



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:07 AM UTC

PDB ID : 5IY9 / pdb_00005iy9
EMDB ID : EMD-8134
Title : Human holo-PIC in the initial transcribing state (no IIS)
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on : 2016-03-24
Resolution : 6.30 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:

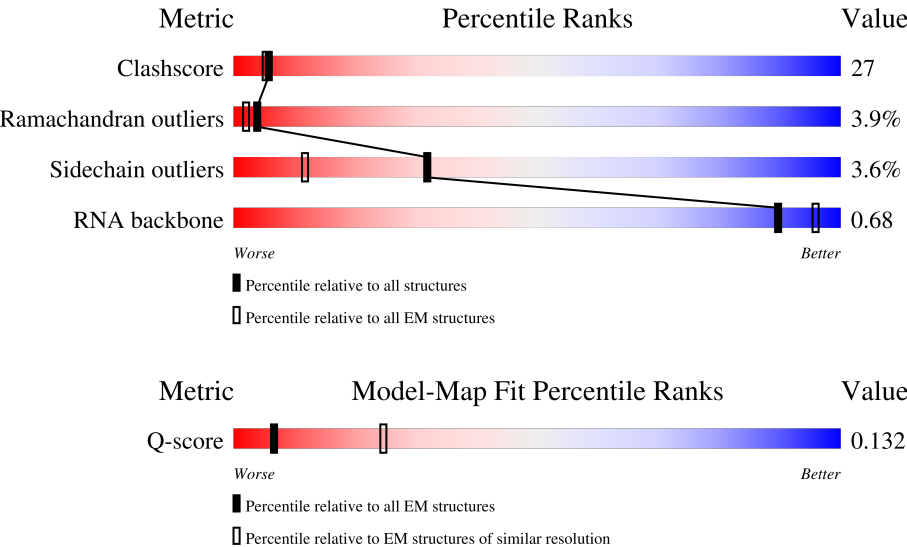
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 6.30 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.



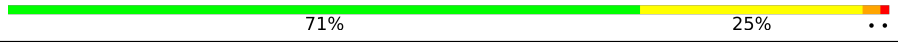
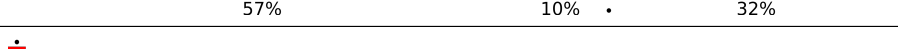
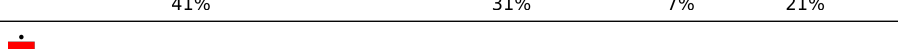
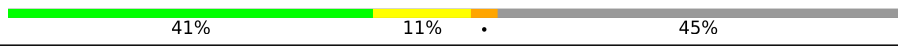
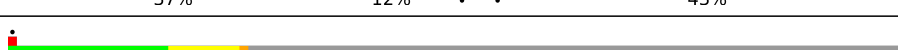
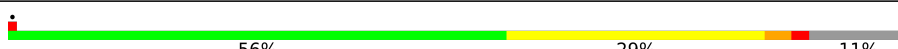
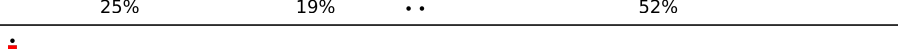
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	550 (5.80 - 6.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	

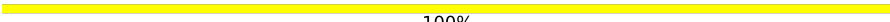
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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	V	782	
22	W	760	
23	0	395	
24	1	71	
25	2	462	
26	3	308	
27	X	83	
28	Y	83	

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Mol	Chain	Length	Quality of chain
29	Z	6	 100%

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 61725 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 TFIIH basal transcription factor complex helicase XPB subunit.

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

- Molecule 22 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

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

- Molecule 23 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	188	Total	C	N	O	S	0	0
			1479	935	258	276	10		

- Molecule 24 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	62	Total	C	N	O	S	0	0
			491	317	77	93	4		

- Molecule 25 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	274	Total	C	N	O	S	0	0
			2196	1417	377	392	10		

- Molecule 26 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	193	Total	C	N	O	S	0	0
			1526	978	252	284	12		

- Molecule 27 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	83	Total	C	N	O	P	0	0
			1710	815	307	506	82		

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

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

- Molecule 29 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	6	Total	C	N	O	P	0	0
			125	57	23	40	5		

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

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

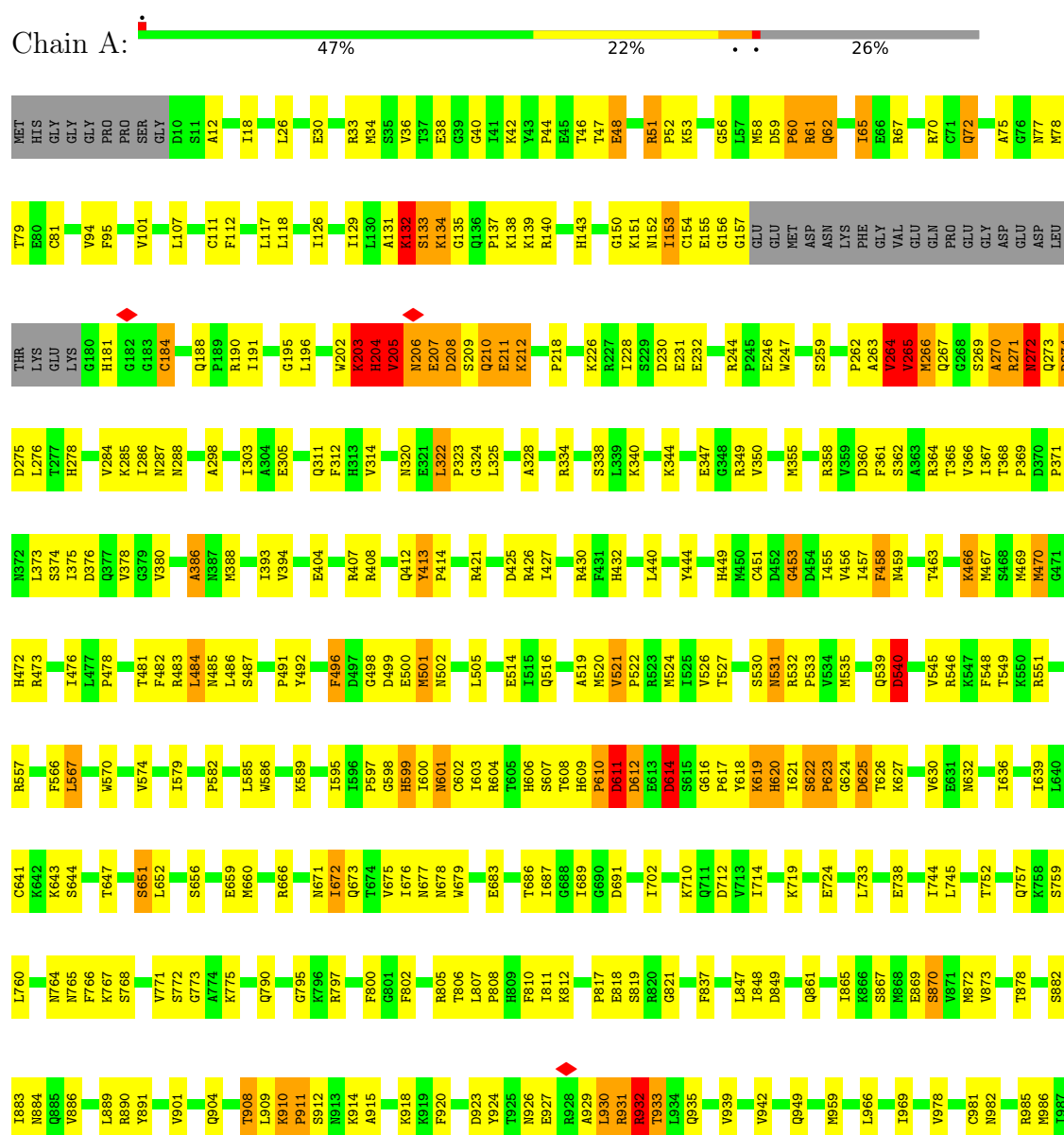
- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

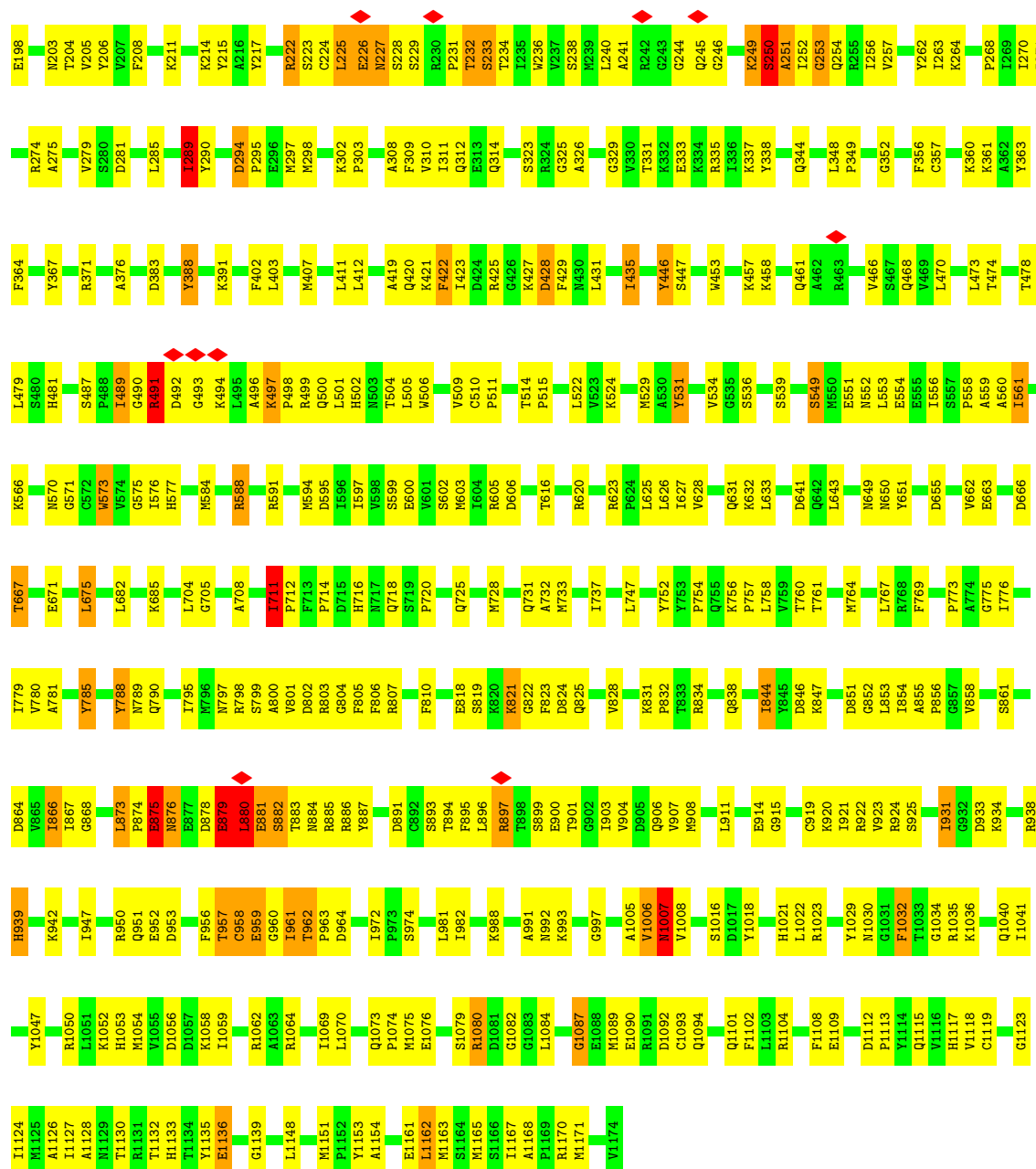
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



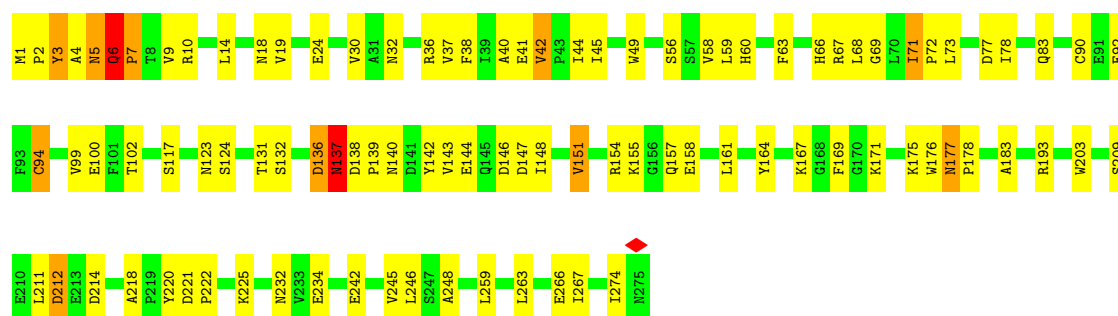


Q90	Q91	Y92	L93	S94	K95	H98	A99	D102	G103	A104	P105	M108	T119	A122	P123	L124	D127	I128	T131	V132	I133	K134	E135	Q139	L140	Q141	Q145	K146	L156	Y160	C161	L162	L163	N164	G165	L166	T167	D168	P169	D170	D180	P181	T187	K192	F200		
MET	TYR	ASP	ALA	ASP	GLU	ASP	GLN	Y10	D11	E12	Q23	E24	A25	I28	S32	Y33	K37	G38	L39	V40	R41	D45	S46	F47	F50	I51	Q52	Q56	R57	L58	V59	E60	D61	A62	P63	P64	I65	H73	A74	E77	V78	E79	E80	P81	P82	L86	F90



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

Chain C: 64% 31%



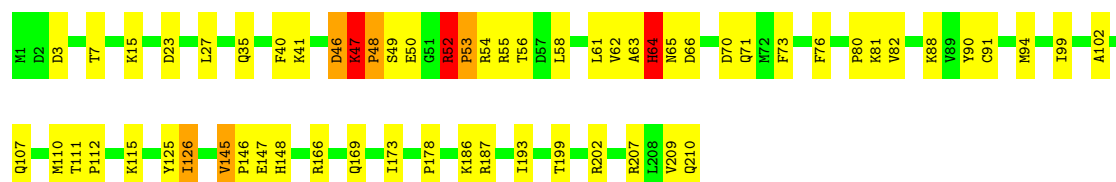
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 



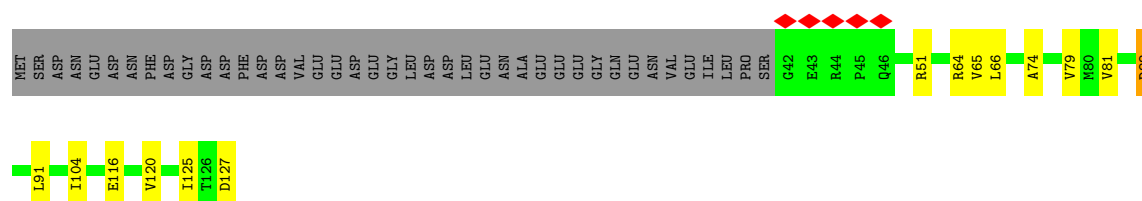
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5

Chain E: 



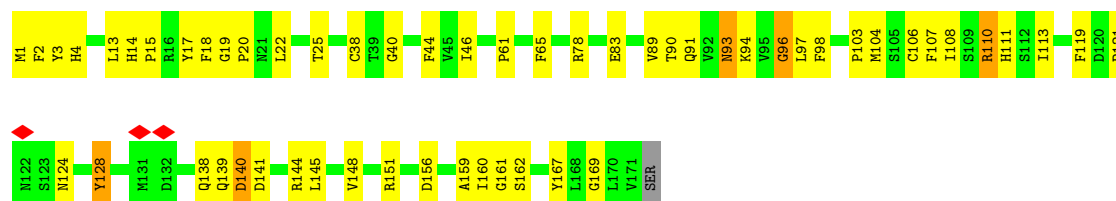
- Molecule 6: DNA-directed RNA polymerase II subunit RPB6

Chain F: 



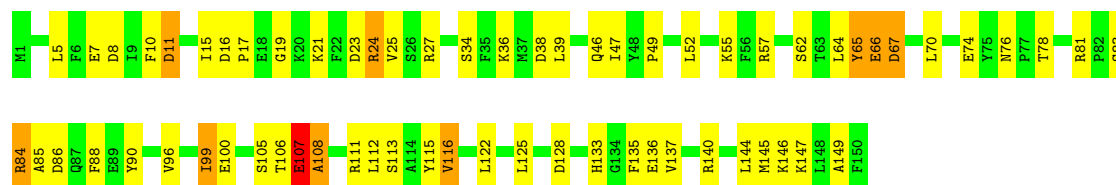
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 

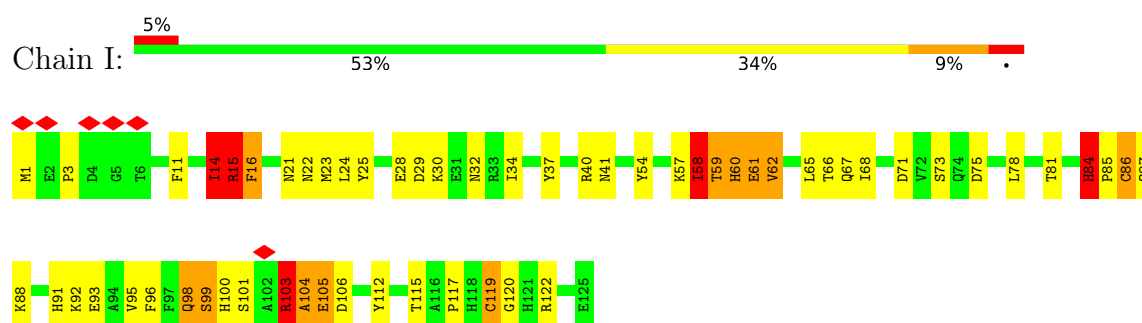


- Molecule 8: DNA-directed RNA polymerase II subunit RPB8

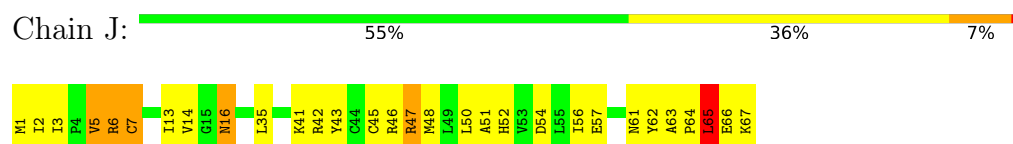
Chain H: 



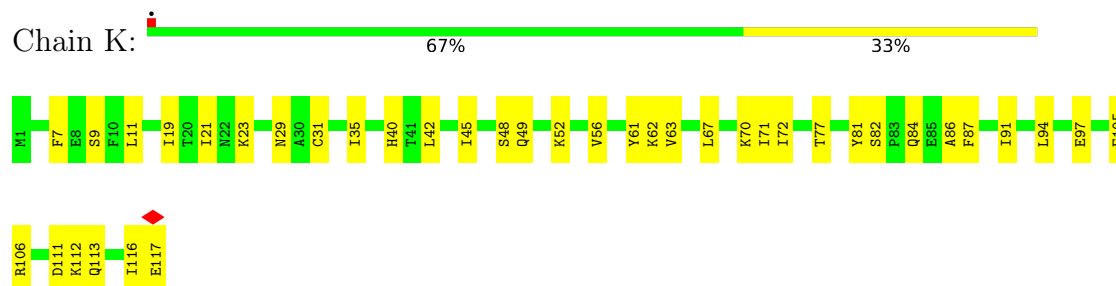
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



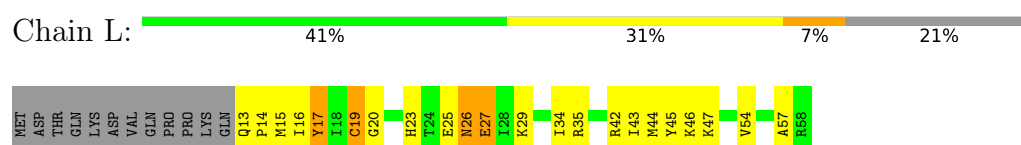
- Molecule 10: DNA-directed RNA polymerase II subunit RPB10



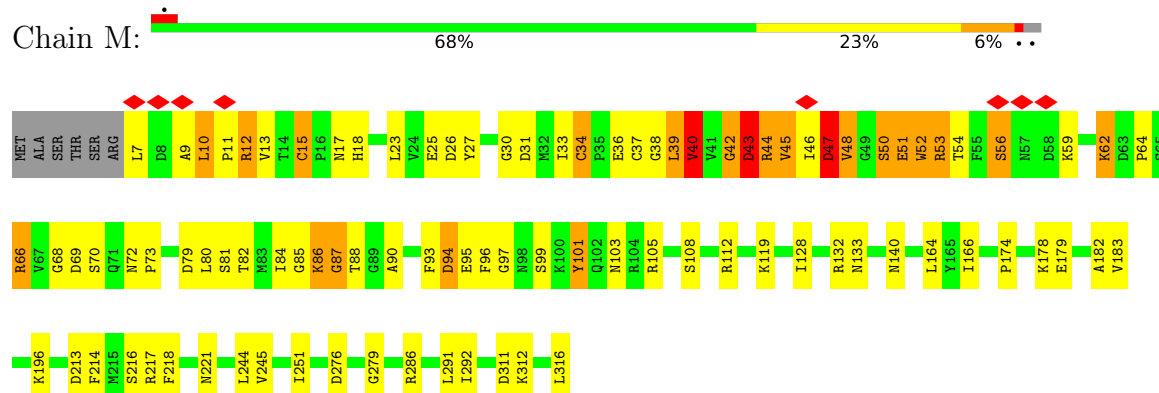
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



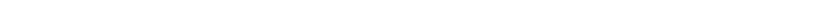
- Molecule 12: DNA-directed RNA polymerase II subunit RPB12

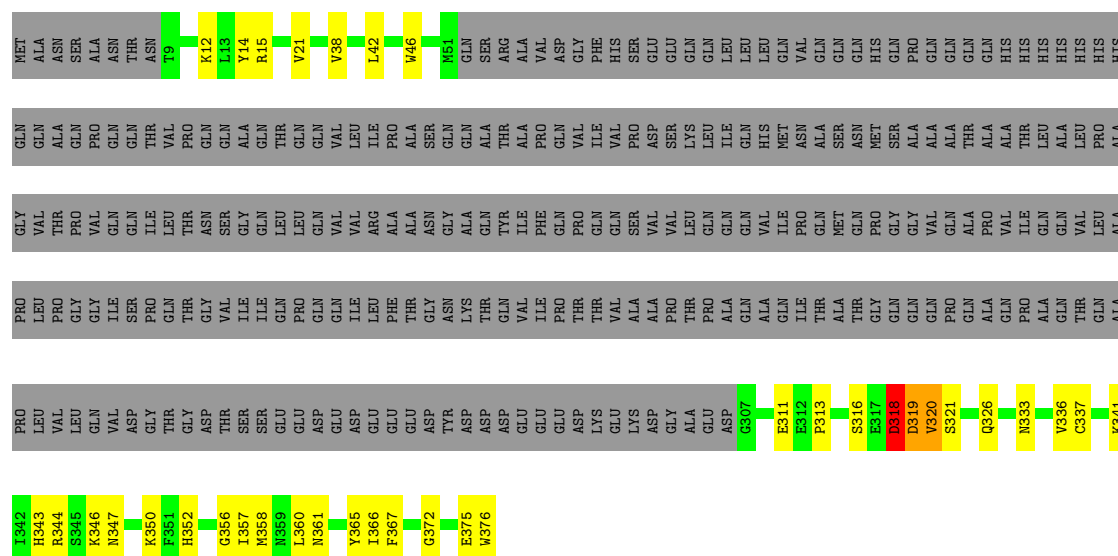


- Molecule 13: Transcription initiation factor IIB



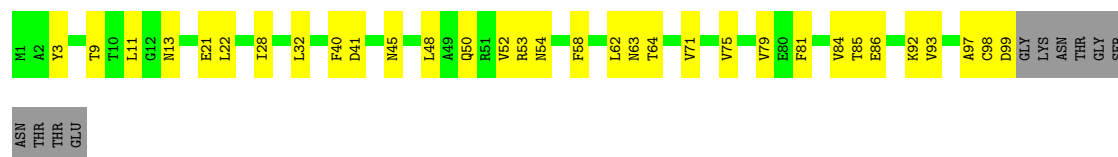
- Molecule 14: Transcription initiation factor IIA subunit 1

Chain N:  20% 9% 70%

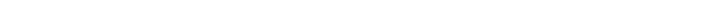


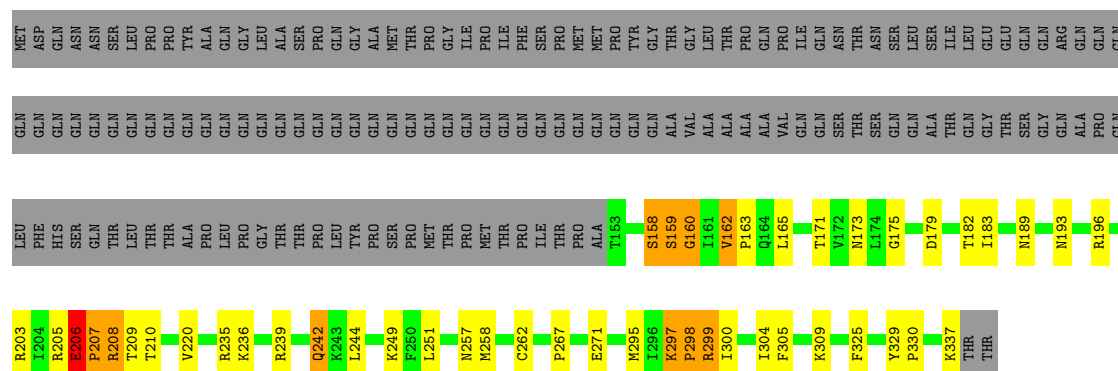
- Molecule 15: Transcription initiation factor IIA subunit 2

Chain 0: 61% 29% 9%

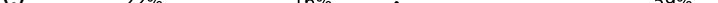


- Molecule 16: TATA-box-binding protein

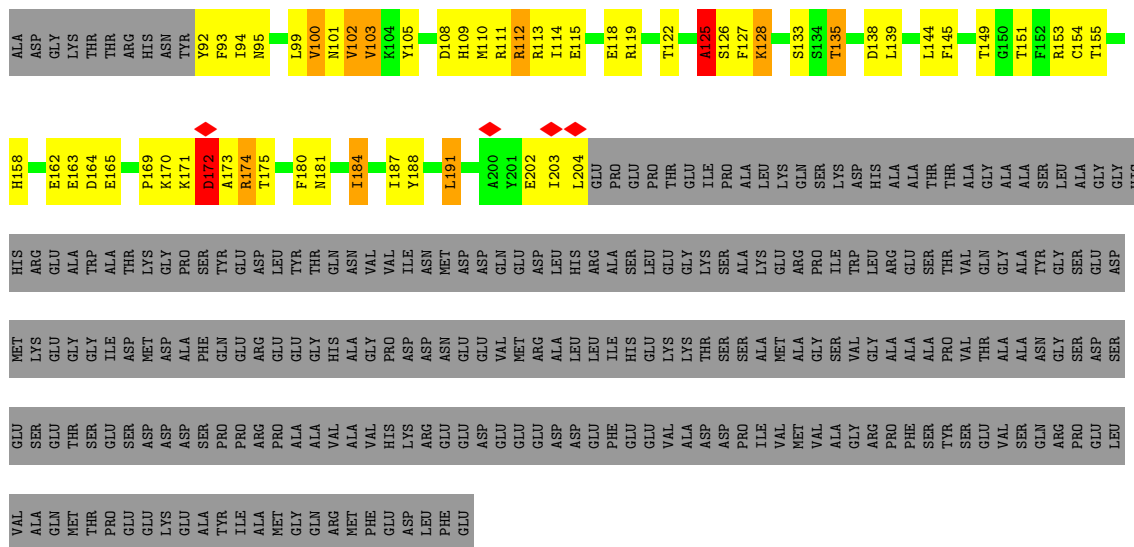
Chain P:  41% 11% . 45%



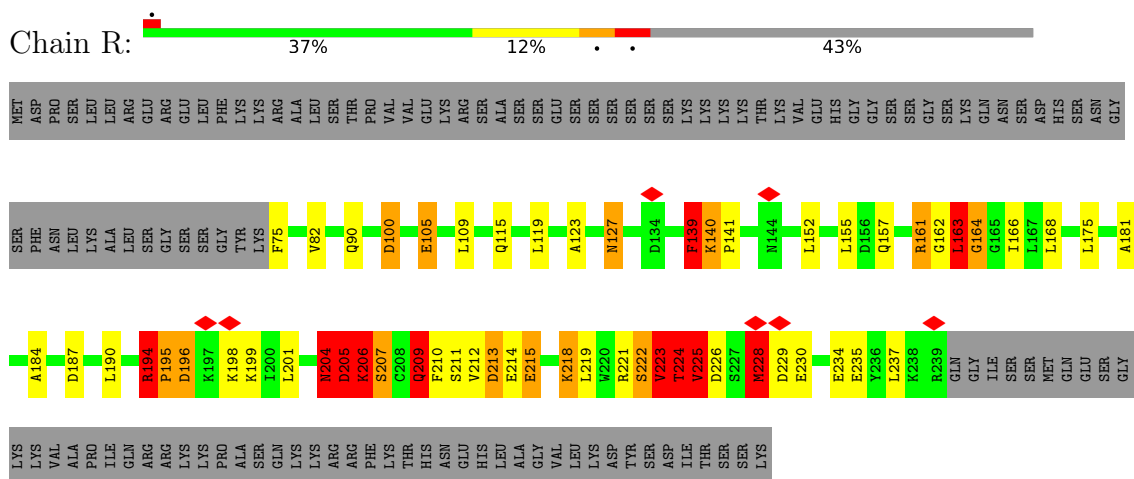
- Molecule 17: General transcription factor IIE subunit 1

Chain Q:  22% 16% 59%

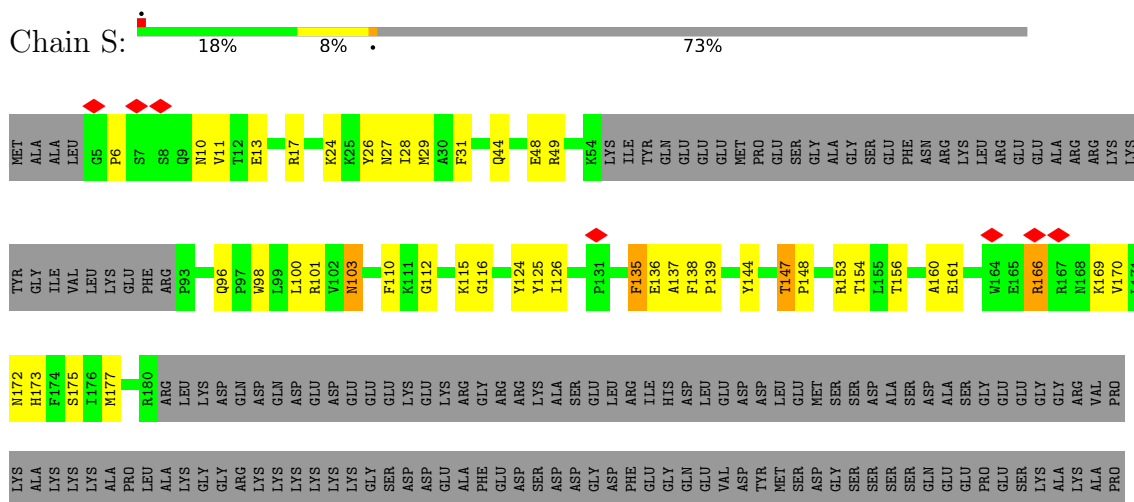


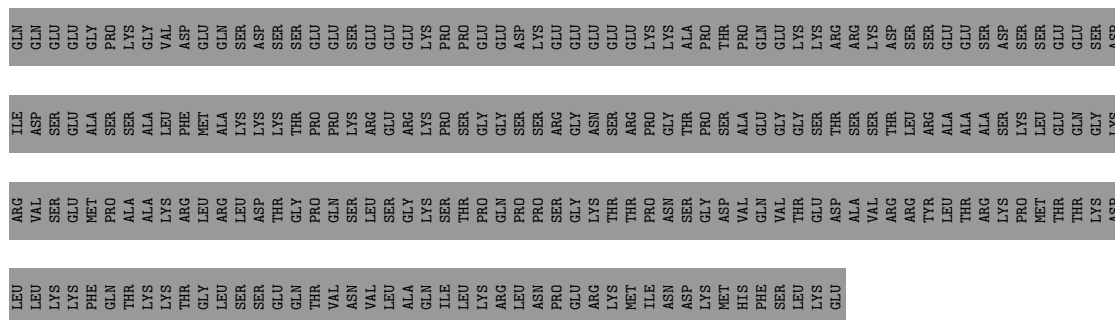


- Molecule 18: Transcription initiation factor IIE subunit beta

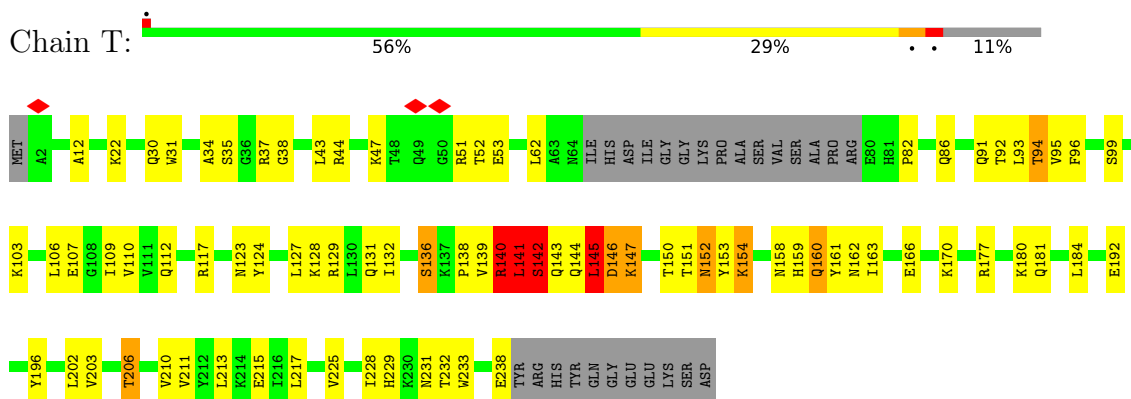


- Molecule 19: General transcription factor IIF subunit 1

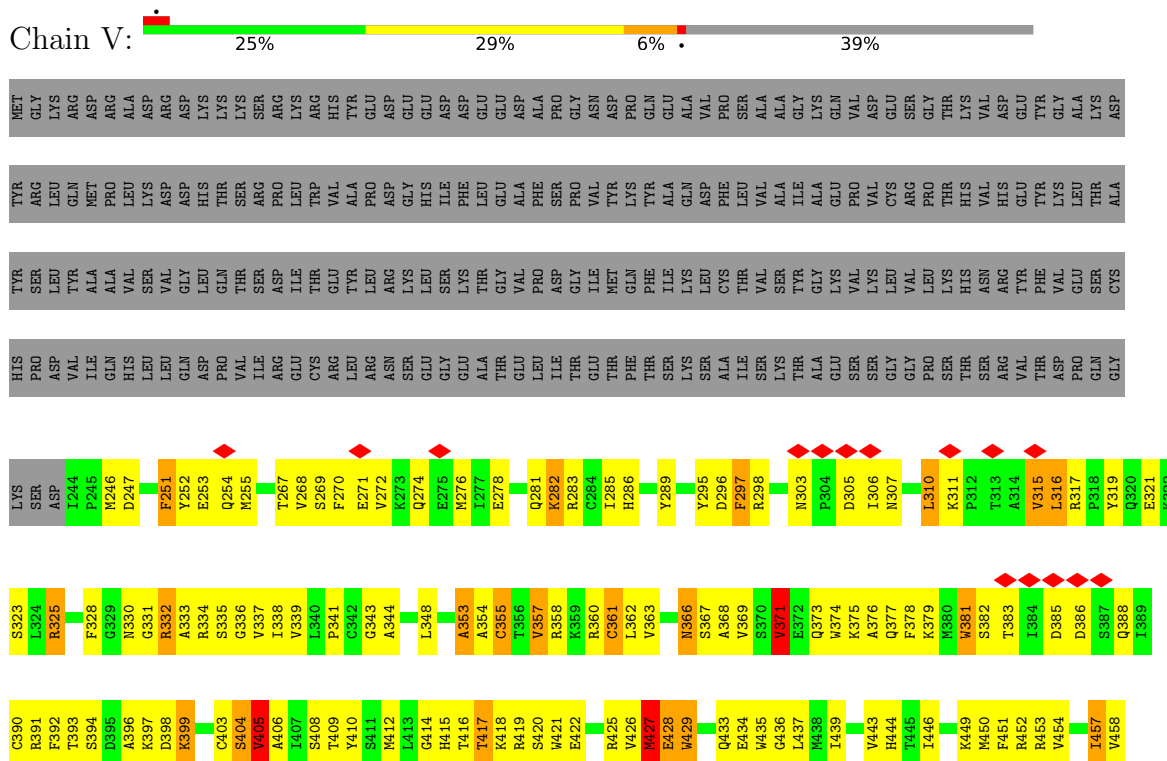


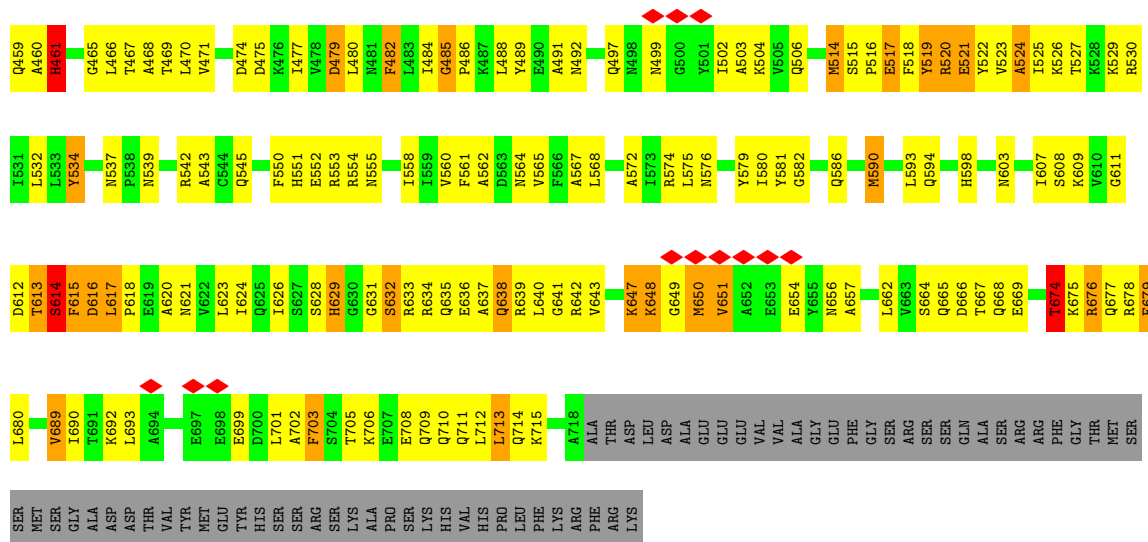


- Molecule 20: General transcription factor IIF subunit 2

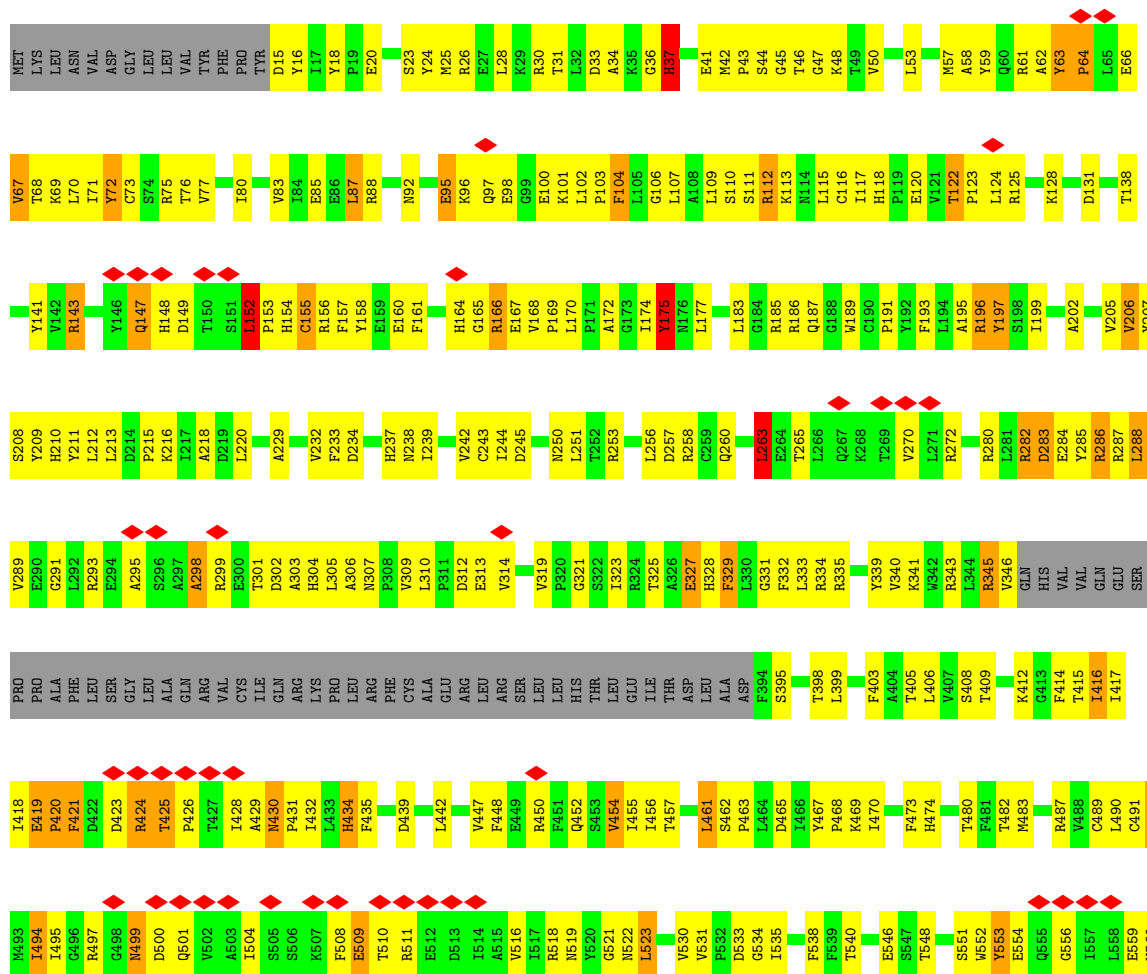


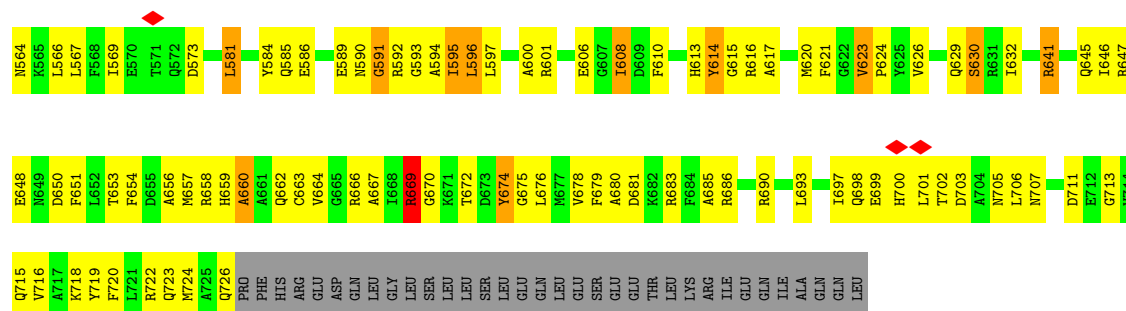
- Molecule 21: TFIIH basal transcription factor complex helicase XPB subunit



