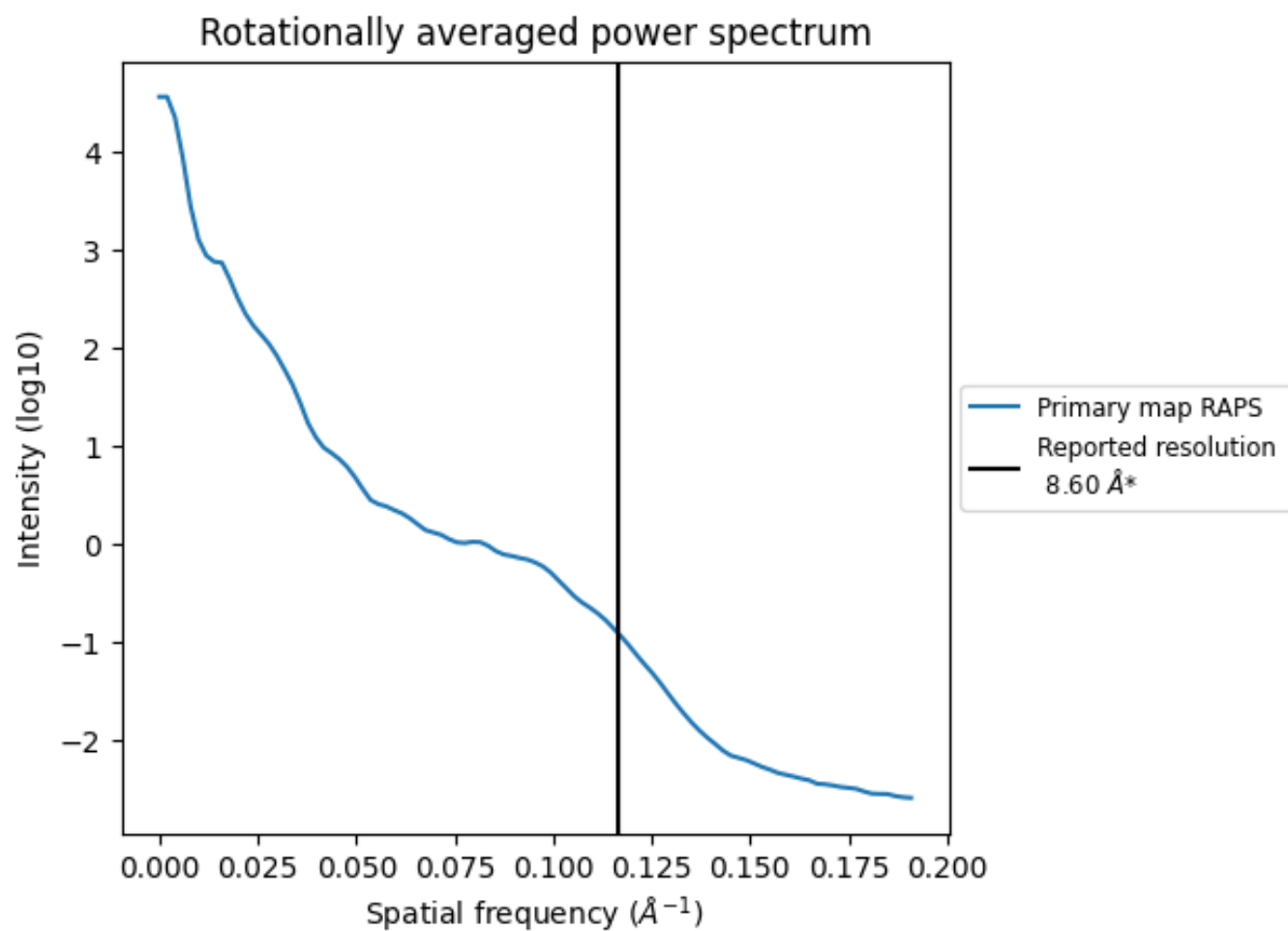
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