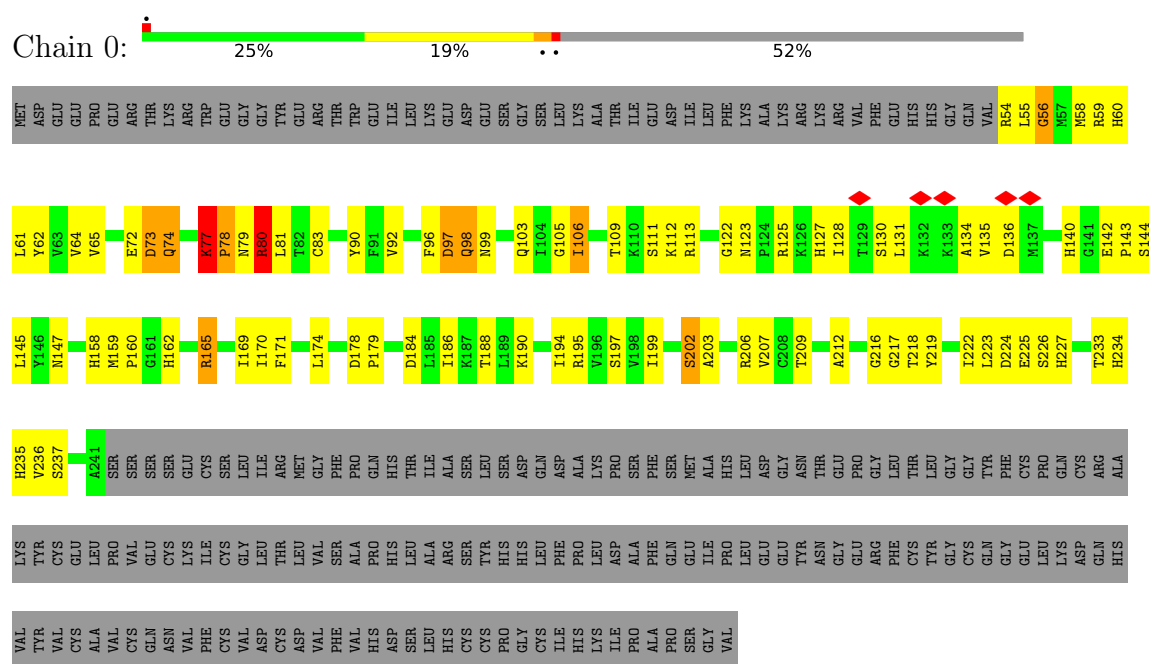


• Molecule 22: TFIIF basal transcription factor complex helicase XPD subunit

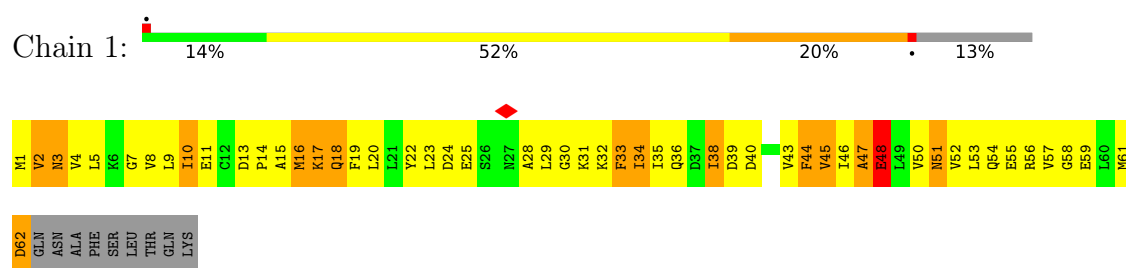




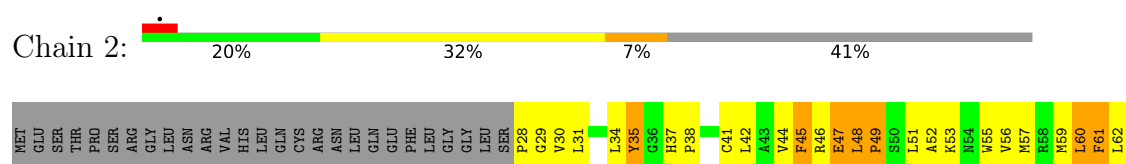
• Molecule 23: General transcription factor IIH subunit 2



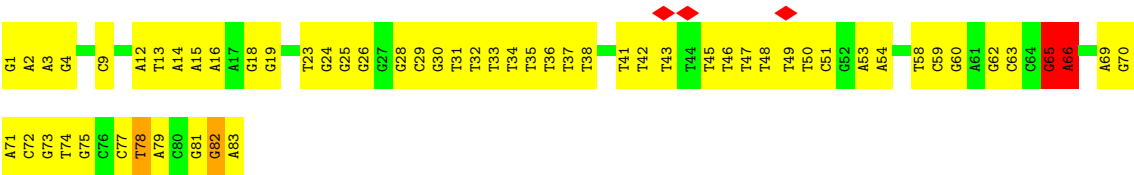
• Molecule 24: General transcription factor IIH subunit 5



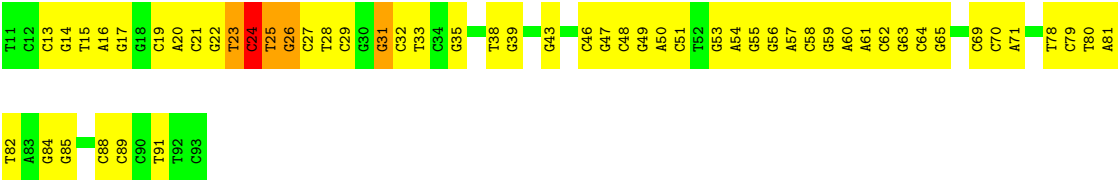
• Molecule 25: General transcription factor IIH subunit 4



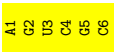
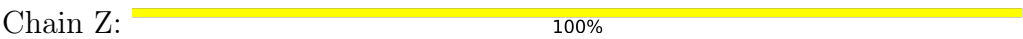




● Molecule 28: SCP-Y



● Molecule 29: RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91642	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	0.276	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	503.03998, 503.03998, 503.03998	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.62, 2.62, 2.62	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.74	4/11727 (0.0%)	1.21	95/15833 (0.6%)
2	B	0.85	1/9503 (0.0%)	1.26	61/12831 (0.5%)
3	C	0.74	0/2259	1.16	14/3073 (0.5%)
4	D	0.34	0/1077	0.91	2/1446 (0.1%)
5	E	0.55	0/1753	1.14	6/2368 (0.3%)
6	F	0.59	0/700	1.04	2/946 (0.2%)
7	G	0.41	0/1382	0.99	9/1874 (0.5%)
8	H	0.52	0/1227	0.98	2/1654 (0.1%)
9	I	0.43	0/1038	1.20	8/1407 (0.6%)
10	J	0.78	0/542	1.26	5/730 (0.7%)
11	K	0.66	0/956	1.08	6/1294 (0.5%)
12	L	0.65	0/394	1.10	2/524 (0.4%)
13	M	0.56	0/2429	1.18	20/3281 (0.6%)
14	N	0.31	0/945	0.93	2/1274 (0.2%)
15	O	0.38	0/816	0.88	0/1105
16	P	0.41	0/1489	1.00	5/2005 (0.2%)
17	Q	0.41	0/1507	1.03	5/2023 (0.2%)
18	R	0.90	4/1380 (0.3%)	1.53	18/1854 (1.0%)
19	S	0.34	0/1167	0.84	3/1576 (0.2%)
20	T	0.38	0/1817	1.05	10/2445 (0.4%)
21	V	1.92	81/3931 (2.1%)	2.37	254/5298 (4.8%)
22	W	2.05	130/5460 (2.4%)	2.43	354/7390 (4.8%)
23	0	2.08	32/1506 (2.1%)	2.31	71/2038 (3.5%)
24	1	1.30	1/496 (0.2%)	1.80	13/669 (1.9%)
25	2	1.23	0/2243	1.70	38/3024 (1.3%)
26	3	1.28	0/1548	1.56	15/2090 (0.7%)
27	X	0.65	2/1917 (0.1%)	1.04	14/2962 (0.5%)
28	Y	0.66	2/1880 (0.1%)	1.05	23/2896 (0.8%)
29	Z	0.19	0/139	0.32	0/215
All	All	1.07	257/63228 (0.4%)	1.47	1057/86125 (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	2
8	H	0	1
15	O	0	1
16	P	0	1
17	Q	0	2
18	R	0	20
20	T	0	1
21	V	0	16
22	W	0	18
23	0	0	2
24	1	0	1
25	2	0	8
27	X	0	3
28	Y	0	3
All	All	0	79

All (257) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	206	LYS	CA-C	11.31	1.67	1.53
23	0	142	GLU	N-CA	-10.03	1.37	1.45
23	0	158	HIS	CA-C	9.99	1.65	1.52
23	0	99	ASN	CA-CB	9.65	1.63	1.53
22	W	465	ASP	CA-C	9.09	1.64	1.52
18	R	205	ASP	CA-C	9.08	1.66	1.53
21	V	590	MET	CA-C	8.86	1.64	1.52
21	V	376	ALA	CA-C	8.67	1.63	1.52
18	R	206	LYS	N-CA	8.66	1.57	1.46
23	0	122	GLY	N-CA	8.55	1.55	1.45
28	Y	25	DT	O3'-P	8.48	1.73	1.61
21	V	255	MET	N-CA	8.44	1.54	1.47
18	R	205	ASP	N-CA	8.44	1.57	1.46
23	0	142	GLU	CA-C	8.37	1.60	1.52
22	W	237	HIS	CE1-NE2	8.30	1.40	1.32
21	V	374	TRP	CA-CB	8.20	1.66	1.53
23	0	235	HIS	CE1-NE2	7.92	1.40	1.32
22	W	670	GLY	CA-C	7.73	1.59	1.52
23	0	135	VAL	N-CA	7.70	1.55	1.46
23	0	186	ILE	N-CA	7.67	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	302	ASP	CA-C	7.65	1.62	1.53
21	V	289	TYR	N-CA	7.65	1.54	1.46
22	W	606	GLU	CA-CB	7.55	1.65	1.53
21	V	554	ARG	NE-CZ	7.33	1.41	1.33
21	V	391	ARG	CZ-NH2	-7.30	1.24	1.33
22	W	168	VAL	CA-CB	7.28	1.58	1.54
23	O	112	LYS	N-CA	7.27	1.56	1.46
22	W	566	LEU	CA-C	7.26	1.61	1.52
28	Y	31	DG	O3'-P	-7.22	1.50	1.61
22	W	556	GLY	N-CA	7.19	1.52	1.45
21	V	417	THR	CA-C	7.18	1.62	1.52
23	O	203	ALA	CA-C	7.18	1.61	1.52
22	W	521	GLY	N-CA	7.17	1.55	1.45
22	W	706	LEU	CA-C	7.15	1.62	1.52
23	O	169	ILE	CA-CB	7.14	1.63	1.54
21	V	626	ILE	N-CA	7.07	1.55	1.46
22	W	272	ARG	CA-CB	7.06	1.64	1.53
22	W	327	GLU	CA-C	7.00	1.61	1.52
22	W	546	GLU	C-N	6.97	1.43	1.33
21	V	676	ARG	N-CA	6.90	1.54	1.46
22	W	531	VAL	C-N	6.85	1.39	1.33
22	W	272	ARG	N-CA	6.79	1.54	1.45
22	W	615	GLY	N-CA	6.74	1.52	1.44
22	W	429	ALA	CA-C	6.71	1.61	1.52
22	W	474	HIS	CD2-NE2	-6.67	1.30	1.37
21	V	353	ALA	C-N	6.66	1.42	1.33
22	W	698	GLN	N-CA	6.65	1.54	1.46
23	O	188	THR	N-CA	6.65	1.54	1.46
2	B	939	HIS	CA-C	-6.60	1.45	1.53
21	V	706	LYS	N-CA	-6.60	1.38	1.46
22	W	115	LEU	N-CA	6.59	1.54	1.46
22	W	683	ARG	CZ-NH2	-6.58	1.24	1.33
22	W	674	TYR	N-CA	6.58	1.54	1.45
21	V	425	ARG	C-O	-6.57	1.16	1.24
21	V	382	SER	N-CA	6.55	1.54	1.46
22	W	494	ILE	C-O	-6.54	1.17	1.24
23	O	171	PHE	CA-C	6.52	1.60	1.52
22	W	321	GLY	N-CA	6.51	1.54	1.45
22	W	522	ASN	CA-C	6.50	1.61	1.52
23	O	96	PHE	CA-C	6.45	1.61	1.52
23	O	202	SER	CA-C	6.45	1.62	1.53
21	V	414	GLY	CA-C	6.41	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	712	LEU	CA-C	6.40	1.61	1.52
1	A	1291	ASN	CA-CB	6.39	1.63	1.53
21	V	348	LEU	C-O	-6.39	1.16	1.24
22	W	291	GLY	CA-C	6.38	1.59	1.52
21	V	453	ARG	CZ-NH2	-6.34	1.25	1.33
22	W	245	ASP	N-CA	6.32	1.53	1.46
22	W	265	THR	N-CA	6.27	1.54	1.46
22	W	301	THR	N-CA	6.27	1.54	1.45
21	V	479	ASP	N-CA	-6.27	1.38	1.46
22	W	523	LEU	N-CA	6.24	1.53	1.46
22	W	47	GLY	N-CA	6.20	1.54	1.45
21	V	618	PRO	C-O	6.18	1.31	1.23
22	W	693	LEU	CA-CB	6.18	1.61	1.54
22	W	490	LEU	CA-C	6.18	1.59	1.52
23	O	142	GLU	CA-CB	-6.16	1.46	1.54
22	W	158	TYR	N-CA	6.16	1.54	1.46
21	V	252	TYR	CA-CB	6.16	1.62	1.53
23	O	128	ILE	CA-C	6.15	1.60	1.52
22	W	432	ILE	CA-CB	6.14	1.62	1.54
22	W	608	ILE	CA-CB	6.13	1.63	1.54
22	W	685	ALA	N-CA	6.13	1.53	1.46
21	V	332	ARG	CA-C	6.13	1.60	1.52
22	W	67	VAL	N-CA	6.10	1.53	1.46
22	W	69	LYS	CA-C	6.09	1.60	1.52
21	V	609	LYS	N-CA	6.08	1.54	1.46
23	O	199	ILE	C-N	6.07	1.41	1.33
22	W	18	TYR	CA-CB	6.05	1.62	1.53
22	W	511	ARG	NE-CZ	-6.03	1.26	1.33
21	V	647	LYS	CA-C	6.00	1.60	1.52
21	V	383	THR	CB-OG1	-6.00	1.34	1.43
22	W	559	GLU	C-O	-6.00	1.16	1.23
22	W	701	LEU	N-CA	6.00	1.54	1.46
22	W	491	CYS	N-CA	5.97	1.52	1.46
21	V	620	ALA	N-CA	5.97	1.54	1.46
22	W	698	GLN	CA-C	5.97	1.60	1.52
22	W	83	VAL	CA-C	5.96	1.60	1.52
23	O	171	PHE	N-CA	-5.94	1.39	1.46
21	V	306	ILE	N-CA	-5.93	1.39	1.46
22	W	244	ILE	CA-CB	5.93	1.61	1.54
22	W	632	ILE	N-CA	5.93	1.53	1.46
22	W	492	PRO	CA-C	5.92	1.59	1.52
21	V	286	HIS	N-CA	5.92	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	325	ARG	CZ-NH1	-5.91	1.24	1.32
21	V	633	ARG	CZ-NH1	-5.91	1.24	1.32
21	V	551	HIS	CA-C	5.87	1.60	1.52
21	V	468	ALA	N-CA	5.87	1.53	1.46
21	V	269	SER	N-CA	5.87	1.53	1.46
21	V	638	GLN	N-CA	5.86	1.53	1.46
21	V	286	HIS	CB-CG	5.85	1.58	1.50
22	W	242	VAL	N-CA	5.84	1.53	1.46
22	W	648	GLU	C-N	5.84	1.41	1.33
22	W	508	PHE	CA-CB	5.82	1.57	1.53
22	W	705	ASN	C-O	-5.80	1.16	1.24
22	W	106	GLY	CA-C	5.80	1.56	1.51
1	A	484	LEU	CA-C	-5.79	1.45	1.52
21	V	534	TYR	N-CA	5.76	1.53	1.46
22	W	666	ARG	NE-CZ	-5.76	1.26	1.33
21	V	690	ILE	CA-CB	5.75	1.61	1.54
22	W	448	PHE	CA-C	5.74	1.60	1.52
23	0	162	HIS	CA-C	5.74	1.60	1.52
22	W	237	HIS	CA-C	5.74	1.60	1.52
22	W	152	LEU	N-CA	5.73	1.54	1.46
22	W	703	ASP	CA-C	5.73	1.60	1.53
23	0	207	VAL	CA-CB	5.72	1.61	1.54
22	W	42	MET	CA-C	5.72	1.60	1.52
22	W	343	ARG	CA-C	5.72	1.60	1.52
21	V	437	LEU	C-N	5.71	1.41	1.33
23	0	147	ASN	CA-C	5.68	1.60	1.52
22	W	160	GLU	CA-C	5.68	1.60	1.52
22	W	256	LEU	C-N	-5.67	1.26	1.33
21	V	452	ARG	CZ-NH2	-5.66	1.26	1.33
1	A	1290	SER	C-O	5.66	1.30	1.24
21	V	332	ARG	CZ-NH2	-5.65	1.26	1.33
21	V	657	ALA	CA-C	5.65	1.59	1.52
22	W	286	ARG	CZ-NH2	-5.64	1.26	1.33
22	W	645	GLN	N-CA	5.63	1.53	1.46
21	V	461	HIS	CG-CD2	5.61	1.42	1.35
24	1	47	ALA	CA-C	-5.61	1.48	1.53
22	W	334	ARG	CZ-NH2	-5.59	1.26	1.33
21	V	629	HIS	CE1-NE2	5.59	1.38	1.32
23	0	190	LYS	N-CA	5.58	1.53	1.46
22	W	283	ASP	CA-CB	5.57	1.61	1.53
22	W	155	CYS	C-N	5.57	1.43	1.34
22	W	291	GLY	C-N	5.57	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	474	ASP	N-CA	5.56	1.53	1.46
21	V	639	ARG	N-CA	5.56	1.53	1.46
21	V	252	TYR	C-N	5.55	1.41	1.33
1	A	806	THR	CA-CB	-5.55	1.45	1.53
21	V	640	LEU	CA-C	5.55	1.60	1.52
21	V	392	PHE	C-N	5.55	1.38	1.33
22	W	663	CYS	N-CA	-5.54	1.39	1.46
22	W	600	ALA	N-CA	5.53	1.53	1.46
22	W	331	GLY	N-CA	-5.52	1.39	1.45
21	V	415	HIS	CD2-NE2	5.51	1.44	1.37
21	V	565	VAL	N-CA	5.51	1.53	1.46
21	V	323	SER	CA-C	5.50	1.59	1.52
23	0	131	LEU	CA-C	5.50	1.60	1.52
22	W	552	TRP	C-O	-5.47	1.17	1.24
21	V	310	LEU	CA-C	5.46	1.60	1.52
23	0	195	ARG	CA-CB	5.46	1.61	1.53
21	V	705	THR	CB-OG1	-5.45	1.35	1.43
22	W	110	SER	CA-CB	5.44	1.63	1.53
21	V	560	VAL	N-CA	-5.44	1.39	1.46
21	V	626	ILE	CB-CG1	5.42	1.64	1.53
22	W	405	THR	N-CA	5.41	1.52	1.46
22	W	229	ALA	N-CA	5.39	1.52	1.46
22	W	693	LEU	N-CA	5.38	1.51	1.45
22	W	185	ARG	CA-CB	5.38	1.62	1.53
21	V	332	ARG	NE-CZ	-5.37	1.27	1.33
22	W	630	SER	CA-C	5.37	1.59	1.52
23	0	136	ASP	N-CA	5.37	1.52	1.46
21	V	296	ASP	CA-C	5.36	1.59	1.52
22	W	518	ARG	CZ-NH2	-5.35	1.26	1.33
22	W	48	LYS	N-CA	5.33	1.52	1.46
22	W	77	VAL	CA-C	5.32	1.57	1.52
21	V	699	GLU	CA-C	5.32	1.59	1.52
22	W	85	GLU	CA-C	5.32	1.59	1.52
22	W	298	ALA	CA-C	5.31	1.59	1.52
22	W	592	ARG	CD-NE	5.30	1.53	1.46
22	W	412	LYS	N-CA	5.28	1.53	1.46
23	0	217	GLY	N-CA	5.28	1.53	1.45
27	X	71	DA	P-O5'	-5.28	1.49	1.60
21	V	386	ASP	N-CA	5.28	1.51	1.46
22	W	510	THR	CA-C	-5.28	1.45	1.52
21	V	692	LYS	CA-C	5.28	1.59	1.52
21	V	618	PRO	CA-CB	5.28	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	561	PHE	C-N	5.27	1.40	1.33
22	W	154	HIS	CA-CB	5.27	1.62	1.53
22	W	263	LEU	N-CA	5.27	1.52	1.46
23	0	97	ASP	N-CA	5.26	1.52	1.46
22	W	713	GLY	CA-C	5.25	1.57	1.52
22	W	95	GLU	CA-C	5.23	1.58	1.52
22	W	310	LEU	CA-CB	5.23	1.60	1.53
22	W	148	HIS	CE1-NE2	5.22	1.37	1.32
22	W	72	TYR	CA-C	5.22	1.59	1.52
21	V	636	GLU	N-CA	5.22	1.52	1.46
22	W	75	ARG	CZ-NH2	-5.21	1.26	1.33
22	W	341	LYS	CA-CB	5.21	1.61	1.53
22	W	548	THR	N-CA	5.20	1.52	1.46
22	W	426	PRO	CA-CB	-5.19	1.47	1.53
22	W	658	ARG	CZ-NH2	-5.18	1.26	1.33
23	0	140	HIS	ND1-CE1	5.18	1.37	1.32
21	V	303	ASN	C-N	5.18	1.37	1.33
27	X	66	DA	C1'-N9	5.18	1.56	1.46
21	V	693	LEU	CA-C	5.17	1.59	1.53
23	0	197	SER	N-CA	-5.17	1.39	1.46
22	W	122	THR	CA-C	5.17	1.58	1.52
21	V	398	ASP	N-CA	5.16	1.52	1.45
22	W	96	LYS	N-CA	5.16	1.52	1.46
22	W	482	THR	N-CA	5.16	1.52	1.46
21	V	420	SER	N-CA	5.16	1.52	1.46
22	W	66	GLU	N-CA	5.16	1.53	1.46
22	W	672	THR	N-CA	5.16	1.52	1.46
21	V	316	LEU	CA-CB	5.15	1.61	1.53
21	V	410	TYR	N-CA	5.15	1.52	1.46
22	W	675	GLY	N-CA	5.14	1.52	1.45
21	V	598	HIS	CB-CG	5.14	1.57	1.50
22	W	257	ASP	CA-C	5.14	1.59	1.52
22	W	501	GLN	CA-C	5.14	1.59	1.52
22	W	567	LEU	N-CA	-5.13	1.40	1.45
21	V	607	ILE	C-O	-5.12	1.18	1.24
22	W	398	THR	CB-OG1	-5.12	1.35	1.43
21	V	623	LEU	C-O	-5.12	1.18	1.24
21	V	617	LEU	N-CA	5.12	1.51	1.45
21	V	408	SER	CA-C	-5.11	1.46	1.52
22	W	491	CYS	CA-C	5.11	1.58	1.53
22	W	30	ARG	N-CA	5.11	1.52	1.46
23	0	195	ARG	CZ-NH1	-5.11	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	532	LEU	CA-CB	5.11	1.61	1.53
22	W	303	ALA	CA-C	5.11	1.59	1.52
22	W	452	GLN	CA-CB	5.11	1.61	1.53
22	W	699	GLU	N-CA	5.11	1.52	1.46
21	V	521	GLU	CA-CB	5.10	1.61	1.53
22	W	210	HIS	CE1-NE2	5.09	1.37	1.32
22	W	418	ILE	N-CA	5.09	1.52	1.46
22	W	328	HIS	ND1-CE1	5.08	1.37	1.32
22	W	104	PHE	CG-CD1	5.08	1.49	1.38
21	V	367	SER	N-CA	-5.08	1.39	1.46
22	W	651	PHE	N-CA	-5.08	1.40	1.46
22	W	185	ARG	NE-CZ	-5.07	1.27	1.33
23	O	61	LEU	N-CA	5.07	1.52	1.46
22	W	626	VAL	N-CA	5.07	1.52	1.46
22	W	679	PHE	CA-CB	5.07	1.62	1.53
22	W	61	ARG	CA-C	5.06	1.59	1.52
21	V	420	SER	CA-C	-5.06	1.46	1.52
22	W	531	VAL	C-O	-5.05	1.18	1.24
22	W	286	ARG	CZ-NH1	-5.05	1.25	1.32
22	W	20	GLU	C-N	-5.04	1.27	1.33
22	W	168	VAL	N-CA	5.04	1.52	1.46
21	V	338	ILE	CA-C	5.03	1.58	1.52
22	W	335	ARG	CA-C	-5.03	1.46	1.52
22	W	417	ILE	CA-C	-5.03	1.46	1.52
22	W	629	GLN	N-CA	-5.02	1.39	1.46
21	V	633	ARG	N-CA	5.02	1.52	1.46
21	V	333	ALA	CA-C	-5.00	1.45	1.52

All (1057) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	84	HIS	C-N-CD	-16.35	57.95	125.00
13	M	94	ASP	N-CA-C	-15.28	90.41	114.09
18	R	206	LYS	N-CA-C	15.18	128.07	107.73
2	B	882	SER	N-CA-C	-14.44	91.01	111.81
1	A	413	TYR	CA-C-N	-13.85	106.70	120.83
1	A	413	TYR	C-N-CA	-13.85	106.70	120.83
27	X	62	DG	O3'-P-O5'	-13.52	83.72	104.00
5	E	52	ARG	C-N-CD	-13.23	70.76	125.00
28	Y	31	DG	O3'-P-O5'	13.09	123.63	104.00
23	O	77	LYS	C-N-CD	-12.96	71.87	125.00
26	3	71	TYR	C-N-CD	-12.22	74.91	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	622	SER	C-N-CD	-12.16	75.13	125.00
18	R	162	GLY	N-CA-C	11.95	127.11	110.74
21	V	520	ARG	O-C-N	11.70	135.56	122.11
9	I	61	GLU	N-CA-C	-11.68	99.40	112.72
22	W	26	ARG	NE-CZ-NH2	11.64	129.67	119.20
21	V	520	ARG	CA-C-N	-11.51	100.90	120.58
21	V	520	ARG	C-N-CA	-11.51	100.90	120.58
25	2	236	PHE	CA-CB-CG	-11.13	102.67	113.80
21	V	550	PHE	CA-CB-CG	11.08	124.88	113.80
21	V	358	ARG	NE-CZ-NH2	11.07	129.16	119.20
22	W	335	ARG	NE-CZ-NH1	-11.01	110.49	121.50
16	P	159	SER	N-CA-C	-10.87	100.25	113.19
18	R	205	ASP	N-CA-C	10.72	126.38	109.65
21	V	270	PHE	CA-CB-CG	10.61	124.41	113.80
18	R	194	ARG	C-N-CD	-10.60	81.55	125.00
9	I	103	ARG	N-CA-C	-10.53	88.38	110.80
22	W	167	GLU	CA-C-N	10.48	128.71	120.33
22	W	167	GLU	C-N-CA	10.48	128.71	120.33
20	T	141	LEU	N-CA-C	-10.46	88.52	110.80
22	W	287	ARG	NE-CZ-NH2	9.89	128.10	119.20
22	W	26	ARG	NH1-CZ-NH2	-9.82	106.54	119.30
3	C	137	ASN	N-CA-C	-9.79	97.71	111.81
22	W	117	ILE	N-CA-C	9.75	119.69	110.53
21	V	586	GLN	OE1-CD-NE2	-9.74	112.86	122.60
21	V	638	GLN	OE1-CD-NE2	-9.62	112.98	122.60
24	1	44	PHE	CA-CB-CG	-9.61	104.19	113.80
22	W	645	GLN	OE1-CD-NE2	-9.55	113.05	122.60
21	V	388	GLN	OE1-CD-NE2	-9.51	113.09	122.60
22	W	147	GLN	OE1-CD-NE2	-9.44	113.16	122.60
21	V	621	ASN	CA-CB-CG	9.43	122.03	112.60
21	V	634	ARG	NE-CZ-NH2	9.38	127.64	119.20
21	V	377	GLN	OE1-CD-NE2	-9.36	113.24	122.60
21	V	444	HIS	CB-CG-CD2	-9.33	119.06	131.20
10	J	65	LEU	N-CA-C	-9.12	102.30	113.15
22	W	335	ARG	NE-CZ-NH2	9.11	127.40	119.20
26	3	231	PHE	CA-CB-CG	-9.09	104.71	113.80
1	A	211	GLU	N-CA-C	-8.98	100.65	111.69
21	V	668	GLN	OE1-CD-NE2	-8.98	113.62	122.60
21	V	334	ARG	CD-NE-CZ	8.96	136.94	124.40
22	W	530	VAL	N-CA-CB	8.96	120.77	110.65
21	V	421	TRP	CD2-CE3-CZ3	8.94	130.23	118.60
25	2	61	PHE	CB-CA-C	-8.92	97.12	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	492	ASP	N-CA-C	8.91	124.30	111.56
27	X	65	DG	C4'-C3'-O3'	8.90	123.35	110.00
22	W	270	VAL	CA-C-O	8.81	131.80	120.78
22	W	112	ARG	CA-C-N	8.77	132.03	120.28
22	W	112	ARG	C-N-CA	8.77	132.03	120.28
21	V	665	GLN	OE1-CD-NE2	-8.76	113.84	122.60
1	A	1314	THR	N-CA-C	-8.75	103.19	114.04
22	W	76	THR	CA-CB-OG1	8.74	122.72	109.60
24	1	34	ILE	CA-C-N	-8.71	111.79	123.12
24	1	34	ILE	C-N-CA	-8.71	111.79	123.12
9	I	15	ARG	N-CA-C	-8.69	92.30	110.80
22	W	332	PHE	CA-CB-CG	8.68	122.48	113.80
28	Y	14	DG	O4'-C1'-N9	8.66	121.39	108.40
2	B	80	GLU	CA-C-N	-8.62	111.50	120.38
2	B	80	GLU	C-N-CA	-8.62	111.50	120.38
25	2	268	PHE	CA-CB-CG	-8.61	105.19	113.80
22	W	343	ARG	NE-CZ-NH2	8.57	126.91	119.20
24	1	47	ALA	CB-CA-C	-8.54	106.72	116.54
22	W	469	LYS	CA-C-N	8.52	131.46	120.56
22	W	469	LYS	C-N-CA	8.52	131.46	120.56
2	B	588	ARG	CB-CG-CD	-8.50	91.75	111.30
1	A	601	ASN	N-CA-C	8.49	122.48	107.80
21	V	484	ILE	N-CA-C	8.47	119.09	111.81
1	A	614	ASP	CA-C-N	-8.44	108.27	122.11
1	A	614	ASP	C-N-CA	-8.44	108.27	122.11
22	W	263	LEU	N-CA-CB	-8.41	97.75	110.12
12	L	26	ASN	N-CA-C	-8.40	101.36	111.69
22	W	193	PHE	CA-CB-CG	8.34	122.14	113.80
22	W	77	VAL	N-CA-CB	-8.32	105.26	110.50
2	B	880	LEU	N-CA-C	8.31	128.51	110.80
13	M	43	ASP	N-CA-C	-8.30	93.12	110.80
22	W	157	PHE	CA-CB-CG	8.27	122.07	113.80
2	B	1008	VAL	N-CA-C	8.16	118.20	110.53
22	W	521	GLY	CA-C-N	8.15	131.03	120.44
22	W	521	GLY	C-N-CA	8.15	131.03	120.44
27	X	66	DA	P-O5'-C5'	8.14	132.22	120.00
22	W	106	GLY	CA-C-O	-8.13	114.50	121.57
21	V	392	PHE	CA-CB-CG	8.12	121.92	113.80
25	2	47	GLU	N-CA-C	8.12	120.04	111.03
21	V	433	GLN	N-CA-C	8.08	121.70	112.57
22	W	667	ALA	N-CA-C	8.04	119.67	111.07
22	W	697	ILE	N-CA-C	8.03	120.98	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	148	HIS	CE1-NE2-CD2	-8.02	100.98	109.00
22	W	700	HIS	CB-CG-CD2	-7.96	120.85	131.20
20	T	140	ARG	N-CA-C	7.93	122.93	110.32
1	A	672	ILE	N-CA-C	7.92	118.70	110.62
2	B	62	ALA	CA-C-N	-7.91	112.23	120.38
2	B	62	ALA	C-N-CA	-7.91	112.23	120.38
22	W	395	SER	CA-C-O	-7.91	110.67	118.34
21	V	421	TRP	CE2-CD2-CE3	-7.89	110.91	118.80
21	V	394	SER	N-CA-C	7.89	122.00	112.38
21	V	333	ALA	N-CA-C	7.88	121.83	111.75
16	P	162	VAL	CA-C-N	7.85	127.91	119.90
16	P	162	VAL	C-N-CA	7.85	127.91	119.90
1	A	150	GLY	N-CA-C	7.85	123.89	113.37
7	G	46	ILE	N-CA-C	7.85	117.91	110.53
22	W	345	ARG	N-CA-C	7.84	122.19	112.47
25	2	160	LEU	N-CA-C	-7.83	102.75	111.28
2	B	80	GLU	N-CA-C	7.81	127.06	109.81
1	A	744	ILE	N-CA-C	7.80	117.91	110.42
22	W	16	TYR	N-CA-C	7.80	118.28	108.45
13	M	51	GLU	N-CA-C	7.79	119.78	111.28
21	V	415	HIS	CG-CD2-NE2	-7.79	99.41	107.20
22	W	499	ASN	OD1-CG-ND2	-7.76	114.84	122.60
1	A	1385	VAL	N-CA-C	7.73	118.50	110.62
1	A	1483	GLY	N-CA-C	7.72	122.65	112.77
1	A	476	ILE	N-CA-C	7.68	118.90	109.30
22	W	724	MET	CA-C-N	7.66	130.54	120.28
22	W	724	MET	C-N-CA	7.66	130.54	120.28
21	V	640	LEU	O-C-N	7.65	130.27	122.08
9	I	84	HIS	N-CA-C	7.65	126.72	109.81
25	2	162	PHE	CA-CB-CG	-7.64	106.16	113.80
21	V	710	GLN	CA-C-N	7.62	130.35	120.44
21	V	710	GLN	C-N-CA	7.62	130.35	120.44
22	W	497	ARG	CD-NE-CZ	7.61	135.06	124.40
27	X	78	DT	N1-C1'-C2'	7.59	124.89	113.50
21	V	422	GLU	CA-C-O	7.59	128.82	119.11
22	W	304	HIS	CB-CG-CD2	-7.59	121.33	131.20
22	W	700	HIS	ND1-CG-CD2	7.59	113.69	106.10
23	0	237	SER	CA-C-N	7.58	128.19	120.38
23	0	237	SER	C-N-CA	7.58	128.19	120.38
26	3	182	PHE	CA-CB-CG	-7.57	106.23	113.80
20	T	142	SER	N-CA-C	7.56	126.90	110.80
22	W	295	ALA	N-CA-C	7.55	119.29	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	428	GLU	N-CA-C	7.52	120.81	107.80
22	W	329	PHE	CA-CB-CG	7.52	121.32	113.80
22	W	41	GLU	O-C-N	7.51	131.76	123.27
13	M	9	ALA	N-CA-C	7.50	122.62	111.81
1	A	932	ARG	CA-C-N	-7.50	106.95	121.58
1	A	932	ARG	C-N-CA	-7.50	106.95	121.58
22	W	250	ASN	OD1-CG-ND2	-7.49	115.11	122.60
26	3	127	GLN	N-CA-C	-7.48	103.20	111.36
21	V	355	CYS	CA-C-N	7.48	130.61	120.44
21	V	355	CYS	C-N-CA	7.48	130.61	120.44
22	W	509	GLU	N-CA-C	7.47	122.06	112.34
25	2	35	TYR	CA-CB-CG	-7.47	100.46	113.90
23	0	123	ASN	CA-C-N	7.44	127.46	119.28
23	0	123	ASN	C-N-CA	7.44	127.46	119.28
22	W	165	GLY	CA-C-N	7.43	130.85	120.29
22	W	165	GLY	C-N-CA	7.43	130.85	120.29
21	V	669	GLU	CA-C-N	7.42	131.59	120.31
21	V	669	GLU	C-N-CA	7.42	131.59	120.31
23	0	206	ARG	NH1-CZ-NH2	-7.41	109.67	119.30
25	2	245	LEU	N-CA-C	-7.41	101.30	110.41
2	B	223	SER	N-CA-C	7.36	120.31	110.88
23	0	98	GLN	OE1-CD-NE2	-7.36	115.24	122.60
26	3	16	ASP	CA-C-N	7.35	133.00	120.72
26	3	16	ASP	C-N-CA	7.35	133.00	120.72
22	W	487	ARG	N-CA-C	7.33	120.15	111.71
23	0	92	VAL	O-C-N	7.32	129.09	121.91
22	W	302	ASP	CA-C-O	7.31	126.76	119.08
28	Y	21	DC	C6-N1-C1'	7.31	130.66	119.70
23	0	165	ARG	NE-CZ-NH2	-7.29	112.64	119.20
22	W	654	PHE	CA-C-N	7.25	130.00	120.28
22	W	654	PHE	C-N-CA	7.25	130.00	120.28
9	I	86	CYS	N-CA-C	-7.22	99.19	109.96
2	B	294	ASP	CA-C-N	7.22	127.23	119.28
2	B	294	ASP	C-N-CA	7.22	127.23	119.28
21	V	580	ILE	CA-C-O	7.22	128.01	120.36
22	W	288	LEU	O-C-N	-7.21	114.53	122.03
22	W	683	ARG	NE-CZ-NH2	7.19	125.67	119.20
21	V	486	PRO	CA-C-N	7.18	132.68	121.99
21	V	486	PRO	C-N-CA	7.18	132.68	121.99
22	W	690	ARG	NE-CZ-NH2	7.16	125.64	119.20
13	M	93	PHE	N-CA-C	7.15	120.60	110.23
2	B	46	SER	N-CA-C	7.14	119.07	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	0	195	ARG	NE-CZ-NH1	7.14	128.64	121.50
22	W	323	ILE	CA-C-N	7.13	129.83	120.28
22	W	323	ILE	C-N-CA	7.13	129.83	120.28
22	W	24	TYR	N-CA-C	7.12	121.21	112.23
28	Y	21	DC	C2-N1-C1'	-7.12	109.02	119.70
21	V	598	HIS	CB-CG-CD2	-7.11	121.96	131.20
3	C	42	VAL	CA-C-N	-7.11	113.35	120.31
3	C	42	VAL	C-N-CA	-7.11	113.35	120.31
25	2	89	LEU	N-CA-C	-7.10	103.62	111.36
13	M	50	SER	CA-C-N	7.09	129.78	120.28
13	M	50	SER	C-N-CA	7.09	129.78	120.28
22	W	232	VAL	CA-CB-CG1	7.08	122.44	110.40
28	Y	29	DC	O5'-C5'-C4'	7.07	121.40	110.80
21	V	393	THR	O-C-N	-7.05	113.86	122.68
25	2	193	PRO	N-CA-C	7.05	119.30	110.70
21	V	267	THR	CA-C-O	-7.05	112.00	120.32
25	2	225	SER	N-CA-C	-7.04	103.54	111.14
3	C	136	ASP	N-CA-C	7.04	121.03	107.44
21	V	421	TRP	NE1-CE2-CD2	-7.04	98.25	107.40
22	W	653	THR	CA-C-N	7.04	129.71	120.28
22	W	653	THR	C-N-CA	7.04	129.71	120.28
22	W	419	GLU	C-N-CD	-7.03	96.17	125.00
27	X	82	DG	C4'-C3'-O3'	-6.97	99.54	110.00
22	W	340	VAL	CA-C-N	6.96	129.60	120.28
22	W	340	VAL	C-N-CA	6.96	129.60	120.28
23	0	147	ASN	OD1-CG-ND2	-6.95	115.65	122.60
22	W	343	ARG	NE-CZ-NH1	-6.93	114.57	121.50
21	V	558	ILE	N-CA-CB	-6.92	101.42	111.52
22	W	97	GLN	OE1-CD-NE2	-6.90	115.70	122.60
13	M	62	LYS	N-CA-C	-6.90	105.41	114.31
24	1	45	VAL	CA-C-N	-6.90	113.47	122.51
24	1	45	VAL	C-N-CA	-6.90	113.47	122.51
27	X	83	DA	O4'-C1'-N9	6.90	118.75	108.40
22	W	715	GLN	OE1-CD-NE2	-6.90	115.70	122.60
22	W	186	ARG	NE-CZ-NH1	6.89	128.39	121.50
22	W	98	GLU	CA-C-N	6.88	130.20	122.15
22	W	98	GLU	C-N-CA	6.88	130.20	122.15
21	V	274	GLN	O-C-N	-6.88	116.65	123.46
22	W	328	HIS	CB-CG-CD2	-6.87	122.27	131.20
21	V	444	HIS	CA-C-N	6.87	130.75	120.31
21	V	444	HIS	C-N-CA	6.87	130.75	120.31
22	W	462	SER	CA-C-N	6.86	126.55	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	462	SER	C-N-CA	6.86	126.55	119.82
21	V	715	LYS	N-CA-C	6.86	118.75	111.28
16	P	158	SER	N-CA-C	-6.84	102.31	111.96
22	W	562	GLN	OE1-CD-NE2	-6.84	115.76	122.60
25	2	193	PRO	CA-N-CD	-6.83	102.43	112.00
1	A	548	PHE	N-CA-C	6.82	118.79	111.36
23	0	145	LEU	N-CA-C	6.81	118.71	111.28
2	B	802	ASP	N-CA-C	6.81	118.35	111.07
21	V	348	LEU	CA-C-O	-6.80	113.34	120.55
21	V	641	GLY	N-CA-C	6.79	120.88	112.73
22	W	595	ILE	CB-CA-C	6.79	122.42	111.29
22	W	659	HIS	CA-CB-CG	6.79	120.59	113.80
22	W	66	GLU	CA-C-N	6.79	134.19	121.97
22	W	66	GLU	C-N-CA	6.79	134.19	121.97
22	W	703	ASP	N-CA-C	6.78	120.89	111.74
21	V	317	ARG	CA-C-O	-6.78	113.03	120.69
22	W	34	ALA	CA-C-N	6.77	132.43	122.82
22	W	34	ALA	C-N-CA	6.77	132.43	122.82
22	W	497	ARG	NE-CZ-NH1	6.77	128.27	121.50
22	W	473	PHE	CA-CB-CG	-6.76	107.04	113.80
14	N	319	ASP	N-CA-C	6.75	121.28	113.38
21	V	608	SER	O-C-N	-6.72	113.87	122.20
22	W	131	ASP	CA-C-N	6.72	127.44	119.98
22	W	131	ASP	C-N-CA	6.72	127.44	119.98
22	W	263	LEU	O-C-N	-6.72	115.00	122.12
22	W	270	VAL	CA-C-N	6.72	130.51	120.17
22	W	270	VAL	C-N-CA	6.72	130.51	120.17
13	M	251	ILE	N-CA-C	6.71	116.86	110.42
1	A	458	PHE	N-CA-CB	-6.71	99.15	110.83
1	A	1405	MET	N-CA-C	6.70	119.59	111.82
21	V	331	GLY	CA-C-N	6.69	129.25	120.28
21	V	331	GLY	C-N-CA	6.69	129.25	120.28
1	A	1199	MET	CA-C-N	6.69	128.20	119.84
1	A	1199	MET	C-N-CA	6.69	128.20	119.84
22	W	467	TYR	CA-C-N	6.68	126.63	119.28
22	W	467	TYR	C-N-CA	6.68	126.63	119.28
21	V	711	GLN	OE1-CD-NE2	-6.68	115.92	122.60
23	0	236	VAL	CA-CB-CG1	6.68	121.75	110.40
22	W	591	GLY	CA-C-O	-6.67	113.79	121.47
22	W	613	HIS	CA-C-N	6.67	129.21	120.28
22	W	613	HIS	C-N-CA	6.67	129.21	120.28
22	W	723	GLN	OE1-CD-NE2	-6.67	115.93	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	142	SER	CA-C-N	-6.66	111.97	121.83
20	T	142	SER	C-N-CA	-6.66	111.97	121.83
12	L	19	CYS	N-CA-C	6.65	118.43	110.19
23	0	64	VAL	O-C-N	-6.63	116.10	123.26
23	0	92	VAL	CA-C-O	-6.63	114.14	121.17
22	W	629	GLN	CA-C-O	-6.63	113.73	120.96
21	V	629	HIS	CB-CG-CD2	-6.62	122.59	131.20
22	W	540	THR	O-C-N	-6.62	114.13	122.27
21	V	598	HIS	CB-CG-ND1	6.62	132.63	122.70
17	Q	172	ASP	N-CA-C	6.61	124.88	110.80
1	A	133	SER	N-CA-C	6.61	124.88	110.80
23	0	59	ARG	NE-CZ-NH2	6.59	125.14	119.20
21	V	714	GLN	OE1-CD-NE2	-6.58	116.02	122.60
22	W	80	ILE	N-CA-CB	6.58	119.49	110.54
22	W	187	GLN	OE1-CD-NE2	-6.58	116.02	122.60
25	2	272	PHE	CA-CB-CG	-6.58	107.22	113.80
25	2	242	PHE	CA-CB-CG	-6.57	107.23	113.80
21	V	358	ARG	NH1-CZ-NH2	-6.57	110.76	119.30
21	V	374	TRP	O-C-N	-6.57	114.66	122.15
21	V	553	ARG	NE-CZ-NH2	6.56	125.10	119.20
22	W	120	GLU	CA-C-N	6.55	128.95	120.56
22	W	120	GLU	C-N-CA	6.55	128.95	120.56
21	V	701	LEU	O-C-N	-6.55	115.57	123.10
21	V	388	GLN	CG-CD-NE2	6.54	126.22	116.40
21	V	418	LYS	CA-C-O	-6.54	114.16	120.90
22	W	33	ASP	N-CA-C	6.54	119.23	111.71
22	W	152	LEU	O-C-N	-6.52	113.82	121.32
22	W	314	VAL	N-CA-CB	6.52	118.18	110.55
21	V	624	ILE	N-CA-CB	-6.51	103.18	111.64
22	W	698	GLN	OE1-CD-NE2	-6.51	116.09	122.60
21	V	366	ASN	CA-CB-CG	6.50	119.10	112.60
21	V	709	GLN	CA-C-N	6.49	128.98	120.28
21	V	709	GLN	C-N-CA	6.49	128.98	120.28
22	W	138	THR	CA-C-O	-6.49	113.67	120.55
1	A	527	THR	CA-C-N	6.48	127.04	120.04
1	A	527	THR	C-N-CA	6.48	127.04	120.04
22	W	406	LEU	CA-C-O	-6.48	114.20	121.00
1	A	1470	CYS	N-CA-C	6.47	121.03	113.20
21	V	409	THR	CA-C-N	6.47	131.04	120.63
21	V	409	THR	C-N-CA	6.47	131.04	120.63
21	V	467	THR	N-CA-C	6.46	118.67	108.79
22	W	166	ARG	CD-NE-CZ	6.46	133.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	14	ILE	N-CA-C	6.45	117.90	109.58
1	A	1454	VAL	N-CA-C	6.44	116.59	110.53
1	A	807	LEU	CA-C-N	-6.44	113.17	119.87
1	A	807	LEU	C-N-CA	-6.44	113.17	119.87
21	V	454	VAL	CA-C-N	6.44	129.43	120.29
21	V	454	VAL	C-N-CA	6.44	129.43	120.29
21	V	434	GLU	N-CA-C	6.44	118.38	111.36
28	Y	23	DT	N1-C1'-C2'	6.44	123.16	113.50
1	A	501	MET	CA-CB-CG	6.43	126.97	114.10
1	A	539	GLN	CA-C-N	6.43	128.90	120.28
1	A	539	GLN	C-N-CA	6.43	128.90	120.28
22	W	88	ARG	CA-C-N	6.43	129.42	120.29
22	W	88	ARG	C-N-CA	6.43	129.42	120.29
2	B	962	THR	CA-C-N	6.42	126.38	119.76
2	B	962	THR	C-N-CA	6.42	126.38	119.76
21	V	328	PHE	CA-C-N	6.42	134.00	121.41
21	V	328	PHE	C-N-CA	6.42	134.00	121.41
22	W	491	CYS	CA-C-N	6.42	126.79	119.92
22	W	491	CYS	C-N-CA	6.42	126.79	119.92
23	O	105	GLY	CA-C-O	-6.41	115.99	121.57
1	A	614	ASP	N-CA-C	6.41	124.45	110.80
2	B	58	ILE	N-CA-C	6.41	116.57	110.42
22	W	196	ARG	CA-C-N	6.41	128.86	120.28
22	W	196	ARG	C-N-CA	6.41	128.86	120.28
22	W	161	PHE	CA-CB-CG	6.40	120.20	113.80
22	W	210	HIS	ND1-CG-CD2	6.40	112.50	106.10
21	V	643	VAL	CA-CB-CG1	6.39	121.27	110.40
9	I	98	GLN	N-CA-C	6.39	119.12	108.96
21	V	373	GLN	OE1-CD-NE2	-6.38	116.22	122.60
21	V	281	GLN	O-C-N	6.38	128.73	122.09
1	A	203	LYS	N-CA-C	6.38	121.13	107.67
18	R	163	LEU	CA-C-N	-6.38	108.91	121.41
18	R	163	LEU	C-N-CA	-6.38	108.91	121.41
26	3	218	PRO	N-CA-C	-6.38	99.13	111.69
21	V	396	ALA	CA-C-N	6.37	132.98	121.89
21	V	396	ALA	C-N-CA	6.37	132.98	121.89
17	Q	66	LEU	N-CA-C	6.37	118.22	111.28
21	V	391	ARG	NE-CZ-NH1	-6.37	115.13	121.50
23	O	58	MET	O-C-N	6.37	131.04	123.27
22	W	299	ARG	NE-CZ-NH1	6.37	127.86	121.50
22	W	416	ILE	CA-C-N	6.36	131.84	123.06
22	W	416	ILE	C-N-CA	6.36	131.84	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	447	VAL	O-C-N	6.35	128.03	121.87
22	W	511	ARG	NE-CZ-NH2	6.35	124.91	119.20
18	R	204	ASN	O-C-N	-6.34	115.56	122.79
22	W	83	VAL	CA-C-N	6.34	128.55	120.56
22	W	83	VAL	C-N-CA	6.34	128.55	120.56
22	W	416	ILE	O-C-N	-6.34	115.72	122.95
7	G	110	ARG	N-CA-C	6.34	119.86	111.75
26	3	181	ILE	CB-CA-C	-6.33	103.86	111.97
22	W	552	TRP	N-CA-C	-6.33	104.30	111.14
22	W	662	GLN	OE1-CD-NE2	-6.33	116.27	122.60
22	W	258	ARG	CA-C-O	-6.33	113.71	120.42
11	K	9	SER	N-CA-C	6.33	120.10	112.38
2	B	711	ILE	CA-C-N	6.32	126.82	119.99
2	B	711	ILE	C-N-CA	6.32	126.82	119.99
23	0	111	SER	CA-C-N	6.32	132.97	123.05
23	0	111	SER	C-N-CA	6.32	132.97	123.05
25	2	238	PHE	CA-CB-CG	-6.31	107.49	113.80
23	0	224	ASP	N-CA-CB	-6.31	101.59	111.56
21	V	545	GLN	N-CA-C	6.31	118.15	111.28
22	W	257	ASP	CA-CB-CG	-6.30	106.30	112.60
21	V	341	PRO	CB-CA-C	-6.29	103.34	111.39
22	W	70	LEU	CA-C-O	-6.29	113.63	120.36
21	V	689	VAL	O-C-N	-6.29	116.58	123.18
22	W	238	ASN	OD1-CG-ND2	-6.27	116.33	122.60
22	W	242	VAL	CA-C-O	-6.26	114.21	120.85
21	V	449	LYS	N-CA-C	6.26	118.11	111.28
21	V	480	LEU	CA-C-N	6.25	128.66	120.28
21	V	480	LEU	C-N-CA	6.25	128.66	120.28
22	W	113	LYS	CA-C-O	-6.25	113.92	120.55
28	Y	15	DT	O4'-C1'-N1	6.25	117.78	108.40
1	A	886	VAL	CB-CA-C	-6.25	103.77	111.08
22	W	299	ARG	N-CA-C	-6.25	104.87	113.18
21	V	443	VAL	O-C-N	-6.24	115.60	121.90
22	W	592	ARG	NH1-CZ-NH2	-6.23	111.20	119.30
28	Y	28	DT	C6-N1-C1'	6.22	128.68	119.35
28	Y	28	DT	C2-N1-C1'	-6.22	110.02	119.35
3	C	221	ASP	CA-C-N	6.22	125.84	119.56
3	C	221	ASP	C-N-CA	6.22	125.84	119.56
11	K	62	LYS	CA-C-N	-6.22	118.37	122.60
11	K	62	LYS	C-N-CA	-6.22	118.37	122.60
22	W	125	ARG	CD-NE-CZ	6.22	133.10	124.40
2	B	844	ILE	N-CA-C	6.21	117.36	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	63	TYR	CA-C-N	6.21	126.11	119.28
22	W	63	TYR	C-N-CA	6.21	126.11	119.28
23	0	62	TYR	CA-C-O	6.21	127.00	120.54
4	D	115	ILE	CA-C-N	6.20	126.67	119.47
4	D	115	ILE	C-N-CA	6.20	126.67	119.47
22	W	286	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	A	620	HIS	N-CA-C	6.20	123.14	113.72
22	W	50	VAL	CA-CB-CG1	6.20	120.94	110.40
2	B	421	LYS	N-CA-C	6.20	118.03	111.28
25	2	229	ASP	CA-CB-CG	-6.19	106.41	112.60
21	V	524	ALA	N-CA-C	6.19	118.03	111.28
22	W	662	GLN	CG-CD-NE2	6.19	125.68	116.40
21	V	251	PHE	CA-C-N	6.19	130.35	121.50
21	V	251	PHE	C-N-CA	6.19	130.35	121.50
22	W	461	LEU	CA-C-N	6.18	128.74	120.58
22	W	461	LEU	C-N-CA	6.18	128.74	120.58
22	W	272	ARG	NH1-CZ-NH2	-6.18	111.27	119.30
27	X	81	DG	C4-N9-C1'	-6.18	117.73	127.00
1	A	1190	GLN	N-CA-C	6.17	118.01	111.28
3	C	92	GLU	CB-CA-C	-6.17	109.44	116.54
7	G	107	PHE	N-CA-C	6.17	119.00	109.07
21	V	341	PRO	N-CA-CB	6.17	108.50	103.32
22	W	585	GLN	O-C-N	6.16	130.24	122.23
28	Y	19	DC	P-O5'-C5'	6.16	129.24	120.00
21	V	474	ASP	CA-C-N	6.15	133.29	121.54
21	V	474	ASP	C-N-CA	6.15	133.29	121.54
21	V	337	VAL	CA-C-N	6.15	131.54	122.99
21	V	337	VAL	C-N-CA	6.15	131.54	122.99
21	V	529	LYS	O-C-N	-6.14	115.19	122.20
22	W	345	ARG	CD-NE-CZ	6.14	133.00	124.40
23	0	206	ARG	NE-CZ-NH1	6.14	127.64	121.50
22	W	312	ASP	N-CA-C	6.13	117.77	111.14
21	V	330	ASN	CA-C-O	-6.13	113.44	120.24
21	V	337	VAL	CA-C-O	-6.12	115.57	121.63
23	0	123	ASN	OD1-CG-ND2	-6.12	116.48	122.60
22	W	332	PHE	O-C-N	-6.12	115.63	122.12
22	W	463	PRO	N-CA-CB	6.11	109.33	103.52
23	0	140	HIS	CB-CG-CD2	-6.10	123.27	131.20
23	0	184	ASP	CA-CB-CG	6.10	118.70	112.60
21	V	286	HIS	CE1-NE2-CD2	-6.10	102.90	109.00
21	V	367	SER	CA-C-N	6.10	128.95	120.29
21	V	367	SER	C-N-CA	6.10	128.95	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	210	HIS	CB-CG-CD2	-6.09	123.28	131.20
25	2	79	PHE	CA-CB-CG	-6.09	107.71	113.80
1	A	672	ILE	CB-CA-C	-6.08	103.94	112.14
22	W	301	THR	CA-C-N	6.08	130.38	120.23
22	W	301	THR	C-N-CA	6.08	130.38	120.23
1	A	496	PHE	N-CA-C	-6.06	104.06	112.30
22	W	30	ARG	CD-NE-CZ	6.06	132.88	124.40
2	B	919	CYS	N-CA-C	6.04	119.33	109.24
22	W	183	LEU	CA-C-N	6.04	126.65	120.00
22	W	183	LEU	C-N-CA	6.04	126.65	120.00
2	B	922	ARG	N-CA-C	6.04	119.09	109.24
28	Y	24	DC	C2-N1-C1'	-6.04	110.65	119.70
5	E	46	ASP	N-CA-C	6.03	123.65	110.80
21	V	651	VAL	CA-C-O	-6.03	113.24	120.78
21	V	713	LEU	CA-C-O	-6.02	114.46	120.90
22	W	122	THR	CA-C-N	6.02	127.37	119.84
22	W	122	THR	C-N-CA	6.02	127.37	119.84
22	W	148	HIS	CG-CD2-NE2	6.02	113.22	107.20
22	W	314	VAL	N-CA-C	6.01	116.19	110.42
25	2	203	PHE	CA-CB-CG	-6.01	107.79	113.80
21	V	404	SER	CB-CA-C	6.01	122.38	110.42
2	B	164	ASN	N-CA-C	6.01	119.71	112.38
3	C	225	LYS	CA-C-N	-6.00	113.35	120.13
3	C	225	LYS	C-N-CA	-6.00	113.35	120.13
13	M	81	SER	N-CA-C	6.00	116.16	108.24
19	S	147	THR	CA-C-N	6.00	125.95	119.78
19	S	147	THR	C-N-CA	6.00	125.95	119.78
21	V	278	GLU	CA-C-O	-6.00	112.70	120.25
22	W	569	ILE	N-CA-CB	-5.99	105.24	112.07
22	W	592	ARG	NE-CZ-NH1	5.99	127.49	121.50
25	2	171	VAL	CB-CA-C	-5.99	104.30	111.97
1	A	759	SER	N-CA-C	5.99	119.84	112.54
23	0	235	HIS	CB-CG-CD2	-5.99	123.42	131.20
21	V	603	ASN	CA-CB-CG	5.99	118.59	112.60
27	X	66	DA	O4'-C1'-C2'	-5.99	97.42	106.40
23	0	130	SER	N-CA-C	5.98	117.88	111.36
22	W	590	ASN	N-CA-C	5.98	119.82	110.32
22	W	164	HIS	CB-CG-CD2	-5.97	123.43	131.20
21	V	410	TYR	CA-C-N	5.97	129.60	120.82
21	V	410	TYR	C-N-CA	5.97	129.60	120.82
21	V	709	GLN	OE1-CD-NE2	-5.97	116.63	122.60
21	V	403	CYS	N-CA-CB	-5.97	101.99	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	561	PHE	O-C-N	-5.96	116.53	123.27
1	A	910	LYS	CA-C-N	5.96	127.29	119.84
1	A	910	LYS	C-N-CA	5.96	127.29	119.84
21	V	379	LYS	N-CA-C	5.96	119.38	111.75
21	V	307	ASN	CA-CB-CG	5.96	118.56	112.60
21	V	607	ILE	CA-CB-CG1	5.96	120.52	110.40
23	O	158	HIS	CB-CG-CD2	-5.96	123.46	131.20
22	W	621	PHE	CA-CB-CG	-5.95	107.85	113.80
23	O	74	GLN	OE1-CD-NE2	-5.95	116.65	122.60
22	W	470	ILE	CB-CG1-CD1	-5.95	101.31	113.80
22	W	650	ASP	CA-C-O	-5.94	114.58	120.70
21	V	459	GLN	CA-C-N	5.94	132.89	121.54
21	V	459	GLN	C-N-CA	5.94	132.89	121.54
22	W	416	ILE	CA-C-O	5.94	127.42	120.71
3	C	66	HIS	N-CA-C	5.93	117.42	111.07
17	Q	174	ARG	N-CA-C	5.93	117.74	111.28
22	W	207	TYR	CA-C-O	-5.92	115.08	121.36
22	W	480	THR	CA-CB-OG1	5.92	118.48	109.60
1	A	539	GLN	N-CA-C	5.92	116.75	108.00
1	A	322	LEU	CA-C-N	5.91	125.85	119.76
1	A	322	LEU	C-N-CA	5.91	125.85	119.76
22	W	20	GLU	CA-C-O	-5.91	114.28	120.55
28	Y	19	DC	O5'-C5'-C4'	5.91	119.67	110.80
2	B	497	LYS	CA-C-N	-5.91	110.72	120.88
2	B	497	LYS	C-N-CA	-5.91	110.72	120.88
1	A	986	MET	N-CA-C	5.90	117.38	111.07
2	B	435	ILE	N-CA-C	5.90	116.02	108.12
1	A	1160	ARG	N-CA-C	5.90	117.71	111.28
10	J	45	CYS	N-CA-C	-5.89	104.98	111.82
21	V	633	ARG	NE-CZ-NH2	-5.89	113.90	119.20
26	3	153	ASP	N-CA-C	-5.89	104.86	111.28
22	W	161	PHE	O-C-N	-5.89	115.97	122.09
22	W	289	VAL	N-CA-C	5.89	116.62	110.62
21	V	369	VAL	CA-CB-CG1	5.88	120.40	110.40
27	X	81	DG	C8-N9-C1'	5.88	135.82	127.00
22	W	442	LEU	CA-C-N	5.88	128.64	120.29
22	W	442	LEU	C-N-CA	5.88	128.64	120.29
1	A	920	PHE	N-CA-C	5.87	120.60	112.45
23	O	203	ALA	N-CA-C	5.87	119.04	108.48
22	W	37	HIS	N-CA-C	5.86	117.76	108.79
7	G	19	GLY	CA-C-N	5.86	125.23	118.85
7	G	19	GLY	C-N-CA	5.86	125.23	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	606	GLU	O-C-N	-5.85	115.38	122.22
21	V	485	GLY	CA-C-N	5.85	126.17	119.92
21	V	485	GLY	C-N-CA	5.85	126.17	119.92
22	W	716	VAL	N-CA-CB	5.84	119.34	110.58
25	2	175	LEU	N-CA-CB	5.84	119.22	110.22
10	J	50	LEU	N-CA-C	5.84	118.42	111.71
21	V	335	SER	N-CA-C	5.84	117.94	109.07
1	A	678	ASN	N-CA-C	5.84	117.64	111.28
22	W	92	ASN	OD1-CG-ND2	-5.84	116.76	122.60
22	W	623	VAL	N-CA-C	-5.84	103.61	108.63
24	1	34	ILE	N-CA-C	5.84	116.02	110.42
1	A	848	ILE	N-CA-C	5.83	116.61	110.72
23	0	190	LYS	N-CA-C	-5.83	105.01	111.36
21	V	461	HIS	CB-CG-CD2	-5.82	123.63	131.20
21	V	594	GLN	O-C-N	-5.82	115.80	122.09
13	M	42	GLY	N-CA-C	5.82	126.96	113.18
22	W	152	LEU	CA-C-N	5.81	125.75	119.76
22	W	152	LEU	C-N-CA	5.81	125.75	119.76
21	V	527	THR	CA-C-O	-5.81	115.37	121.99
2	B	1162	LEU	N-CA-C	5.80	117.61	111.28
22	W	213	LEU	N-CA-C	5.80	118.38	111.71
22	W	722	ARG	CD-NE-CZ	5.80	132.51	124.40
1	A	72	GLN	CB-CA-C	-5.79	109.35	117.23
22	W	685	ALA	N-CA-C	5.79	118.34	111.33
21	V	674	THR	CA-C-N	5.79	127.97	120.44
21	V	674	THR	C-N-CA	5.79	127.97	120.44
22	W	672	THR	N-CA-C	5.79	119.97	113.02
21	V	281	GLN	N-CA-C	5.79	118.06	111.11
22	W	702	THR	N-CA-C	5.79	119.96	113.01
26	3	64	ILE	CB-CA-C	-5.79	104.56	111.97
28	Y	25	DT	O3'-P-O5'	-5.79	95.32	104.00
22	W	586	GLU	N-CA-C	5.78	117.26	111.07
22	W	683	ARG	CD-NE-CZ	5.78	132.50	124.40
5	E	102	ALA	N-CA-C	5.78	117.83	108.41
22	W	447	VAL	CA-C-O	-5.78	114.94	120.95
1	A	521	VAL	N-CA-C	5.78	121.36	108.88
1	A	677	ASN	N-CA-C	5.78	117.58	111.28
20	T	136	SER	N-CA-C	5.77	117.92	110.65
21	V	332	ARG	NE-CZ-NH1	5.77	127.27	121.50
22	W	154	HIS	CB-CG-ND1	5.77	131.35	122.70
22	W	206	VAL	CA-CB-CG1	5.77	120.20	110.40
22	W	280	ARG	CA-C-O	-5.77	114.31	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	312	ASP	N-CA-CB	-5.77	101.71	110.07
22	W	548	THR	CA-C-O	-5.76	114.77	120.82
22	W	92	ASN	CB-CG-ND2	5.76	125.04	116.40
21	V	614	SER	N-CA-C	5.75	123.06	110.80
13	M	34	CYS	CA-C-N	5.75	127.03	119.84
13	M	34	CYS	C-N-CA	5.75	127.03	119.84
2	B	785	TYR	CA-C-N	-5.75	113.52	122.37
2	B	785	TYR	C-N-CA	-5.75	113.52	122.37
21	V	276	MET	CA-C-O	-5.75	114.82	121.26
22	W	218	ALA	N-CA-C	5.75	117.55	111.28
21	V	488	LEU	N-CA-C	5.75	117.62	111.36
22	W	239	ILE	N-CA-C	5.75	116.48	110.62
21	V	416	THR	CB-CA-C	-5.75	99.65	109.65
23	0	160	PRO	CA-C-N	5.74	132.66	121.41
23	0	160	PRO	C-N-CA	5.74	132.66	121.41
21	V	338	ILE	CA-C-O	-5.73	114.28	120.36
18	R	127	ASN	OD1-CG-ND2	-5.73	116.87	122.60
22	W	112	ARG	NE-CZ-NH1	5.73	127.23	121.50
21	V	520	ARG	NE-CZ-NH2	5.73	124.36	119.20
21	V	393	THR	N-CA-C	5.73	115.58	108.19
13	M	52	TRP	N-CA-C	-5.72	105.13	111.71
22	W	415	THR	CA-C-O	5.72	127.58	120.54
24	1	48	GLU	N-CA-C	-5.72	98.61	110.80
22	W	177	LEU	N-CA-C	5.72	117.19	111.07
25	2	403	PHE	CA-C-N	5.72	132.73	122.09
25	2	403	PHE	C-N-CA	5.72	132.73	122.09
21	V	421	TRP	NE1-CE2-CZ2	5.71	138.67	130.10
21	V	444	HIS	CA-C-O	-5.71	112.87	119.61
23	0	56	GLY	CA-C-N	5.71	131.59	122.10
23	0	56	GLY	C-N-CA	5.71	131.59	122.10
2	B	1082	GLY	N-CA-C	5.71	122.05	112.85
22	W	175	TYR	O-C-N	5.71	129.75	123.01
23	0	92	VAL	CB-CA-C	-5.71	104.67	111.97
3	C	123	ASN	N-CA-C	-5.71	105.14	111.36
21	V	656	ASN	CA-CB-CG	5.71	118.31	112.60
21	V	679	PHE	CA-CB-CG	5.70	119.50	113.80
22	W	593	GLY	CA-C-N	5.70	132.80	122.02
22	W	593	GLY	C-N-CA	5.70	132.80	122.02
21	V	354	ALA	N-CA-C	5.70	117.50	111.28
21	V	497	GLN	OE1-CD-NE2	-5.70	116.90	122.60
22	W	216	LYS	CA-C-O	-5.70	114.51	120.55
25	2	444	THR	CA-CB-OG1	5.70	118.14	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	567	ALA	CA-C-N	5.70	128.23	120.54
21	V	567	ALA	C-N-CA	5.70	128.23	120.54
21	V	412	MET	O-C-N	-5.69	115.15	122.21
21	V	479	ASP	N-CA-C	5.69	118.42	111.82
22	W	651	PHE	CA-CB-CG	5.69	119.49	113.80
22	W	44	SER	CA-C-O	5.69	126.37	119.49
23	O	178	ASP	O-C-N	-5.69	116.24	121.30
28	Y	15	DT	O3'-P-O5'	5.69	112.53	104.00
13	M	44	ARG	N-CA-C	5.68	118.57	110.10
22	W	109	LEU	CA-C-N	5.68	133.45	121.91
22	W	109	LEU	C-N-CA	5.68	133.45	121.91
21	V	702	ALA	N-CA-CB	-5.68	102.52	110.25
22	W	669	ARG	NE-CZ-NH1	5.68	127.18	121.50
21	V	295	TYR	N-CA-C	5.68	118.03	110.53
22	W	272	ARG	NE-CZ-NH1	5.68	127.18	121.50
21	V	420	SER	O-C-N	-5.67	116.22	122.07
22	W	339	TYR	CA-C-N	5.67	128.48	120.42
22	W	339	TYR	C-N-CA	5.67	128.48	120.42
21	V	435	TRP	CE2-CD2-CE3	-5.67	113.13	118.80
21	V	526	LYS	CA-C-N	5.67	131.72	121.06
21	V	526	LYS	C-N-CA	5.67	131.72	121.06
21	V	665	GLN	CG-CD-NE2	5.67	124.91	116.40
21	V	579	TYR	N-CA-C	5.67	118.46	109.50
22	W	193	PHE	N-CA-C	5.67	117.46	111.28
28	Y	24	DC	O4'-C1'-N1	5.67	116.90	108.40
21	V	506	GLN	OE1-CD-NE2	-5.67	116.93	122.60
5	E	145	VAL	N-CA-C	5.66	113.48	107.76
7	G	124	ASN	CA-C-N	-5.66	114.55	120.38
7	G	124	ASN	C-N-CA	-5.66	114.55	120.38
22	W	414	PHE	CA-CB-CG	5.66	119.46	113.80
2	B	132	VAL	N-CA-C	5.66	115.75	107.37
21	V	307	ASN	N-CA-CB	-5.66	102.21	111.66
21	V	532	LEU	N-CA-C	5.66	118.38	111.82
8	H	85	ALA	N-CA-C	-5.66	105.20	111.71
18	R	115	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	847	LEU	N-CA-C	5.65	117.44	111.28
21	V	477	ILE	CA-CB-CG1	5.65	120.00	110.40
21	V	375	LYS	CA-C-N	5.64	127.78	120.44
21	V	375	LYS	C-N-CA	5.64	127.78	120.44
26	3	120	THR	CA-C-N	5.64	127.84	120.28
26	3	120	THR	C-N-CA	5.64	127.84	120.28
22	W	154	HIS	CA-CB-CG	-5.64	108.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	527	THR	N-CA-C	5.64	117.34	110.41
21	V	636	GLU	N-CA-C	-5.63	105.04	111.07
22	W	104	PHE	CA-CB-CG	5.63	119.43	113.80
1	A	432	HIS	CA-C-N	5.63	125.74	119.32
1	A	432	HIS	C-N-CA	5.63	125.74	119.32
2	B	77	GLU	N-CA-C	5.63	122.78	110.80
22	W	434	HIS	CB-CG-CD2	-5.62	123.89	131.20
2	B	163	LEU	N-CA-C	5.62	119.24	112.38
1	A	206	ASN	CA-C-N	-5.62	110.82	121.54
1	A	206	ASN	C-N-CA	-5.62	110.82	121.54
10	J	43	TYR	N-CA-C	5.62	119.39	112.54
22	W	421	PHE	CA-C-N	-5.62	114.15	122.35
22	W	421	PHE	C-N-CA	-5.62	114.15	122.35
22	W	215	PRO	CA-C-N	5.61	127.80	120.28
22	W	215	PRO	C-N-CA	5.61	127.80	120.28
8	H	66	GLU	N-CA-C	5.61	122.75	110.80
18	R	139	PHE	CA-C-N	5.61	131.80	121.70
18	R	139	PHE	C-N-CA	5.61	131.80	121.70
21	V	551	HIS	CA-CB-CG	-5.61	108.19	113.80
21	V	439	ILE	CB-CG1-CD1	5.61	125.57	113.80
22	W	103	PRO	CB-CA-C	5.61	120.81	111.56
22	W	220	LEU	O-C-N	-5.60	115.76	122.15
22	W	16	TYR	CA-C-N	5.60	129.84	122.51
22	W	16	TYR	C-N-CA	5.60	129.84	122.51
22	W	53	LEU	CA-C-O	-5.60	114.62	120.55
21	V	703	PHE	N-CA-CB	-5.60	103.50	111.84
25	2	61	PHE	N-CA-CB	5.59	118.09	109.98
22	W	305	LEU	CA-C-N	5.59	127.77	120.28
22	W	305	LEU	C-N-CA	5.59	127.77	120.28
21	V	677	GLN	N-CA-C	5.59	117.05	111.07
21	V	355	CYS	O-C-N	-5.59	116.20	122.12
22	W	207	TYR	CA-CB-CG	5.59	123.96	113.90
22	W	270	VAL	O-C-N	-5.58	115.59	122.57
21	V	405	VAL	CB-CA-C	5.58	120.44	111.29
22	W	197	TYR	CA-C-O	5.58	126.46	120.55
22	W	703	ASP	CA-C-N	5.58	132.19	121.54
22	W	703	ASP	C-N-CA	5.58	132.19	121.54
16	P	325	PHE	N-CA-C	5.57	117.43	111.36
22	W	68	THR	CA-C-O	-5.57	115.75	121.87
23	0	113	ARG	N-CA-C	5.57	117.87	109.41
21	V	429	TRP	CA-C-N	5.57	133.21	122.53
21	V	429	TRP	C-N-CA	5.57	133.21	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	262	LEU	CB-CA-C	-5.56	102.15	110.88
23	0	99	ASN	N-CA-C	5.56	119.92	110.02
22	W	590	ASN	CA-C-N	5.55	129.05	121.83
22	W	590	ASN	C-N-CA	5.55	129.05	121.83
28	Y	20	DA	N9-C1'-C2'	5.55	121.83	113.50
1	A	101	VAL	N-CA-C	5.55	115.74	110.42
22	W	306	ALA	CA-C-O	-5.54	114.67	120.55
22	W	468	PRO	CA-N-CD	-5.54	104.24	112.00
23	0	194	ILE	CA-C-O	5.54	127.17	120.74
22	W	334	ARG	N-CA-CB	-5.53	101.99	110.01
21	V	675	LYS	N-CA-C	5.52	116.98	111.07
21	V	457	ILE	N-CA-CB	-5.52	102.12	111.23
22	W	685	ALA	CA-C-O	5.52	126.59	120.63
22	W	251	LEU	CB-CA-C	5.51	119.46	109.37
5	E	126	ILE	N-CA-C	5.51	115.89	108.17
22	W	265	THR	CA-C-N	5.51	129.42	120.60
22	W	265	THR	C-N-CA	5.51	129.42	120.60
21	V	567	ALA	O-C-N	5.51	128.43	122.15
22	W	439	ASP	CA-C-O	5.51	127.21	120.60
23	0	98	GLN	CA-C-O	5.50	126.25	120.42
21	V	268	VAL	CA-C-N	5.50	129.06	120.75
21	V	268	VAL	C-N-CA	5.50	129.06	120.75
21	V	637	ALA	N-CA-C	5.50	118.20	111.82
21	V	572	ALA	N-CA-C	5.50	117.28	111.28
17	Q	103	VAL	N-CA-C	5.50	116.54	111.81
22	W	494	ILE	O-C-N	-5.50	117.22	123.10
22	W	601	ARG	NE-CZ-NH2	-5.50	114.25	119.20
18	R	161	ARG	CA-C-N	-5.50	113.41	120.72
18	R	161	ARG	C-N-CA	-5.50	113.41	120.72
18	R	90	GLN	OE1-CD-NE2	-5.49	117.11	122.60
22	W	726	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	886	VAL	N-CA-C	5.49	116.66	108.54
23	0	227	HIS	CA-CB-CG	5.48	119.28	113.80
22	W	606	GLU	CA-C-O	5.47	126.28	120.10
25	2	182	ALA	N-CA-C	-5.47	102.78	110.50
21	V	514	MET	CB-CA-C	5.47	118.89	110.14
1	A	75	ALA	CB-CA-C	-5.46	110.25	116.54
10	J	7	CYS	N-CA-C	5.46	118.40	110.42
7	G	96	GLY	N-CA-C	5.46	117.55	110.45
23	0	226	SER	N-CA-CB	-5.46	102.09	110.12
27	X	79	DA	C2'-C3'-O3'	5.46	119.69	111.50
22	W	463	PRO	CA-C-N	5.46	131.97	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	463	PRO	C-N-CA	5.46	131.97	121.54
25	2	267	GLU	CA-C-N	-5.46	115.74	122.84
25	2	267	GLU	C-N-CA	-5.46	115.74	122.84
21	V	662	LEU	N-CA-CB	-5.46	101.53	110.43
22	W	57	MET	CA-C-N	5.46	129.34	120.60
22	W	57	MET	C-N-CA	5.46	129.34	120.60
1	A	675	VAL	CB-CA-C	-5.46	104.99	111.97
22	W	454	VAL	CA-C-N	5.45	131.05	122.33
22	W	454	VAL	C-N-CA	5.45	131.05	122.33
23	0	123	ASN	O-C-N	-5.44	114.92	121.12
1	A	394	VAL	N-CA-C	5.44	116.07	108.89
2	B	161	CYS	N-CA-C	-5.44	103.52	110.53
2	B	192	LYS	N-CA-C	-5.44	99.57	108.76
1	A	380	VAL	CA-C-N	5.43	125.43	119.89
1	A	380	VAL	C-N-CA	5.43	125.43	119.89
21	V	542	ARG	NE-CZ-NH2	5.43	124.08	119.20
22	W	197	TYR	O-C-N	-5.43	116.37	122.12
25	2	98	THR	CA-C-N	5.43	128.09	120.28
25	2	98	THR	C-N-CA	5.43	128.09	120.28
21	V	433	GLN	OE1-CD-NE2	-5.42	117.18	122.60
2	B	1087	GLY	N-CA-C	5.42	119.52	112.25
21	V	360	ARG	CD-NE-CZ	5.42	131.99	124.40
22	W	489	CYS	CA-C-N	5.42	130.41	122.39
22	W	489	CYS	C-N-CA	5.42	130.41	122.39
23	0	134	ALA	CA-C-O	5.42	126.16	120.42
23	0	142	GLU	O-C-N	5.42	125.78	121.55
24	1	51	ASN	CA-CB-CG	-5.42	107.18	112.60
1	A	456	VAL	CA-C-N	-5.42	115.17	122.91
1	A	456	VAL	C-N-CA	-5.42	115.17	122.91
22	W	487	ARG	NH1-CZ-NH2	-5.41	112.26	119.30
1	A	267	GLN	CB-CA-C	-5.41	110.36	116.63
1	A	867	SER	N-CA-C	5.41	117.03	111.03
2	B	407	MET	N-CA-C	5.41	117.25	111.36
1	A	470	MET	N-CA-C	5.40	117.40	109.24
21	V	427	MET	N-CA-C	5.40	122.31	110.80
22	W	75	ARG	NE-CZ-NH1	5.40	126.90	121.50
22	W	455	ILE	N-CA-C	5.40	115.66	108.27
21	V	253	GLU	CA-C-N	5.39	131.84	121.54
21	V	253	GLU	C-N-CA	5.39	131.84	121.54
25	2	45	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	566	PHE	N-CA-C	5.39	119.48	113.01
23	0	186	ILE	N-CA-C	5.39	116.12	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	660	MET	N-CA-C	5.39	119.84	113.16
22	W	141	TYR	N-CA-C	5.39	117.15	111.28
22	W	645	GLN	CA-C-N	5.39	131.67	121.97
22	W	645	GLN	C-N-CA	5.39	131.67	121.97
23	O	236	VAL	CB-CA-C	-5.39	104.86	112.14
2	B	39	LEU	N-CA-C	5.39	118.95	112.38
2	B	95	LYS	CA-C-N	5.38	126.57	119.84
2	B	95	LYS	C-N-CA	5.38	126.57	119.84
6	F	88	ASP	CA-C-N	5.38	125.03	119.05
6	F	88	ASP	C-N-CA	5.38	125.03	119.05
25	2	35	TYR	CB-CA-C	5.38	121.00	110.67
22	W	76	THR	N-CA-C	5.38	117.25	109.07
27	X	81	DG	C2'-C3'-O3'	5.38	119.57	111.50
21	V	677	GLN	OE1-CD-NE2	-5.38	117.22	122.60
22	W	560	ASN	CA-CB-CG	-5.37	107.23	112.60
24	1	33	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	540	ASP	CB-CA-C	5.37	119.70	110.79
22	W	156	ARG	CD-NE-CZ	5.37	131.92	124.40
22	W	313	GLU	N-CA-C	5.37	116.81	111.07
23	O	131	LEU	O-C-N	-5.37	115.67	122.27
27	X	65	DG	O3'-P-O5'	-5.37	95.95	104.00
1	A	386	ALA	N-CA-C	5.36	118.04	111.82
1	A	539	GLN	CB-CA-C	-5.36	108.83	116.34
14	N	346	LYS	CB-CA-C	-5.36	109.94	117.23
21	V	564	ASN	CA-C-N	5.36	127.80	120.46
21	V	564	ASN	C-N-CA	5.36	127.80	120.46
21	V	339	VAL	CA-C-O	5.36	126.01	120.39
1	A	288	ASN	N-CA-C	-5.35	105.52	111.36
23	O	73	ASP	CA-CB-CG	5.35	117.95	112.60
22	W	202	ALA	N-CA-C	5.35	118.26	109.76
22	W	282	ARG	CA-C-N	5.34	127.44	120.28
22	W	282	ARG	C-N-CA	5.34	127.44	120.28
13	M	25	GLU	N-CA-C	5.34	117.33	108.20
22	W	149	ASP	O-C-N	-5.34	116.46	122.12
23	O	178	ASP	CA-C-N	5.34	124.85	119.19
23	O	178	ASP	C-N-CA	5.34	124.85	119.19
21	V	469	THR	CA-C-N	5.34	131.73	121.54
21	V	469	THR	C-N-CA	5.34	131.73	121.54
22	W	148	HIS	ND1-CE1-NE2	5.34	113.74	108.40
2	B	963	PRO	CA-C-O	-5.33	115.26	121.34
22	W	600	ALA	CA-C-N	5.33	127.96	120.28
22	W	600	ALA	C-N-CA	5.33	127.96	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	79	DA	C1'-O4'-C4'	-5.33	101.70	109.70
21	V	381	TRP	CZ3-CH2-CZ2	-5.33	114.57	121.50
22	W	118	HIS	CB-CG-CD2	-5.33	124.27	131.20
21	V	286	HIS	CG-CD2-NE2	5.33	112.53	107.20
22	W	686	ARG	CA-C-N	5.33	126.98	120.22
22	W	686	ARG	C-N-CA	5.33	126.98	120.22
22	W	669	ARG	NH1-CZ-NH2	-5.32	112.38	119.30
2	B	1006	VAL	CA-C-N	5.32	131.70	121.54
2	B	1006	VAL	C-N-CA	5.32	131.70	121.54
21	V	366	ASN	N-CA-C	5.32	119.49	112.89
21	V	555	ASN	N-CA-C	5.32	118.78	111.54
21	V	361	CYS	N-CA-CB	-5.32	101.58	110.83
2	B	250	SER	N-CA-C	5.32	117.13	110.91
21	V	703	PHE	N-CA-C	5.32	118.77	111.54
22	W	435	PHE	CA-C-N	5.31	128.39	120.95
22	W	435	PHE	C-N-CA	5.31	128.39	120.95
22	W	562	GLN	CB-CG-CD	5.31	121.63	112.60
28	Y	22	DG	C2'-C3'-O3'	5.31	119.47	111.50
1	A	636	ILE	N-CA-C	5.31	115.97	110.82
21	V	576	ASN	N-CA-CB	-5.31	103.93	111.84
23	O	99	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	1121	VAL	N-CA-C	5.30	120.34	108.88
7	G	93	ASN	N-CA-C	5.30	117.25	109.24
22	W	621	PHE	O-C-N	5.30	129.38	122.38
22	W	450	ARG	N-CA-C	5.30	122.08	110.80
1	A	1093	GLN	N-CA-C	5.29	117.96	111.82
21	V	272	VAL	O-C-N	5.29	127.00	121.87
22	W	37	HIS	CA-C-N	5.29	127.80	120.92
22	W	37	HIS	C-N-CA	5.29	127.80	120.92
23	O	237	SER	N-CA-C	5.29	116.08	109.57
21	V	552	GLU	N-CA-C	5.29	117.80	111.71
21	V	332	ARG	CA-CB-CG	5.29	124.67	114.10
21	V	576	ASN	CA-C-O	5.28	127.67	121.54
22	W	169	PRO	N-CA-CB	5.28	109.09	103.39
22	W	455	ILE	CA-C-O	-5.28	114.99	120.64
23	O	170	ILE	CA-CB-CG1	5.28	119.38	110.40
1	A	1076	PHE	N-CA-C	5.28	117.03	111.28
2	B	757	PRO	CA-C-O	-5.28	115.40	121.36
22	W	253	ARG	N-CA-C	5.28	117.03	111.28
23	O	90	TYR	CA-C-N	5.28	127.35	120.28
23	O	90	TYR	C-N-CA	5.28	127.35	120.28
21	V	317	ARG	O-C-N	5.27	127.34	121.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	27	DC	C6-N1-C1'	5.27	127.61	119.70
22	W	516	VAL	N-CA-C	5.27	116.00	110.62
1	A	1369	LEU	N-CA-C	5.27	119.71	113.28
3	C	71	ILE	CA-C-N	5.27	125.03	119.76
3	C	71	ILE	C-N-CA	5.27	125.03	119.76
22	W	319	VAL	CA-C-N	5.27	126.42	119.84
22	W	319	VAL	C-N-CA	5.27	126.42	119.84
26	3	50	PHE	CA-CB-CG	-5.26	108.54	113.80
2	B	667	THR	N-CA-C	5.26	117.76	111.71
22	W	564	ASN	OD1-CG-ND2	-5.26	117.34	122.60
21	V	435	TRP	CA-C-O	-5.26	114.89	121.46
21	V	575	LEU	CA-C-N	5.26	129.59	122.07
21	V	575	LEU	C-N-CA	5.26	129.59	122.07
1	A	1482	TYR	CA-C-N	5.25	125.78	120.00
1	A	1482	TYR	C-N-CA	5.25	125.78	120.00
21	V	332	ARG	NH1-CZ-NH2	-5.25	112.47	119.30
28	Y	21	DC	C1'-O4'-C4'	-5.25	101.82	109.70
2	B	1054	MET	N-CA-C	5.25	117.96	109.40
21	V	282	LYS	CG-CD-CE	5.25	123.38	111.30
21	V	699	GLU	N-CA-C	5.25	116.78	108.96
22	W	46	THR	CA-CB-OG1	5.25	117.47	109.60
22	W	457	THR	N-CA-CB	-5.25	103.42	111.56
28	Y	24	DC	C6-N1-C1'	5.25	127.57	119.70
1	A	81	CYS	CA-C-N	5.25	125.33	119.87
1	A	81	CYS	C-N-CA	5.25	125.33	119.87
22	W	454	VAL	N-CA-CB	-5.25	105.83	112.60
21	V	315	VAL	CA-C-O	-5.25	114.88	120.39
21	V	562	ALA	CA-C-N	5.24	131.56	121.54
21	V	562	ALA	C-N-CA	5.24	131.56	121.54
23	0	135	VAL	N-CA-C	5.24	115.97	110.62
22	W	284	GLU	N-CA-CB	5.24	117.61	110.01
21	V	341	PRO	N-CA-C	5.24	119.44	111.11
1	A	60	PRO	N-CA-C	-5.24	107.32	113.86
22	W	50	VAL	O-C-N	5.23	127.22	121.83
22	W	711	ASP	CA-CB-CG	-5.23	107.37	112.60
22	W	87	LEU	CB-CA-C	5.23	119.74	110.85
21	V	525	ILE	CA-C-O	-5.23	114.53	120.65
22	W	534	GLY	O-C-N	-5.23	118.91	122.62
22	W	102	LEU	CA-C-N	5.23	126.37	119.84
22	W	102	LEU	C-N-CA	5.23	126.37	119.84
23	0	179	PRO	CA-C-O	-5.23	111.66	119.34
2	B	788	TYR	CA-C-N	-5.22	114.32	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	788	TYR	C-N-CA	-5.22	114.32	122.73
11	K	82	SER	CA-C-N	5.22	124.72	119.19
11	K	82	SER	C-N-CA	5.22	124.72	119.19
13	M	216	SER	N-CA-C	5.22	116.66	110.97
18	R	139	PHE	O-C-N	-5.22	116.52	122.89
21	V	297	PHE	N-CA-C	5.22	117.00	109.07
28	Y	14	DG	C4-N9-C1'	-5.22	119.17	127.00
21	V	574	ARG	O-C-N	-5.21	116.21	122.15
25	2	60	LEU	CB-CA-C	-5.21	102.69	110.88
22	W	128	LYS	CA-C-N	5.21	128.11	120.71
22	W	128	LYS	C-N-CA	5.21	128.11	120.71
27	X	79	DA	P-O3'-C3'	5.21	128.02	120.20
21	V	443	VAL	CA-C-N	5.21	129.02	120.63
21	V	443	VAL	C-N-CA	5.21	129.02	120.63
25	2	261	PHE	CB-CA-C	-5.21	102.70	110.88
21	V	399	LYS	CA-C-N	5.20	124.81	119.56
21	V	399	LYS	C-N-CA	5.20	124.81	119.56
21	V	545	GLN	CA-C-N	5.20	127.25	120.28
21	V	545	GLN	C-N-CA	5.20	127.25	120.28
1	A	287	ASN	N-CA-C	5.20	116.94	111.28
22	W	153	PRO	CB-CA-C	5.20	118.17	111.46
21	V	251	PHE	N-CA-C	5.20	116.97	109.07
22	W	24	TYR	CA-C-N	5.20	127.19	120.44
22	W	24	TYR	C-N-CA	5.20	127.19	120.44
22	W	205	VAL	CA-C-N	5.20	130.28	123.11
22	W	205	VAL	C-N-CA	5.20	130.28	123.11
1	A	651	SER	N-CA-C	5.19	117.23	110.53
23	0	59	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
21	V	341	PRO	CA-C-N	5.19	129.87	122.08
21	V	341	PRO	C-N-CA	5.19	129.87	122.08
2	B	997	GLY	N-CA-C	5.19	120.80	111.62
21	V	283	ARG	NE-CZ-NH2	-5.19	114.53	119.20
21	V	252	TYR	O-C-N	-5.19	116.97	123.04
21	V	634	ARG	NE-CZ-NH1	-5.19	116.31	121.50
22	W	152	LEU	N-CA-C	5.19	121.27	109.81
2	B	388	TYR	CA-CB-CG	-5.18	104.57	113.90
21	V	678	ARG	CA-C-O	-5.18	115.06	120.55
25	2	402	ARG	N-CA-C	5.18	117.55	110.24
21	V	639	ARG	NE-CZ-NH2	5.18	123.86	119.20
22	W	707	ASN	OD1-CG-ND2	-5.18	117.42	122.60
21	V	421	TRP	CE2-CD2-CG	5.18	113.41	107.20
22	W	87	LEU	CA-C-N	5.18	127.22	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	87	LEU	C-N-CA	5.18	127.22	120.28
20	T	136	SER	CA-C-N	-5.17	115.89	122.98
20	T	136	SER	C-N-CA	-5.17	115.89	122.98
1	A	933	THR	N-CA-C	-5.17	106.92	113.18
1	A	1128	ILE	N-CA-C	5.17	115.38	110.42
22	W	399	LEU	CA-C-O	-5.17	115.38	120.70
22	W	96	LYS	N-CA-C	5.17	121.80	110.80
21	V	305	ASP	CA-C-N	5.16	131.26	121.97
21	V	305	ASP	C-N-CA	5.16	131.26	121.97
21	V	285	ILE	CA-CB-CG2	5.16	119.28	110.50
2	B	169	ARG	N-CA-C	5.16	116.98	111.36
20	T	94	THR	CA-C-N	-5.16	115.94	123.06
20	T	94	THR	C-N-CA	-5.16	115.94	123.06
21	V	366	ASN	OD1-CG-ND2	5.16	127.75	122.60
18	R	163	LEU	N-CA-C	5.15	123.82	113.31
23	O	65	VAL	CA-CB-CG1	5.15	119.15	110.40
21	V	363	VAL	CA-C-N	-5.14	115.90	123.00
21	V	363	VAL	C-N-CA	-5.14	115.90	123.00
18	R	218	LYS	CA-C-N	5.14	127.12	120.44
18	R	218	LYS	C-N-CA	5.14	127.12	120.44
22	W	538	PHE	O-C-N	5.14	129.12	123.16
21	V	628	SER	CA-C-N	5.14	131.35	121.54
21	V	628	SER	C-N-CA	5.14	131.35	121.54
2	B	866	ILE	N-CA-C	5.14	116.60	111.00
22	W	660	ALA	CA-C-N	5.14	127.67	120.28
22	W	660	ALA	C-N-CA	5.14	127.67	120.28
21	V	452	ARG	CA-CB-CG	5.13	124.36	114.10
21	V	465	GLY	CA-C-O	-5.13	115.91	120.94
21	V	344	ALA	N-CA-CB	-5.13	101.39	111.60
21	V	564	ASN	CB-CA-C	5.13	118.52	109.80
22	W	154	HIS	CG-CD2-NE2	5.13	112.33	107.20
22	W	641	ARG	CD-NE-CZ	5.13	131.58	124.40
25	2	128	ALA	CA-C-N	-5.13	115.53	123.17
25	2	128	ALA	C-N-CA	-5.13	115.53	123.17
21	V	580	ILE	O-C-N	-5.12	117.67	123.20
21	V	397	LYS	CA-CB-CG	5.12	124.33	114.10
26	3	169	ASP	CA-CB-CG	-5.12	107.48	112.60
22	W	199	ILE	O-C-N	-5.11	116.91	121.87
22	W	693	LEU	CB-CA-C	5.11	116.90	109.08
13	M	166	ILE	CB-CA-C	-5.11	105.43	111.97
21	V	357	VAL	N-CA-CB	5.11	117.49	110.54
21	V	419	ARG	CD-NE-CZ	5.11	131.56	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	69	LYS	CG-CD-CE	5.11	123.05	111.30
28	Y	27	DC	C2-N1-C1'	-5.11	112.03	119.70
2	B	780	VAL	N-CA-C	5.11	115.84	108.48
22	W	31	THR	CA-CB-CG2	5.11	119.18	110.50
21	V	680	LEU	N-CA-C	5.11	116.85	111.28
22	W	71	ILE	N-CA-C	5.11	115.83	108.48
23	O	80	ARG	CD-NE-CZ	5.11	131.55	124.40
3	C	83	GLN	N-CA-C	5.10	117.39	110.35
22	W	143	ARG	CA-CB-CG	-5.10	103.90	114.10
23	O	233	THR	CA-CB-OG1	5.10	117.25	109.60
21	V	708	GLU	O-C-N	5.10	127.52	122.12
22	W	511	ARG	CA-C-N	5.10	131.29	122.32
22	W	511	ARG	C-N-CA	5.10	131.29	122.32
5	E	64	HIS	N-CA-C	5.09	120.88	113.40
22	W	64	PRO	CA-N-CD	-5.09	104.88	112.00
22	W	98	GLU	O-C-N	-5.09	115.82	122.59
23	O	212	ALA	CA-C-N	5.09	127.36	120.44
23	O	212	ALA	C-N-CA	5.09	127.36	120.44
1	A	1117	VAL	N-CA-C	-5.09	98.76	109.34
22	W	175	TYR	CA-C-O	-5.08	115.25	121.05
22	W	260	GLN	CA-C-N	5.08	125.62	119.98
22	W	260	GLN	C-N-CA	5.08	125.62	119.98
22	W	672	THR	CA-C-N	5.08	130.72	122.53
22	W	672	THR	C-N-CA	5.08	130.72	122.53
17	Q	184	ILE	N-CA-C	5.08	115.80	110.62
19	S	103	ASN	CB-CA-C	-5.08	110.33	117.23
28	Y	21	DC	C4'-C3'-O3'	-5.08	102.39	110.00
22	W	720	PHE	CA-CB-CG	5.07	118.87	113.80
25	2	48	LEU	N-CA-C	5.07	121.02	109.81
22	W	483	MET	N-CA-CB	-5.07	102.71	110.42
23	O	234	HIS	CA-CB-CG	5.07	118.87	113.80
1	A	204	HIS	N-CA-C	5.07	121.60	110.80
22	W	170	LEU	O-C-N	-5.07	115.97	120.48
22	W	699	GLU	CB-CA-C	5.07	118.42	109.80
26	3	9	ASN	CA-CB-CG	-5.07	107.53	112.60
2	B	942	LYS	N-CA-C	-5.07	102.27	110.32
22	W	519	ASN	CA-CB-CG	5.07	117.67	112.60
22	W	205	VAL	CA-CB-CG1	5.06	119.00	110.40
23	O	207	VAL	CA-C-N	5.06	127.48	120.29
23	O	207	VAL	C-N-CA	5.06	127.48	120.29
13	M	15	CYS	CA-C-N	5.06	124.67	119.05
13	M	15	CYS	C-N-CA	5.06	124.67	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1141	VAL	N-CA-C	5.06	115.37	107.99
22	W	434	HIS	CA-C-N	5.06	131.66	123.37
22	W	434	HIS	C-N-CA	5.06	131.66	123.37
2	B	531	TYR	CA-C-N	-5.06	115.42	122.75
2	B	531	TYR	C-N-CA	-5.06	115.42	122.75
24	1	62	ASP	CA-CB-CG	-5.05	107.55	112.60
22	W	158	TYR	CA-C-N	5.05	127.55	120.28
22	W	158	TYR	C-N-CA	5.05	127.55	120.28
21	V	466	LEU	N-CA-CB	-5.05	102.07	110.80
22	W	23	SER	CB-CA-C	-5.05	102.96	110.88
21	V	634	ARG	N-CA-C	5.04	117.67	111.82
22	W	553	TYR	CB-CA-C	5.04	118.84	110.78
1	A	639	ILE	N-CA-C	5.04	116.08	109.58
21	V	543	ALA	N-CA-C	5.04	116.77	111.28
21	V	371	VAL	CA-C-N	5.03	127.44	120.29
21	V	371	VAL	C-N-CA	5.03	127.44	120.29
22	W	243	CYS	CA-C-O	-5.03	115.52	120.70
1	A	848	ILE	CB-CA-C	-5.03	105.28	112.22
24	1	3	ASN	CA-C-N	-5.03	115.13	122.58
24	1	3	ASN	C-N-CA	-5.03	115.13	122.58
21	V	252	TYR	N-CA-C	5.02	117.75	109.76
22	W	138	THR	N-CA-C	-5.02	105.80	111.28
22	W	189	TRP	NE1-CE2-CD2	-5.02	100.87	107.40
22	W	43	PRO	CA-C-N	5.02	128.63	120.60
22	W	43	PRO	C-N-CA	5.02	128.63	120.60
22	W	718	LYS	CA-C-N	5.02	127.00	120.28
22	W	718	LYS	C-N-CA	5.02	127.00	120.28
11	K	21	ILE	N-CA-C	5.02	115.07	107.75
1	A	1372	GLU	N-CA-C	5.01	116.82	111.36
2	B	205	VAL	N-CA-C	5.01	115.50	108.89
2	B	364	PHE	N-CA-C	5.01	116.74	111.28
22	W	172	ALA	CA-C-N	5.01	131.23	121.41
22	W	172	ALA	C-N-CA	5.01	131.23	121.41
23	0	106	ILE	CA-C-N	5.01	130.66	122.69
23	0	106	ILE	C-N-CA	5.01	130.66	122.69
21	V	316	LEU	CB-CA-C	-5.01	101.59	111.60
22	W	195	ALA	O-C-N	5.01	127.23	122.07
22	W	629	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (79) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	0	143	PRO	Mainchain
23	0	165	ARG	Sidechain
24	1	17	LYS	Mainchain
25	2	389	ASP	Mainchain,Sidechain
25	2	399	ASP	Sidechain
25	2	403	PHE	Mainchain,Peptide
25	2	406	GLY	Peptide
25	2	409	TYR	Sidechain
25	2	425	ALA	Mainchain
1	A	1291	ASN	Sidechain
1	A	210	GLN	Mainchain
8	H	99	ILE	Peptide
15	O	86	GLU	Sidechain
16	P	242	GLN	Sidechain
17	Q	112	ARG	Sidechain
17	Q	125	ALA	Peptide
18	R	100	ASP	Sidechain
18	R	105	GLU	Sidechain
18	R	109	LEU	Mainchain
18	R	139	PHE	Mainchain,Peptide
18	R	204	ASN	Mainchain
18	R	209	GLN	Sidechain
18	R	213	ASP	Peptide,Sidechain
18	R	215	GLU	Mainchain
18	R	222	SER	Peptide
18	R	223	VAL	Mainchain,Peptide
18	R	224	THR	Mainchain,Peptide
18	R	225	VAL	Mainchain
18	R	228	MET	Mainchain,Peptide
18	R	229	ASP	Sidechain
18	R	235	GLU	Sidechain
20	T	123	ASN	Peptide
21	V	247	ASP	Mainchain
21	V	251	PHE	Sidechain
21	V	319	TYR	Sidechain
21	V	378	PHE	Sidechain
21	V	417	THR	Peptide
21	V	427	MET	Mainchain,Peptide
21	V	489	TYR	Sidechain
21	V	503	ALA	Peptide
21	V	519	TYR	Sidechain
21	V	530	ARG	Sidechain
21	V	534	TYR	Sidechain