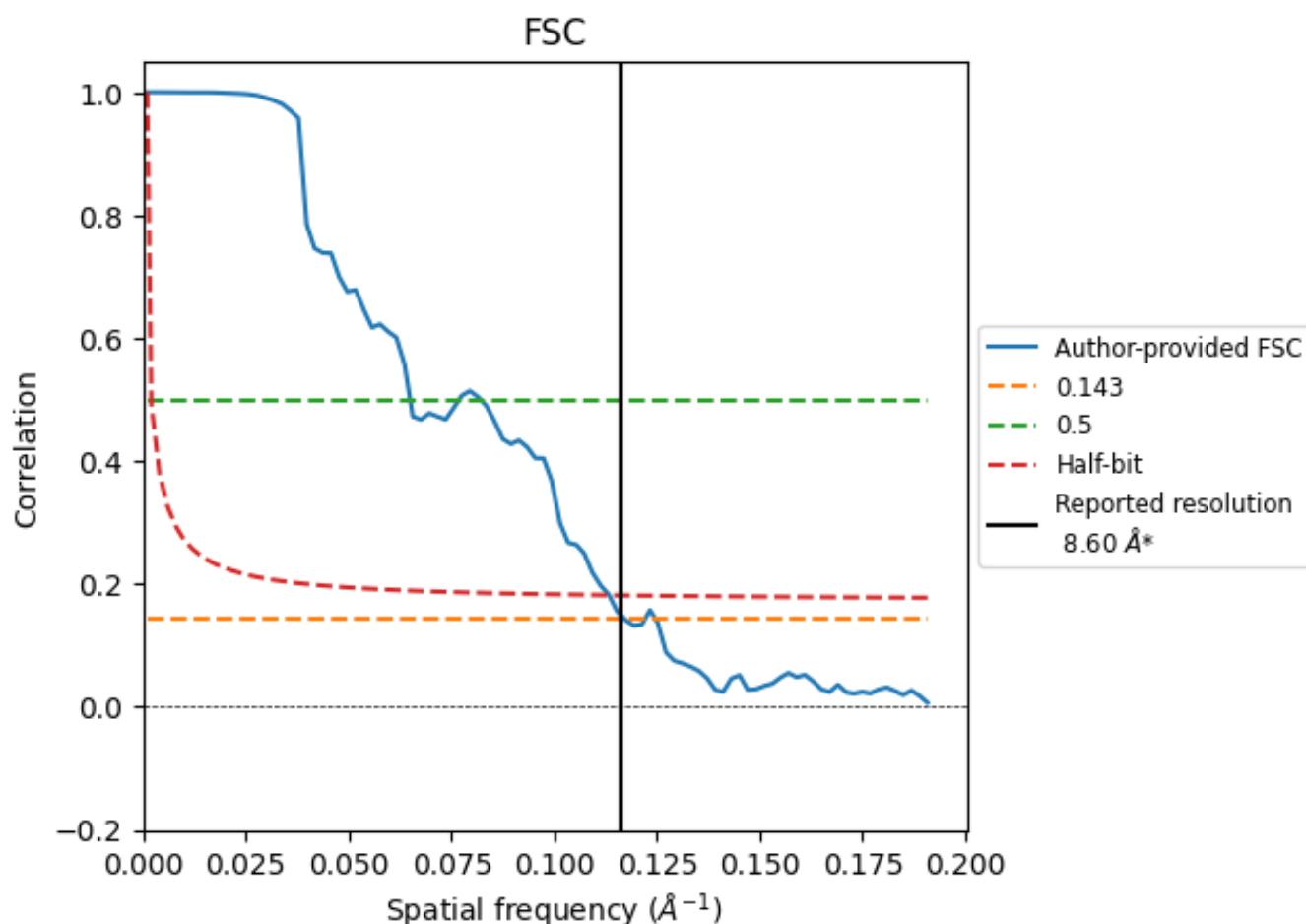


*Reported resolution corresponds to spatial frequency of 0.116 Å⁻¹

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 0.116 Å⁻¹

8.2 Resolution estimates [i](#)

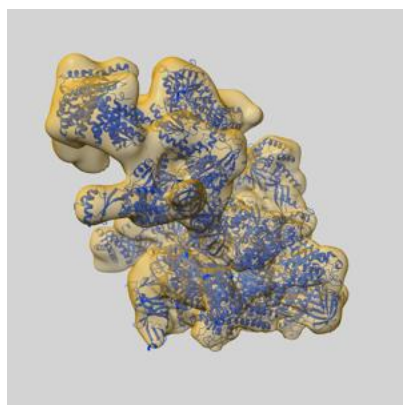
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.60	-	-
Author-provided FSC curve	8.55	15.38	8.82
Unmasked-calculated*	-	-	-

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

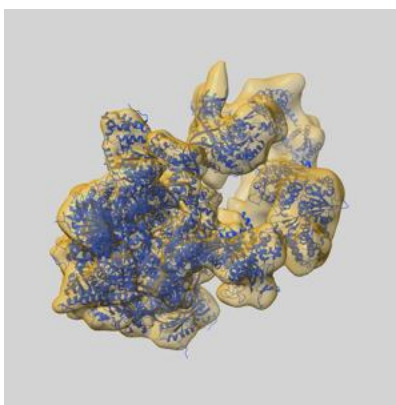
9 Map-model fit [i](#)

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

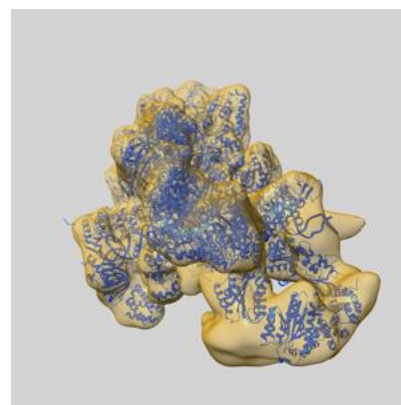
9.1 Map-model overlay [i](#)



X



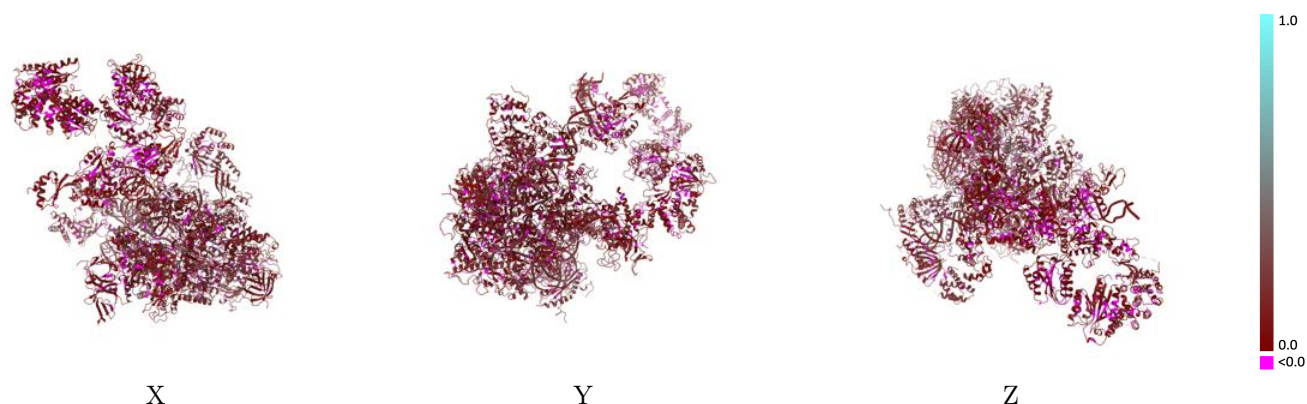
Y



Z

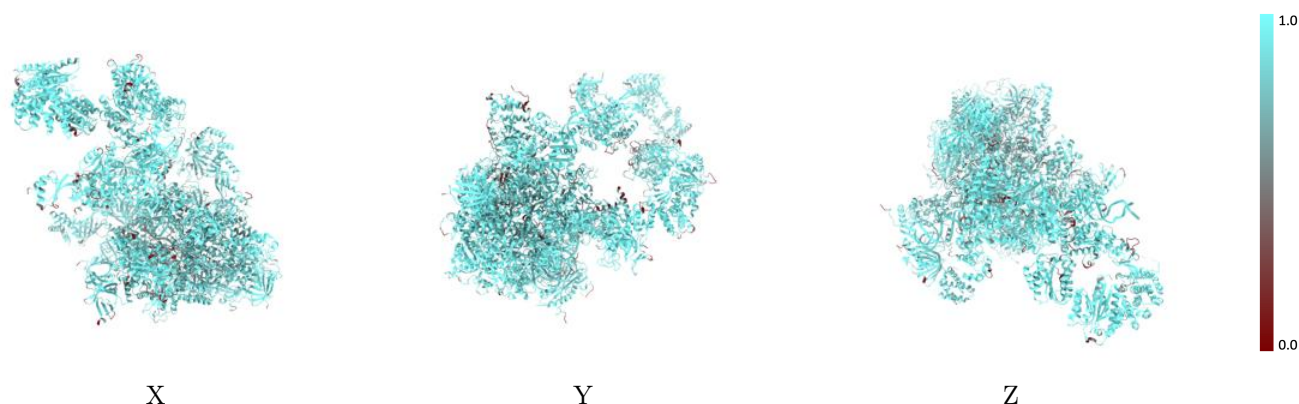
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