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Mol	Chain	Res	Type	Group
21	V	674	THR	Mainchain
21	V	676	ARG	Sidechain
21	V	679	PHE	Sidechain
21	V	703	PHE	Sidechain
22	W	104	PHE	Sidechain
22	W	175	TYR	Sidechain
22	W	197	TYR	Sidechain
22	W	206	VAL	Mainchain
22	W	208	SER	Mainchain
22	W	211	TYR	Sidechain
22	W	282	ARG	Sidechain
22	W	286	ARG	Sidechain
22	W	293	ARG	Sidechain
22	W	409	THR	Peptide
22	W	553	TYR	Sidechain
22	W	614	TYR	Sidechain
22	W	616	ARG	Sidechain
22	W	641	ARG	Sidechain
22	W	669	ARG	Sidechain
22	W	674	TYR	Sidechain
22	W	719	TYR	Sidechain
22	W	72	TYR	Sidechain
27	X	65	DG	Sidechain
27	X	66	DA	Sidechain
27	X	72	DC	Sidechain
28	Y	23	DT	Sidechain
28	Y	24	DC	Sidechain
28	Y	26	DG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11608	544	0
2	B	9317	0	9307	427	0
3	C	2213	0	2153	99	0
4	D	1062	0	1042	15	0
5	E	1723	0	1745	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	689	0	715	11	0
7	G	1351	0	1358	42	0
8	H	1205	0	1167	50	0
9	I	1013	0	930	83	0
10	J	533	0	553	41	0
11	K	937	0	959	26	0
12	L	388	0	393	27	0
13	M	2391	0	2410	166	0
14	N	930	0	888	34	0
15	O	806	0	818	25	0
16	P	1462	0	1548	54	0
17	Q	1484	0	1498	216	0
18	R	1357	0	1381	228	0
19	S	1138	0	1103	42	0
20	T	1788	0	1819	97	0
21	V	3855	0	3871	137	0
22	W	5348	0	5373	124	0
23	0	1479	0	1524	45	0
24	1	491	0	507	237	0
25	2	2196	0	2206	586	0
26	3	1526	0	1561	476	0
27	X	1710	0	941	67	0
28	Y	1681	0	932	55	0
29	Z	125	0	67	10	0
30	A	2	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	Q	1	0	0	0	0
All	All	61725	0	60377	3267	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 (3267) 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)
26:3:59:VAL:HG12	26:3:71:TYR:CD1	1.24	1.66
21:V:516:PRO:CG	24:1:15:ALA:HB3	1.21	1.65
1:A:1171:ALA:CB	9:I:59:THR:HG21	1.18	1.59
18:R:223:VAL:CG2	18:R:224:THR:HG21	1.29	1.59
21:V:315:VAL:HG13	22:W:500:ASP:CB	1.21	1.57
13:M:34:CYS:CB	13:M:39:LEU:HD23	1.28	1.56
26:3:59:VAL:CG1	26:3:71:TYR:HD1	1.15	1.56
23:0:54:ARG:HG3	26:3:182:PHE:CE1	1.42	1.55
18:R:223:VAL:CA	18:R:224:THR:HG23	1.09	1.53
25:2:31:LEU:HD11	26:3:33:THR:CB	1.39	1.52
21:V:516:PRO:HG3	24:1:15:ALA:CB	1.11	1.52
13:M:34:CYS:HB3	13:M:39:LEU:CD2	1.35	1.51
16:P:206:GLU:HB3	16:P:207:PRO:CD	1.34	1.50
1:A:202:TRP:CD1	1:A:212:LYS:HE2	1.47	1.47
1:A:1171:ALA:HB1	9:I:59:THR:CG2	1.42	1.47
21:V:315:VAL:CG1	22:W:500:ASP:HB2	1.01	1.47
18:R:223:VAL:CG2	18:R:224:THR:CG2	1.84	1.46
25:2:117:ASN:ND2	26:3:108:ASN:CB	1.76	1.46
3:C:157:GLN:NE2	10:J:65:LEU:HB3	1.29	1.45
25:2:117:ASN:HD21	26:3:108:ASN:CB	1.27	1.45
13:M:37:CYS:SG	13:M:39:LEU:HD22	1.53	1.45
21:V:321:GLU:HB3	22:W:499:ASN:CG	1.38	1.45
25:2:31:LEU:HD11	26:3:33:THR:CG2	1.42	1.44
25:2:117:ASN:CG	26:3:108:ASN:HB2	1.39	1.44
25:2:28:PRO:N	26:3:25:GLN:HA	1.29	1.43
17:Q:113:ARG:NE	18:R:222:SER:HB3	1.24	1.42
21:V:321:GLU:HB3	22:W:499:ASN:ND2	1.25	1.42
17:Q:113:ARG:HE	18:R:222:SER:CB	1.33	1.41
5:E:40:PHE:CE2	5:E:46:ASP:OD2	1.72	1.40
23:0:54:ARG:CG	26:3:182:PHE:HE1	1.35	1.38
1:A:1171:ALA:CB	9:I:59:THR:CG2	1.95	1.38
17:Q:180:PHE:CE2	18:R:213:ASP:OD1	1.76	1.37
25:2:29:GLY:N	26:3:25:GLN:HG3	1.32	1.37
18:R:223:VAL:CA	18:R:224:THR:CG2	1.75	1.36
27:X:15:DA:H61	28:Y:79:DC:N4	1.23	1.35
25:2:31:LEU:HD21	26:3:33:THR:N	1.34	1.34
17:Q:113:ARG:HD3	18:R:221:ARG:C	1.50	1.34
25:2:117:ASN:OD1	26:3:108:ASN:ND2	1.57	1.34
17:Q:188:TYR:CE2	18:R:210:PHE:CD1	2.15	1.34
25:2:30:VAL:HG23	26:3:25:GLN:CB	1.57	1.33
1:A:202:TRP:CD1	1:A:212:LYS:CE	2.11	1.33
1:A:152:ASN:O	1:A:153:ILE:CG1	1.75	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:325:ARG:NH2	22:W:499:ASN:HB3	1.02	1.32
25:2:118:LEU:CD2	26:3:39:ASP:OD1	1.75	1.32
27:X:15:DA:N6	28:Y:79:DC:H42	1.25	1.32
21:V:615:PHE:O	21:V:617:LEU:N	1.60	1.32
25:2:118:LEU:HD22	26:3:39:ASP:OD1	1.16	1.31
21:V:321:GLU:HB3	22:W:499:ASN:OD1	1.30	1.30
24:1:1:MET:O	25:2:413:LEU:HG	1.28	1.30
18:R:194:ARG:HB3	18:R:195:PRO:CD	1.57	1.30
13:M:178:LYS:O	20:T:154:LYS:HB3	1.22	1.30
18:R:194:ARG:CB	18:R:195:PRO:HD3	1.58	1.29
18:R:223:VAL:C	18:R:224:THR:HG23	1.52	1.29
25:2:28:PRO:N	26:3:25:GLN:CA	1.94	1.29
1:A:1171:ALA:CA	9:I:59:THR:CG2	2.09	1.28
21:V:321:GLU:CB	22:W:499:ASN:HD21	1.45	1.28
1:A:202:TRP:CB	1:A:212:LYS:HB3	1.64	1.28
17:Q:113:ARG:CD	18:R:221:ARG:C	2.06	1.28
21:V:325:ARG:NH2	22:W:499:ASN:CB	1.97	1.27
9:I:103:ARG:O	9:I:105:GLU:N	1.66	1.27
17:Q:21:VAL:O	18:R:210:PHE:CE2	1.87	1.26
17:Q:188:TYR:CE2	18:R:210:PHE:HD1	1.51	1.26
25:2:118:LEU:HD21	26:3:39:ASP:O	1.23	1.25
25:2:30:VAL:CG2	26:3:25:GLN:HB3	1.66	1.25
23:0:97:ASP:O	26:3:208:ASP:HB3	1.12	1.25
21:V:523:VAL:HG11	24:1:20:LEU:CD2	1.64	1.24
26:3:59:VAL:CG1	26:3:71:TYR:CD1	1.98	1.24
21:V:321:GLU:OE2	22:W:500:ASP:CB	1.85	1.24
1:A:202:TRP:CG	1:A:212:LYS:HD2	1.71	1.24
18:R:223:VAL:HB	18:R:224:THR:CB	1.68	1.24
2:B:51:ILE:O	20:T:141:LEU:HD23	1.34	1.23
13:M:34:CYS:CB	13:M:39:LEU:CD2	2.03	1.23
17:Q:113:ARG:HD3	18:R:221:ARG:O	1.36	1.23
5:E:7:THR:OG1	5:E:47:LYS:HD3	1.35	1.23
22:W:59:TYR:CZ	22:W:62:ALA:CB	2.21	1.22
21:V:321:GLU:CB	22:W:499:ASN:OD1	1.88	1.22
26:3:58:ALA:N	26:3:71:TYR:OH	1.74	1.21
21:V:674:THR:HG23	25:2:392:ARG:NH2	1.53	1.21
25:2:31:LEU:CD1	26:3:33:THR:HB	1.69	1.21
1:A:608:THR:C	1:A:610:PRO:HD2	1.66	1.21
17:Q:188:TYR:CZ	18:R:210:PHE:CD1	2.29	1.21
2:B:56:GLN:CG	20:T:140:ARG:HG3	1.68	1.20
17:Q:113:ARG:HD2	18:R:221:ARG:CB	1.70	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:180:PHE:HE2	18:R:213:ASP:OD1	1.05	1.20
22:W:209:TYR:OH	22:W:233:PHE:HA	1.37	1.20
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.71	1.19
1:A:202:TRP:HB2	1:A:212:LYS:CB	1.71	1.19
22:W:59:TYR:CZ	22:W:62:ALA:HB1	1.76	1.19
24:1:59:GLU:OE2	25:2:402:ARG:NH2	1.75	1.19
1:A:1098:PRO:O	1:A:1101:GLN:NE2	1.74	1.18
21:V:516:PRO:CG	24:1:15:ALA:CB	1.91	1.18
17:Q:188:TYR:CZ	18:R:210:PHE:HD1	1.61	1.18
26:3:66:GLU:HA	26:3:132:LEU:HD12	1.22	1.18
2:B:880:LEU:O	2:B:881:GLU:HB2	1.37	1.17
25:2:31:LEU:CD1	26:3:33:THR:CG2	2.21	1.17
2:B:225:LEU:HB3	2:B:228:SER:CB	1.73	1.17
25:2:117:ASN:ND2	26:3:108:ASN:HB2	0.85	1.16
2:B:225:LEU:CB	2:B:228:SER:HB3	1.76	1.16
10:J:63:ALA:HB3	10:J:64:PRO:HD3	1.17	1.16
21:V:325:ARG:HH22	22:W:499:ASN:CB	1.55	1.16
16:P:206:GLU:HB3	16:P:207:PRO:HD2	1.17	1.16
25:2:30:VAL:HB	26:3:25:GLN:O	1.46	1.16
26:3:57:LEU:O	26:3:71:TYR:HE2	1.28	1.16
1:A:1171:ALA:CA	9:I:59:THR:HG22	1.73	1.16
17:Q:113:ARG:CZ	18:R:222:SER:HB3	1.76	1.16
13:M:37:CYS:SG	13:M:39:LEU:CD2	2.34	1.16
24:1:2:VAL:CG1	25:2:456:LYS:HG2	1.74	1.16
21:V:613:THR:O	21:V:614:SER:HB2	1.44	1.15
25:2:211:GLN:HG3	25:2:257:SER:HB3	1.28	1.15
23:0:77:LYS:HB2	23:0:83:CYS:HB2	1.18	1.15
24:1:28:ALA:HB1	24:1:31:LYS:HD2	1.27	1.14
1:A:206:ASN:O	1:A:207:GLU:CB	1.92	1.14
5:E:47:LYS:HB3	5:E:48:PRO:HD3	1.23	1.14
17:Q:23:ARG:NH2	18:R:207:SER:O	1.78	1.14
8:H:107:GLU:O	8:H:108:ALA:O	1.66	1.14
16:P:206:GLU:CB	16:P:207:PRO:CD	2.25	1.14
24:1:1:MET:CG	25:2:413:LEU:HB3	1.76	1.14
2:B:56:GLN:HG2	20:T:140:ARG:CG	1.77	1.13
21:V:321:GLU:CB	22:W:499:ASN:ND2	2.05	1.13
22:W:419:GLU:HB3	22:W:420:PRO:CD	1.77	1.13
21:V:516:PRO:HB3	24:1:15:ALA:HB1	1.25	1.13
24:1:2:VAL:HG13	25:2:422:LEU:HD11	1.20	1.13
26:3:59:VAL:N	26:3:71:TYR:CE1	2.15	1.13
1:A:265:VAL:C	1:A:272:ASN:CG	2.17	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:59:TYR:CE2	22:W:62:ALA:CB	2.32	1.12
23:O:54:ARG:CG	26:3:182:PHE:CE1	2.17	1.13
25:2:28:PRO:N	26:3:25:GLN:C	2.07	1.12
1:A:156:GLY:HA2	1:A:181:HIS:ND1	1.62	1.12
16:P:206:GLU:HB3	16:P:207:PRO:HD3	1.18	1.12
24:1:13:ASP:CG	24:1:14:PRO:HD2	1.74	1.12
24:1:9:LEU:HD13	24:1:48:GLU:HA	1.32	1.12
26:3:33:THR:HG23	26:3:36:LYS:H	1.13	1.12
1:A:426:ARG:O	13:M:40:VAL:HG22	1.49	1.12
2:B:225:LEU:HD13	2:B:228:SER:OG	1.49	1.12
2:B:133:ILE:HG23	2:B:139:GLN:HG2	1.29	1.11
26:3:57:LEU:C	26:3:71:TYR:OH	1.93	1.11
17:Q:113:ARG:NE	18:R:222:SER:CB	1.97	1.11
17:Q:184:ILE:HD11	18:R:213:ASP:CG	1.76	1.11
24:1:5:LEU:CD2	25:2:408:LEU:HD13	1.80	1.11
17:Q:187:ILE:HG21	18:R:211:SER:HA	1.20	1.10
17:Q:187:ILE:HG22	18:R:210:PHE:O	1.49	1.10
18:R:194:ARG:O	18:R:196:ASP:N	1.84	1.10
18:R:223:VAL:CG1	18:R:224:THR:CG2	2.30	1.10
17:Q:188:TYR:OH	18:R:210:PHE:CE1	2.02	1.10
25:2:31:LEU:CD1	26:3:33:THR:CB	2.27	1.10
25:2:42:LEU:HD21	25:2:55:TRP:HB2	1.20	1.10
25:2:192:GLU:HG3	25:2:193:PRO:HD2	1.33	1.10
3:C:157:GLN:CD	10:J:65:LEU:HB3	1.76	1.09
21:V:315:VAL:CG1	22:W:500:ASP:CB	1.94	1.09
24:1:2:VAL:HG11	25:2:456:LYS:CG	1.81	1.09
24:1:5:LEU:HD11	25:2:408:LEU:HB3	1.17	1.09
1:A:118:LEU:HD21	1:A:151:LYS:O	1.48	1.09
1:A:206:ASN:O	1:A:207:GLU:HB2	1.34	1.09
1:A:426:ARG:HB3	13:M:40:VAL:HG21	1.31	1.09
2:B:879:GLU:O	2:B:880:LEU:HB2	1.32	1.09
25:2:160:LEU:HD23	25:2:206:LEU:HD21	1.25	1.09
17:Q:113:ARG:NH1	18:R:218:LYS:O	1.86	1.09
21:V:321:GLU:OE2	22:W:500:ASP:HB3	0.91	1.09
24:1:18:GLN:HB2	24:1:44:PHE:CE2	1.86	1.09
25:2:31:LEU:HD11	26:3:33:THR:HB	1.15	1.09
26:3:137:LEU:HB3	26:3:180:VAL:HG11	1.34	1.09
21:V:516:PRO:CB	24:1:15:ALA:HB1	1.81	1.08
26:3:59:VAL:HB	26:3:71:TYR:CE1	1.89	1.08
25:2:171:VAL:HG22	25:2:213:TRP:HA	1.27	1.08
2:B:225:LEU:CB	2:B:228:SER:CB	2.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:159:VAL:HG13	25:2:161:HIS:H	1.16	1.08
8:H:64:LEU:HB3	8:H:84:ARG:HD3	1.14	1.08
25:2:163:MET:HE2	25:2:206:LEU:HD12	1.30	1.08
1:A:152:ASN:O	1:A:153:ILE:HG12	0.91	1.08
8:H:64:LEU:HB3	8:H:84:ARG:CD	1.84	1.08
17:Q:188:TYR:OH	18:R:210:PHE:CD1	2.07	1.08
24:1:5:LEU:HD21	25:2:408:LEU:CD1	1.82	1.08
1:A:202:TRP:CD1	1:A:212:LYS:HD2	1.89	1.07
26:3:49:LEU:HB3	26:3:101:TYR:HB3	1.14	1.07
26:3:59:VAL:HG13	26:3:70:LEU:HB2	1.27	1.07
24:1:2:VAL:HG11	25:2:456:LYS:HG2	1.09	1.07
1:A:1171:ALA:HA	9:I:59:THR:HG22	1.08	1.06
2:B:225:LEU:HB3	2:B:228:SER:HB2	1.32	1.06
23:0:97:ASP:O	26:3:208:ASP:CB	2.02	1.06
22:W:424:ARG:O	22:W:425:THR:HG23	1.52	1.06
1:A:202:TRP:CD1	1:A:212:LYS:CD	2.37	1.06
23:0:54:ARG:HB2	26:3:209:ILE:HG23	1.36	1.06
1:A:203:LYS:O	1:A:204:HIS:HB2	1.39	1.06
1:A:1117:VAL:O	1:A:1119:LEU:N	1.87	1.06
1:A:131:ALA:O	1:A:133:SER:N	1.87	1.06
25:2:234:LEU:HD21	25:2:237:LEU:HD12	1.36	1.06
24:1:1:MET:CB	25:2:413:LEU:HB3	1.86	1.05
22:W:419:GLU:CB	22:W:420:PRO:HD2	1.78	1.05
21:V:674:THR:HG23	25:2:392:ARG:CZ	1.85	1.05
17:Q:184:ILE:HD13	18:R:211:SER:HB2	1.36	1.04
24:1:4:VAL:HG12	25:2:411:GLN:O	1.55	1.04
26:3:57:LEU:O	26:3:71:TYR:CE2	2.10	1.04
18:R:194:ARG:CB	18:R:195:PRO:CD	2.20	1.04
17:Q:110:MET:HG2	18:R:222:SER:HB2	1.08	1.04
1:A:609:HIS:N	1:A:610:PRO:HD2	1.72	1.03
25:2:28:PRO:CD	26:3:25:GLN:HA	1.88	1.03
1:A:1116:ASN:HD21	1:A:1138:SER:HB3	1.20	1.03
13:M:179:GLU:HA	20:T:154:LYS:HG2	1.38	1.03
16:P:297:LYS:CB	16:P:298:PRO:CD	2.34	1.03
17:Q:187:ILE:HG21	18:R:211:SER:CA	1.88	1.03
24:1:5:LEU:HD12	25:2:409:TYR:O	1.56	1.03
25:2:81:LYS:HE3	25:2:93:LEU:HD21	1.40	1.03
17:Q:113:ARG:HD2	18:R:221:ARG:HB2	1.32	1.03
21:V:523:VAL:HG11	24:1:20:LEU:HD21	1.06	1.03
13:M:94:ASP:OD2	13:M:97:GLY:O	1.76	1.02
1:A:273:GLN:O	1:A:274:ASP:O	1.76	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:54:ARG:CD	26:3:182:PHE:HE1	1.72	1.02
23:0:54:ARG:NE	26:3:182:PHE:CE1	2.26	1.02
25:2:31:LEU:HD11	26:3:33:THR:HG22	1.37	1.02
3:C:157:GLN:NE2	10:J:65:LEU:CB	2.23	1.02
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.06	1.02
17:Q:188:TYR:CE1	18:R:211:SER:HB3	1.93	1.02
21:V:516:PRO:CB	24:1:15:ALA:CB	2.37	1.02
21:V:315:VAL:HG11	22:W:500:ASP:HB2	1.42	1.01
25:2:199:ALA:HB3	25:2:202:GLN:HE22	1.22	1.01
13:M:178:LYS:O	20:T:154:LYS:CB	2.07	1.01
26:3:196:LEU:HD21	26:3:223:LEU:HD23	1.42	1.01
22:W:59:TYR:CE2	22:W:62:ALA:HB3	1.94	1.01
13:M:46:ILE:O	13:M:47:ASP:HB2	1.54	1.01
21:V:515:SER:HB3	21:V:539:ASN:HD21	1.26	1.01
26:3:59:VAL:CB	26:3:71:TYR:CE1	2.44	1.01
2:B:875:GLU:O	2:B:876:ASN:HB2	1.57	1.00
13:M:94:ASP:HB2	13:M:99:SER:H	1.26	1.00
22:W:419:GLU:HB3	22:W:420:PRO:HD2	1.03	1.00
24:1:34:ILE:HG12	24:1:50:VAL:HG11	1.39	1.00
1:A:1171:ALA:HB2	9:I:59:THR:HG21	1.41	1.00
26:3:58:ALA:CA	26:3:71:TYR:CZ	2.44	1.00
1:A:67:ARG:NH2	13:M:45:VAL:O	1.94	1.00
16:P:298:PRO:O	16:P:300:ILE:HG12	1.61	1.00
17:Q:20:TYR:O	18:R:210:PHE:CD2	2.14	1.00
9:I:59:THR:O	9:I:60:HIS:CG	2.14	1.00
17:Q:105:TYR:OH	18:R:234:GLU:OE1	1.80	1.00
1:A:265:VAL:N	1:A:272:ASN:CB	2.25	1.00
2:B:225:LEU:HB2	2:B:228:SER:HB3	1.39	1.00
17:Q:113:ARG:CD	18:R:222:SER:N	2.25	1.00
26:3:59:VAL:HB	26:3:71:TYR:HE1	1.24	1.00
1:A:211:GLU:O	1:A:212:LYS:HB2	1.62	0.99
16:P:206:GLU:CB	16:P:207:PRO:HD3	1.88	0.99
1:A:263:ALA:O	1:A:265:VAL:N	1.96	0.99
25:2:117:ASN:CG	26:3:108:ASN:CB	2.20	0.99
22:W:209:TYR:OH	22:W:233:PHE:CA	2.09	0.99
2:B:225:LEU:O	2:B:227:ASN:N	1.94	0.99
26:3:148:ASN:HB2	26:3:157:MET:HE2	1.42	0.99
18:R:223:VAL:CG1	18:R:224:THR:HG21	1.93	0.99
13:M:94:ASP:CB	13:M:99:SER:H	1.76	0.99
1:A:1171:ALA:HA	9:I:59:THR:CG2	1.80	0.98
10:J:63:ALA:CB	10:J:64:PRO:HD3	1.89	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:1:MET:HE1	25:2:440:LEU:HD13	1.44	0.98
1:A:79:THR:HG21	13:M:43:ASP:HB2	1.46	0.98
25:2:196:ILE:HD11	25:2:210:ALA:HB2	1.45	0.98
1:A:133:SER:O	1:A:135:GLY:N	1.94	0.98
17:Q:188:TYR:HE2	18:R:210:PHE:CD1	1.76	0.98
25:2:100:LEU:HD11	25:2:119:ARG:HG3	1.46	0.98
25:2:118:LEU:CD2	26:3:39:ASP:O	2.12	0.98
22:W:584:TYR:CD1	22:W:594:ALA:HB2	1.99	0.98
13:M:34:CYS:HB3	13:M:39:LEU:CG	1.94	0.98
5:E:47:LYS:CB	5:E:48:PRO:HD3	1.94	0.97
13:M:34:CYS:SG	13:M:39:LEU:HD23	2.02	0.97
25:2:29:GLY:N	26:3:25:GLN:CG	2.27	0.97
26:3:165:LYS:HD2	26:3:195:VAL:HG22	1.44	0.97
18:R:223:VAL:HG21	18:R:224:THR:HG21	1.47	0.97
1:A:1116:ASN:O	1:A:1117:VAL:HG23	1.64	0.97
1:A:265:VAL:O	1:A:272:ASN:OD1	1.81	0.97
17:Q:113:ARG:CZ	18:R:218:LYS:O	2.13	0.97
23:0:77:LYS:CB	23:0:83:CYS:HB2	1.95	0.97
25:2:176:ALA:HB1	25:2:178:LEU:HD13	1.47	0.97
1:A:265:VAL:N	1:A:272:ASN:HB3	1.76	0.97
17:Q:180:PHE:CE2	18:R:213:ASP:CG	2.27	0.97
13:M:34:CYS:CB	13:M:39:LEU:CG	2.42	0.96
26:3:173:GLN:HA	26:3:176:ASN:HD21	1.28	0.96
17:Q:184:ILE:HD12	18:R:218:LYS:NZ	1.81	0.96
26:3:59:VAL:CB	26:3:71:TYR:CD1	2.48	0.96
22:W:59:TYR:CE1	22:W:62:ALA:HB1	2.01	0.96
23:0:77:LYS:HA	23:0:77:LYS:HE3	1.43	0.96
26:3:133:LEU:HD23	26:3:177:PHE:CD1	2.01	0.96
1:A:156:GLY:HA2	1:A:181:HIS:CG	2.01	0.96
21:V:321:GLU:CA	22:W:499:ASN:HD21	1.78	0.96
18:R:163:LEU:O	18:R:164:GLY:C	2.05	0.95
21:V:612:ASP:OD2	21:V:635:GLN:OE1	1.83	0.95
22:W:209:TYR:HH	22:W:233:PHE:HA	1.30	0.95
25:2:118:LEU:HD11	26:3:43:VAL:CG2	1.95	0.95
25:2:211:GLN:HA	25:2:261:PHE:CZ	2.01	0.95
24:1:13:ASP:OD2	24:1:17:LYS:HB3	1.65	0.95
25:2:29:GLY:CA	26:3:25:GLN:HG3	1.95	0.95
21:V:631:GLY:O	21:V:632:SER:CB	2.14	0.95
1:A:79:THR:CG2	13:M:43:ASP:HB2	1.96	0.94
24:1:1:MET:HB3	25:2:413:LEU:CG	1.98	0.94
25:2:35:TYR:CE1	25:2:62:LEU:HG	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:2:VAL:CG1	25:2:422:LEU:HD11	1.96	0.94
25:2:117:ASN:N	26:3:104:LEU:HD21	1.83	0.94
13:M:34:CYS:HB2	13:M:39:LEU:HG	1.49	0.94
17:Q:113:ARG:NE	18:R:222:SER:CA	2.31	0.94
2:B:51:ILE:O	20:T:141:LEU:CD2	2.15	0.94
18:R:194:ARG:C	18:R:196:ASP:H	1.71	0.94
1:A:47:THR:O	1:A:48:GLU:HG2	1.68	0.94
17:Q:24:GLY:N	18:R:210:PHE:CD2	2.35	0.94
21:V:325:ARG:HH21	22:W:499:ASN:HB3	1.19	0.94
25:2:31:LEU:CD2	26:3:33:THR:N	2.30	0.94
17:Q:187:ILE:CG2	18:R:210:PHE:O	2.15	0.93
26:3:133:LEU:HD13	26:3:133:LEU:H	1.33	0.93
21:V:515:SER:CB	21:V:539:ASN:HD21	1.80	0.93
17:Q:24:GLY:CA	18:R:210:PHE:CE2	2.51	0.93
1:A:1116:ASN:ND2	1:A:1138:SER:CB	2.30	0.93
2:B:879:GLU:O	2:B:880:LEU:CB	2.16	0.93
9:I:59:THR:O	9:I:60:HIS:CB	2.17	0.93
24:1:8:VAL:HG11	24:1:45:VAL:CG1	1.99	0.93
17:Q:113:ARG:HE	18:R:222:SER:CA	1.82	0.93
25:2:177:GLN:HA	25:2:220:LEU:CD2	1.99	0.93
17:Q:24:GLY:HA3	18:R:210:PHE:CD2	2.04	0.93
17:Q:110:MET:HG2	18:R:222:SER:CB	1.98	0.93
2:B:133:ILE:O	2:B:134:LYS:O	1.86	0.92
1:A:202:TRP:HD1	1:A:212:LYS:HE2	0.83	0.92
25:2:29:GLY:H	26:3:25:GLN:CG	1.83	0.92
24:1:9:LEU:HD22	24:1:51:ASN:HD22	1.34	0.92
26:3:11:LEU:HD22	26:3:160:ARG:HG2	1.51	0.92
26:3:187:GLN:HG3	26:3:189:ILE:HG12	1.51	0.92
18:R:223:VAL:HG23	18:R:224:THR:CG2	1.98	0.92
26:3:190:LEU:HA	26:3:210:THR:HG22	1.50	0.92
21:V:516:PRO:HA	24:1:15:ALA:O	1.67	0.92
5:E:47:LYS:HB3	5:E:48:PRO:CD	1.97	0.92
1:A:426:ARG:O	13:M:40:VAL:CG2	2.17	0.92
24:1:18:GLN:HB2	24:1:44:PHE:HE2	1.26	0.92
25:2:118:LEU:HD22	26:3:39:ASP:CG	1.94	0.92
26:3:165:LYS:HE3	26:3:200:SER:CB	2.00	0.92
14:N:319:ASP:O	14:N:321:SER:N	2.03	0.91
25:2:118:LEU:HD23	26:3:42:MET:HB2	1.50	0.91
1:A:265:VAL:H	1:A:272:ASN:HB3	1.30	0.91
20:T:142:SER:OG	20:T:143:GLN:OE1	1.87	0.91
25:2:159:VAL:HG22	25:2:160:LEU:HD12	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:24:GLY:N	18:R:210:PHE:CE2	2.38	0.91
17:Q:188:TYR:CE2	18:R:210:PHE:CE1	2.58	0.91
1:A:265:VAL:HA	1:A:272:ASN:HB2	1.52	0.91
1:A:202:TRP:CG	1:A:212:LYS:CD	2.52	0.91
22:W:59:TYR:CE1	22:W:62:ALA:CB	2.52	0.91
25:2:81:LYS:HD2	25:2:89:LEU:HD21	1.52	0.91
26:3:58:ALA:C	26:3:71:TYR:CZ	2.49	0.91
17:Q:109:HIS:CE1	18:R:225:VAL:HG21	2.05	0.91
17:Q:184:ILE:HD11	18:R:213:ASP:OD2	1.68	0.91
1:A:265:VAL:CA	1:A:272:ASN:CB	2.49	0.90
16:P:206:GLU:O	16:P:208:ARG:N	2.01	0.90
17:Q:113:ARG:HH22	18:R:218:LYS:HG2	1.34	0.90
25:2:81:LYS:CE	25:2:93:LEU:HD21	2.00	0.90
23:0:98:GLN:OE1	26:3:209:ILE:HA	1.70	0.90
2:B:880:LEU:O	2:B:881:GLU:CB	2.15	0.90
5:E:46:ASP:O	5:E:47:LYS:HB2	1.71	0.90
1:A:133:SER:C	1:A:135:GLY:H	1.79	0.90
18:R:223:VAL:CB	18:R:224:THR:CG2	0.90	0.90
17:Q:58:GLN:OE1	18:R:194:ARG:HD2	1.71	0.90
17:Q:110:MET:CG	18:R:222:SER:HB2	1.99	0.90
23:0:54:ARG:HG3	26:3:182:PHE:CZ	2.05	0.90
23:0:97:ASP:OD1	26:3:208:ASP:OD1	1.88	0.90
1:A:265:VAL:CA	1:A:272:ASN:CG	2.35	0.90
26:3:137:LEU:CB	26:3:180:VAL:HG11	2.01	0.90
2:B:132:VAL:HG23	2:B:141:GLN:HG3	1.54	0.90
1:A:202:TRP:HE3	1:A:212:LYS:O	1.54	0.90
1:A:426:ARG:CB	13:M:40:VAL:HG21	2.02	0.90
17:Q:188:TYR:CE1	18:R:211:SER:CB	2.55	0.90
25:2:160:LEU:HB3	25:2:206:LEU:HD11	1.53	0.90
22:W:430:ASN:HB3	22:W:431:PRO:HD2	1.54	0.89
1:A:1098:PRO:C	1:A:1101:GLN:HE21	1.80	0.89
17:Q:113:ARG:HD2	18:R:221:ARG:C	1.90	0.89
21:V:315:VAL:HG13	22:W:500:ASP:CA	2.03	0.89
24:1:8:VAL:HG11	24:1:45:VAL:HG13	1.55	0.89
26:3:165:LYS:HG3	26:3:203:LEU:HD12	1.52	0.89
1:A:265:VAL:O	1:A:272:ASN:CG	2.14	0.89
24:1:47:ALA:CB	24:1:50:VAL:HB	2.03	0.89
3:C:132:SER:HB3	3:C:147:ASP:HB2	1.54	0.89
26:3:177:PHE:CD2	26:3:181:ILE:HD11	2.08	0.89
9:I:103:ARG:C	9:I:105:GLU:H	1.80	0.89
1:A:1171:ALA:HB1	9:I:59:THR:HG23	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:ASN:HB3	3:C:7:PRO:HD3	1.55	0.89
1:A:926:ASN:OD1	1:A:931:ARG:HG2	1.71	0.89
1:A:1307:VAL:HG11	1:A:1339:ASP:HB3	1.52	0.88
26:3:58:ALA:HA	26:3:71:TYR:CE2	2.08	0.88
24:1:4:VAL:HG11	25:2:412:PHE:HD2	1.36	0.88
3:C:157:GLN:HE21	10:J:65:LEU:HB3	1.07	0.88
21:V:615:PHE:O	21:V:616:ASP:C	2.16	0.88
26:3:70:LEU:HD13	26:3:115:ILE:HD11	1.55	0.88
26:3:71:TYR:CD2	26:3:72:PRO:HD2	2.08	0.88
26:3:177:PHE:CE2	26:3:181:ILE:HD11	2.08	0.88
25:2:117:ASN:CB	26:3:42:MET:CE	2.51	0.88
5:E:40:PHE:HE2	5:E:46:ASP:OD2	1.52	0.88
13:M:94:ASP:HB2	13:M:97:GLY:O	1.74	0.88
25:2:163:MET:SD	25:2:196:ILE:HG21	2.14	0.88
1:A:265:VAL:C	1:A:272:ASN:ND2	2.30	0.88
16:P:159:SER:HB3	16:P:329:TYR:CE2	2.08	0.88
17:Q:101:ASN:C	17:Q:103:VAL:H	1.81	0.88
24:1:1:MET:HB3	25:2:413:LEU:CB	2.04	0.88
1:A:929:ALA:O	1:A:931:ARG:N	2.06	0.88
24:1:1:MET:O	25:2:413:LEU:CG	2.21	0.88
25:2:243:SER:CB	25:2:258:LEU:HD22	2.04	0.88
24:1:28:ALA:CB	24:1:31:LYS:HD2	2.04	0.87
25:2:118:LEU:HD11	26:3:43:VAL:HG22	1.56	0.87
25:2:160:LEU:CB	25:2:206:LEU:HD11	2.04	0.87
1:A:265:VAL:HA	1:A:272:ASN:CB	2.04	0.87
5:E:49:SER:O	5:E:52:ARG:NH1	2.07	0.87
17:Q:187:ILE:HD13	18:R:211:SER:HA	1.57	0.87
1:A:609:HIS:N	1:A:610:PRO:CD	2.37	0.87
2:B:549:SER:HG	2:B:577:HIS:HE2	1.19	0.87
21:V:523:VAL:CG1	24:1:20:LEU:CD2	2.53	0.87
25:2:160:LEU:CA	25:2:206:LEU:HD11	2.04	0.87
26:3:59:VAL:CG1	26:3:70:LEU:HB2	2.03	0.87
24:1:2:VAL:HG13	25:2:422:LEU:CD1	2.03	0.87
25:2:218:GLN:HB3	25:2:264:HIS:CD2	2.08	0.87
2:B:716:HIS:HD2	2:B:982:ILE:HG13	1.38	0.87
8:H:66:GLU:O	8:H:67:ASP:HB2	1.72	0.87
25:2:224:GLN:HB2	25:2:268:PHE:CZ	2.10	0.87
5:E:15:LYS:NZ	5:E:35:GLN:O	2.07	0.87
17:Q:21:VAL:C	18:R:210:PHE:CE2	2.52	0.87
22:W:37:HIS:CE1	22:W:454:VAL:HG13	2.09	0.87
22:W:59:TYR:CG	22:W:62:ALA:HB2	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:28:PRO:HD2	26:3:25:GLN:NE2	1.89	0.87
25:2:160:LEU:CD2	25:2:206:LEU:HD21	2.04	0.87
17:Q:21:VAL:O	18:R:210:PHE:HE2	1.36	0.87
24:1:1:MET:HB3	25:2:413:LEU:HB3	1.52	0.87
25:2:45:PHE:HB2	25:2:51:LEU:HD13	1.56	0.87
25:2:117:ASN:OD1	26:3:108:ASN:CB	2.23	0.87
13:M:46:ILE:O	13:M:47:ASP:CB	2.21	0.87
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.09	0.86
25:2:138:PRO:HG3	25:2:189:GLU:HG3	1.57	0.86
25:2:29:GLY:H	26:3:25:GLN:HG3	1.12	0.86
2:B:225:LEU:C	2:B:227:ASN:H	1.81	0.86
5:E:41:LYS:HA	5:E:46:ASP:HB2	1.56	0.86
26:3:64:ILE:HG13	26:3:123:ASP:HB3	1.57	0.86
1:A:1116:ASN:ND2	1:A:1138:SER:HB3	1.89	0.86
25:2:221:GLN:HG2	25:2:268:PHE:CZ	2.11	0.86
21:V:516:PRO:CG	24:1:15:ALA:HB1	1.96	0.86
26:3:178:MET:HE2	26:3:202:LEU:CD1	2.05	0.86
14:N:313:PRO:HG2	16:P:235:ARG:HH22	1.41	0.86
20:T:154:LYS:HD2	20:T:154:LYS:H	1.41	0.86
17:Q:188:TYR:HE1	18:R:211:SER:CB	1.89	0.86
25:2:117:ASN:OD1	26:3:108:ASN:CG	2.18	0.86
26:3:69:PHE:CZ	26:3:139:LYS:HB3	2.10	0.86
1:A:1114:ALA:HB2	1:A:1309:MET:HE1	1.56	0.86
25:2:48:LEU:HB3	25:2:49:PRO:HD3	1.57	0.86
26:3:165:LYS:HE3	26:3:200:SER:HB2	1.56	0.86
26:3:190:LEU:HA	26:3:210:THR:CG2	2.05	0.86
21:V:316:LEU:HB2	21:V:321:GLU:HG3	1.58	0.85
25:2:81:LYS:CD	25:2:89:LEU:HD21	2.05	0.85
26:3:160:ARG:HB3	26:3:190:LEU:HD21	1.57	0.85
21:V:631:GLY:O	21:V:632:SER:HB2	1.76	0.85
25:2:218:GLN:HB3	25:2:264:HIS:HD2	1.38	0.85
22:W:59:TYR:CD2	22:W:62:ALA:HB2	2.11	0.85
25:2:118:LEU:CD2	26:3:42:MET:HB2	2.06	0.85
25:2:171:VAL:HG22	25:2:213:TRP:CA	2.06	0.85
1:A:890:ARG:HH21	1:A:1023:VAL:HG13	1.42	0.85
23:O:77:LYS:HB2	23:O:83:CYS:CB	2.04	0.85
24:1:1:MET:SD	25:2:415:GLN:O	2.34	0.85
25:2:177:GLN:HA	25:2:220:LEU:HD21	1.56	0.85
26:3:14:VAL:HG21	26:3:163:VAL:HG22	1.57	0.85
26:3:59:VAL:HG12	26:3:71:TYR:CG	2.07	0.85
2:B:880:LEU:HD12	2:B:881:GLU:OE1	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:24:GLY:CA	18:R:210:PHE:CD2	2.59	0.85
17:Q:113:ARG:HE	18:R:222:SER:HB3	0.68	0.85
2:B:874:PRO:O	2:B:876:ASN:N	2.09	0.85
25:2:81:LYS:CD	25:2:93:LEU:HD21	2.07	0.85
26:3:178:MET:HE2	26:3:202:LEU:HD12	1.57	0.85
1:A:79:THR:HG21	13:M:43:ASP:CB	2.06	0.85
26:3:59:VAL:HG11	26:3:71:TYR:HD1	1.39	0.85
26:3:124:ILE:HD13	26:3:125:LYS:N	1.91	0.85
1:A:202:TRP:CE3	1:A:212:LYS:O	2.30	0.84
3:C:157:GLN:CG	10:J:65:LEU:CB	2.55	0.84
5:E:3:ASP:O	5:E:47:LYS:HE3	1.77	0.84
25:2:31:LEU:CD1	26:3:33:THR:HG22	1.96	0.84
25:2:167:PRO:O	25:2:171:VAL:HG23	1.76	0.84
1:A:1116:ASN:HD21	1:A:1138:SER:CB	1.89	0.84
1:A:1307:VAL:HG11	1:A:1339:ASP:CB	2.07	0.84
24:1:2:VAL:CG1	25:2:422:LEU:CD1	2.55	0.84
26:3:100:LYS:HB3	26:3:103:LEU:HD13	1.58	0.84
26:3:184:ALA:HA	26:3:187:GLN:HG2	1.57	0.84
1:A:1117:VAL:C	1:A:1119:LEU:H	1.86	0.84
17:Q:113:ARG:NH2	18:R:222:SER:HB3	1.92	0.84
2:B:250:SER:O	2:B:251:ALA:CB	2.25	0.84
12:L:26:ASN:HB2	12:L:44:MET:HE2	1.59	0.84
17:Q:20:TYR:O	18:R:210:PHE:HD2	1.57	0.84
25:2:160:LEU:HD23	25:2:206:LEU:CD2	2.07	0.84
25:2:176:ALA:CB	25:2:178:LEU:HD13	2.07	0.84
25:2:211:GLN:HG3	25:2:257:SER:CB	2.05	0.84
23:0:79:ASN:O	23:0:81:LEU:N	2.10	0.84
25:2:159:VAL:HG22	25:2:160:LEU:H	1.41	0.84
25:2:229:ASP:O	25:2:233:ILE:HG12	1.78	0.84
24:1:52:VAL:HG23	24:1:53:LEU:HD12	1.59	0.83
25:2:118:LEU:HD12	25:2:119:ARG:N	1.92	0.83
26:3:49:LEU:CB	26:3:101:TYR:HB3	2.05	0.83
26:3:58:ALA:C	26:3:71:TYR:CE1	2.57	0.83
8:H:107:GLU:O	8:H:108:ALA:C	2.18	0.83
25:2:159:VAL:HG22	25:2:160:LEU:CD1	2.08	0.83
1:A:1246:ILE:HD11	1:A:1258:ARG:HD2	1.60	0.83
25:2:78:GLU:O	25:2:81:LYS:HG2	1.77	0.83
2:B:56:GLN:HG2	20:T:140:ARG:HG3	0.85	0.83
5:E:52:ARG:HH21	5:E:54:ARG:CG	1.90	0.83
19:S:31:PHE:HB2	20:T:92:THR:HB	1.60	0.83
21:V:366:ASN:HD21	21:V:613:THR:HG22	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:118:LEU:CD2	26:3:39:ASP:HA	2.08	0.83
26:3:57:LEU:HD23	26:3:58:ALA:N	1.91	0.83
21:V:321:GLU:HB2	22:W:499:ASN:OD1	1.77	0.83
25:2:57:MET:HA	25:2:60:LEU:CD1	2.09	0.83
25:2:86:SER:HB3	25:2:140:LYS:HE2	1.60	0.83
24:1:9:LEU:HB2	24:1:51:ASN:HD21	1.44	0.82
2:B:61:ASP:HB3	2:B:63:PRO:HD3	1.61	0.82
2:B:803:ARG:NH2	3:C:177:ASN:OD1	2.10	0.82
18:R:223:VAL:HB	18:R:224:THR:CG2	0.49	0.82
24:1:9:LEU:CD1	24:1:48:GLU:HA	2.09	0.82
2:B:289:ILE:HG12	2:B:297:MET:HG2	1.61	0.82
25:2:221:GLN:NE2	25:2:230:LEU:HB2	1.93	0.82
25:2:259:LEU:HD12	25:2:260:ASN:N	1.94	0.82
24:1:47:ALA:HB2	24:1:50:VAL:HB	1.61	0.82
26:3:12:VAL:HG21	26:3:161:ILE:HG12	1.61	0.82
17:Q:21:VAL:O	18:R:210:PHE:CZ	2.32	0.82
25:2:174:ASP:O	25:2:220:LEU:HD23	1.79	0.82
5:E:52:ARG:HH21	5:E:54:ARG:HG2	1.45	0.82
17:Q:113:ARG:HD3	18:R:222:SER:N	1.90	0.82
25:2:160:LEU:O	25:2:164:VAL:HG23	1.79	0.82
26:3:49:LEU:HB3	26:3:101:TYR:CB	2.05	0.82
17:Q:105:TYR:CZ	18:R:234:GLU:OE1	2.33	0.82
17:Q:113:ARG:HD2	18:R:221:ARG:CA	2.10	0.82
26:3:196:LEU:HD21	26:3:223:LEU:CD2	2.09	0.82
24:1:52:VAL:CG2	24:1:53:LEU:HD12	2.09	0.82
1:A:623:PRO:O	1:A:625:ASP:N	2.12	0.82
21:V:523:VAL:HG11	24:1:20:LEU:HD23	1.62	0.82
1:A:266:MET:HG2	1:A:272:ASN:OD1	1.79	0.81
1:A:269:SER:O	1:A:270:ALA:HB3	1.79	0.81
2:B:92:TYR:CB	20:T:145:LEU:HD12	2.10	0.81
2:B:957:THR:O	2:B:960:GLY:N	2.10	0.81
9:I:14:ILE:HG13	9:I:16:PHE:CZ	2.14	0.81
24:1:59:GLU:OE1	25:2:402:ARG:NH1	2.13	0.81
25:2:221:GLN:OE1	25:2:224:GLN:HA	1.80	0.81
26:3:12:VAL:CG2	26:3:161:ILE:HG12	2.10	0.81
1:A:156:GLY:CA	1:A:181:HIS:ND1	2.43	0.81
1:A:659:GLU:OE1	1:A:985:ARG:NH1	2.13	0.81
2:B:92:TYR:HB2	20:T:145:LEU:HD12	1.61	0.81
5:E:126:ILE:HD13	5:E:186:LYS:HE3	1.60	0.81
12:L:26:ASN:HB2	12:L:44:MET:CE	2.09	0.81
21:V:315:VAL:HG12	22:W:500:ASP:HB2	1.54	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:100:LEU:HG	25:2:119:ARG:HE	1.45	0.81
18:R:195:PRO:O	18:R:196:ASP:HB2	1.81	0.81
2:B:133:ILE:HG23	2:B:139:GLN:CG	2.09	0.81
21:V:674:THR:CG2	25:2:392:ARG:CZ	2.59	0.81
17:Q:112:ARG:NH2	18:R:237:LEU:HB2	1.95	0.81
22:W:59:TYR:CD1	22:W:62:ALA:HB2	2.16	0.81
26:3:216:LYS:H	26:3:216:LYS:HD2	1.43	0.81
25:2:37:HIS:HB3	25:2:38:PRO:HD3	1.61	0.81
25:2:174:ASP:OD1	25:2:179:LEU:HD12	1.80	0.81
25:2:175:LEU:HB3	25:2:216:MET:SD	2.20	0.81
25:2:251:VAL:HG11	25:2:254:MET:HG3	1.62	0.81
3:C:6:GLN:N	3:C:7:PRO:HD3	1.95	0.81
3:C:157:GLN:CG	10:J:65:LEU:HB3	2.10	0.81
17:Q:24:GLY:H	18:R:210:PHE:HD2	1.28	0.81
21:V:516:PRO:HA	24:1:15:ALA:C	2.05	0.81
25:2:177:GLN:CD	25:2:220:LEU:HD22	2.06	0.81
24:1:34:ILE:HG22	24:1:46:ILE:HD11	1.63	0.81
9:I:14:ILE:HG13	9:I:16:PHE:CE2	2.15	0.80
26:3:165:LYS:HE2	26:3:167:ALA:O	1.81	0.80
2:B:73:HIS:O	2:B:74:ALA:HB3	1.82	0.80
9:I:57:LYS:C	9:I:58:ILE:HG12	2.05	0.80
25:2:256:ASP:O	25:2:259:LEU:HG	1.81	0.80
26:3:121:LYS:O	26:3:124:ILE:HB	1.81	0.80
5:E:40:PHE:CD2	5:E:46:ASP:OD2	2.35	0.80
5:E:64:HIS:C	5:E:66:ASP:H	1.89	0.80
21:V:612:ASP:C	21:V:614:SER:H	1.87	0.80
26:3:144:ILE:CD1	26:3:147:MET:HE3	2.11	0.80
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.63	0.80
1:A:1171:ALA:HB1	9:I:59:THR:HG21	0.82	0.80
26:3:214:TYR:O	26:3:215:LEU:HD23	1.82	0.80
3:C:157:GLN:CD	10:J:65:LEU:CB	2.54	0.80
13:M:34:CYS:SG	13:M:39:LEU:CD2	2.64	0.80
24:1:50:VAL:HG12	24:1:54:GLN:HG2	1.62	0.80
25:2:52:ALA:O	25:2:56:VAL:HG13	1.81	0.80
25:2:224:GLN:HB2	25:2:268:PHE:CE2	2.17	0.80
1:A:1117:VAL:C	1:A:1119:LEU:N	2.35	0.80
17:Q:109:HIS:ND1	18:R:225:VAL:HG21	1.96	0.80
20:T:145:LEU:O	20:T:147:LYS:N	2.14	0.80
25:2:117:ASN:HB3	26:3:42:MET:HE3	1.62	0.80
26:3:11:LEU:CD2	26:3:160:ARG:HG2	2.12	0.80
26:3:64:ILE:HG23	26:3:128:HIS:CD2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:SER:O	1:A:270:ALA:CB	2.30	0.80
25:2:42:LEU:HD12	25:2:59:MET:CE	2.11	0.80
2:B:225:LEU:HD13	2:B:228:SER:CB	2.12	0.80
25:2:93:LEU:HA	25:2:96:TRP:CD1	2.17	0.80
1:A:204:HIS:O	1:A:205:VAL:O	1.99	0.79
1:A:623:PRO:C	1:A:625:ASP:H	1.88	0.79
17:Q:113:ARG:NH2	18:R:222:SER:CB	2.45	0.79
24:1:1:MET:CB	25:2:413:LEU:CB	2.60	0.79
25:2:35:TYR:CD1	25:2:62:LEU:HG	2.16	0.79
25:2:117:ASN:CG	26:3:42:MET:CE	2.55	0.79
17:Q:180:PHE:HE2	18:R:213:ASP:CG	1.68	0.79
22:W:419:GLU:CB	22:W:420:PRO:CD	2.46	0.79
1:A:608:THR:OG1	1:A:610:PRO:CG	2.30	0.79
2:B:132:VAL:CG2	2:B:141:GLN:HG3	2.13	0.79
16:P:207:PRO:O	16:P:209:THR:HG23	1.83	0.79
18:R:194:ARG:HB3	18:R:195:PRO:HD3	0.82	0.79
25:2:221:GLN:HE22	25:2:230:LEU:HB2	1.47	0.79
26:3:57:LEU:C	26:3:71:TYR:CZ	2.61	0.79
1:A:926:ASN:HD22	1:A:932:ARG:HG3	1.47	0.79
5:E:52:ARG:NH2	5:E:54:ARG:CG	2.44	0.79
18:R:223:VAL:CB	18:R:224:THR:HG21	0.92	0.79
24:1:1:MET:HA	25:2:414:SER:H	1.46	0.79
23:0:77:LYS:O	23:0:79:ASN:N	2.15	0.79
25:2:205:LEU:O	25:2:209:PRO:HD2	1.81	0.79
26:3:58:ALA:N	26:3:71:TYR:CZ	2.51	0.79
25:2:190:PRO:O	25:2:194:PRO:HD2	1.83	0.79
5:E:52:ARG:HG3	5:E:53:PRO:N	1.98	0.79
1:A:926:ASN:ND2	1:A:932:ARG:CG	2.46	0.79
25:2:159:VAL:HG13	25:2:161:HIS:N	1.96	0.79
26:3:222:SER:O	26:3:225:GLN:HG2	1.83	0.79
18:R:223:VAL:CB	18:R:224:THR:CB	2.41	0.78
26:3:14:VAL:CG2	26:3:163:VAL:HG22	2.13	0.78
8:H:64:LEU:CB	8:H:84:ARG:HD3	2.07	0.78
13:M:10:LEU:HB3	13:M:13:VAL:O	1.84	0.78
25:2:118:LEU:CD1	26:3:39:ASP:OD1	2.31	0.78
9:I:59:THR:O	9:I:60:HIS:HB2	1.83	0.78
17:Q:184:ILE:CD1	18:R:218:LYS:NZ	2.45	0.78
24:1:1:MET:HB3	25:2:413:LEU:HD23	1.65	0.78
24:1:13:ASP:OD1	24:1:14:PRO:HD2	1.82	0.78
1:A:206:ASN:O	1:A:207:GLU:CG	2.31	0.78
13:M:34:CYS:HB2	13:M:39:LEU:CG	2.07	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:298:ALA:HA	22:W:421:PHE:CD2	2.19	0.78
25:2:181:GLN:OE1	25:2:229:ASP:HB2	1.83	0.78
25:2:203:PHE:CD2	25:2:205:LEU:HD23	2.18	0.78
26:3:151:VAL:HG12	26:3:155:GLN:O	1.84	0.78
18:R:195:PRO:O	18:R:196:ASP:CB	2.31	0.78
25:2:207:ASP:O	25:2:211:GLN:HG2	1.84	0.78
1:A:926:ASN:OD1	1:A:931:ARG:CG	2.30	0.78
2:B:80:GLU:O	2:B:82:PRO:HD3	1.83	0.78
13:M:94:ASP:CB	13:M:97:GLY:O	2.32	0.78
18:R:223:VAL:CG2	18:R:224:THR:HG23	1.77	0.78
25:2:118:LEU:CG	26:3:39:ASP:OD1	2.32	0.78
24:1:13:ASP:OD2	24:1:17:LYS:CB	2.31	0.78
25:2:53:LYS:O	25:2:56:VAL:HG22	1.84	0.78
25:2:196:ILE:CD1	25:2:210:ALA:HB2	2.13	0.78
16:P:206:GLU:C	16:P:208:ARG:H	1.91	0.78
21:V:516:PRO:CD	24:1:15:ALA:HB3	2.11	0.78
25:2:77:LYS:HD3	25:2:78:GLU:N	1.97	0.78
25:2:234:LEU:O	25:2:234:LEU:HD23	1.83	0.78
1:A:478:PRO:O	1:A:483:ARG:NH2	2.16	0.78
1:A:926:ASN:HD21	1:A:932:ARG:HG2	1.47	0.78
24:1:1:MET:HG3	25:2:415:GLN:O	1.84	0.78
25:2:34:LEU:O	25:2:38:PRO:HD2	1.84	0.78
26:3:147:MET:O	26:3:151:VAL:HG23	1.84	0.78
17:Q:113:ARG:HH21	18:R:222:SER:CB	1.96	0.78
24:1:34:ILE:CG2	24:1:46:ILE:HD11	2.13	0.77
24:1:38:ILE:HA	24:1:44:PHE:HD1	1.47	0.77
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.83	0.77
24:1:25:GLU:CD	24:1:35:ILE:HG12	2.09	0.77
25:2:30:VAL:H	26:3:25:GLN:HB3	1.49	0.77
26:3:58:ALA:HA	26:3:71:TYR:CZ	2.18	0.77
1:A:129:ILE:O	1:A:132:LYS:HB2	1.84	0.77
23:0:54:ARG:NE	26:3:182:PHE:HE1	1.73	0.77
2:B:1080:ARG:HH21	13:M:50:SER:HB3	1.49	0.77
23:0:54:ARG:HB2	26:3:209:ILE:CG2	2.14	0.77
25:2:30:VAL:HG23	26:3:25:GLN:HB3	0.80	0.77
26:3:57:LEU:C	26:3:71:TYR:CE2	2.62	0.77
3:C:6:GLN:N	3:C:7:PRO:CD	2.48	0.77
7:G:151:ARG:HG3	17:Q:139:LEU:HD22	1.66	0.77
13:M:15:CYS:SG	13:M:39:LEU:HD21	2.25	0.77
25:2:179:LEU:HB3	25:2:184:LEU:HD11	1.65	0.77
26:3:185:GLN:HA	26:3:185:GLN:HE21	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:279:GLY:HA2	20:T:153:TYR:HE1	1.49	0.77
21:V:519:TYR:CE2	24:1:20:LEU:HG	2.20	0.77
24:1:10:ILE:CG2	25:2:407:VAL:HG21	2.15	0.77
25:2:211:GLN:CG	25:2:257:SER:HB3	2.13	0.77
28:Y:24:DC:H2"	28:Y:25:DT:H72	1.67	0.77
25:2:189:GLU:HB2	25:2:190:PRO:HD3	1.66	0.76
25:2:211:GLN:HA	25:2:261:PHE:HZ	1.49	0.76
26:3:185:GLN:NE2	26:3:210:THR:HA	2.00	0.76
17:Q:187:ILE:CD1	18:R:212:VAL:H	1.99	0.76
25:2:117:ASN:CG	26:3:42:MET:HE2	2.09	0.76
26:3:147:MET:HE1	26:3:157:MET:SD	2.25	0.76
1:A:211:GLU:O	1:A:212:LYS:CB	2.33	0.76
2:B:490:GLY:O	2:B:491:ARG:HB2	1.84	0.76
24:1:1:MET:CE	25:2:440:LEU:HD13	2.16	0.76
24:1:38:ILE:HG22	24:1:44:PHE:CD1	2.19	0.76
1:A:1116:ASN:O	1:A:1117:VAL:CG2	2.33	0.76
17:Q:113:ARG:NE	18:R:222:SER:N	2.32	0.76
25:2:44:VAL:HG13	25:2:45:PHE:CD1	2.20	0.76
25:2:163:MET:CE	25:2:206:LEU:HD12	2.14	0.76
26:3:14:VAL:CG2	26:3:163:VAL:HA	2.16	0.76
13:M:10:LEU:N	13:M:10:LEU:HD22	2.01	0.76
2:B:958:CYS:SG	2:B:959:GLU:N	2.56	0.76
3:C:157:GLN:CG	10:J:65:LEU:HB2	2.16	0.76
9:I:57:LYS:O	9:I:58:ILE:HG12	1.85	0.76
14:N:343:HIS:NE2	27:X:9:DC:OP1	2.19	0.76
17:Q:184:ILE:HD13	18:R:211:SER:CB	2.15	0.76
24:1:1:MET:HE3	25:2:415:GLN:C	2.10	0.76
25:2:234:LEU:CD2	25:2:237:LEU:HD12	2.14	0.76
2:B:222:ARG:HB3	2:B:222:ARG:HH11	1.49	0.76
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.15	0.76
24:1:38:ILE:H	24:1:38:ILE:HD13	1.51	0.76
25:2:163:MET:HE2	25:2:206:LEU:CD1	2.15	0.76
26:3:133:LEU:HD23	26:3:177:PHE:HD1	1.49	0.76
1:A:360:ASP:OD1	1:A:361:PHE:N	2.17	0.76
18:R:223:VAL:CA	18:R:224:THR:HG22	1.78	0.76
21:V:674:THR:CG2	25:2:392:ARG:NH2	2.43	0.76
24:1:1:MET:SD	25:2:413:LEU:HB3	2.25	0.76
25:2:208:THR:HG23	25:2:209:PRO:CD	2.16	0.76
26:3:172:LEU:HD13	26:3:172:LEU:O	1.86	0.76
25:2:118:LEU:HD22	26:3:39:ASP:HA	1.65	0.76
2:B:225:LEU:CB	2:B:228:SER:HB2	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:1:MET:HB3	25:2:413:LEU:CD2	2.15	0.75
24:1:24:ASP:OD2	24:1:57:VAL:HG11	1.85	0.75
26:3:190:LEU:HD23	26:3:190:LEU:H	1.51	0.75
13:M:53:ARG:HH22	28:Y:54:DA:H61	1.34	0.75
17:Q:113:ARG:CD	18:R:221:ARG:CB	2.60	0.75
25:2:42:LEU:HD21	25:2:55:TRP:CB	2.10	0.75
25:2:208:THR:HG23	25:2:209:PRO:HD3	1.66	0.75
2:B:496:ALA:HB1	2:B:498:PRO:HD2	1.66	0.75
2:B:875:GLU:O	2:B:876:ASN:CB	2.35	0.75
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.65	0.75
25:2:243:SER:HB3	25:2:258:LEU:HD22	1.69	0.75
26:3:8:LEU:HD23	26:3:54:SER:HB3	1.68	0.75
1:A:1305:SER:C	1:A:1306:LYS:HG3	2.10	0.75
13:M:10:LEU:C	13:M:12:ARG:H	1.90	0.75
1:A:202:TRP:CD2	1:A:212:LYS:HD2	2.21	0.75
21:V:523:VAL:HG21	24:1:20:LEU:HG	1.68	0.75
5:E:47:LYS:CB	5:E:48:PRO:CD	2.59	0.75
25:2:53:LYS:HE3	25:2:95:ILE:HD11	1.67	0.75
25:2:86:SER:HB3	25:2:140:LYS:CE	2.16	0.75
25:2:218:GLN:NE2	25:2:265:LEU:HA	2.00	0.75
2:B:132:VAL:HG21	2:B:141:GLN:OE1	1.86	0.75
10:J:65:LEU:HD13	10:J:65:LEU:N	2.01	0.75
17:Q:188:TYR:HE2	18:R:210:PHE:CE1	2.00	0.75
25:2:35:TYR:CD2	25:2:62:LEU:HB3	2.22	0.75
25:2:100:LEU:CD1	25:2:119:ARG:HG3	2.16	0.75
25:2:196:ILE:HD11	25:2:210:ALA:CB	2.17	0.75
2:B:428:ASP:OD1	20:T:158:ASN:ND2	2.18	0.75
2:B:1040:GLN:OE1	2:B:1040:GLN:N	2.20	0.75
26:3:11:LEU:HD22	26:3:160:ARG:CG	2.16	0.75
17:Q:184:ILE:HD12	18:R:218:LYS:HZ3	1.51	0.74
21:V:612:ASP:CG	21:V:635:GLN:CD	2.55	0.74
25:2:180:SER:O	25:2:184:LEU:HG	1.87	0.74
26:3:38:ILE:O	26:3:41:VAL:HG12	1.87	0.74
1:A:679:TRP:CH2	1:A:683:GLU:HG3	2.22	0.74
18:R:163:LEU:O	18:R:164:GLY:O	2.05	0.74
9:I:92:LYS:NZ	9:I:93:GLU:OE2	2.20	0.74
17:Q:113:ARG:NH2	18:R:222:SER:OG	2.21	0.74
22:W:73:CYS:HB2	22:W:209:TYR:CZ	2.22	0.74
27:X:41:DT:H3'	27:X:42:DT:H4'	1.67	0.74
1:A:1171:ALA:C	9:I:59:THR:CG2	2.59	0.74
2:B:250:SER:O	2:B:251:ALA:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:VAL:HG13	19:S:161:GLU:HB3	1.70	0.74
26:3:24:LYS:O	26:3:25:GLN:O	2.06	0.74
26:3:148:ASN:CB	26:3:157:MET:HE2	2.17	0.74
2:B:907:VAL:HG13	2:B:921:ILE:HG22	1.69	0.74
1:A:263:ALA:C	1:A:265:VAL:H	1.94	0.74
17:Q:113:ARG:CZ	18:R:222:SER:CB	2.51	0.74
21:V:321:GLU:OE1	22:W:499:ASN:OD1	2.06	0.74
24:1:1:MET:HB2	25:2:418:PHE:CB	2.18	0.74
22:W:430:ASN:HB3	22:W:431:PRO:CD	2.17	0.74
14:N:319:ASP:O	14:N:320:VAL:C	2.28	0.74
25:2:117:ASN:HD21	26:3:108:ASN:HB3	1.47	0.74
2:B:91:ILE:HD11	2:B:124:LEU:HD21	1.69	0.74
22:W:59:TYR:CD2	22:W:62:ALA:CB	2.70	0.74
22:W:298:ALA:HA	22:W:421:PHE:HD2	1.50	0.74
22:W:424:ARG:O	22:W:425:THR:CG2	2.32	0.74
25:2:51:LEU:HD23	25:2:51:LEU:O	1.87	0.74
1:A:1439:LEU:HD13	2:B:1162:LEU:HD21	1.70	0.73
18:R:223:VAL:HG23	18:R:224:THR:OG1	1.88	0.73
25:2:127:LYS:N	25:2:178:LEU:HD23	2.01	0.73
26:3:141:LEU:O	26:3:144:ILE:HG22	1.88	0.73
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.21	0.73
13:M:94:ASP:CG	13:M:97:GLY:O	2.30	0.73
1:A:152:ASN:C	1:A:153:ILE:HG12	2.04	0.73
22:W:584:TYR:HD1	22:W:594:ALA:HB2	1.52	0.73
24:1:1:MET:C	25:2:413:LEU:HG	2.12	0.73
26:3:12:VAL:HG23	26:3:161:ILE:HG23	1.70	0.73
26:3:59:VAL:CA	26:3:71:TYR:CE1	2.69	0.73
26:3:144:ILE:HG12	26:3:147:MET:HE3	1.70	0.73
26:3:214:TYR:HE2	26:3:216:LYS:HE2	1.53	0.73
12:L:19:CYS:SG	12:L:20:GLY:N	2.62	0.73
24:1:18:GLN:CB	24:1:44:PHE:HE2	2.01	0.73
24:1:34:ILE:HD13	24:1:54:GLN:OE1	1.88	0.73
1:A:18:ILE:HD12	2:B:1171:MET:HB2	1.69	0.73
1:A:1307:VAL:CG1	1:A:1339:ASP:HB3	2.18	0.73
17:Q:122:THR:HA	17:Q:169:PRO:HD2	1.70	0.73
25:2:251:VAL:HG11	25:2:254:MET:CG	2.18	0.73
26:3:33:THR:HG23	26:3:36:LYS:N	1.98	0.73
1:A:47:THR:O	1:A:48:GLU:CG	2.37	0.73
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.69	0.73
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.70	0.73
3:C:157:GLN:HE21	10:J:65:LEU:CB	1.94	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:LYS:O	5:E:49:SER:N	2.22	0.73
24:1:34:ILE:HG12	24:1:50:VAL:CG1	2.18	0.73
25:2:41:CYS:O	25:2:44:VAL:HG12	1.88	0.73
1:A:1223:ASP:OD2	1:A:1224:ARG:NH1	2.22	0.73
19:S:49:ARG:NH1	19:S:96:GLN:O	2.21	0.73
22:W:73:CYS:C	22:W:209:TYR:CE2	2.67	0.73
24:1:2:VAL:CG1	25:2:456:LYS:CG	2.53	0.73
25:2:60:LEU:HD11	25:2:95:ILE:HB	1.71	0.73
25:2:160:LEU:HA	25:2:206:LEU:HD11	1.70	0.73
8:H:99:ILE:HG22	8:H:136:GLU:HG3	1.70	0.73
14:N:333:ASN:HB3	14:N:360:LEU:HA	1.71	0.73
25:2:30:VAL:CB	26:3:25:GLN:O	2.34	0.73
1:A:61:ARG:HB3	1:A:72:GLN:HG2	1.69	0.73
22:W:59:TYR:CE2	22:W:62:ALA:HB2	2.22	0.73
25:2:172:SER:HA	25:2:175:LEU:CD2	2.19	0.73
21:V:522:TYR:HE2	24:1:62:ASP:CG	1.96	0.72
25:2:132:ASP:O	25:2:135:GLN:HG2	1.88	0.72
26:3:222:SER:HB2	26:3:226:TYR:HE2	1.54	0.72
1:A:691:ASP:HB3	1:A:766:PHE:HB2	1.71	0.72
2:B:73:HIS:O	2:B:74:ALA:CB	2.37	0.72
2:B:89:GLU:HB3	2:B:127:ASP:HB3	1.70	0.72
2:B:906:GLN:HG2	12:L:45:TYR:HE1	1.52	0.72
21:V:667:THR:HA	24:1:62:ASP:OD1	1.89	0.72
24:1:1:MET:HG3	25:2:418:PHE:HB2	1.69	0.72
24:1:9:LEU:HD22	24:1:51:ASN:ND2	2.04	0.72
26:3:111:ILE:HG13	26:3:112:VAL:N	2.02	0.72
24:1:1:MET:HG2	25:2:413:LEU:C	2.14	0.72
26:3:66:GLU:CA	26:3:132:LEU:HD12	2.13	0.72
26:3:226:TYR:HA	26:3:230:VAL:HG23	1.71	0.72
1:A:926:ASN:ND2	1:A:932:ARG:HG2	2.05	0.72
2:B:487:SER:OG	2:B:524:LYS:NZ	2.22	0.72
10:J:3:ILE:H	10:J:3:ILE:HD12	1.54	0.72
17:Q:101:ASN:C	17:Q:103:VAL:N	2.45	0.72
17:Q:188:TYR:CE1	18:R:211:SER:OG	2.42	0.72
25:2:118:LEU:HD21	26:3:39:ASP:C	2.12	0.72
25:2:35:TYR:CG	25:2:62:LEU:HD12	2.25	0.72
1:A:426:ARG:HD2	13:M:40:VAL:HG11	1.72	0.72
1:A:926:ASN:ND2	1:A:932:ARG:HG3	2.04	0.72
17:Q:187:ILE:CG2	18:R:210:PHE:C	2.62	0.72
21:V:689:VAL:HB	25:2:391:ILE:HD11	1.70	0.72
24:1:5:LEU:HD21	25:2:408:LEU:HD13	0.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:134:SER:O	25:2:138:PRO:HD2	1.89	0.72
25:2:218:GLN:HE22	25:2:265:LEU:HA	1.54	0.72
25:2:243:SER:HB2	25:2:258:LEU:HD22	1.71	0.72
26:3:69:PHE:CE1	26:3:139:LYS:HD2	2.25	0.72
1:A:1101:GLN:OE1	1:A:1389:ASP:OD2	2.07	0.72
22:W:209:TYR:HE1	22:W:233:PHE:CD1	2.07	0.72
25:2:175:LEU:HD22	25:2:216:MET:SD	2.29	0.72
2:B:51:ILE:CG2	20:T:141:LEU:HD21	2.18	0.72
1:A:426:ARG:CA	13:M:40:VAL:HG21	2.20	0.72
17:Q:184:ILE:HD11	18:R:213:ASP:OD1	1.90	0.72
24:1:1:MET:HE2	25:2:413:LEU:O	1.90	0.72
25:2:117:ASN:ND2	26:3:42:MET:HE1	2.03	0.72
25:2:117:ASN:HB3	26:3:42:MET:CE	2.18	0.72
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.72	0.72
21:V:504:LYS:HB3	21:V:654:GLU:O	1.90	0.72
25:2:117:ASN:HB2	26:3:104:LEU:HD11	1.71	0.72
26:3:165:LYS:HG3	26:3:203:LEU:CD1	2.20	0.72
3:C:193:ARG:HH12	3:C:218:ALA:HB1	1.54	0.71
17:Q:188:TYR:CZ	18:R:210:PHE:CE1	2.65	0.71
24:1:2:VAL:HG12	25:2:422:LEU:HD13	1.72	0.71
26:3:217:VAL:HG13	26:3:226:TYR:CZ	2.25	0.71
14:N:319:ASP:C	14:N:321:SER:N	2.46	0.71
28:Y:53:DG:H2''	28:Y:55:DG:H5'	1.73	0.71
25:2:171:VAL:HG12	25:2:216:MET:SD	2.31	0.71
25:2:237:LEU:O	25:2:240:LEU:HD13	1.88	0.71
25:2:118:LEU:CD2	26:3:39:ASP:CA	2.68	0.71
1:A:1171:ALA:CA	9:I:59:THR:HG21	1.91	0.71
21:V:611:GLY:HA2	21:V:615:PHE:HB3	1.71	0.71
25:2:86:SER:CB	25:2:140:LYS:HE2	2.20	0.71
25:2:118:LEU:HD22	26:3:39:ASP:CA	2.19	0.71
26:3:18:ASN:CG	26:3:20:ILE:HD13	2.15	0.71
24:1:1:MET:HG2	25:2:413:LEU:HB3	1.71	0.71
25:2:199:ALA:HB3	25:2:202:GLN:NE2	2.02	0.71
27:X:42:DT:H3'	27:X:43:DT:H5''	1.72	0.71
27:X:47:DT:H3'	27:X:48:DT:H5''	1.71	0.71
22:W:209:TYR:OH	22:W:234:ASP:N	2.23	0.71
13:M:10:LEU:C	13:M:12:ARG:N	2.48	0.71
14:N:316:SER:OG	16:P:235:ARG:NH1	2.23	0.71
16:P:159:SER:HB3	16:P:329:TYR:CD2	2.25	0.71
22:W:589:GLU:O	22:W:594:ALA:HB1	1.91	0.71
2:B:356:PHE:HB3	19:S:116:GLY:HA2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:648:LYS:O	21:V:650:MET:N	2.24	0.71
7:G:97:LEU:HB2	7:G:108:ILE:HB	1.71	0.70
8:H:147:LYS:HE2	8:H:149:ALA:HA	1.73	0.70
22:W:59:TYR:CE1	22:W:62:ALA:HB2	2.26	0.70
24:1:29:LEU:HD23	24:1:30:GLY:N	2.06	0.70
25:2:163:MET:O	25:2:167:PRO:HD2	1.91	0.70
1:A:1192:TRP:HE1	1:A:1249:ASP:H	1.35	0.70
13:M:279:GLY:HA2	20:T:153:TYR:CE1	2.27	0.70
21:V:315:VAL:HG12	22:W:500:ASP:CB	2.16	0.70
23:0:74:GLN:HA	23:0:78:PRO:O	1.92	0.70
1:A:491:PRO:HG3	1:A:535:MET:HE2	1.73	0.70
2:B:854:ILE:HD11	2:B:921:ILE:HD12	1.73	0.70
9:I:101:SER:O	9:I:104:ALA:HB2	1.91	0.70
25:2:42:LEU:HD12	25:2:59:MET:HE1	1.71	0.70
25:2:192:GLU:HG3	25:2:193:PRO:CD	2.18	0.70
24:1:28:ALA:HB3	24:1:31:LYS:HB2	1.71	0.70
25:2:199:ALA:CB	25:2:202:GLN:HE22	2.02	0.70
3:C:212:ASP:C	3:C:214:ASP:N	2.49	0.70
23:0:54:ARG:NE	26:3:182:PHE:CD1	2.60	0.70
24:1:2:VAL:HG12	25:2:456:LYS:HE2	1.74	0.70
26:3:177:PHE:CZ	26:3:203:LEU:HD23	2.27	0.70
13:M:178:LYS:C	20:T:154:LYS:HB3	2.14	0.70
1:A:79:THR:HG21	13:M:43:ASP:CA	2.22	0.70
1:A:190:ARG:NH2	27:X:58:DT:OP2	2.24	0.70
2:B:102:ASP:OD1	2:B:103:GLY:N	2.24	0.70
2:B:514:THR:HG22	2:B:524:LYS:HA	1.72	0.70
3:C:212:ASP:C	3:C:214:ASP:H	1.99	0.70
17:Q:114:ILE:HD11	18:R:218:LYS:HE3	1.74	0.70
26:3:162:LEU:HA	26:3:192:ASP:OD1	1.92	0.70
28:Y:49:DG:H2'	28:Y:50:DA:H8	1.56	0.70
1:A:203:LYS:O	1:A:204:HIS:CB	2.25	0.70
2:B:51:ILE:HG22	20:T:141:LEU:HD21	1.71	0.70
2:B:225:LEU:C	2:B:227:ASN:N	2.39	0.70
21:V:321:GLU:CB	22:W:499:ASN:CG	2.32	0.70
25:2:126:GLY:C	25:2:178:LEU:HD23	2.16	0.70
25:2:185:MET:SD	25:2:232:GLU:HB2	2.32	0.70
26:3:51:MET:HE3	26:3:52:ASN:ND2	2.07	0.70
26:3:69:PHE:CZ	26:3:139:LYS:HD2	2.27	0.70
28:Y:24:DC:H2''	28:Y:25:DT:C7	2.22	0.70
24:1:53:LEU:HD12	24:1:53:LEU:H	1.57	0.70
25:2:218:GLN:OE1	25:2:265:LEU:HA	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:ALA:C	1:A:931:ARG:H	2.00	0.69
2:B:851:ASP:HB2	12:L:14:PRO:HG3	1.72	0.69
8:H:106:THR:C	8:H:108:ALA:H	1.99	0.69
14:N:311:GLU:HG2	16:P:251:LEU:HD21	1.72	0.69
25:2:218:GLN:CD	25:2:265:LEU:HA	2.17	0.69
21:V:515:SER:HB3	21:V:539:ASN:ND2	2.05	0.69
2:B:1076:GLU:HG3	13:M:54:THR:OG1	1.93	0.69
7:G:93:ASN:ND2	17:Q:151:THR:HA	2.08	0.69
13:M:7:LEU:CD1	13:M:10:LEU:HD11	2.22	0.69
21:V:674:THR:OG1	25:2:392:ARG:NE	2.26	0.69
13:M:11:PRO:O	13:M:12:ARG:HB3	1.91	0.69
17:Q:24:GLY:HA2	18:R:209:GLN:CD	2.17	0.69
24:1:1:MET:CG	25:2:415:GLN:O	2.41	0.69
13:M:7:LEU:HD11	13:M:10:LEU:HD11	1.74	0.69
24:1:34:ILE:CG1	24:1:50:VAL:HG11	2.21	0.69
25:2:189:GLU:HA	25:2:192:GLU:HG2	1.71	0.69
17:Q:187:ILE:HD13	18:R:212:VAL:H	1.56	0.69
25:2:81:LYS:HD2	25:2:89:LEU:CD2	2.20	0.69
26:3:144:ILE:CG1	26:3:147:MET:HE3	2.23	0.69
26:3:215:LEU:HD12	26:3:230:VAL:CG1	2.23	0.69
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.75	0.69
5:E:52:ARG:NE	5:E:54:ARG:HG3	2.06	0.69
25:2:81:LYS:HE3	25:2:93:LEU:CD2	2.20	0.69
24:1:8:VAL:HG11	24:1:45:VAL:HG12	1.74	0.69
25:2:130:SER:O	25:2:133:THR:HG22	1.92	0.69
25:2:140:LYS:HD3	25:2:162:PHE:HE1	1.58	0.69
2:B:834:ARG:O	2:B:885:ARG:NH1	2.24	0.69
24:1:55:GLU:OE2	25:2:402:ARG:HG3	1.93	0.69
26:3:133:LEU:HD22	26:3:134:ALA:H	1.56	0.69
13:M:7:LEU:CG	13:M:10:LEU:HD11	2.23	0.69
13:M:94:ASP:HB3	13:M:99:SER:H	1.57	0.69
17:Q:109:HIS:ND1	18:R:225:VAL:CG2	2.55	0.69
25:2:117:ASN:CG	26:3:108:ASN:ND2	2.50	0.69
25:2:118:LEU:HD11	26:3:43:VAL:HG23	1.75	0.69
2:B:80:GLU:O	2:B:82:PRO:CD	2.41	0.68
3:C:157:GLN:HG2	10:J:65:LEU:CB	2.22	0.68
13:M:108:SER:HB3	13:M:112:ARG:HH11	1.58	0.68
26:3:33:THR:HG22	26:3:36:LYS:HB2	1.73	0.68
26:3:34:LEU:O	26:3:34:LEU:HD13	1.92	0.68
25:2:28:PRO:CA	26:3:25:GLN:C	2.66	0.68
25:2:163:MET:CE	25:2:206:LEU:HB3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:ASN:C	1:A:1117:VAL:HG23	2.18	0.68
5:E:52:ARG:CG	5:E:53:PRO:N	2.50	0.68
21:V:612:ASP:C	21:V:614:SER:N	2.49	0.68
25:2:181:GLN:HG3	25:2:229:ASP:CG	2.17	0.68
25:2:251:VAL:HG12	25:2:254:MET:H	1.58	0.68
2:B:329:GLY:H	2:B:335:ARG:HH21	1.39	0.68
5:E:71:GLN:HE21	5:E:99:ILE:HA	1.59	0.68
26:3:114:GLU:O	26:3:118:LEU:HD23	1.92	0.68
25:2:48:LEU:CB	25:2:49:PRO:HD3	2.19	0.68
25:2:118:LEU:HD13	26:3:39:ASP:OD1	1.93	0.68
26:3:130:GLU:HB2	26:3:173:GLN:NE2	2.09	0.68
12:L:26:ASN:O	12:L:27:GLU:HB3	1.94	0.68
26:3:59:VAL:N	26:3:71:TYR:CD1	2.62	0.68
25:2:211:GLN:HA	25:2:261:PHE:CE1	2.28	0.68
26:3:187:GLN:HG3	26:3:189:ILE:CG1	2.24	0.68
5:E:52:ARG:HE	5:E:54:ARG:HG3	1.59	0.68
9:I:119:CYS:SG	9:I:120:GLY:N	2.64	0.68
21:V:355:CYS:HG	21:V:381:TRP:CD1	2.12	0.68
1:A:1086:MET:O	1:A:1088:GLY:N	2.27	0.67
20:T:154:LYS:HD2	20:T:154:LYS:N	2.08	0.67
24:1:39:ASP:OD1	24:1:43:VAL:HB	1.94	0.67
26:3:18:ASN:CG	26:3:64:ILE:HD11	2.19	0.67
1:A:112:PHE:H	1:A:188:GLN:HE22	1.40	0.67
1:A:153:ILE:O	1:A:155:GLU:HG2	1.94	0.67
2:B:1029:TYR:HE1	2:B:1036:LYS:HE2	1.59	0.67
24:1:4:VAL:CG1	25:2:411:GLN:O	2.39	0.67
25:2:30:VAL:H	26:3:25:GLN:CB	2.07	0.67
25:2:170:ALA:HB1	25:2:213:TRP:CZ3	2.29	0.67
1:A:207:GLU:O	1:A:209:SER:N	2.27	0.67
2:B:775:GLY:N	2:B:1047:TYR:OH	2.28	0.67
2:B:875:GLU:OE2	2:B:875:GLU:HA	1.92	0.67
18:R:223:VAL:HB	18:R:224:THR:HG22	0.75	0.67
18:R:223:VAL:CB	18:R:224:THR:HG22	1.24	0.67
21:V:516:PRO:HB3	24:1:15:ALA:CB	2.05	0.67
25:2:211:GLN:HB3	25:2:261:PHE:HE1	1.59	0.67
1:A:358:ARG:NH2	2:B:1076:GLU:OE1	2.23	0.67
18:R:223:VAL:CG1	18:R:224:THR:HG22	2.07	0.67
26:3:159:SER:OG	26:3:189:ILE:HD12	1.94	0.67
2:B:895:PHE:O	2:B:897:ARG:NE	2.27	0.67
13:M:10:LEU:HD23	13:M:10:LEU:O	1.95	0.67
25:2:176:ALA:HB1	25:2:178:LEU:CD1	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:111:ILE:O	26:3:115:ILE:HD13	1.94	0.67
1:A:271:ARG:HG2	13:M:73:PRO:HG3	1.76	0.67
1:A:923:ASP:O	1:A:932:ARG:NH1	2.28	0.67
2:B:882:SER:HB2	2:B:887:TYR:CZ	2.30	0.67
20:T:228:ILE:HG22	27:X:29:DC:H1'	1.75	0.67
21:V:612:ASP:CG	21:V:635:GLN:OE1	2.37	0.67
24:1:10:ILE:HG21	25:2:407:VAL:HG21	1.76	0.67
25:2:117:ASN:HD21	26:3:108:ASN:CA	2.04	0.67
25:2:172:SER:O	25:2:175:LEU:HD23	1.95	0.67
25:2:181:GLN:CD	25:2:229:ASP:HB2	2.20	0.67
2:B:588:ARG:NH1	2:B:603:MET:HE2	2.09	0.67
13:M:62:LYS:HB2	29:Z:1:A:H5''	1.76	0.67
21:V:516:PRO:HG3	24:1:15:ALA:HB2	1.58	0.67
21:V:667:THR:HA	24:1:62:ASP:CG	2.19	0.67
26:3:187:GLN:CG	26:3:189:ILE:HG12	2.24	0.67
14:N:319:ASP:C	14:N:321:SER:H	2.03	0.67
24:1:1:MET:HE3	25:2:415:GLN:CA	2.24	0.67
24:1:59:GLU:OE2	25:2:402:ARG:CZ	2.41	0.67
26:3:24:LYS:HE2	26:3:220:MET:SD	2.33	0.67
25:2:56:VAL:HG11	25:2:91:SER:HB2	1.77	0.67
11:K:111:ASP:O	11:K:113:GLN:N	2.29	0.67
16:P:206:GLU:CG	16:P:207:PRO:HD3	2.23	0.67
1:A:775:LYS:HB3	2:B:974:SER:OG	1.96	0.66
14:N:358:MET:HB2	14:N:365:TYR:HB2	1.78	0.66
17:Q:188:TYR:HH	18:R:210:PHE:HE1	1.29	0.66
21:V:631:GLY:O	21:V:632:SER:HB3	1.95	0.66