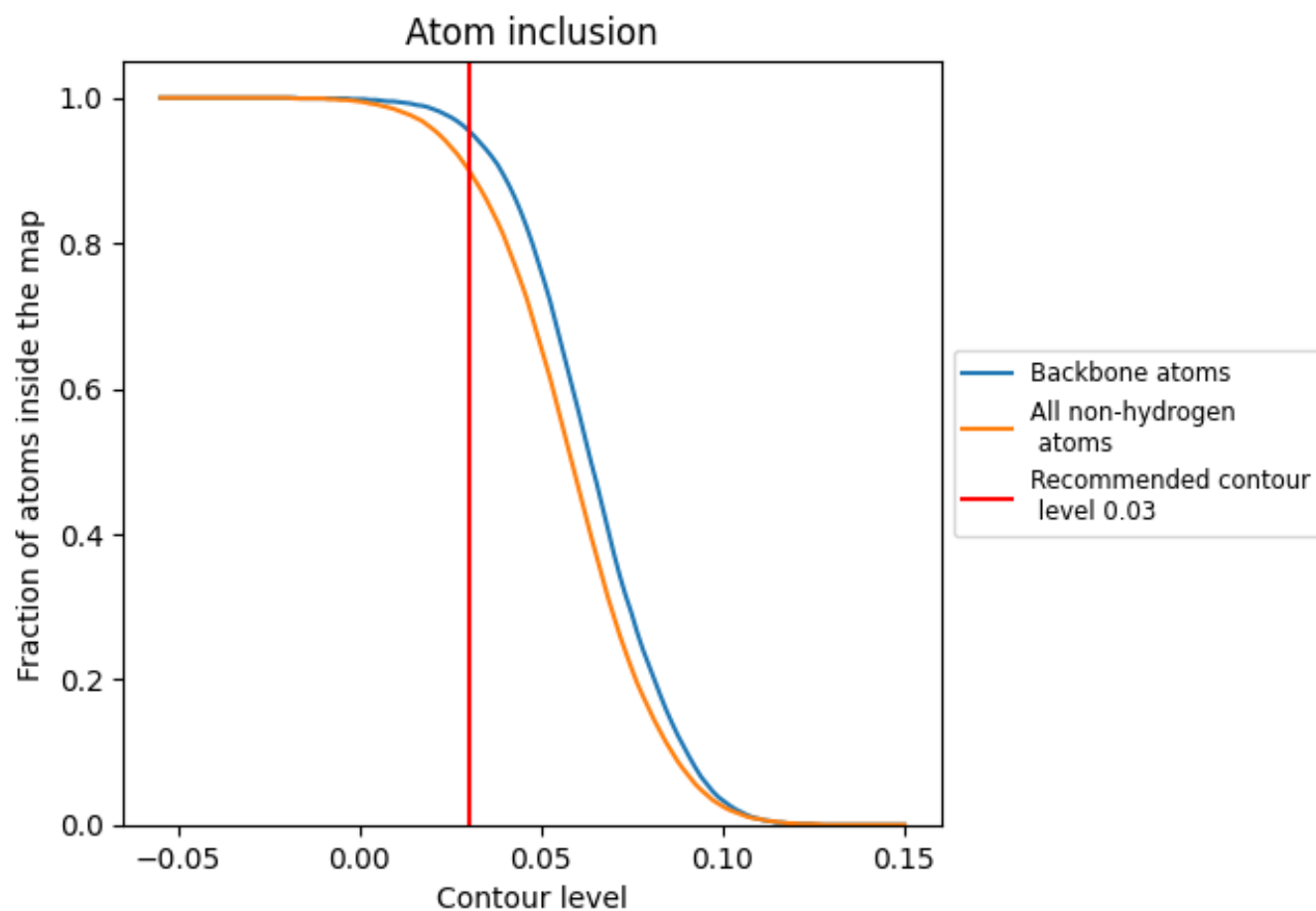
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.1050
0	 0.9280	 0.0520
1	 0.8260	 0.0650
2	 0.9350	 0.0720
3	 0.9520	 0.0610
A	 0.8900	 0.1260
B	 0.8750	 0.1170
C	 0.9330	 0.1170
D	 0.8990	 0.1120
E	 0.9240	 0.1250
F	 0.8040	 0.1300
G	 0.9370	 0.1050
H	 0.9380	 0.1170
I	 0.8730	 0.0950
J	 0.9650	 0.1190
K	 0.9420	 0.1420
L	 0.9460	 0.1240
M	 0.8860	 0.1170
N	 0.9040	 0.0930
O	 0.9590	 0.0820
P	 0.9660	 0.1140
Q	 0.9340	 0.1030
R	 0.8850	 0.1030
S	 0.8970	 0.0720
T	 0.8800	 0.1030
U	 0.6410	 0.0780
V	 0.9220	 0.0640
W	 0.9130	 0.0670
X	 0.9430	 0.1560
Y	 0.9160	 0.1590