25:2:56:VAL:O	25:2:60:LEU:HG	1.94	0.66
1:A:228:ILE:O	1:A:244:ARG:NH2	2.26	0.66
25:2:160:LEU:HD12	25:2:160:LEU:H	1.60	0.66
26:3:146:ARG:O	26:3:149:LYS:HG2	1.95	0.66
1:A:355:MET:HE1	1:A:1431:SER:HB2	1.78	0.66
3:C:267:ILE:HG21	11:K:84:GLN:HE22	1.60	0.66
17:Q:23:ARG:NH2	18:R:206:LYS:O	2.27	0.66
18:R:223:VAL:CB	18:R:224:THR:HG23	1.10	0.66
27:X:69:DA:C2	28:Y:26:DG:C2	2.84	0.66
1:A:79:THR:HG21	13:M:43:ASP:HA	1.78	0.66
13:M:52:TRP:CD1	13:M:52:TRP:O	2.48	0.66
14:N:318:ASP:OD1	16:P:239:ARG:NE	2.28	0.66
26:3:207:CYS:SG	26:3:214:TYR:HB2	2.34	0.66
24:1:35:ILE:HG22	24:1:46:ILE:HD12	1.78	0.66
25:2:218:GLN:CG	25:2:268:PHE:HB3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:217:VAL:HG13	26:3:226:TYR:CE2	2.30	0.66
1:A:611:ASP:O	1:A:612:ASP:HB2	1.95	0.66
1:A:1481:LYS:HA	1:A:1484:MET:HE2	1.78	0.66
2:B:224:CYS:O	2:B:226:GLU:OE1	2.12	0.66
17:Q:109:HIS:CE1	18:R:225:VAL:CG2	2.79	0.66
17:Q:113:ARG:HH12	18:R:218:LYS:CG	2.09	0.66
2:B:225:LEU:HD13	2:B:228:SER:HG	1.59	0.66
24:1:8:VAL:HG12	24:1:9:LEU:N	2.10	0.66
11:K:81:TYR:HE2	11:K:86:ALA:HB2	1.61	0.66
13:M:7:LEU:HG	13:M:10:LEU:HD11	1.77	0.66
13:M:178:LYS:C	20:T:154:LYS:CB	2.69	0.66
16:P:205:ARG:O	16:P:206:GLU:O	2.13	0.66
17:Q:42:CYS:C	17:Q:95:ASN:HD21	2.04	0.66
24:1:19:PHE:O	24:1:22:TYR:HB3	1.96	0.66
25:2:117:ASN:CB	26:3:42:MET:HE3	2.22	0.66
26:3:33:THR:CG2	26:3:36:LYS:HB2	2.26	0.66
26:3:45:GLY:O	26:3:49:LEU:HD23	1.96	0.66
26:3:144:ILE:O	26:3:147:MET:HG3	1.96	0.66
26:3:184:ALA:CA	26:3:187:GLN:HG2	2.25	0.66
1:A:421:ARG:NH2	1:A:425:ASP:OD2	2.29	0.65
2:B:801:VAL:HA	2:B:805:PHE:HB3	1.77	0.65
2:B:873:LEU:H	2:B:874:PRO:HD2	1.61	0.65
16:P:239:ARG:NH1	16:P:242:GLN:OE1	2.29	0.65
17:Q:113:ARG:CD	18:R:221:ARG:O	2.22	0.65
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.61	0.65
24:1:1:MET:SD	25:2:419:GLU:HB2	2.37	0.65
2:B:490:GLY:O	2:B:491:ARG:CB	2.43	0.65
16:P:206:GLU:CB	16:P:207:PRO:HD2	2.10	0.65
25:2:270:LEU:HD23	25:2:273:GLN:HE21	1.62	0.65
1:A:486:LEU:HD22	2:B:790:GLN:CD	2.22	0.65
2:B:309:PHE:CE2	9:I:40:ARG:HD2	2.31	0.65
24:1:13:ASP:CG	24:1:14:PRO:CD	2.61	0.65
25:2:42:LEU:CD2	25:2:55:TRP:HB2	2.13	0.65
25:2:173:GLN:CD	25:2:179:LEU:HD21	2.22	0.65
26:3:137:LEU:HB3	26:3:180:VAL:CG1	2.20	0.65
17:Q:68:GLY:O	18:R:226:ASP:OD2	2.14	0.65
25:2:171:VAL:HG13	25:2:216:MET:CB	2.26	0.65
24:1:10:ILE:HG22	25:2:407:VAL:HG21	1.79	0.65
25:2:44:VAL:HG13	25:2:45:PHE:HD1	1.59	0.65
26:3:106:SER:O	26:3:110:VAL:HG23	1.97	0.65
1:A:610:PRO:HB2	1:A:626:THR:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:584:TYR:CE1	22:W:614:TYR:O	2.46	0.65
24:1:22:TYR:HD1	24:1:23:LEU:HD23	1.61	0.65
25:2:117:ASN:ND2	26:3:108:ASN:CA	2.57	0.65
27:X:32:DT:H4'	27:X:33:DT:H5'	1.78	0.65
2:B:249:LYS:O	2:B:249:LYS:HG2	1.96	0.65
10:J:63:ALA:HB3	10:J:64:PRO:CD	2.11	0.65
1:A:266:MET:CG	1:A:272:ASN:OD1	2.45	0.65
17:Q:101:ASN:O	17:Q:103:VAL:N	2.29	0.65
25:2:189:GLU:HA	25:2:192:GLU:CG	2.26	0.65
25:2:270:LEU:HD23	25:2:270:LEU:O	1.96	0.65
8:H:105:SER:HB2	8:H:108:ALA:HB2	1.79	0.65
25:2:57:MET:HA	25:2:60:LEU:HD11	1.77	0.65
1:A:152:ASN:O	1:A:153:ILE:CB	2.44	0.65
1:A:890:ARG:NH2	1:A:1023:VAL:HG13	2.12	0.64
25:2:236:PHE:CZ	25:2:262:LEU:HD22	2.32	0.64
1:A:202:TRP:HB2	1:A:212:LYS:HB3	0.75	0.64
1:A:610:PRO:HB2	1:A:626:THR:HG21	1.79	0.64
1:A:738:GLU:OE2	1:A:797:ARG:HD3	1.97	0.64
2:B:241:ALA:HA	2:B:253:GLY:HA2	1.78	0.64
2:B:326:ALA:HB2	2:B:338:TYR:HE2	1.61	0.64
2:B:908:MET:HE3	2:B:920:LYS:HB2	1.77	0.64
26:3:17:ALA:CB	26:3:63:HIS:HD2	2.10	0.64
2:B:489:ILE:HG21	2:B:522:LEU:HD13	1.79	0.64
2:B:1005:ALA:C	2:B:1007:ASN:H	2.04	0.64
3:C:67:ARG:NH2	10:J:3:ILE:O	2.28	0.64
24:1:13:ASP:OD1	24:1:14:PRO:CD	2.46	0.64
25:2:117:ASN:ND2	26:3:42:MET:CE	2.60	0.64
25:2:266:ARG:O	25:2:270:LEU:HB2	1.97	0.64
26:3:131:THR:O	26:3:133:LEU:HD13	1.97	0.64
26:3:192:ASP:HB2	26:3:231:PHE:CE1	2.32	0.64
1:A:157:GLY:H	1:A:181:HIS:CE1	2.15	0.64
1:A:375:ILE:HB	1:A:666:ARG:HD2	1.80	0.64
25:2:211:GLN:CB	25:2:261:PHE:HE1	2.11	0.64
26:3:149:LYS:HG3	26:3:150:GLU:N	2.12	0.64
2:B:312:GLN:HB3	19:S:153:ARG:HH22	1.62	0.64
2:B:881:GLU:C	2:B:883:THR:H	2.05	0.64
3:C:3:TYR:O	11:K:52:LYS:HE3	1.96	0.64
21:V:523:VAL:CG1	24:1:20:LEU:HD23	2.21	0.64
23:0:54:ARG:CD	26:3:182:PHE:CE1	2.60	0.64
24:1:35:ILE:HG22	24:1:46:ILE:CD1	2.27	0.64
25:2:31:LEU:CD1	26:3:33:THR:HG21	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:45:PHE:HB2	25:2:51:LEU:CD1	2.26	0.64
26:3:14:VAL:HG22	26:3:163:VAL:HA	1.78	0.64
1:A:426:ARG:HB3	13:M:40:VAL:CG2	2.19	0.64
2:B:934:LYS:NZ	29:Z:6:C:OP1	2.31	0.64
17:Q:188:TYR:HE1	18:R:211:SER:OG	1.80	0.64
26:3:58:ALA:CA	26:3:71:TYR:OH	2.39	0.64
21:V:517:GLU:HB2	21:V:713:LEU:HD22	1.80	0.64
25:2:258:LEU:HG	25:2:262:LEU:CD2	2.28	0.64
26:3:64:ILE:HB	26:3:123:ASP:OD2	1.98	0.64
26:3:130:GLU:HB2	26:3:173:GLN:HE22	1.61	0.64
1:A:686:THR:OG1	1:A:687:ILE:N	2.26	0.64
2:B:602:SER:OG	2:B:620:ARG:NH1	2.31	0.64
2:B:1124:ILE:HG22	2:B:1126:ALA:H	1.63	0.64
7:G:94:LYS:NZ	17:Q:162:GLU:OE2	2.30	0.64
13:M:17:ASN:OD1	13:M:18:HIS:N	2.30	0.64
17:Q:113:ARG:HD2	18:R:221:ARG:HB3	1.75	0.64
22:W:423:ASP:C	22:W:425:THR:H	2.04	0.64
25:2:140:LYS:HG2	25:2:162:PHE:CE1	2.33	0.64
17:Q:113:ARG:NH2	18:R:218:LYS:HG2	2.10	0.64
1:A:467:MET:SD	1:A:524:MET:HB3	2.37	0.63
25:2:220:LEU:O	25:2:220:LEU:HD13	1.98	0.63
26:3:17:ALA:HB1	26:3:63:HIS:HD2	1.63	0.63
1:A:367:ILE:HG21	1:A:501:MET:CG	2.28	0.63
18:R:127:ASN:ND2	20:T:238:GLU:OE1	2.31	0.63
22:W:581:LEU:HD21	22:W:608:ILE:HG21	1.78	0.63
24:1:35:ILE:HA	24:1:46:ILE:HG13	1.80	0.63
25:2:159:VAL:HG11	25:2:161:HIS:HD2	1.62	0.63
1:A:271:ARG:HG2	13:M:73:PRO:CG	2.28	0.63
1:A:271:ARG:CG	13:M:73:PRO:HG3	2.29	0.63
1:A:1192:TRP:CD1	1:A:1248:ASN:HA	2.34	0.63
25:2:177:GLN:OE1	25:2:220:LEU:HD22	1.98	0.63
25:2:202:GLN:HE21	25:2:202:GLN:H	1.44	0.63
2:B:52:GLN:OE1	2:B:160:TYR:OH	2.15	0.63
8:H:57:ARG:HD3	8:H:146:LYS:HD3	1.78	0.63
11:K:56:VAL:HA	11:K:77:THR:HG22	1.81	0.63
24:1:38:ILE:HB	24:1:44:PHE:HE1	1.63	0.63
26:3:70:LEU:HD13	26:3:115:ILE:CD1	2.28	0.63
26:3:214:TYR:CE2	26:3:216:LYS:HE2	2.32	0.63
1:A:691:ASP:OD2	1:A:765:ASN:HB2	1.98	0.63
13:M:10:LEU:CB	13:M:13:VAL:O	2.47	0.63
13:M:44:ARG:HH11	13:M:46:ILE:HG22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:77:LYS:HG2	23:0:225:GLU:OE2	1.99	0.63
25:2:35:TYR:CZ	25:2:62:LEU:HG	2.34	0.63
25:2:100:LEU:HG	25:2:119:ARG:NE	2.13	0.63
26:3:134:ALA:HB2	26:3:176:ASN:OD1	1.99	0.63
26:3:144:ILE:HD13	26:3:147:MET:HE3	1.80	0.63
26:3:64:ILE:CG1	26:3:123:ASP:HB3	2.29	0.63
2:B:453:TRP:CE3	2:B:466:VAL:HG21	2.33	0.63
8:H:23:ASP:O	8:H:25:VAL:N	2.31	0.63
24:1:18:GLN:NE2	24:1:44:PHE:HZ	1.97	0.63
25:2:123:LEU:O	25:2:123:LEU:HD23	1.99	0.63
26:3:59:VAL:CB	26:3:71:TYR:HE1	1.94	0.63
26:3:184:ALA:HA	26:3:187:GLN:CG	2.29	0.63
27:X:42:DT:H2'	27:X:43:DT:H71	1.81	0.63
1:A:131:ALA:C	1:A:133:SER:H	2.00	0.63
1:A:1116:ASN:OD1	1:A:1136:THR:O	2.17	0.63
2:B:95:LYS:HD3	2:B:162:LEU:HD21	1.80	0.63
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.32	0.63
6:F:125:ILE:HG22	6:F:127:ASP:H	1.63	0.63
8:H:7:GLU:OE2	8:H:57:ARG:NH2	2.32	0.63
20:T:12:ALA:HB2	20:T:106:LEU:HD23	1.81	0.63
24:1:59:GLU:CD	25:2:402:ARG:NH1	2.56	0.63
1:A:157:GLY:N	1:A:181:HIS:CE1	2.68	0.62
2:B:882:SER:O	2:B:887:TYR:CG	2.52	0.62
13:M:34:CYS:HB3	13:M:39:LEU:CB	2.29	0.62
13:M:34:CYS:HB3	13:M:39:LEU:HD23	0.64	0.62
17:Q:112:ARG:HH21	18:R:237:LEU:HD22	1.63	0.62
25:2:60:LEU:HD11	25:2:95:ILE:CB	2.29	0.62
25:2:197:THR:HG21	25:2:239:GLN:CD	2.24	0.62
1:A:455:ILE:HD13	1:A:520:MET:HE1	1.81	0.62
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.79	0.62
9:I:99:SER:OG	9:I:100:HIS:N	2.32	0.62
21:V:612:ASP:OD2	21:V:635:GLN:CD	2.42	0.62
1:A:208:ASP:OD1	1:A:209:SER:N	2.32	0.62
3:C:42:VAL:HB	3:C:178:PRO:HG2	1.81	0.62
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.64	0.62
22:W:59:TYR:OH	22:W:63:TYR:CE2	2.52	0.62
24:1:2:VAL:HG12	25:2:422:LEU:CD1	2.27	0.62
25:2:30:VAL:CG2	26:3:25:GLN:CB	2.48	0.62
25:2:160:LEU:HB3	25:2:206:LEU:CD1	2.27	0.62
26:3:165:LYS:O	26:3:165:LYS:HD3	1.98	0.62
8:H:106:THR:O	8:H:108:ALA:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:99:LEU:O	17:Q:101:ASN:N	2.25	0.62
17:Q:184:ILE:CD1	18:R:211:SER:HB2	2.20	0.62
18:R:194:ARG:C	18:R:196:ASP:N	2.40	0.62
24:1:1:MET:HB2	25:2:418:PHE:HB3	1.81	0.62
26:3:18:ASN:O	26:3:21:TRP:HD1	1.82	0.62
2:B:881:GLU:C	2:B:883:THR:N	2.55	0.62
2:B:956:PHE:HB3	2:B:962:THR:HG22	1.81	0.62
22:W:584:TYR:CG	22:W:594:ALA:HB2	2.34	0.62
25:2:173:GLN:HG2	25:2:179:LEU:HG	1.81	0.62
21:V:516:PRO:CA	24:1:15:ALA:O	2.45	0.62
25:2:93:LEU:HA	25:2:96:TRP:HD1	1.64	0.62
26:3:46:ASN:CG	26:3:104:LEU:HD22	2.25	0.62
26:3:58:ALA:CA	26:3:71:TYR:CE2	2.78	0.62
26:3:160:ARG:NH2	26:3:190:LEU:HD12	2.13	0.62
25:2:31:LEU:CG	26:3:33:THR:HB	2.28	0.62
25:2:203:PHE:HD2	25:2:205:LEU:HD23	1.64	0.62
25:2:218:GLN:HG2	25:2:268:PHE:HB3	1.82	0.62
26:3:133:LEU:HD22	26:3:134:ALA:N	2.14	0.62
26:3:216:LYS:H	26:3:216:LYS:CD	2.13	0.62
1:A:47:THR:O	1:A:48:GLU:CB	2.47	0.62
2:B:810:PHE:N	2:B:925:SER:O	2.29	0.62
12:L:35:ARG:NH1	12:L:42:ARG:HH21	1.98	0.62
17:Q:35:ASP:OD2	18:R:161:ARG:NH2	2.26	0.62
17:Q:114:ILE:CD1	18:R:218:LYS:HE3	2.29	0.62
24:1:50:VAL:HA	24:1:53:LEU:HD13	1.82	0.62
1:A:531:ASN:HD22	1:A:901:VAL:HG23	1.65	0.62
1:A:1372:GLU:HG3	5:E:193:ILE:HD13	1.81	0.62
24:1:38:ILE:HB	24:1:44:PHE:CE1	2.34	0.62
25:2:46:ARG:CD	25:2:85:GLU:HB2	2.30	0.62
25:2:89:LEU:HD23	25:2:89:LEU:O	1.99	0.62
25:2:189:GLU:O	25:2:193:PRO:HD2	2.00	0.62
2:B:899:SER:O	2:B:901:THR:N	2.33	0.61
6:F:65:VAL:HG22	6:F:104:ILE:HD11	1.81	0.61
21:V:613:THR:O	21:V:614:SER:CB	2.30	0.61
22:W:37:HIS:CE1	22:W:454:VAL:CG1	2.82	0.61
25:2:118:LEU:CD2	26:3:39:ASP:C	2.72	0.61
1:A:1480:CYS:O	1:A:1484:MET:HG3	2.00	0.61
10:J:64:PRO:C	10:J:66:GLU:H	2.08	0.61
21:V:612:ASP:O	21:V:614:SER:N	2.33	0.61
24:1:1:MET:HG2	25:2:414:SER:N	2.15	0.61
1:A:935:GLN:HG2	1:A:1059:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:PHE:CD1	2:B:422:PHE:C	2.77	0.61
2:B:1115:GLN:HB2	2:B:1148:LEU:HD21	1.82	0.61
10:J:67:LYS:NZ	12:L:20:GLY:O	2.32	0.61
24:1:8:VAL:O	25:2:407:VAL:HG12	1.99	0.61
25:2:60:LEU:CD1	25:2:95:ILE:HB	2.31	0.61
2:B:225:LEU:CD1	2:B:228:SER:CB	2.78	0.61
13:M:7:LEU:HD11	13:M:10:LEU:CD1	2.31	0.61
15:O:41:ASP:OD1	15:O:45:ASN:ND2	2.33	0.61
17:Q:165:GLU:HB3	17:Q:170:LYS:HE2	1.82	0.61
25:2:236:PHE:CE2	25:2:262:LEU:HD13	2.36	0.61
2:B:329:GLY:O	2:B:335:ARG:NE	2.34	0.61
21:V:368:ALA:O	21:V:371:VAL:HG22	2.00	0.61
22:W:209:TYR:OH	22:W:233:PHE:C	2.42	0.61
22:W:584:TYR:HB2	22:W:594:ALA:HB2	1.81	0.61
26:3:9:ASN:O	26:3:56:LYS:HD3	1.99	0.61
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.82	0.61
2:B:489:ILE:HG13	2:B:490:GLY:H	1.65	0.61
2:B:529:MET:HE2	2:B:623:ARG:HB2	1.82	0.61
8:H:65:TYR:HE1	8:H:84:ARG:HE	1.47	0.61
18:R:163:LEU:O	18:R:163:LEU:HD12	2.01	0.61
26:3:8:LEU:HA	26:3:54:SER:HB3	1.83	0.61
26:3:70:LEU:CD1	26:3:115:ILE:HD11	2.27	0.61
28:Y:24:DC:C2'	28:Y:25:DT:H72	2.30	0.61
1:A:202:TRP:CB	1:A:212:LYS:CB	2.53	0.61
1:A:1116:ASN:ND2	1:A:1138:SER:HB2	2.14	0.61
3:C:5:ASN:C	3:C:7:PRO:HD3	2.25	0.61
5:E:166:ARG:HB2	5:E:169:GLN:HG3	1.80	0.61
8:H:65:TYR:CE2	8:H:70:LEU:HB3	2.36	0.61
12:L:15:MET:HB3	12:L:29:LYS:HB3	1.83	0.61
21:V:316:LEU:HB2	21:V:321:GLU:CG	2.29	0.61
21:V:366:ASN:HD21	21:V:613:THR:CG2	2.11	0.61
24:1:1:MET:HA	25:2:414:SER:N	2.15	0.61
25:2:28:PRO:HD2	26:3:25:GLN:CD	2.25	0.61
25:2:30:VAL:HG23	26:3:25:GLN:HB2	1.74	0.61
26:3:190:LEU:H	26:3:190:LEU:CD2	2.12	0.61
28:Y:49:DG:N2	29:Z:4:C:O2	2.34	0.61
1:A:60:PRO:HD2	1:A:62:GLN:HG2	1.83	0.61
1:A:608:THR:CB	1:A:610:PRO:HD2	2.30	0.61
4:D:70:ARG:NH2	7:G:140:ASP:O	2.33	0.61
16:P:206:GLU:HG3	16:P:207:PRO:HD3	1.82	0.61
24:1:47:ALA:HB1	24:1:50:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:173:GLN:CA	26:3:176:ASN:HD21	2.10	0.61
1:A:206:ASN:O	1:A:207:GLU:HG3	1.99	0.61
1:A:426:ARG:CD	13:M:40:VAL:HG11	2.31	0.61
13:M:27:TYR:HE2	13:M:46:ILE:CD1	2.14	0.61
21:V:520:ARG:HD3	24:1:19:PHE:HB3	1.82	0.61
21:V:523:VAL:CB	24:1:20:LEU:HD23	2.31	0.61
25:2:83:GLN:OE1	25:2:83:GLN:HA	2.01	0.61
2:B:1130:THR:HB	2:B:1133:HIS:HB2	1.83	0.61
10:J:3:ILE:HG13	10:J:52:HIS:CE1	2.36	0.61
13:M:52:TRP:O	13:M:54:THR:N	2.31	0.61
22:W:73:CYS:CB	22:W:209:TYR:CZ	2.84	0.61
22:W:209:TYR:CE1	22:W:233:PHE:CD1	2.89	0.61
25:2:117:ASN:CG	26:3:108:ASN:CG	2.65	0.61
25:2:251:VAL:CG1	25:2:254:MET:HG3	2.30	0.61
26:3:143:TYR:O	26:3:146:ARG:HG2	2.01	0.61
2:B:461:GLN:NE2	27:X:43:DT:O2	2.34	0.60
16:P:297:LYS:HB2	16:P:298:PRO:HD2	1.82	0.60
17:Q:113:ARG:NH1	18:R:218:LYS:C	2.59	0.60
21:V:520:ARG:HG3	24:1:23:LEU:HD11	1.82	0.60
25:2:164:VAL:HG13	25:2:209:PRO:HG2	1.83	0.60
26:3:100:LYS:HG3	26:3:101:TYR:N	2.16	0.60
1:A:608:THR:OG1	1:A:610:PRO:HG3	2.01	0.60
1:A:865:ILE:O	1:A:869:GLU:HB3	2.01	0.60
9:I:14:ILE:HG13	9:I:16:PHE:CE1	2.36	0.60
16:P:158:SER:C	16:P:160:GLY:H	2.07	0.60
17:Q:108:ASP:OD2	18:R:237:LEU:HD22	2.01	0.60
22:W:423:ASP:O	22:W:425:THR:N	2.34	0.60
26:3:24:LYS:O	26:3:25:GLN:C	2.44	0.60
26:3:222:SER:HB2	26:3:226:TYR:CE2	2.36	0.60
2:B:553:LEU:HD13	2:B:573:TRP:CZ3	2.36	0.60
9:I:29:ASP:OD2	9:I:32:ASN:ND2	2.28	0.60
25:2:42:LEU:HD12	25:2:59:MET:HE3	1.83	0.60
25:2:159:VAL:HG13	25:2:160:LEU:N	2.17	0.60
9:I:58:ILE:HG22	9:I:58:ILE:O	2.00	0.60
20:T:94:THR:HG23	20:T:109:ILE:HG22	1.83	0.60
22:W:584:TYR:CE2	22:W:614:TYR:HB2	2.36	0.60
24:1:1:MET:HA	25:2:413:LEU:HA	1.83	0.60
2:B:80:GLU:OE1	2:B:134:LYS:HE2	2.00	0.60
10:J:63:ALA:CB	10:J:64:PRO:CD	2.73	0.60
18:R:223:VAL:CG2	18:R:224:THR:CB	2.77	0.60
24:1:10:ILE:C	24:1:10:ILE:HD13	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:712:PRO:O	2:B:939:HIS:HE1	1.84	0.60
20:T:146:ASP:O	20:T:147:LYS:HB3	2.01	0.60
25:2:30:VAL:HG12	25:2:34:LEU:HD23	1.82	0.60
1:A:931:ARG:O	1:A:933:THR:N	2.35	0.60
17:Q:171:LYS:O	17:Q:173:ALA:N	2.35	0.60
19:S:28:ILE:HD13	20:T:95:VAL:HG22	1.82	0.60
21:V:366:ASN:ND2	21:V:613:THR:CG2	2.65	0.60
24:1:1:MET:HB3	25:2:413:LEU:HG	1.83	0.60
24:1:9:LEU:CB	24:1:51:ASN:HD21	2.14	0.60
26:3:42:MET:HE2	26:3:108:ASN:CG	2.27	0.60
2:B:861:SER:N	2:B:864:ASP:OD2	2.34	0.60
18:R:166:ILE:HG22	18:R:168:LEU:H	1.66	0.60
2:B:959:GLU:OE2	2:B:961:ILE:HB	2.01	0.60
17:Q:113:ARG:CD	18:R:222:SER:CA	2.77	0.60
21:V:366:ASN:ND2	21:V:613:THR:HG22	2.15	0.60
23:0:55:LEU:HD12	26:3:178:MET:CE	2.31	0.60
25:2:206:LEU:HD22	25:2:206:LEU:N	2.17	0.60
2:B:552:ASN:OD1	2:B:553:LEU:N	2.35	0.60
13:M:10:LEU:HD22	13:M:10:LEU:H	1.65	0.60
13:M:94:ASP:O	13:M:96:PHE:N	2.35	0.60
20:T:82:PRO:HG2	20:T:117:ARG:HB2	1.83	0.60
26:3:21:TRP:O	26:3:24:LYS:HB2	2.02	0.60
1:A:47:THR:C	1:A:48:GLU:CG	2.75	0.59
1:A:1188:GLU:HG3	9:I:1:MET:HG2	1.83	0.59
2:B:51:ILE:HG22	20:T:141:LEU:CD2	2.32	0.59
2:B:866:ILE:HD12	2:B:921:ILE:HD11	1.82	0.59
13:M:36:GLU:N	13:M:36:GLU:OE1	2.34	0.59
24:1:53:LEU:HD12	24:1:53:LEU:N	2.17	0.59
25:2:171:VAL:HG13	25:2:216:MET:HB2	1.83	0.59
26:3:14:VAL:HG23	26:3:163:VAL:HA	1.84	0.59
26:3:174:TYR:CE1	26:3:178:MET:HE3	2.37	0.59
1:A:263:ALA:HA	1:A:272:ASN:O	2.02	0.59
1:A:545:VAL:HG22	1:A:676:ILE:HG13	1.84	0.59
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.67	0.59
9:I:15:ARG:HD2	9:I:37:TYR:CD2	2.37	0.59
24:1:18:GLN:HB2	24:1:44:PHE:CZ	2.37	0.59
25:2:202:GLN:NE2	25:2:202:GLN:H	2.00	0.59
26:3:213:LEU:HD23	26:3:230:VAL:HG12	1.84	0.59
28:Y:49:DG:H2'	28:Y:50:DA:C8	2.37	0.59
1:A:930:LEU:O	1:A:931:ARG:O	2.19	0.59
1:A:1026:ASP:O	1:A:1031:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:LEU:HB3	2:B:228:SER:HB3	1.49	0.59
8:H:96:VAL:HG22	8:H:116:VAL:HG13	1.84	0.59
13:M:86:LYS:HA	13:M:86:LYS:HE3	1.83	0.59
18:R:223:VAL:HA	18:R:224:THR:HG22	1.79	0.59
22:W:584:TYR:HB2	22:W:594:ALA:CB	2.32	0.59
26:3:110:VAL:O	26:3:114:GLU:HG2	2.02	0.59
28:Y:48:DC:H2'	28:Y:49:DG:C8	2.37	0.59
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.85	0.59
14:N:347:ASN:ND2	14:N:375:GLU:OE2	2.35	0.59
20:T:158:ASN:HB3	20:T:161:TYR:HB2	1.84	0.59
22:W:37:HIS:ND1	22:W:454:VAL:HG13	2.15	0.59
25:2:56:VAL:HG11	25:2:91:SER:CB	2.31	0.59
5:E:52:ARG:NH2	5:E:54:ARG:HD3	2.18	0.59
13:M:59:LYS:HB2	29:Z:1:A:H5'	1.83	0.59
17:Q:187:ILE:HG21	18:R:210:PHE:C	2.27	0.59
1:A:67:ARG:H	1:A:78:MET:HE1	1.67	0.59
1:A:1022:ILE:HG23	1:A:1023:VAL:HG23	1.84	0.59
2:B:226:GLU:O	2:B:227:ASN:HB2	2.00	0.59
2:B:631:GLN:HB3	2:B:685:LYS:NZ	2.18	0.59
8:H:106:THR:C	8:H:108:ALA:N	2.60	0.59
17:Q:24:GLY:HA2	18:R:209:GLN:HG2	1.83	0.59
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	1.85	0.59
1:A:926:ASN:OD1	1:A:931:ARG:CB	2.51	0.59
3:C:154:ARG:NH2	10:J:61:ASN:OD1	2.35	0.59
25:2:215:PHE:CD2	25:2:264:HIS:HB2	2.38	0.59
1:A:133:SER:C	1:A:135:GLY:N	2.45	0.59
1:A:386:ALA:HA	1:A:449:HIS:CD2	2.38	0.59
3:C:4:ALA:HA	11:K:52:LYS:HZ2	1.68	0.59
3:C:147:ASP:O	10:J:16:ASN:HB3	2.03	0.59
25:2:30:VAL:CB	26:3:25:GLN:HB3	2.32	0.59
26:3:215:LEU:CD1	26:3:230:VAL:HG13	2.32	0.59
1:A:131:ALA:C	1:A:133:SER:N	2.57	0.59
2:B:226:GLU:O	2:B:226:GLU:HG2	2.01	0.59
19:S:44:GLN:HB2	19:S:103:ASN:HA	1.84	0.59
24:1:38:ILE:H	24:1:38:ILE:CD1	2.16	0.59
1:A:51:ARG:H	1:A:52:PRO:HD2	1.66	0.59
1:A:154:CYS:O	1:A:184:CYS:O	2.21	0.59
1:A:486:LEU:HD22	2:B:790:GLN:OE1	2.03	0.59
1:A:1116:ASN:O	1:A:1117:VAL:CB	2.51	0.59
2:B:419:ALA:O	2:B:423:ILE:HG12	2.03	0.59
17:Q:184:ILE:CD1	18:R:218:LYS:HZ3	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:29:LEU:HD23	24:1:29:LEU:C	2.27	0.59
24:1:34:ILE:HG22	24:1:46:ILE:CD1	2.32	0.59
26:3:131:THR:HG23	26:3:133:LEU:CD1	2.33	0.59
19:S:10:ASN:OD1	19:S:11:VAL:N	2.36	0.58
25:2:160:LEU:HD12	25:2:160:LEU:N	2.18	0.58
25:2:196:ILE:HA	25:2:202:GLN:OE1	2.02	0.58
25:2:217:LEU:HD23	25:2:233:ILE:CD1	2.32	0.58
25:2:259:LEU:HD12	25:2:259:LEU:C	2.27	0.58
26:3:169:ASP:CG	26:3:202:LEU:HD23	2.28	0.58
2:B:798:ARG:O	2:B:801:VAL:HG22	2.03	0.58
2:B:1162:LEU:HD23	2:B:1165:MET:HE3	1.86	0.58
5:E:7:THR:HG1	5:E:47:LYS:HD3	1.61	0.58
9:I:14:ILE:HG13	9:I:16:PHE:CD2	2.37	0.58
24:1:2:VAL:HB	25:2:456:LYS:HD3	1.86	0.58
26:3:21:TRP:CD2	26:3:34:LEU:HD23	2.38	0.58
2:B:133:ILE:CG2	2:B:139:GLN:HG2	2.18	0.58
2:B:225:LEU:HD22	2:B:228:SER:HB2	1.85	0.58
2:B:470:LEU:HD21	2:B:478:THR:HG23	1.83	0.58
2:B:1079:SER:O	2:B:1080:ARG:HD2	2.03	0.58
2:B:1117:HIS:HB2	2:B:1127:ILE:HG12	1.84	0.58
13:M:311:ASP:OD2	13:M:312:LYS:NZ	2.36	0.58
24:1:2:VAL:CG1	25:2:456:LYS:CD	2.82	0.58
24:1:19:PHE:O	24:1:23:LEU:HG	2.02	0.58
24:1:34:ILE:O	24:1:46:ILE:HG13	2.03	0.58
25:2:177:GLN:HE22	25:2:220:LEU:HA	1.68	0.58
25:2:203:PHE:CE2	25:2:205:LEU:HD23	2.38	0.58
13:M:27:TYR:HE2	13:M:46:ILE:HD13	1.68	0.58
25:2:28:PRO:HA	26:3:33:THR:HB	1.85	0.58
26:3:215:LEU:HD12	26:3:230:VAL:HG13	1.85	0.58
1:A:155:GLU:C	1:A:181:HIS:HD1	2.12	0.58
2:B:510:CYS:HB2	2:B:705:GLY:HA3	1.84	0.58
3:C:4:ALA:HA	11:K:52:LYS:NZ	2.18	0.58
13:M:179:GLU:HA	20:T:154:LYS:CG	2.24	0.58
25:2:62:LEU:HD13	25:2:62:LEU:C	2.28	0.58
26:3:59:VAL:HB	26:3:71:TYR:CD1	2.25	0.58
1:A:152:ASN:C	1:A:153:ILE:CG1	2.63	0.58
1:A:320:ASN:HB2	1:A:338:SER:OG	2.03	0.58
1:A:1171:ALA:C	9:I:59:THR:HG23	2.27	0.58
1:A:1464:ALA:O	1:A:1469:GLY:HA3	2.03	0.58
2:B:357:CYS:HB2	2:B:360:LYS:HD2	1.85	0.58
17:Q:113:ARG:HH22	18:R:218:LYS:CG	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:419:GLU:O	22:W:420:PRO:O	2.20	0.58
23:O:79:ASN:O	23:O:80:ARG:C	2.46	0.58
26:3:131:THR:CG2	26:3:133:LEU:HD12	2.33	0.58
2:B:906:GLN:CG	12:L:45:TYR:HE1	2.17	0.58
3:C:274:ILE:HD11	11:K:31:CYS:SG	2.43	0.58
13:M:27:TYR:CE2	13:M:46:ILE:HD13	2.39	0.58
23:O:109:THR:HB	23:O:144:SER:H	1.67	0.58
25:2:236:PHE:CZ	25:2:258:LEU:HD11	2.39	0.58
1:A:30:GLU:OE1	1:A:33:ARG:NH2	2.24	0.58
2:B:880:LEU:O	2:B:881:GLU:OE1	2.22	0.58
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.86	0.58
25:2:220:LEU:HD13	25:2:220:LEU:C	2.29	0.58
1:A:1372:GLU:OE2	5:E:207:ARG:NH1	2.36	0.58
25:2:44:VAL:HG13	25:2:45:PHE:N	2.17	0.58
26:3:169:ASP:CB	26:3:202:LEU:HD23	2.33	0.58
1:A:79:THR:HG23	13:M:43:ASP:HB2	1.81	0.58
1:A:1307:VAL:HG11	1:A:1339:ASP:HB2	1.86	0.58
13:M:59:LYS:HG3	13:M:64:PRO:HG2	1.84	0.58
26:3:16:ASP:O	26:3:21:TRP:NE1	2.27	0.58
26:3:160:ARG:HB3	26:3:190:LEU:CD2	2.32	0.58
1:A:47:THR:C	1:A:48:GLU:HG2	2.28	0.57
2:B:290:TYR:OH	2:B:566:LYS:NZ	2.36	0.57
7:G:144:ARG:N	7:G:169:GLY:O	2.34	0.57
13:M:94:ASP:HB2	13:M:99:SER:N	2.09	0.57
17:Q:113:ARG:HD3	18:R:222:SER:CA	2.34	0.57
22:W:584:TYR:CB	22:W:594:ALA:HB2	2.33	0.57
25:2:30:VAL:N	26:3:25:GLN:HB3	2.19	0.57
26:3:190:LEU:HD23	26:3:190:LEU:N	2.18	0.57
2:B:80:GLU:O	2:B:82:PRO:N	2.37	0.57
16:P:207:PRO:O	16:P:208:ARG:C	2.47	0.57
25:2:35:TYR:CB	25:2:62:LEU:HD12	2.33	0.57
25:2:118:LEU:HD12	25:2:118:LEU:C	2.28	0.57
26:3:196:LEU:CD2	26:3:223:LEU:HD23	2.25	0.57
1:A:426:ARG:H	13:M:40:VAL:HG21	1.69	0.57
2:B:92:TYR:HE2	2:B:146:LYS:HE2	1.69	0.57
2:B:446:TYR:HB2	28:Y:59:DG:OP1	2.05	0.57
2:B:895:PHE:O	2:B:897:ARG:HG3	2.04	0.57
16:P:171:THR:HG22	16:P:220:VAL:HG22	1.87	0.57
26:3:44:LEU:HD13	26:3:44:LEU:C	2.30	0.57
26:3:210:THR:HG22	26:3:210:THR:O	2.04	0.57
2:B:92:TYR:HB3	20:T:145:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:SER:O	2:B:122:ALA:HB1	2.04	0.57
12:L:26:ASN:CB	12:L:44:MET:HE2	2.33	0.57
24:1:8:VAL:HG12	24:1:9:LEU:H	1.69	0.57
24:1:18:GLN:CD	24:1:44:PHE:HZ	2.12	0.57
25:2:29:GLY:CA	26:3:25:GLN:CG	2.78	0.57
1:A:935:GLN:HA	1:A:1059:ARG:HH22	1.67	0.57
1:A:1123:ARG:NH2	1:A:1381:GLU:OE1	2.31	0.57
2:B:81:PRO:HD2	2:B:135:GLU:HG3	1.87	0.57
25:2:82:ALA:HA	25:2:89:LEU:HD11	1.85	0.57
26:3:14:VAL:HG23	26:3:163:VAL:HG13	1.86	0.57
27:X:49:DT:H2'	27:X:50:DT:H4'	1.86	0.57
1:A:334:ARG:NH2	13:M:66:ARG:O	2.37	0.57
1:A:608:THR:OG1	1:A:610:PRO:CD	2.52	0.57
17:Q:24:GLY:HA2	18:R:209:GLN:CG	2.34	0.57
26:3:144:ILE:HG12	26:3:147:MET:CE	2.34	0.57
26:3:187:GLN:NE2	26:3:189:ILE:HG13	2.20	0.57
1:A:618:TYR:C	1:A:620:HIS:H	2.12	0.57
1:A:927:GLU:HB3	1:A:931:ARG:HD3	1.87	0.57
2:B:761:THR:OG1	2:B:764:MET:HG3	2.05	0.57
3:C:90:CYS:SG	3:C:94:CYS:HB3	2.43	0.57
5:E:64:HIS:C	5:E:66:ASP:N	2.56	0.57
6:F:88:ASP:OD1	6:F:91:LEU:N	2.33	0.57
21:V:321:GLU:HA	22:W:499:ASN:HD21	1.65	0.57
23:0:54:ARG:C	26:3:209:ILE:HD11	2.25	0.57
25:2:29:GLY:H	26:3:25:GLN:CD	2.12	0.57
25:2:117:ASN:HD22	26:3:42:MET:HE1	1.70	0.57
1:A:805:ARG:NH2	2:B:671:GLU:O	2.37	0.57
2:B:133:ILE:C	2:B:134:LYS:O	2.46	0.57
1:A:426:ARG:N	13:M:40:VAL:HG21	2.20	0.57
2:B:1075:MET:HE1	13:M:51:GLU:HG2	1.87	0.57
3:C:5:ASN:N	11:K:97:GLU:OE2	2.38	0.57
5:E:52:ARG:CZ	5:E:54:ARG:HG3	2.35	0.57
5:E:91:CYS:HA	5:E:94:MET:HE3	1.87	0.57
25:2:47:GLU:HG3	25:2:48:LEU:N	2.20	0.57
25:2:60:LEU:HD11	25:2:95:ILE:CG2	2.35	0.57
25:2:185:MET:HB2	25:2:229:ASP:OD1	2.04	0.57
2:B:1053:HIS:CE1	2:B:1058:LYS:HG3	2.40	0.57
21:V:514:MET:SD	21:V:537:ASN:ND2	2.78	0.57
1:A:355:MET:CE	1:A:1431:SER:HB2	2.35	0.56
1:A:1123:ARG:NH2	1:A:1360:ASN:HB2	2.19	0.56
9:I:15:ARG:O	9:I:24:LEU:HD12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.86	0.56
18:R:155:LEU:HD13	18:R:204:ASN:HD22	1.70	0.56
25:2:160:LEU:H	25:2:160:LEU:CD1	2.18	0.56
26:3:195:VAL:HG21	26:3:214:TYR:OH	2.05	0.56
1:A:322:LEU:HD12	1:A:323:PRO:HD2	1.87	0.56
1:A:567:LEU:HG	1:A:671:ASN:OD1	2.04	0.56
2:B:232:THR:HG23	2:B:233:SER:H	1.69	0.56
2:B:716:HIS:CD2	2:B:982:ILE:HG13	2.30	0.56
2:B:1029:TYR:CE1	2:B:1036:LYS:HE2	2.38	0.56
3:C:175:LYS:HZ2	12:L:57:ALA:HB3	1.70	0.56
10:J:7:CYS:SG	10:J:48:MET:HE3	2.45	0.56
12:L:17:TYR:HB3	12:L:44:MET:HE3	1.86	0.56
17:Q:125:ALA:HB1	17:Q:138:ASP:HB3	1.87	0.56
1:A:904:GLN:NE2	1:A:982:ASN:HA	2.20	0.56
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.87	0.56
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.39	0.56
14:N:313:PRO:HG2	16:P:235:ARG:NH2	2.17	0.56
17:Q:77:ARG:HB2	17:Q:93:PHE:HB3	1.86	0.56
17:Q:115:GLU:HA	17:Q:118:GLU:HB3	1.88	0.56
24:1:59:GLU:CD	25:2:402:ARG:HH12	2.13	0.56
25:2:117:ASN:HB2	26:3:104:LEU:CD1	2.35	0.56
25:2:423:ALA:HA	25:2:426:ARG:HE	1.70	0.56
1:A:1466:ALA:O	1:A:1469:GLY:N	2.39	0.56
13:M:72:ASN:HB2	28:Y:58:DC:H42	1.70	0.56
17:Q:21:VAL:HA	18:R:210:PHE:CE2	2.40	0.56
26:3:165:LYS:HD3	26:3:165:LYS:C	2.31	0.56
1:A:455:ILE:HG12	1:A:473:ARG:HG2	1.87	0.56
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.88	0.56
1:A:1211:LEU:HD11	1:A:1258:ARG:HG3	1.86	0.56
16:P:257:ASN:ND2	27:X:14:DA:N3	2.54	0.56
26:3:42:MET:SD	26:3:111:ILE:HD13	2.46	0.56
26:3:57:LEU:HD23	26:3:58:ALA:C	2.31	0.56
26:3:223:LEU:HD11	26:3:227:LEU:HD11	1.87	0.56
1:A:375:ILE:HB	1:A:666:ARG:CD	2.35	0.56
1:A:1154:ALA:HB1	1:A:1310:HIS:CE1	2.41	0.56
1:A:1289:GLU:HG2	1:A:1292:MET:HE2	1.87	0.56
2:B:166:LEU:HB3	2:B:170:ASP:HB2	1.87	0.56
2:B:758:LEU:HD13	2:B:991:ALA:HB2	1.88	0.56
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.69	0.56
21:V:426:VAL:HG13	21:V:427:MET:H	1.69	0.56
26:3:19:PRO:HG2	26:3:123:ASP:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:GLN:HE22	1:A:821:GLY:HA3	1.71	0.56
1:A:1188:GLU:O	1:A:1192:TRP:HZ3	1.87	0.56
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.86	0.56
24:1:1:MET:CB	25:2:418:PHE:HB2	2.35	0.56
24:1:17:LYS:O	24:1:20:LEU:HB3	2.05	0.56
25:2:130:SER:HB2	25:2:173:GLN:OE1	2.06	0.56
25:2:206:LEU:HD22	25:2:206:LEU:H	1.71	0.56
26:3:172:LEU:HD13	26:3:172:LEU:C	2.29	0.56
26:3:223:LEU:O	26:3:223:LEU:HD13	2.06	0.56
1:A:139:LYS:HE2	1:A:143:HIS:NE2	2.20	0.56
7:G:94:LYS:O	7:G:110:ARG:NH1	2.34	0.56
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.39	0.56
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.39	0.56
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.86	0.56
23:O:73:ASP:O	23:O:79:ASN:HA	2.06	0.56
2:B:206:TYR:HD1	2:B:208:PHE:HE1	1.54	0.56
2:B:625:LEU:HD13	2:B:675:LEU:HD11	1.87	0.56
3:C:157:GLN:HG2	10:J:65:LEU:HB2	1.83	0.56
26:3:178:MET:SD	26:3:181:ILE:HD12	2.46	0.56
2:B:584:MET:HE3	2:B:588:ARG:HH12	1.70	0.56
2:B:605:ARG:NH2	9:I:71:ASP:OD2	2.39	0.56
5:E:62:VAL:O	5:E:63:ALA:HB2	2.05	0.56
8:H:17:PRO:C	8:H:19:GLY:H	2.13	0.56
9:I:96:PHE:HB3	9:I:112:TYR:HD1	1.72	0.56
17:Q:70:LYS:HZ2	18:R:226:ASP:HA	1.71	0.56
18:R:181:ALA:HA	18:R:184:ALA:HB3	1.88	0.56
18:R:184:ALA:HA	18:R:187:ASP:HB3	1.87	0.56
1:A:264:VAL:HG21	13:M:68:GLY:HA3	1.88	0.55
2:B:270:ILE:HG21	2:B:308:ALA:HB2	1.87	0.55
17:Q:149:THR:HG23	17:Q:151:THR:H	1.72	0.55
24:1:1:MET:CG	25:2:418:PHE:HB2	2.35	0.55
24:1:52:VAL:HG22	24:1:53:LEU:HD12	1.87	0.55
1:A:458:PHE:HE1	1:A:501:MET:HE3	1.71	0.55
2:B:474:THR:HG23	2:B:732:ALA:O	2.05	0.55
3:C:154:ARG:NH1	10:J:61:ASN:HA	2.21	0.55
5:E:64:HIS:O	5:E:66:ASP:N	2.37	0.55
8:H:16:ASP:HB3	8:H:19:GLY:HA2	1.89	0.55
13:M:94:ASP:HB3	13:M:99:SER:N	2.21	0.55
17:Q:25:PHE:N	18:R:210:PHE:CE2	2.74	0.55
17:Q:108:ASP:O	17:Q:111:ARG:HG2	2.06	0.55
19:S:27:ASN:O	20:T:95:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:423:ASP:C	22:W:425:THR:N	2.63	0.55
24:1:34:ILE:HG23	24:1:50:VAL:HG11	1.89	0.55
25:2:37:HIS:HB3	25:2:38:PRO:CD	2.35	0.55
25:2:159:VAL:HG22	25:2:160:LEU:N	2.16	0.55
26:3:133:LEU:H	26:3:133:LEU:CD1	2.10	0.55
1:A:298:ALA:H	17:Q:60:ARG:HE	1.53	0.55
1:A:644:SER:O	1:A:651:SER:HB3	2.06	0.55
5:E:52:ARG:NH2	5:E:54:ARG:CD	2.70	0.55
7:G:138:GLN:HG2	7:G:139:GLN:HG2	1.89	0.55
1:A:930:LEU:O	1:A:931:ARG:C	2.49	0.55
1:A:1287:CYS:HA	2:B:250:SER:HB2	1.88	0.55
2:B:225:LEU:CG	2:B:228:SER:CB	2.84	0.55
25:2:181:GLN:HA	25:2:181:GLN:HE21	1.70	0.55
1:A:138:LYS:N	1:A:1445:HIS:HE1	2.04	0.55
1:A:1036:ASN:ND2	5:E:202:ARG:O	2.29	0.55
2:B:133:ILE:O	2:B:133:ILE:HG22	2.06	0.55
13:M:27:TYR:CD2	13:M:46:ILE:CG2	2.89	0.55
17:Q:112:ARG:HH22	18:R:237:LEU:HB2	1.72	0.55
18:R:204:ASN:OD1	18:R:205:ASP:N	2.39	0.55
20:T:93:LEU:HB2	20:T:110:VAL:HB	1.89	0.55
27:X:70:DG:N2	28:Y:25:DT:O2	2.39	0.55
19:S:6:PRO:HG3	19:S:10:ASN:HD22	1.71	0.55
24:1:1:MET:HB2	25:2:418:PHE:HB2	1.88	0.55
24:1:3:ASN:CB	25:2:412:PHE:O	2.54	0.55
24:1:31:LYS:O	24:1:32:LYS:HB2	2.06	0.55
24:1:36:GLN:HB3	24:1:45:VAL:HG12	1.88	0.55
1:A:263:ALA:O	1:A:265:VAL:HG22	2.07	0.55
1:A:546:ARG:NH1	1:A:768:SER:OG	2.39	0.55
1:A:1373:ALA:HB2	5:E:145:VAL:HG22	1.88	0.55
2:B:906:GLN:HG2	12:L:45:TYR:CE1	2.39	0.55
20:T:177:ARG:NH2	27:X:19:DG:OP1	2.39	0.55
1:A:328:ALA:HA	13:M:84:ILE:HG22	1.89	0.55
2:B:45:ASP:HB3	2:B:534:VAL:HG11	1.88	0.55
2:B:649:ASN:OD1	2:B:650:ASN:N	2.40	0.55
3:C:274:ILE:O	11:K:23:LYS:NZ	2.33	0.55
17:Q:188:TYR:OH	18:R:210:PHE:HE1	1.79	0.55
20:T:203:VAL:HG11	20:T:210:VAL:HG22	1.88	0.55
26:3:44:LEU:HD13	26:3:44:LEU:O	2.06	0.55
1:A:265:VAL:HG21	13:M:48:VAL:HB	1.88	0.55
1:A:601:ASN:HD21	1:A:632:ASN:H	1.55	0.55
2:B:894:THR:HG23	2:B:897:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1087:GLY:HA3	28:Y:48:DC:OP1	2.07	0.55
9:I:60:HIS:C	9:I:62:VAL:H	2.15	0.55
13:M:119:LYS:HD3	28:Y:60:DA:H62	1.72	0.55
17:Q:170:LYS:HG2	17:Q:171:LYS:H	1.72	0.55
23:O:72:GLU:O	23:O:79:ASN:CB	2.55	0.55
24:1:38:ILE:HA	24:1:44:PHE:CD1	2.37	0.55
25:2:177:GLN:NE2	25:2:220:LEU:HA	2.22	0.55
25:2:211:GLN:HB3	25:2:261:PHE:CE1	2.40	0.55
1:A:611:ASP:OD1	1:A:626:THR:HG23	2.07	0.54
21:V:325:ARG:HH22	22:W:499:ASN:HB3	0.72	0.54
21:V:504:LYS:HD2	21:V:654:GLU:O	2.07	0.54
25:2:123:LEU:HD21	25:2:178:LEU:CD1	2.38	0.54
1:A:196:LEU:HB2	1:A:325:LEU:HD21	1.90	0.54
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.47	0.54
24:1:34:ILE:HG21	24:1:54:GLN:CD	2.32	0.54
24:1:52:VAL:HG23	24:1:53:LEU:N	2.21	0.54
25:2:208:THR:O	25:2:212:LEU:HG	2.07	0.54
25:2:214:TYR:CD2	25:2:261:PHE:CD2	2.95	0.54
26:3:64:ILE:HG23	26:3:128:HIS:CG	2.42	0.54
27:X:42:DT:H3'	27:X:43:DT:C5'	2.37	0.54
28:Y:64:DC:H2''	28:Y:65:DG:H5'	1.89	0.54
1:A:129:ILE:HG22	1:A:140:ARG:HG3	1.90	0.54
1:A:608:THR:CA	1:A:610:PRO:HD2	2.37	0.54
1:A:930:LEU:C	1:A:931:ARG:O	2.50	0.54
2:B:855:ALA:O	2:B:858:VAL:HG12	2.07	0.54
17:Q:23:ARG:CZ	18:R:207:SER:O	2.51	0.54
25:2:123:LEU:CD2	25:2:178:LEU:HD11	2.37	0.54
8:H:88:PHE:HD2	8:H:144:LEU:HB3	1.72	0.54
16:P:158:SER:C	16:P:160:GLY:N	2.60	0.54
16:P:163:PRO:HA	16:P:262:CYS:HB3	1.88	0.54
16:P:206:GLU:C	16:P:208:ARG:N	2.55	0.54
1:A:285:LYS:HD2	13:M:80:LEU:HD23	1.89	0.54
1:A:870:SER:HB2	1:A:882:SER:HB3	1.90	0.54
3:C:157:GLN:HG2	10:J:65:LEU:HB3	1.85	0.54
3:C:209:SER:O	3:C:211:LEU:N	2.41	0.54
9:I:15:ARG:HD2	9:I:37:TYR:HD2	1.72	0.54
13:M:174:PRO:HD2	13:M:213:ASP:HB3	1.89	0.54
26:3:100:LYS:O	26:3:103:LEU:HB2	2.08	0.54
26:3:106:SER:O	26:3:109:GLU:HG3	2.08	0.54
26:3:223:LEU:HD13	26:3:227:LEU:HG	1.89	0.54
27:X:69:DA:C2	28:Y:26:DG:N2	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:LEU:HD13	1:A:767:LYS:HB2	1.89	0.54
2:B:198:GLU:OE2	2:B:391:LYS:NZ	2.35	0.54
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.90	0.54
7:G:108:ILE:HG23	7:G:162:SER:HA	1.90	0.54
13:M:27:TYR:CD2	13:M:46:ILE:HG21	2.43	0.54
17:Q:187:ILE:HG21	18:R:211:SER:N	2.21	0.54
20:T:177:ARG:HH22	27:X:19:DG:P	2.31	0.54
25:2:53:LYS:CE	25:2:95:ILE:HD11	2.36	0.54
25:2:199:ALA:HB1	25:2:201:PHE:CD2	2.43	0.54
1:A:373:LEU:O	1:A:485:ASN:ND2	2.41	0.54
12:L:26:ASN:O	12:L:27:GLU:CB	2.55	0.54
21:V:667:THR:HA	24:1:62:ASP:OD2	2.07	0.54
27:X:24:DG:H2''	27:X:25:DG:H5'	1.89	0.54
1:A:271:ARG:CG	13:M:73:PRO:CG	2.86	0.54
13:M:182:ALA:HB2	20:T:154:LYS:HA	1.89	0.54
26:3:22:TRP:O	26:3:25:GLN:NE2	2.39	0.54
26:3:223:LEU:HD13	26:3:223:LEU:C	2.33	0.54
28:Y:31:DG:C5	28:Y:32:DC:C4	2.96	0.54
1:A:522:PRO:HB3	1:A:666:ARG:HB2	1.89	0.54
2:B:132:VAL:HG23	2:B:141:GLN:CG	2.31	0.54
2:B:252:ILE:O	2:B:254:GLN:N	2.35	0.54
3:C:6:GLN:O	3:C:7:PRO:C	2.51	0.54
5:E:52:ARG:NH2	5:E:54:ARG:HG3	2.21	0.54
20:T:140:ARG:O	20:T:142:SER:N	2.41	0.54
21:V:638:GLN:O	21:V:642:ARG:HG2	2.08	0.54
22:W:209:TYR:CZ	22:W:233:PHE:HA	2.38	0.54
24:1:25:GLU:HG2	24:1:32:LYS:HA	1.89	0.54
1:A:206:ASN:C	1:A:207:GLU:HG3	2.33	0.53
2:B:911:LEU:HD13	2:B:915:GLY:HA2	1.90	0.53
2:B:1053:HIS:HE1	2:B:1058:LYS:HG3	1.73	0.53
7:G:106:CYS:HA	7:G:159:ALA:O	2.08	0.53
9:I:86:CYS:O	9:I:87:GLN:C	2.50	0.53
13:M:45:VAL:CG1	13:M:48:VAL:HG13	2.38	0.53
13:M:94:ASP:CB	13:M:99:SER:N	2.58	0.53
19:S:13:GLU:OE1	20:T:44:ARG:NH1	2.41	0.53
19:S:48:GLU:OE1	19:S:101:ARG:NH2	2.41	0.53
26:3:58:ALA:C	26:3:71:TYR:OH	2.50	0.53
26:3:133:LEU:HD13	26:3:133:LEU:N	2.14	0.53
1:A:1253:GLU:HG2	9:I:3:PRO:HB2	1.89	0.53
2:B:752:TYR:CG	3:C:63:PHE:HE1	2.26	0.53
17:Q:105:TYR:OH	18:R:234:GLU:CD	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:4:VAL:HG12	25:2:411:GLN:C	2.30	0.53
24:1:8:VAL:CG1	24:1:45:VAL:HG13	2.35	0.53
25:2:86:SER:O	25:2:90:LEU:HD13	2.09	0.53
25:2:141:HIS:HA	25:2:162:PHE:CE2	2.43	0.53
26:3:105:THR:HG23	26:3:106:SER:N	2.23	0.53
1:A:375:ILE:HG13	1:A:666:ARG:HH11	1.74	0.53
1:A:611:ASP:CG	1:A:626:THR:OG1	2.51	0.53
2:B:309:PHE:HE2	9:I:40:ARG:HD2	1.72	0.53
2:B:352:GLY:HA3	2:B:357:CYS:SG	2.48	0.53
2:B:708:ALA:O	2:B:711:ILE:HG23	2.08	0.53
17:Q:144:LEU:HD22	17:Q:154:CYS:HA	1.91	0.53
19:S:172:ASN:HD21	19:S:175:SER:HB2	1.72	0.53
25:2:81:LYS:HG3	25:2:82:ALA:N	2.21	0.53
25:2:160:LEU:CG	25:2:206:LEU:HD21	2.39	0.53
1:A:263:ALA:C	1:A:265:VAL:N	2.58	0.53
25:2:222:THR:HG23	25:2:222:THR:O	2.07	0.53
1:A:65:ILE:HA	1:A:78:MET:HE2	1.89	0.53
1:A:153:ILE:HG22	1:A:155:GLU:OE2	2.08	0.53
1:A:358:ARG:HE	2:B:1076:GLU:CD	2.16	0.53
2:B:92:TYR:CE2	2:B:146:LYS:HE2	2.42	0.53
11:K:116:ILE:HG13	11:K:117:GLU:HG3	1.90	0.53
1:A:485:ASN:C	1:A:485:ASN:OD1	2.52	0.53
1:A:1204:VAL:HA	1:A:1207:ILE:HG12	1.89	0.53
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.91	0.53
26:3:191:ILE:N	26:3:210:THR:HG21	2.24	0.53
1:A:273:GLN:O	1:A:274:ASP:C	2.49	0.53
1:A:1188:GLU:HA	9:I:1:MET:HE2	1.91	0.53
17:Q:21:VAL:CA	18:R:210:PHE:CE2	2.91	0.53
22:W:428:ILE:HA	22:W:430:ASN:ND2	2.24	0.53
24:1:2:VAL:HG12	25:2:456:LYS:HG2	1.79	0.53
25:2:241:SER:O	25:2:245:LEU:HD23	2.09	0.53
26:3:18:ASN:O	26:3:21:TRP:CD1	2.62	0.53
27:X:45:DT:O2	27:X:46:DT:N3	2.41	0.53
29:Z:1:A:H2'	29:Z:2:G:O4'	2.08	0.53
1:A:156:GLY:CA	1:A:181:HIS:CE1	2.92	0.53
2:B:627:ILE:HD11	2:B:663:GLU:HB2	1.89	0.53
7:G:93:ASN:HD22	17:Q:151:THR:HA	1.73	0.53
12:L:13:GLN:C	12:L:15:MET:H	2.17	0.53
17:Q:25:PHE:HA	18:R:219:LEU:HD13	1.91	0.53
17:Q:113:ARG:HD3	18:R:222:SER:HA	1.91	0.53
25:2:211:GLN:HE21	25:2:257:SER:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:O	1:A:272:ASN:N	2.42	0.53
1:A:426:ARG:H	13:M:40:VAL:CG2	2.21	0.53
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	1.91	0.53
4:D:33:LEU:HD12	4:D:80:ILE:HG23	1.91	0.53
4:D:135:GLN:HA	4:D:138:ARG:HG2	1.91	0.53
17:Q:180:PHE:CE1	18:R:214:GLU:N	2.70	0.53
24:1:35:ILE:O	24:1:35:ILE:HG13	2.08	0.53
26:3:15:VAL:HG23	26:3:15:VAL:O	2.08	0.53
26:3:160:ARG:NH2	26:3:192:ASP:HB3	2.23	0.53
1:A:367:ILE:HG21	1:A:501:MET:HG2	1.91	0.53
1:A:557:ARG:HA	1:A:586:TRP:CZ3	2.44	0.53
2:B:800:ALA:O	2:B:805:PHE:HB2	2.09	0.53
17:Q:203:ILE:HG23	17:Q:204:LEU:HG	1.91	0.53
24:1:1:MET:CE	25:2:415:GLN:C	2.80	0.53
26:3:34:LEU:HD13	26:3:34:LEU:C	2.33	0.53
1:A:360:ASP:CG	2:B:1064:ARG:H	2.17	0.52
1:A:440:LEU:HB2	1:A:444:TYR:HD2	1.73	0.52
23:0:54:ARG:CG	26:3:182:PHE:CZ	2.80	0.52
25:2:138:PRO:O	25:2:139:ASP:HB2	2.08	0.52
25:2:159:VAL:CG1	25:2:161:HIS:H	2.06	0.52
26:3:100:LYS:HG3	26:3:101:TYR:H	1.74	0.52
1:A:455:ILE:HG21	1:A:520:MET:HE1	1.91	0.52
1:A:1477:ALA:HB2	7:G:22:LEU:HD23	1.90	0.52
2:B:295:PRO:HB3	9:I:11:PHE:HD2	1.75	0.52
2:B:712:PRO:HD2	2:B:939:HIS:CE1	2.44	0.52
19:S:125:TYR:CD1	19:S:139:PRO:HA	2.44	0.52
21:V:689:VAL:CB	25:2:391:ILE:HD11	2.39	0.52
1:A:205:VAL:HG21	1:A:212:LYS:NZ	2.24	0.52
2:B:51:ILE:HG23	20:T:141:LEU:HD21	1.90	0.52
2:B:489:ILE:HA	27:X:47:DT:O2	2.09	0.52
13:M:34:CYS:SG	13:M:39:LEU:HD21	2.46	0.52
17:Q:102:VAL:HG23	17:Q:102:VAL:O	2.09	0.52
23:0:54:ARG:CB	26:3:209:ILE:CG2	2.87	0.52
25:2:221:GLN:CD	25:2:230:LEU:HB2	2.34	0.52
27:X:26:DG:N2	28:Y:69:DC:N3	2.57	0.52
1:A:469:MET:HE3	2:B:1094:GLN:OE1	2.09	0.52
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.74	0.52
2:B:473:LEU:HD21	2:B:1052:LYS:HB2	1.90	0.52
2:B:838:GLN:O	2:B:891:ASP:N	2.43	0.52
2:B:844:ILE:HG22	2:B:846:ASP:H	1.74	0.52
26:3:204:GLN:HG2	26:3:214:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:ILE:HD13	1:A:1080:ILE:HD12	1.92	0.52
16:P:298:PRO:O	16:P:299:ARG:C	2.52	0.52
20:T:229:HIS:NE2	27:X:28:DG:H1'	2.25	0.52
26:3:14:VAL:HG23	26:3:14:VAL:O	2.09	0.52
2:B:1073:GLN:NE2	2:B:1154:ALA:HB2	2.25	0.52
3:C:157:GLN:HG3	10:J:65:LEU:HB2	1.90	0.52
12:L:35:ARG:HH11	12:L:42:ARG:HH21	1.57	0.52
13:M:196:LYS:NZ	27:X:13:DT:OP1	2.32	0.52
25:2:30:VAL:O	25:2:34:LEU:HD23	2.09	0.52
26:3:10:LEU:HD21	26:3:143:TYR:CD2	2.45	0.52
26:3:222:SER:HB3	26:3:225:GLN:HG2	1.92	0.52
28:Y:48:DC:O2	29:Z:5:G:N2	2.26	0.52
1:A:924:TYR:CZ	1:A:949:GLN:HG3	2.45	0.52
21:V:615:PHE:C	21:V:617:LEU:N	2.57	0.52
22:W:584:TYR:HB2	22:W:591:GLY:HA3	1.92	0.52
25:2:234:LEU:HD23	25:2:234:LEU:C	2.34	0.52
26:3:10:LEU:HD21	26:3:143:TYR:CE2	2.44	0.52
1:A:95:PHE:CE1	1:A:218:PRO:HG3	2.44	0.52
2:B:56:GLN:CD	20:T:140:ARG:HG3	2.31	0.52
2:B:553:LEU:O	2:B:556:ILE:HG12	2.10	0.52
2:B:914:GLU:HG3	13:M:132:ARG:HB3	1.91	0.52
2:B:1053:HIS:CE1	2:B:1058:LYS:HE3	2.45	0.52
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.75	0.52
25:2:257:SER:O	25:2:261:PHE:HD1	1.93	0.52
1:A:926:ASN:OD1	1:A:931:ARG:HB3	2.10	0.52
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.26	0.52
17:Q:172:ASP:HA	17:Q:175:THR:HB	1.91	0.52
17:Q:184:ILE:CD1	18:R:218:LYS:HZ2	2.21	0.52
21:V:504:LYS:CB	21:V:654:GLU:O	2.58	0.52
1:A:926:ASN:CG	1:A:931:ARG:HB3	2.35	0.52
2:B:225:LEU:CG	2:B:228:SER:HB2	2.40	0.52
2:B:854:ILE:HG13	2:B:866:ILE:O	2.10	0.52
2:B:988:LYS:O	2:B:992:ASN:HB2	2.10	0.52
16:P:309:LYS:HD3	28:Y:82:DT:H5''	1.91	0.52
17:Q:24:GLY:HA2	18:R:209:GLN:OE1	2.09	0.52
21:V:520:ARG:NE	21:V:521:GLU:OE2	2.30	0.52
25:2:193:PRO:HB2	25:2:194:PRO:HD3	1.92	0.52
28:Y:80:DT:H2''	28:Y:81:DA:C8	2.45	0.52
1:A:47:THR:HG23	1:A:53:LYS:HA	1.92	0.51
1:A:451:CYS:O	1:A:453:GLY:N	2.38	0.51
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:HIS:HB3	1:A:627:LYS:HA	1.92	0.51
1:A:679:TRP:CZ3	1:A:683:GLU:HG3	2.44	0.51
1:A:1128:ILE:HG23	1:A:1414:ILE:HG13	1.92	0.51
1:A:1305:SER:O	1:A:1306:LYS:HG3	2.10	0.51
2:B:331:THR:O	2:B:333:GLU:N	2.42	0.51
2:B:1053:HIS:ND1	2:B:1058:LYS:HE3	2.25	0.51
9:I:91:HIS:ND1	9:I:92:LYS:O	2.43	0.51
13:M:52:TRP:CD1	13:M:52:TRP:C	2.88	0.51
26:3:10:LEU:HD22	26:3:147:MET:HG2	1.92	0.51
28:Y:53:DG:H4'	28:Y:54:DA:OP1	2.09	0.51
1:A:40:GLY:O	1:A:42:LYS:HG2	2.10	0.51
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.92	0.51
17:Q:112:ARG:NH2	18:R:237:LEU:HD22	2.25	0.51
21:V:611:GLY:HA2	21:V:615:PHE:CB	2.38	0.51
26:3:42:MET:CG	26:3:111:ILE:HD11	2.40	0.51
26:3:64:ILE:HG21	26:3:128:HIS:CB	2.40	0.51
26:3:131:THR:HG23	26:3:133:LEU:HD12	1.92	0.51
1:A:347:GLU:OE1	1:A:347:GLU:N	2.42	0.51
2:B:1016:SER:HB3	2:B:1022:LEU:CB	2.40	0.51
14:N:333:ASN:CG	14:N:361:ASN:H	2.19	0.51
26:3:121:LYS:HD3	26:3:121:LYS:N	2.25	0.51
26:3:226:TYR:O	26:3:230:VAL:HB	2.10	0.51
1:A:44:PRO:HG3	1:A:284:VAL:HG13	1.91	0.51
1:A:1313:GLN:OE1	1:A:1316:ASN:ND2	2.43	0.51
2:B:631:GLN:HB3	2:B:685:LYS:HZ3	1.74	0.51
3:C:99:VAL:HG13	3:C:124:SER:OG	2.10	0.51
3:C:136:ASP:N	3:C:136:ASP:OD1	2.43	0.51
16:P:193:ASN:HD21	16:P:196:ARG:HD3	1.74	0.51
16:P:203:ARG:NH2	16:P:210:THR:OG1	2.43	0.51
25:2:171:VAL:CG2	25:2:213:TRP:HA	2.20	0.51
25:2:181:GLN:HE21	25:2:181:GLN:CA	2.23	0.51
26:3:70:LEU:HD22	26:3:114:GLU:HB3	1.91	0.51
2:B:56:GLN:NE2	2:B:60:GLU:OE2	2.44	0.51
2:B:214:LYS:O	2:B:240:LEU:HD12	2.11	0.51
21:V:523:VAL:HG21	24:1:20:LEU:CG	2.38	0.51
27:X:50:DT:H3'	27:X:51:DC:H5''	1.92	0.51
1:A:26:LEU:HB2	2:B:1168:ALA:HB2	1.92	0.51
1:A:530:SER:O	1:A:532:ARG:N	2.43	0.51
1:A:1304:ILE:HA	1:A:1340:GLY:HA3	1.93	0.51
2:B:250:SER:O	2:B:251:ALA:HB3	2.09	0.51
7:G:13:LEU:HD21	7:G:22:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:111:HIS:CE1	17:Q:125:ALA:H	2.28	0.51
15:O:48:LEU:HD23	15:O:52:VAL:HG21	1.93	0.51
25:2:215:PHE:CE2	25:2:264:HIS:HB2	2.46	0.51
25:2:231:VAL:O	25:2:234:LEU:HB3	2.11	0.51
1:A:1323:THR:HG23	1:A:1325:ASP:H	1.75	0.51
3:C:138:ASP:O	3:C:139:PRO:C	2.52	0.51
6:F:64:ARG:HH12	7:G:61:PRO:HB3	1.75	0.51
10:J:54:ASP:OD2	10:J:57:GLU:HG2	2.11	0.51
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.46	0.51
25:2:31:LEU:HD13	26:3:33:THR:HG22	1.86	0.51
26:3:141:LEU:HG	26:3:187:GLN:HE22	1.75	0.51
27:X:24:DG:H2'	27:X:25:DG:C8	2.45	0.51
2:B:234:THR:O	2:B:236:TRP:HD1	1.93	0.51
2:B:881:GLU:HA	2:B:883:THR:HG23	1.92	0.51
17:Q:46:GLU:OE2	17:Q:56:ARG:NH1	2.34	0.51
25:2:51:LEU:CD2	25:2:55:TRP:CD1	2.94	0.51
25:2:138:PRO:HG3	25:2:189:GLU:CG	2.35	0.51
25:2:160:LEU:HB3	25:2:206:LEU:HD21	1.93	0.51
26:3:165:LYS:HE3	26:3:200:SER:OG	2.09	0.51
1:A:367:ILE:HG12	1:A:499:ASP:O	2.10	0.51
1:A:883:ILE:HG21	1:A:1424:THR:HA	1.92	0.51
2:B:822:GLY:HA3	2:B:825:GLN:HG2	1.92	0.51
9:I:86:CYS:O	9:I:88:LYS:N	2.43	0.51
13:M:45:VAL:HG11	13:M:48:VAL:HG13	1.93	0.51
17:Q:42:CYS:O	17:Q:95:ASN:ND2	2.40	0.51
17:Q:184:ILE:CD1	18:R:213:ASP:OD1	2.59	0.51
25:2:236:PHE:CE2	25:2:262:LEU:CD1	2.94	0.51
26:3:216:LYS:O	26:3:216:LYS:HG2	2.11	0.51
27:X:23:DT:H2''	27:X:24:DG:H8	1.75	0.51
1:A:616:GLY:O	1:A:619:LYS:HB2	2.11	0.51
1:A:1264:SER:OG	1:A:1267:ASN:ND2	2.38	0.51
3:C:56:SER:OG	3:C:158:GLU:N	2.28	0.51
13:M:34:CYS:HB3	13:M:39:LEU:HB2	1.93	0.51
1:A:152:ASN:OD1	1:A:188:GLN:HB2	2.11	0.50
1:A:202:TRP:N	1:A:212:LYS:O	2.33	0.50
1:A:710:LYS:HE3	1:A:818:GLU:OE2	2.11	0.50
5:E:40:PHE:CZ	5:E:46:ASP:OD2	2.54	0.50
6:F:51:ARG:HA	6:F:116:GLU:OE1	2.10	0.50
13:M:87:GLY:O	13:M:88:THR:CB	2.59	0.50
22:W:581:LEU:C	22:W:581:LEU:HD13	2.36	0.50
25:2:46:ARG:HD3	25:2:85:GLU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:140:LYS:CG	25:2:162:PHE:CE1	2.94	0.50
25:2:236:PHE:CE1	25:2:261:PHE:CB	2.94	0.50
26:3:64:ILE:CG2	26:3:128:HIS:HB3	2.42	0.50
9:I:93:GLU:O	9:I:115:THR:HG22	2.10	0.50
13:M:94:ASP:HB3	13:M:99:SER:C	2.36	0.50
17:Q:44:LYS:HG3	17:Q:46:GLU:H	1.76	0.50
17:Q:180:PHE:CE1	18:R:212:VAL:O	2.65	0.50
18:R:223:VAL:HG23	18:R:224:THR:CB	2.40	0.50
20:T:138:PRO:O	20:T:140:ARG:N	2.44	0.50
23:0:55:LEU:HD12	26:3:178:MET:HE3	1.93	0.50
1:A:603:ILE:HG12	1:A:604:ARG:H	1.76	0.50
13:M:10:LEU:N	13:M:10:LEU:CD2	2.73	0.50
17:Q:23:ARG:HH12	18:R:206:LYS:HB3	1.75	0.50
17:Q:113:ARG:HH12	18:R:218:LYS:CA	2.25	0.50
17:Q:184:ILE:CD1	18:R:211:SER:CB	2.86	0.50
25:2:77:LYS:CD	25:2:78:GLU:HG3	2.41	0.50
25:2:181:GLN:HE22	25:2:220:LEU:HD12	1.76	0.50
25:2:207:ASP:OD2	25:2:254:MET:HE2	2.10	0.50
26:3:12:VAL:HG12	26:3:58:ALA:HB3	1.92	0.50
28:Y:48:DC:H2'	28:Y:49:DG:H8	1.76	0.50
1:A:710:LYS:O	1:A:714:ILE:HG12	2.11	0.50
2:B:98:HIS:HB2	2:B:108:MET:HE3	1.93	0.50
2:B:312:GLN:HB3	19:S:153:ARG:NH2	2.24	0.50
2:B:1029:TYR:CE1	2:B:1036:LYS:HG3	2.46	0.50
5:E:53:PRO:HB2	5:E:56:THR:HB	1.92	0.50
22:W:73:CYS:O	22:W:209:TYR:CE2	2.63	0.50
22:W:116:CYS:SG	22:W:191:PRO:HD2	2.51	0.50
25:2:57:MET:HA	25:2:60:LEU:HG	1.93	0.50
25:2:192:GLU:CG	25:2:193:PRO:HD2	2.23	0.50
25:2:208:THR:HG23	25:2:209:PRO:HD2	1.91	0.50
25:2:223:ALA:O	25:2:224:GLN:HB3	2.12	0.50
26:3:24:LYS:HE2	26:3:196:LEU:HB3	1.93	0.50
27:X:3:DA:H1'	27:X:4:DG:H5'	1.94	0.50
1:A:1319:LYS:HB2	1:A:1333:GLU:OE2	2.11	0.50
13:M:34:CYS:CB	13:M:39:LEU:CB	2.89	0.50
17:Q:28:ILE:HD12	18:R:190:LEU:HD21	1.92	0.50
25:2:57:MET:HA	25:2:60:LEU:CG	2.41	0.50
26:3:107:ALA:O	26:3:111:ILE:HG23	2.11	0.50
1:A:196:LEU:HD22	1:A:325:LEU:HD21	1.94	0.50
1:A:1114:ALA:CB	1:A:1309:MET:HE1	2.36	0.50
1:A:1361:ASP:OD2	1:A:1364:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1473:LEU:HD13	6:F:104:ILE:HD12	1.94	0.50
2:B:367:TYR:OH	2:B:371:ARG:NH1	2.45	0.50
2:B:747:LEU:HD21	2:B:810:PHE:HE1	1.75	0.50
9:I:15:ARG:O	9:I:16:PHE:O	2.30	0.50
9:I:81:THR:HB	9:I:96:PHE:CE2	2.46	0.50
25:2:30:VAL:CG1	25:2:34:LEU:HD23	2.40	0.50
25:2:51:LEU:HD23	25:2:51:LEU:C	2.37	0.50
25:2:199:ALA:CB	25:2:201:PHE:CE2	2.95	0.50
25:2:245:LEU:HD22	25:2:245:LEU:N	2.27	0.50
26:3:137:LEU:CD1	26:3:177:PHE:CE1	2.95	0.50
26:3:178:MET:HE2	26:3:202:LEU:HD13	1.92	0.50
26:3:202:LEU:HD22	26:3:202:LEU:N	2.27	0.50
27:X:36:DT:H71	27:X:37:DT:H3	1.77	0.50
1:A:298:ALA:N	17:Q:60:ARG:HE	2.09	0.50
1:A:366:VAL:O	1:A:481:THR:HB	2.12	0.50
2:B:302:LYS:HG3	9:I:23:MET:HE1	1.93	0.50
3:C:136:ASP:HB2	3:C:138:ASP:HB2	1.94	0.50
3:C:259:LEU:HD22	11:K:42:LEU:HD21	1.94	0.50
22:W:494:ILE:HD11	22:W:680:ALA:HB2	1.93	0.50
25:2:100:LEU:HD11	25:2:119:ARG:CG	2.31	0.50
1:A:137:PRO:HB2	1:A:1445:HIS:CE1	2.47	0.50
1:A:426:ARG:CG	13:M:40:VAL:HG11	2.42	0.50
1:A:1114:ALA:C	1:A:1116:ASN:H	2.18	0.50
2:B:1075:MET:CE	13:M:51:GLU:HG2	2.40	0.50
3:C:138:ASP:C	3:C:140:ASN:N	2.69	0.50
17:Q:36:ILE:HG21	17:Q:48:MET:HG2	1.93	0.50
21:V:520:ARG:CG	24:1:23:LEU:HD11	2.42	0.50
24:1:22:TYR:O	24:1:25:GLU:HB3	2.11	0.50
25:2:199:ALA:HB1	25:2:201:PHE:CE2	2.47	0.50
25:2:236:PHE:CZ	25:2:262:LEU:CD2	2.94	0.50
26:3:10:LEU:CD2	26:3:143:TYR:HE2	2.25	0.50
26:3:12:VAL:HG23	26:3:12:VAL:O	2.10	0.50
26:3:187:GLN:O	26:3:188:ASN:HB2	2.12	0.50
1:A:772:SER:OG	1:A:773:GLY:N	2.45	0.50
1:A:1207:ILE:HG22	1:A:1262:MET:HG3	1.92	0.50
9:I:28:GLU:HG2	9:I:30:LYS:HG3	1.94	0.50
18:R:195:PRO:HB2	18:R:199:LYS:CD	2.41	0.50
19:S:26:TYR:HB2	19:S:139:PRO:O	2.12	0.50
20:T:34:ALA:O	20:T:37:ARG:HG3	2.12	0.50
20:T:95:VAL:O	20:T:107:GLU:N	2.45	0.50
20:T:181:GLN:HA	20:T:184:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:189:GLU:CA	25:2:192:GLU:HG2	2.41	0.50
26:3:215:LEU:HD12	26:3:230:VAL:CG2	2.42	0.50
27:X:33:DT:H2'	27:X:34:DT:C5	2.47	0.50
1:A:608:THR:C	1:A:610:PRO:CD	2.60	0.49
1:A:802:PHE:CE2	1:A:808:PRO:HD3	2.47	0.49
5:E:46:ASP:O	5:E:47:LYS:CB	2.51	0.49
6:F:79:VAL:HG12	6:F:81:VAL:H	1.77	0.49
22:W:430:ASN:CB	22:W:431:PRO:CD	2.85	0.49
24:1:2:VAL:HG23	24:1:2:VAL:O	2.11	0.49
25:2:35:TYR:CD1	25:2:62:LEU:CD1	2.95	0.49
25:2:176:ALA:O	25:2:177:GLN:HB2	2.12	0.49
25:2:214:TYR:CB	25:2:261:PHE:CE2	2.95	0.49
26:3:10:LEU:CD2	26:3:143:TYR:CE2	2.95	0.49
1:A:60:PRO:O	1:A:61:ARG:HG3	2.12	0.49
1:A:1098:PRO:CA	1:A:1101:GLN:NE2	2.74	0.49
2:B:56:GLN:CD	20:T:140:ARG:HD2	2.38	0.49
2:B:883:THR:O	2:B:885:ARG:N	2.45	0.49
5:E:48:PRO:O	5:E:49:SER:OG	2.29	0.49
5:E:52:ARG:NH2	5:E:54:ARG:HG2	2.19	0.49
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.46	0.49
14:N:326:GLN:OE1	15:O:92:LYS:NZ	2.30	0.49
25:2:89:LEU:HD23	25:2:93:LEU:HG	1.94	0.49
26:3:60:ILE:HG22	26:3:61:ALA:N	2.26	0.49
26:3:166:ALA:O	26:3:198:SER:HB2	2.13	0.49
1:A:111:CYS:SG	1:A:154:CYS:CB	3.01	0.49
1:A:138:LYS:H	1:A:1445:HIS:HE1	1.60	0.49
14:N:344:ARG:HH21	28:Y:78:DT:H3'	1.77	0.49
18:R:75:PHE:HD2	20:T:192:GLU:OE2	1.96	0.49
18:R:82:VAL:HG22	18:R:140:LYS:HE2	1.94	0.49
21:V:315:VAL:CG1	22:W:500:ASP:CG	2.80	0.49
22:W:209:TYR:HH	22:W:234:ASP:H	1.59	0.49
24:1:18:GLN:HG3	24:1:19:PHE:H	1.78	0.49
26:3:53:ARG:HA	26:3:101:TYR:HE1	1.78	0.49
28:Y:46:DC:H2'	28:Y:47:DG:C8	2.48	0.49
1:A:107:LEU:HD23	1:A:191:ILE:HD13	1.94	0.49
2:B:323:SER:HB3	2:B:335:ARG:NH1	2.27	0.49
2:B:468:GLN:OE1	2:B:481:HIS:NE2	2.44	0.49
2:B:882:SER:HB2	2:B:887:TYR:CE1	2.46	0.49
2:B:896:LEU:C	2:B:897:ARG:HG3	2.35	0.49
8:H:10:PHE:CE2	8:H:39:LEU:HD22	2.47	0.49
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:347:ASN:O	14:N:375:GLU:HA	2.11	0.49
25:2:35:TYR:CD2	25:2:62:LEU:CB	2.95	0.49
25:2:81:LYS:CE	25:2:89:LEU:HD21	2.42	0.49
25:2:93:LEU:CD2	25:2:96:TRP:HE1	2.25	0.49
25:2:426:ARG:HD2	25:2:444:THR:CG2	2.43	0.49
26:3:59:VAL:HG13	26:3:59:VAL:O	2.12	0.49
26:3:220:MET:N	26:3:221:PRO:HD2	2.28	0.49
1:A:374:SER:C	1:A:485:ASN:HD22	2.20	0.49
1:A:549:THR:O	1:A:589:LYS:NZ	2.44	0.49
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.39	0.49
2:B:356:PHE:HB3	19:S:116:GLY:CA	2.39	0.49
20:T:132:ILE:O	20:T:136:SER:OG	2.26	0.49
22:W:325:THR:HG22	22:W:329:PHE:CE2	2.47	0.49
25:2:35:TYR:CD1	25:2:35:TYR:N	2.79	0.49
25:2:203:PHE:CE2	25:2:205:LEU:CD2	2.96	0.49
26:3:108:ASN:O	26:3:111:ILE:HG12	2.12	0.49
1:A:641:CYS:SG	1:A:643:LYS:N	2.86	0.49
1:A:1130:ILE:HD13	1:A:1411:LEU:HB3	1.95	0.49
2:B:363:TYR:CD2	2:B:553:LEU:HD11	2.48	0.49
2:B:422:PHE:CE2	2:B:429:PHE:HB2	2.48	0.49
2:B:1079:SER:C	2:B:1080:ARG:HD2	2.38	0.49
3:C:36:ARG:NH2	11:K:40:HIS:HB2	2.28	0.49
3:C:137:ASN:ND2	3:C:137:ASN:H	2.10	0.49
17:Q:25:PHE:CE2	18:R:219:LEU:HD11	2.35	0.49
18:R:163:LEU:C	18:R:164:GLY:O	2.55	0.49
24:1:1:MET:HA	25:2:413:LEU:CA	2.42	0.49
24:1:3:ASN:HB2	25:2:412:PHE:O	2.13	0.49
26:3:21:TRP:HA	26:3:24:LYS:CG	2.42	0.49
1:A:231:GLU:H	1:A:231:GLU:CD	2.19	0.49
1:A:516:GLN:HA	1:A:520:MET:HE2	1.94	0.49
2:B:285:LEU:HD21	2:B:298:MET:HE2	1.94	0.49
2:B:819:SER:HB3	2:B:821:LYS:HB2	1.94	0.49
2:B:880:LEU:C	2:B:881:GLU:OE1	2.56	0.49
3:C:100:GLU:HG3	3:C:164:TYR:CE1	2.48	0.49
3:C:142:TYR:O	3:C:144:GLU:N	2.45	0.49
8:H:99:ILE:HD11	8:H:112:LEU:HD21	1.94	0.49
13:M:178:LYS:HB3	20:T:154:LYS:HB2	1.93	0.49
21:V:667:THR:CA	24:1:62:ASP:OD1	2.59	0.49
22:W:624:PRO:O	22:W:656:ALA:HB1	2.12	0.49
24:1:45:VAL:HG21	25:2:409:TYR:CE2	2.48	0.49
25:2:42:LEU:HD22	25:2:52:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:188:THR:HG23	25:2:189:GLU:N	2.27	0.49
25:2:198:SER:OG	25:2:238:PHE:HE2	1.96	0.49
26:3:174:TYR:HD1	26:3:202:LEU:HD11	1.78	0.49
26:3:190:LEU:HA	26:3:210:THR:HG21	1.91	0.49
1:A:156:GLY:HA2	1:A:181:HIS:CE1	2.38	0.49
1:A:702:ILE:HG12	1:A:752:THR:HG23	1.94	0.49
1:A:1147:SER:HB3	1:A:1157:ILE:HD11	1.95	0.49
2:B:422:PHE:O	2:B:425:ARG:N	2.46	0.49
3:C:146:ASP:O	3:C:148:ILE:N	2.45	0.49
13:M:85:GLY:O	13:M:86:LYS:HB2	2.13	0.49
22:W:596:LEU:HG	22:W:597:LEU:N	2.27	0.49
26:3:12:VAL:HG22	26:3:161:ILE:HA	1.94	0.49
26:3:100:LYS:HB3	26:3:103:LEU:CD1	2.37	0.49
1:A:36:VAL:HG11	1:A:72:GLN:NE2	2.26	0.49
2:B:203:ASN:O	2:B:204:THR:OG1	2.27	0.49
3:C:136:ASP:C	3:C:138:ASP:H	2.20	0.49
13:M:245:VAL:HG12	13:M:291:LEU:HD23	1.95	0.49
17:Q:70:LYS:NZ	18:R:230:GLU:OE2	2.45	0.49
25:2:35:TYR:CE2	25:2:62:LEU:CB	2.96	0.49
26:3:217:VAL:CG1	26:3:226:TYR:CE2	2.95	0.49
28:Y:46:DC:H2'	28:Y:47:DG:H8	1.77	0.49
1:A:459:ASN:C	1:A:459:ASN:OD1	2.56	0.49
1:A:1298:LEU:C	1:A:1300:GLY:H	2.21	0.49
2:B:852:GLY:O	2:B:868:GLY:N	2.31	0.49
2:B:952:GLU:OE2	3:C:40:ALA:HB2	2.13	0.49
2:B:1080:ARG:NH1	13:M:53:ARG:HD2	2.28	0.49
20:T:47:LYS:HG2	20:T:52:THR:HG23	1.95	0.49
20:T:217:LEU:HB3	20:T:233:TRP:CE3	2.48	0.49
24:1:43:VAL:HG12	24:1:44:PHE:N	2.27	0.49
25:2:77:LYS:HD3	25:2:78:GLU:HG3	1.94	0.49
25:2:236:PHE:CZ	25:2:258:LEU:CD1	2.95	0.49
26:3:42:MET:HE2	26:3:108:ASN:CB	2.42	0.49
26:3:195:VAL:HG23	26:3:214:TYR:CE1	2.48	0.49
1:A:1076:PHE:CE2	1:A:1080:ILE:HD11	2.47	0.48
1:A:1463:LEU:HA	2:B:1104:ARG:HD3	1.95	0.48
2:B:58:ILE:O	2:B:61:ASP:HB2	2.13	0.48
2:B:752:TYR:O	10:J:1:MET:HG3	2.13	0.48
9:I:58:ILE:C	9:I:60:HIS:H	2.21	0.48
13:M:56:SER:O	28:Y:51:DC:N4	2.45	0.48
19:S:110:PHE:HD1	19:S:148:PRO:HA	1.78	0.48
24:1:45:VAL:CG2	25:2:409:TYR:CE2	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:PRO:HD2	2:B:788:TYR:CE1	2.48	0.48
1:A:606:HIS:O	1:A:608:THR:N	2.44	0.48
1:A:608:THR:CB	1:A:610:PRO:CD	2.91	0.48
1:A:1020:LEU:HD22	1:A:1076:PHE:CD2	2.48	0.48
2:B:899:SER:C	2:B:901:THR:H	2.21	0.48
17:Q:191:LEU:HD21	18:R:210:PHE:HB2	1.95	0.48
22:W:37:HIS:NE2	22:W:454:VAL:CG1	2.76	0.48
25:2:170:ALA:CB	25:2:213:TRP:CZ3	2.95	0.48
25:2:179:LEU:CB	25:2:184:LEU:HD11	2.40	0.48
25:2:211:GLN:HE21	25:2:257:SER:HB3	1.78	0.48
26:3:12:VAL:CG2	26:3:161:ILE:HA	2.42	0.48
27:X:82:DG:N2	28:Y:13:DC:C2	2.81	0.48
1:A:1020:LEU:HD13	1:A:1041:PHE:HE2	1.76	0.48
2:B:799:SER:HB2	2:B:951:GLN:HB2	1.96	0.48
2:B:838:GLN:HG3	2:B:886:ARG:NH2	2.28	0.48
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.14	0.48
3:C:69:GLY:HA3	12:L:57:ALA:HB1	1.95	0.48
7:G:145:LEU:HD13	7:G:161:GLY:HA3	1.94	0.48
20:T:146:ASP:OD2	20:T:147:LYS:HG2	2.13	0.48
21:V:315:VAL:CG1	22:W:500:ASP:HB3	2.26	0.48
21:V:325:ARG:HH21	22:W:499:ASN:CB	1.95	0.48
23:0:55:LEU:N	26:3:209:ILE:HD11	2.28	0.48
25:2:133:THR:HG23	25:2:134:SER:N	2.28	0.48
25:2:211:GLN:CA	25:2:261:PHE:CE1	2.95	0.48
2:B:89:GLU:HG3	2:B:90:GLN:H	1.78	0.48
2:B:102:ASP:OD1	2:B:104:ALA:N	2.38	0.48
3:C:154:ARG:HG2	3:C:155:LYS:H	1.77	0.48
19:S:110:PHE:CD1	19:S:148:PRO:HA	2.48	0.48
21:V:321:GLU:CA	22:W:499:ASN:ND2	2.57	0.48
24:1:1:MET:HE1	25:2:440:LEU:CD1	2.31	0.48
25:2:35:TYR:CD1	25:2:62:LEU:CG	2.92	0.48
25:2:178:LEU:HD12	25:2:178:LEU:N	2.28	0.48
25:2:211:GLN:CB	25:2:261:PHE:CE1	2.95	0.48
26:3:160:ARG:HE	26:3:190:LEU:HG	1.78	0.48
1:A:77:ASN:OD1	1:A:77:ASN:N	2.47	0.48
1:A:137:PRO:HB2	1:A:1445:HIS:NE2	2.29	0.48
2:B:62:ALA:N	2:B:63:PRO:HD3	2.28	0.48
12:L:25:GLU:OE1	12:L:25:GLU:N	2.36	0.48
15:O:79:VAL:HG21	15:O:93:VAL:HG12	1.96	0.48
17:Q:21:VAL:HA	18:R:210:PHE:CD2	2.49	0.48
17:Q:75:ARG:HB3	17:Q:95:ASN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:113:ARG:HH11	18:R:221:ARG:HB2	1.79	0.48
23:O:55:LEU:HD12	26:3:178:MET:HE1	1.95	0.48
25:2:90:LEU:CD2	25:2:140:LYS:HD3	2.42	0.48
26:3:21:TRP:CG	26:3:34:LEU:HD23	2.48	0.48
26:3:177:PHE:CZ	26:3:203:LEU:CD2	2.95	0.48
27:X:13:DT:H3	28:Y:81:DA:H61	1.60	0.48
1:A:882:SER:C	1:A:884:ASN:H	2.22	0.48
4:D:60:VAL:HG13	7:G:103:PRO:HG3	1.95	0.48
8:H:64:LEU:CB	8:H:84:ARG:CD	2.76	0.48
13:M:86:LYS:HA	13:M:86:LYS:CE	2.42	0.48
18:R:140:LYS:H	18:R:141:PRO:HD2	1.79	0.48
20:T:180:LYS:HE3	20:T:184:LEU:HD11	1.95	0.48
21:V:522:TYR:CE2	24:1:62:ASP:CG	2.69	0.48
22:W:73:CYS:CB	22:W:209:TYR:CE1	2.97	0.48
25:2:89:LEU:CD2	25:2:93:LEU:HG	2.44	0.48
25:2:100:LEU:CG	25:2:119:ARG:HE	2.22	0.48
25:2:117:ASN:CB	26:3:42:MET:HE1	2.42	0.48
25:2:159:VAL:N	25:2:162:PHE:HB3	2.28	0.48
25:2:163:MET:HE1	25:2:206:LEU:HB3	1.94	0.48
1:A:118:LEU:CD2	1:A:151:LYS:O	2.40	0.48
1:A:492:TYR:CD2	1:A:501:MET:HE1	2.49	0.48
1:A:1319:LYS:HD3	1:A:1333:GLU:OE1	2.13	0.48
2:B:274:ARG:NH2	2:B:279:VAL:O	2.47	0.48
2:B:728:MET:HA	2:B:731:GLN:HB2	1.95	0.48
2:B:1162:LEU:HD23	2:B:1165:MET:CE	2.43	0.48
7:G:97:LEU:HG	7:G:113:ILE:HD11	1.95	0.48
9:I:21:ASN:O	9:I:22:ASN:ND2	2.47	0.48
9:I:96:PHE:HB3	9:I:112:TYR:CD1	2.47	0.48
17:Q:58:GLN:NE2	18:R:194:ARG:NH1	2.61	0.48
20:T:166:GLU:O	20:T:170:LYS:HG3	2.13	0.48
22:W:73:CYS:HB2	22:W:209:TYR:CE1	2.48	0.48
22:W:285:TYR:CE1	22:W:403:PHE:CZ	3.01	0.48
23:O:209:THR:HA	23:O:219:TYR:CD1	2.48	0.48
24:1:34:ILE:HG22	24:1:46:ILE:CG1	2.44	0.48
26:3:34:LEU:HD13	26:3:38:ILE:HG12	1.96	0.48
1:A:371:PRO:HD2	2:B:788:TYR:CZ	2.49	0.48
2:B:880:LEU:CD1	2:B:881:GLU:OE1	2.56	0.48
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.96	0.48
8:H:65:TYR:HE1	8:H:84:ARG:NE	2.11	0.48
22:W:28:LEU:HD13	22:W:28:LEU:C	2.38	0.48
22:W:73:CYS:HB3	22:W:209:TYR:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:57:VAL:CG2	24:1:61:MET:HE3	2.44	0.48
25:2:166:SER:HB3	25:2:167:PRO:CD	2.43	0.48
2:B:206:TYR:HD1	2:B:208:PHE:CE1	2.32	0.48
2:B:628:VAL:HG12	2:B:633:LEU:HA	1.94	0.48
14:N:360:LEU:HD11	15:O:81:PHE:HD2	1.79	0.48
17:Q:127:PHE:HA	17:Q:163:GLU:C	2.38	0.48
24:1:38:ILE:HG22	24:1:44:PHE:CE1	2.48	0.48
24:1:38:ILE:CG2	24:1:44:PHE:CE1	2.96	0.48
25:2:251:VAL:HG11	25:2:254:MET:SD	2.53	0.48
26:3:124:ILE:HD13	26:3:124:ILE:C	2.38	0.48
1:A:344:LYS:NZ	28:Y:43:DG:H5''	2.28	0.48
1:A:430:ARG:NH2	13:M:26:ASP:OD2	2.47	0.48
2:B:531:TYR:HE2	2:B:599:SER:HB3	1.79	0.48
2:B:1016:SER:HB3	2:B:1022:LEU:HB3	1.96	0.48
8:H:90:TYR:HB3	8:H:145:MET:HB3	1.96	0.48
13:M:52:TRP:C	13:M:54:THR:H	2.18	0.48
19:S:135:PHE:HE2	20:T:43:LEU:HD23	1.79	0.48
21:V:321:GLU:OE2	22:W:500:ASP:CA	2.59	0.48
24:1:53:LEU:H	24:1:53:LEU:CD1	2.26	0.48
26:3:124:ILE:O	26:3:127:GLN:HB2	2.14	0.48
26:3:174:TYR:HE1	26:3:178:MET:HE3	1.77	0.48
1:A:34:MET:SD	2:B:1124:ILE:HG21	2.54	0.47
2:B:573:TRP:O	2:B:573:TRP:HE3	1.97	0.47
4:D:112:LYS:HD2	4:D:124:ASP:OD1	2.14	0.47
8:H:65:TYR:CE2	8:H:70:LEU:CB	2.96	0.47
14:N:333:ASN:O	15:O:93:VAL:HG23	2.14	0.47
19:S:126:ILE:O	19:S:137:ALA:HA	2.13	0.47
25:2:30:VAL:H	26:3:25:GLN:CG	2.27	0.47
25:2:60:LEU:CD1	25:2:95:ILE:CG2	2.91	0.47
25:2:93:LEU:CA	25:2:96:TRP:CD1	2.94	0.47
26:3:160:ARG:HB2	26:3:190:LEU:HG	1.96	0.47
26:3:165:LYS:NZ	26:3:200:SER:H	2.12	0.47
1:A:614:ASP:O	1:A:618:TYR:CE2	2.67	0.47
1:A:719:LYS:HG2	1:A:724:GLU:OE1	2.13	0.47
2:B:312:GLN:O	19:S:153:ARG:NH2	2.47	0.47
2:B:497:LYS:O	2:B:500:GLN:HG2	2.14	0.47
2:B:1029:TYR:HE1	2:B:1036:LYS:CE	2.25	0.47
2:B:1163:MET:HA	2:B:1167:ILE:O	2.14	0.47
3:C:100:GLU:HG3	3:C:164:TYR:HE1	1.79	0.47
3:C:131:THR:HB	3:C:147:ASP:OD1	2.15	0.47
11:K:67:LEU:HD23	11:K:67:LEU:HA	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:183:ILE:HG12	16:P:244:LEU:HD13	1.96	0.47
21:V:514:MET:SD	21:V:537:ASN:CG	2.97	0.47
22:W:209:TYR:HH	22:W:233:PHE:CA	2.08	0.47
24:1:18:GLN:CD	24:1:44:PHE:CZ	2.92	0.47
25:2:205:LEU:HD22	25:2:205:LEU:N	2.30	0.47
25:2:236:PHE:HE2	25:2:262:LEU:CD1	2.27	0.47
26:3:10:LEU:HA	26:3:56:LYS:HG2	1.96	0.47
26:3:216:LYS:O	26:3:218:PRO:HD3	2.14	0.47
1:A:522:PRO:HG3	1:A:666:ARG:HG2	1.95	0.47
2:B:295:PRO:HB3	9:I:11:PHE:CD2	2.49	0.47
5:E:112:PRO:HA	5:E:115:LYS:HE2	1.95	0.47
8:H:81:ARG:C	8:H:83:SER:H	2.23	0.47
10:J:64:PRO:C	10:J:66:GLU:N	2.69	0.47
17:Q:25:PHE:H	18:R:210:PHE:HE2	1.61	0.47
19:S:172:ASN:OD1	19:S:173:HIS:N	2.45	0.47
20:T:140:ARG:C	20:T:142:SER:N	2.71	0.47
22:W:73:CYS:HB3	22:W:209:TYR:CD1	2.49	0.47
26:3:131:THR:HG23	26:3:133:LEU:HD13	1.95	0.47
1:A:312:PHE:HB2	13:M:101:TYR:OH	2.14	0.47
2:B:1123:GLY:HA3	2:B:1170:ARG:HB3	1.97	0.47
11:K:87:PHE:CE1	11:K:91:ILE:HD11	2.49	0.47
13:M:276:ASP:O	20:T:153:TYR:HD1	1.98	0.47
16:P:206:GLU:HB2	16:P:236:LYS:NZ	2.29	0.47
17:Q:105:TYR:CE1	18:R:234:GLU:CD	2.93	0.47
17:Q:118:GLU:HB2	17:Q:181:ASN:ND2	2.29	0.47
18:R:119:LEU:HA	18:R:123:ALA:HB3	1.97	0.47
24:1:9:LEU:N	24:1:9:LEU:HD12	2.29	0.47
25:2:221:GLN:HG2	25:2:268:PHE:HZ	1.75	0.47
1:A:1067:TRP:CZ2	1:A:1071:GLU:HG3	2.50	0.47
1:A:1305:SER:OG	1:A:1306:LYS:N	2.33	0.47
2:B:257:VAL:HA	2:B:268:PRO:HA	1.97	0.47
4:D:95:PHE:HZ	7:G:83:GLU:HG3	1.80	0.47
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.48	0.47
17:Q:187:ILE:HD13	18:R:212:VAL:N	2.25	0.47
19:S:136:GLU:HG2	19:S:138:PHE:CE1	2.49	0.47
22:W:263:LEU:C	22:W:263:LEU:HD23	2.39	0.47
25:2:85:GLU:O	25:2:89:LEU:HB2	2.14	0.47
25:2:203:PHE:CD2	25:2:204:LEU:N	2.82	0.47
25:2:236:PHE:CD1	25:2:261:PHE:HB3	2.49	0.47
26:3:137:LEU:HD11	26:3:177:PHE:CE1	2.50	0.47
1:A:1171:ALA:C	9:I:59:THR:HG22	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:561:ILE:HD11	2:B:576:ILE:HG21	1.97	0.47
7:G:40:GLY:O	7:G:78:ARG:NH1	2.48	0.47
8:H:24:ARG:NH1	8:H:46:GLN:OE1	2.48	0.47
18:R:194:ARG:O	18:R:196:ASP:O	2.33	0.47
25:2:46:ARG:CD	25:2:85:GLU:CB	2.93	0.47
25:2:201:PHE:CD1	25:2:202:GLN:N	2.83	0.47
26:3:34:LEU:HD22	26:3:37:CYS:SG	2.54	0.47
26:3:71:TYR:CG	26:3:72:PRO:HD2	2.18	0.47
26:3:226:TYR:CA	26:3:230:VAL:HG23	2.42	0.47
28:Y:57:DA:H5''	28:Y:58:DC:H2'	1.95	0.47
1:A:362:SER:OG	2:B:1084:LEU:HD13	2.15	0.47
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.55	0.47
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.96	0.47
2:B:217:TYR:CE2	2:B:376:ALA:HA	2.50	0.47
2:B:595:ASP:OD1	20:T:129:ARG:NH1	2.48	0.47
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.97	0.47
3:C:14:LEU:HD13	3:C:19:VAL:HG23	1.95	0.47
5:E:173:ILE:CG2	5:E:209:VAL:HG22	2.44	0.47
18:R:157:GLN:O	18:R:161:ARG:N	2.47	0.47
21:V:361:CYS:HB3	21:V:405:VAL:HG21	1.96	0.47
24:1:38:ILE:O	24:1:38:ILE:HG12	2.15	0.47
24:1:38:ILE:CB	24:1:44:PHE:CE1	2.98	0.47
25:2:96:TRP:CZ2	25:2:97:HIS:NE2	2.83	0.47
26:3:177:PHE:O	26:3:181:ILE:HG13	2.15	0.47
28:Y:16:DA:H2'	28:Y:17:DG:C8	2.50	0.47
1:A:365:THR:HG22	2:B:1059:ILE:HG22	1.97	0.47
1:A:519:ALA:HA	1:A:524:MET:HE3	1.97	0.47
1:A:540:ASP:HB3	2:B:790:GLN:HG2	1.96	0.47
1:A:810:PHE:CZ	1:A:819:SER:HA	2.50	0.47
2:B:348:LEU:N	2:B:349:PRO:HD3	2.30	0.47
2:B:494:LYS:HG3	27:X:49:DT:C2	2.50	0.47
2:B:804:GLY:HA2	2:B:807:ARG:HE	1.80	0.47
3:C:212:ASP:HB2	3:C:214:ASP:HB2	1.97	0.47
7:G:139:GLN:O	7:G:141:ASP:N	2.47	0.47
9:I:15:ARG:O	9:I:24:LEU:CD1	2.62	0.47
17:Q:108:ASP:CG	18:R:237:LEU:HD22	2.39	0.47
17:Q:169:PRO:HA	17:Q:174:ARG:HG2	1.96	0.47
21:V:689:VAL:CG2	25:2:391:ILE:CD1	2.93	0.47
24:1:53:LEU:O	24:1:57:VAL:HG12	2.15	0.47
25:2:28:PRO:CD	26:3:25:GLN:NE2	2.72	0.47
25:2:138:PRO:HD3	25:2:189:GLU:CD	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:69:PHE:HE1	26:3:139:LYS:HD2	1.77	0.47
26:3:70:LEU:HD22	26:3:114:GLU:CB	2.44	0.47
1:A:322:LEU:HD23	1:A:325:LEU:HD22	1.97	0.47
1:A:1306:LYS:O	1:A:1306:LYS:HD3	2.15	0.47
3:C:5:ASN:CB	3:C:7:PRO:HD3	2.35	0.47
5:E:173:ILE:HG23	5:E:209:VAL:HG22	1.97	0.47
22:W:657:MET:O	22:W:660:ALA:HB3	2.15	0.47
25:2:51:LEU:HD21	25:2:55:TRP:CD1	2.50	0.47
25:2:96:TRP:CH2	25:2:97:HIS:CE1	3.03	0.47
1:A:274:ASP:OD2	1:A:276:LEU:N	2.46	0.47
1:A:745:LEU:HD21	1:A:817:PRO:HB3	1.95	0.47
1:A:800:PHE:HD1	1:A:805:ARG:C	2.23	0.47
3:C:10:ARG:HH21	3:C:24:GLU:CD	2.23	0.47
3:C:100:GLU:CG	3:C:164:TYR:HE1	2.28	0.47
4:D:96:GLU:OE2	4:D:117:SER:OG	2.22	0.47
9:I:66:THR:O	9:I:68:ILE:N	2.44	0.47
22:W:143:ARG:HG2	22:W:143:ARG:HH11	1.80	0.47
26:3:64:ILE:HG21	26:3:128:HIS:HB3	1.97	0.47
28:Y:63:DG:H5'	28:Y:65:DG:OP1	2.15	0.47
1:A:152:ASN:O	1:A:153:ILE:CD1	2.55	0.46
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.98	0.46
1:A:601:ASN:ND2	1:A:992:LYS:HD2	2.30	0.46
2:B:551:GLU:HB2	2:B:576:ILE:HD11	1.97	0.46
2:B:733:MET:HG2	2:B:1050:ARG:O	2.14	0.46
2:B:1022:LEU:HD12	2:B:1023:ARG:HG3	1.97	0.46
5:E:81:LYS:HD3	27:X:63:DC:OP1	2.15	0.46
17:Q:188:TYR:OH	18:R:211:SER:OG	2.19	0.46
17:Q:188:TYR:CD2	17:Q:191:LEU:HD22	2.50	0.46
17:Q:202:GLU:C	17:Q:204:LEU:H	2.23	0.46
25:2:217:LEU:CD2	25:2:233:ILE:HD11	2.45	0.46
25:2:240:LEU:HD12	25:2:240:LEU:N	2.31	0.46
26:3:56:LYS:HD3	26:3:56:LYS:N	2.30	0.46
1:A:597:PRO:O	1:A:599:HIS:N	2.48	0.46
2:B:80:GLU:OE1	2:B:134:LYS:HB3	2.16	0.46
2:B:594:MET:O	20:T:129:ARG:NH1	2.49	0.46
2:B:878:ASP:O	2:B:882:SER:OG	2.33	0.46
11:K:61:TYR:HA	11:K:72:ILE:O	2.15	0.46
14:N:376:TRP:HD1	15:O:62:LEU:O	1.98	0.46
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.15	0.46
24:1:10:ILE:HG12	24:1:43:VAL:CG1	2.45	0.46
26:3:10:LEU:CD1	26:3:56:LYS:HG2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:25:GLN:HA	26:3:25:GLN:NE2	2.30	0.46
27:X:73:DG:C2	27:X:74:DT:C2	3.04	0.46
1:A:133:SER:O	1:A:134:LYS:HB2	2.14	0.46
1:A:891:TYR:CE1	1:A:1087:VAL:HG13	2.49	0.46
2:B:874:PRO:C	2:B:876:ASN:N	2.70	0.46
2:B:924:ARG:HG3	2:B:924:ARG:O	2.15	0.46
2:B:1108:PHE:CD2	2:B:1109:GLU:HG3	2.51	0.46
3:C:56:SER:HG	3:C:158:GLU:H	1.55	0.46
3:C:169:PHE:CE1	3:C:171:LYS:HB3	2.51	0.46
5:E:27:LEU:HB2	5:E:64:HIS:HB3	1.97	0.46
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.97	0.46
9:I:32:ASN:HB2	9:I:34:ILE:HG12	1.98	0.46
9:I:98:GLN:O	9:I:100:HIS:N	2.47	0.46
13:M:53:ARG:NH1	28:Y:55:DG:O6	2.48	0.46
14:N:337:CYS:O	15:O:97:ALA:HA	2.14	0.46
17:Q:113:ARG:CD	18:R:221:ARG:HB3	2.40	0.46
19:S:98:TRP:HB2	19:S:112:GLY:HA3	1.97	0.46
23:O:77:LYS:HA	23:O:77:LYS:CE	2.18	0.46
25:2:218:GLN:HG2	25:2:268:PHE:CB	2.44	0.46
2:B:952:GLU:OE1	2:B:952:GLU:N	2.46	0.46
3:C:68:LEU:HD12	3:C:71:ILE:HD12	1.97	0.46
3:C:117:SER:OG	3:C:147:ASP:HB3	2.14	0.46
7:G:94:LYS:HA	7:G:119:PHE:CD2	2.50	0.46
15:O:41:ASP:O	15:O:45:ASN:ND2	2.37	0.46
15:O:84:VAL:HG13	15:O:85:THR:HG23	1.97	0.46
16:P:249:LYS:HB3	16:P:251:LEU:HG	1.97	0.46
17:Q:23:ARG:HH22	18:R:206:LYS:C	2.21	0.46
20:T:143:GLN:O	20:T:144:GLN:C	2.58	0.46
24:1:2:VAL:HG12	25:2:456:LYS:CE	2.44	0.46
1:A:262:PRO:CG	2:B:1070:LEU:HG	2.46	0.46
1:A:350:VAL:HG21	1:A:1435:THR:HG23	1.98	0.46
1:A:427:ILE:HG23	13:M:38:GLY:HA3	1.98	0.46
1:A:610:PRO:HB2	1:A:626:THR:HG22	1.98	0.46
2:B:312:GLN:OE1	19:S:153:ARG:NH1	2.49	0.46
11:K:49:GLN:HG3	11:K:94:LEU:HB2	1.97	0.46
26:3:10:LEU:N	26:3:56:LYS:HE3	2.31	0.46
1:A:273:GLN:C	1:A:274:ASP:O	2.55	0.46
1:A:687:ILE:HA	1:A:691:ASP:OD2	2.15	0.46
1:A:1252:ALA:HB1	9:I:3:PRO:HB3	1.96	0.46
2:B:344:GLN:O	2:B:361:LYS:NZ	2.38	0.46
2:B:584:MET:HG3	2:B:605:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:138:ASP:O	3:C:140:ASN:N	2.49	0.46
3:C:246:LEU:HD11	11:K:106:ARG:NH2	2.31	0.46
12:L:35:ARG:NH1	12:L:42:ARG:NH2	2.62	0.46
22:W:420:PRO:O	22:W:421:PHE:CG	2.68	0.46
24:1:50:VAL:CG1	24:1:54:GLN:HG2	2.41	0.46
26:3:165:LYS:HZ1	26:3:200:SER:H	1.63	0.46
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.81	0.46
2:B:489:ILE:HG13	2:B:490:GLY:N	2.29	0.46
2:B:561:ILE:HD11	2:B:576:ILE:HG12	1.97	0.46
2:B:1135:TYR:O	2:B:1136:GLU:HG2	2.16	0.46
3:C:72:PRO:HG3	10:J:13:ILE:HD13	1.97	0.46
5:E:73:PHE:HD2	5:E:90:TYR:HH	1.61	0.46
21:V:321:GLU:CG	22:W:499:ASN:ND2	2.76	0.46
25:2:211:GLN:CD	25:2:261:PHE:CE1	2.94	0.46
26:3:71:TYR:HD2	26:3:72:PRO:HD2	1.69	0.46
26:3:196:LEU:HB3	26:3:220:MET:SD	2.56	0.46
27:X:77:DC:H2''	27:X:78:DT:H72	1.98	0.46
1:A:472:HIS:NE2	1:A:521:VAL:HG21	2.30	0.46
1:A:687:ILE:HG13	1:A:691:ASP:OD2	2.16	0.46
2:B:309:PHE:HA	2:B:312:GLN:NE2	2.31	0.46
8:H:96:VAL:HG13	8:H:115:TYR:O	2.16	0.46
18:R:198:LYS:HE3	18:R:199:LYS:HE3	1.98	0.46
20:T:150:THR:C	20:T:152:ASN:H	2.22	0.46
24:1:40:ASP:HB2	24:1:43:VAL:H	1.81	0.46
24:1:57:VAL:HG13	24:1:58:GLY:N	2.31	0.46
25:2:123:LEU:HD23	25:2:123:LEU:C	2.41	0.46
26:3:59:VAL:N	26:3:71:TYR:CZ	2.69	0.46
27:X:31:DT:H2'	27:X:32:DT:C2	2.50	0.46
1:A:455:ILE:CG2	1:A:520:MET:HE1	2.46	0.46
1:A:939:VAL:O	1:A:942:VAL:HG22	2.16	0.46
2:B:99:TRP:NE1	2:B:105:PRO:HB3	2.31	0.46
2:B:950:ARG:HH12	3:C:171:LYS:HG3	1.79	0.46
7:G:98:PHE:CZ	17:Q:145:PHE:HB2	2.51	0.46
9:I:41:ASN:CG	19:S:153:ARG:HD2	2.40	0.46
13:M:217:ARG:O	13:M:221:ASN:ND2	2.46	0.46
20:T:196:TYR:HB2	20:T:232:THR:HB	1.98	0.46
26:3:10:LEU:HB2	26:3:56:LYS:HE3	1.97	0.46
27:X:48:DT:OP1	27:X:48:DT:H4'	2.15	0.46
27:X:60:DG:N3	28:Y:35:DG:N2	2.64	0.46
1:A:567:LEU:HD11	1:A:595:ILE:HG12	1.96	0.46
2:B:959:GLU:OE2	10:J:42:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:LYS:NZ	12:L:57:ALA:HB3	2.30	0.46
11:K:35:ILE:HB	11:K:71:ILE:HG12	1.98	0.46
15:O:50:GLN:O	15:O:53:ARG:NH1	2.49	0.46
22:W:37:HIS:CG	22:W:454:VAL:HG13	2.50	0.46
24:1:38:ILE:CG2	24:1:44:PHE:CD1	2.94	0.46
25:2:164:VAL:HG13	25:2:209:PRO:CG	2.45	0.46
25:2:189:GLU:HB2	25:2:190:PRO:CD	2.43	0.46
26:3:9:ASN:C	26:3:56:LYS:HE3	2.41	0.46
1:A:334:ARG:HE	13:M:66:ARG:HD3	1.80	0.45
1:A:908:THR:C	1:A:910:LYS:H	2.24	0.45
2:B:127:ASP:HA	2:B:145:GLN:O	2.16	0.45
21:V:516:PRO:CA	24:1:15:ALA:C	2.84	0.45
25:2:84:GLU:OE1	25:2:84:GLU:HA	2.15	0.45
25:2:203:PHE:CD2	25:2:205:LEU:CD2	2.95	0.45
26:3:64:ILE:CG2	26:3:128:HIS:CB	2.94	0.45
26:3:125:LYS:C	26:3:127:GLN:H	2.24	0.45
26:3:141:LEU:C	26:3:144:ILE:HG22	2.41	0.45
27:X:30:DG:N2	28:Y:64:DC:O2	2.49	0.45
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.52	0.45
1:A:1128:ILE:HG23	1:A:1414:ILE:CG1	2.46	0.45
2:B:225:LEU:CD2	2:B:228:SER:HB2	2.45	0.45
13:M:59:LYS:HA	29:Z:1:A:N7	2.32	0.45
14:N:46:TRP:CZ2	15:O:11:LEU:HD11	2.51	0.45
16:P:179:ASP:OD2	16:P:182:THR:OG1	2.28	0.45
17:Q:184:ILE:CD1	18:R:213:ASP:OD2	2.53	0.45
20:T:128:LYS:HA	20:T:131:GLN:HB3	1.98	0.45
26:3:228:LEU:HD23	26:3:228:LEU:C	2.41	0.45
27:X:37:DT:H1'	27:X:38:DT:O5'	2.16	0.45
2:B:756:LYS:HG2	10:J:51:ALA:O	2.16	0.45
2:B:972:ILE:HG12	2:B:981:LEU:HD21	1.97	0.45
2:B:1151:MET:HE1	2:B:1171:MET:SD	2.56	0.45
4:D:74:PHE:CZ	4:D:83:VAL:HG21	2.51	0.45
9:I:58:ILE:HB	9:I:61:GLU:OE1	2.16	0.45
17:Q:184:ILE:HG13	18:R:218:LYS:HZ2	1.81	0.45
18:R:139:PHE:HA	18:R:140:LYS:HB2	1.98	0.45
18:R:194:ARG:CB	18:R:195:PRO:HD2	2.30	0.45
24:1:22:TYR:CD1	24:1:22:TYR:C	2.94	0.45
25:2:89:LEU:HD23	25:2:89:LEU:C	2.42	0.45
25:2:118:LEU:HD23	26:3:42:MET:CB	2.34	0.45
26:3:165:LYS:CG	26:3:203:LEU:HD12	2.36	0.45
26:3:219:GLN:OE1	26:3:219:GLN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:HD21	1:A:311:GLN:HG3	1.99	0.45
2:B:65:ILE:HD11	2:B:86:LEU:HD12	1.98	0.45
13:M:286:ARG:HG3	13:M:316:LEU:HD23	1.98	0.45
20:T:211:VAL:O	20:T:215:GLU:HG2	2.15	0.45
24:1:59:GLU:CD	25:2:402:ARG:CZ	2.89	0.45
25:2:187:SER:OG	25:2:190:PRO:HD2	2.16	0.45
25:2:203:PHE:CG	25:2:204:LEU:N	2.84	0.45
1:A:470:MET:HG2	1:A:524:MET:HG3	1.98	0.45
1:A:485:ASN:O	1:A:487:SER:N	2.49	0.45
1:A:600:ILE:HD12	1:A:656:SER:HA	1.99	0.45
1:A:795:GLY:HA3	1:A:1107:PHE:HD2	1.80	0.45
1:A:1160:ARG:NH1	1:A:1349:GLU:OE2	2.50	0.45
2:B:1029:TYR:HD1	2:B:1036:LYS:HA	1.82	0.45
13:M:73:PRO:HB3	13:M:79:ASP:OD1	2.17	0.45
20:T:94:THR:HA	20:T:109:ILE:HA	1.99	0.45
20:T:154:LYS:N	20:T:154:LYS:CD	2.74	0.45
25:2:30:VAL:CG1	25:2:34:LEU:CD2	2.94	0.45
26:3:12:VAL:CG2	26:3:161:ILE:HG23	2.43	0.45
26:3:64:ILE:CG2	26:3:128:HIS:CG	2.99	0.45
26:3:160:ARG:HE	26:3:160:ARG:HB2	1.58	0.45
1:A:455:ILE:HD13	1:A:520:MET:CE	2.46	0.45
1:A:601:ASN:ND2	1:A:988:TRP:HZ3	2.14	0.45
2:B:489:ILE:HD12	27:X:47:DT:O2	2.17	0.45
2:B:957:THR:HG23	2:B:961:ILE:HG23	1.98	0.45
3:C:1:MET:O	3:C:3:TYR:N	2.37	0.45
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.98	0.45
5:E:55:ARG:NE	5:E:107:GLN:OE1	2.46	0.45
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.51	0.45
13:M:34:CYS:H	13:M:39:LEU:CB	2.29	0.45
13:M:244:LEU:HD21	13:M:292:ILE:HA	1.98	0.45
16:P:171:THR:HG21	27:X:16:DA:H4'	1.99	0.45
17:Q:92:TYR:CE2	17:Q:94:ILE:HB	2.52	0.45
20:T:99:SER:HB2	20:T:103:LYS:H	1.81	0.45
21:V:647:LYS:O	21:V:648:LYS:O	2.35	0.45
24:1:4:VAL:HG11	25:2:412:PHE:CD2	2.29	0.45
25:2:170:ALA:C	25:2:213:TRP:CZ3	2.94	0.45
26:3:8:LEU:HD23	26:3:54:SER:CB	2.42	0.45
26:3:42:MET:CG	26:3:111:ILE:CD1	2.95	0.45
27:X:53:DA:C6	27:X:54:DA:C6	3.05	0.45
3:C:161:LEU:C	3:C:161:LEU:HD12	2.42	0.45
12:L:17:TYR:HB2	12:L:26:ASN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:179:GLU:CA	20:T:154:LYS:HG2	2.27	0.45
17:Q:69:ASP:HB3	17:Q:71:PHE:CD2	2.52	0.45
20:T:31:TRP:HD1	20:T:62:LEU:HD21	1.82	0.45
22:W:37:HIS:NE2	22:W:454:VAL:HG11	2.32	0.45
22:W:623:VAL:HG23	22:W:681:ASP:HB2	1.98	0.45
25:2:219:TYR:CD1	25:2:219:TYR:C	2.95	0.45
27:X:65:DG:N1	27:X:66:DA:C2	2.85	0.45
1:A:46:THR:HG23	1:A:58:MET:HG2	1.98	0.45
1:A:112:PHE:H	1:A:188:GLN:NE2	2.09	0.45
1:A:322:LEU:HA	1:A:323:PRO:HD3	1.84	0.45
1:A:1098:PRO:C	1:A:1101:GLN:NE2	2.53	0.45
12:L:19:CYS:HB3	12:L:23:HIS:H	1.81	0.45
16:P:295:MET:HG2	16:P:297:LYS:H	1.81	0.45
17:Q:114:ILE:HD11	18:R:218:LYS:CE	2.43	0.45
20:T:140:ARG:HA	20:T:140:ARG:HD3	1.40	0.45
21:V:514:MET:HE2	21:V:664:SER:HB3	1.99	0.45
25:2:214:TYR:CE1	25:2:233:ILE:HG23	2.51	0.45
27:X:24:DG:H4'	27:X:25:DG:OP1	2.16	0.45
1:A:265:VAL:C	1:A:272:ASN:OD1	2.40	0.45
1:A:531:ASN:ND2	1:A:901:VAL:HG23	2.31	0.45
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.31	0.45
1:A:1411:LEU:HD23	1:A:1411:LEU:HA	1.80	0.45
2:B:225:LEU:O	2:B:228:SER:N	2.49	0.45
2:B:234:THR:O	2:B:236:TRP:CD1	2.69	0.45
5:E:146:PRO:O	5:E:148:HIS:ND1	2.48	0.45
15:O:71:VAL:HG22	15:O:98:CYS:HB3	1.99	0.45
17:Q:112:ARG:NH2	18:R:237:LEU:CB	2.73	0.45
25:2:117:ASN:HB2	26:3:104:LEU:CG	2.46	0.45
25:2:236:PHE:CD1	25:2:239:GLN:CD	2.95	0.45
26:3:144:ILE:O	26:3:144:ILE:HD13	2.17	0.45
26:3:148:ASN:ND2	26:3:157:MET:HG3	2.32	0.45
1:A:810:PHE:CE2	1:A:819:SER:HA	2.52	0.45
1:A:1308:TYR:CD1	1:A:1308:TYR:O	2.71	0.45
1:A:1484:MET:SD	7:G:20:PRO:HA	2.57	0.45
2:B:275:ALA:O	2:B:314:GLN:NE2	2.48	0.45
2:B:556:ILE:O	20:T:91:GLN:NE2	2.49	0.45
2:B:838:GLN:HG3	2:B:886:ARG:HH22	1.82	0.45
3:C:18:ASN:HB2	3:C:234:GLU:HG2	1.99	0.45
7:G:14:HIS:CD2	7:G:65:PHE:HE1	2.35	0.45
7:G:89:VAL:HA	7:G:98:PHE:O	2.17	0.45
9:I:14:ILE:CG1	9:I:16:PHE:CG	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:195:PRO:HG2	18:R:201:LEU:HD21	1.97	0.45
19:S:17:ARG:HG2	20:T:38:GLY:O	2.17	0.45
25:2:90:LEU:HD21	25:2:140:LYS:HD3	1.98	0.45
26:3:15:VAL:HG12	26:3:164:ILE:HD12	1.97	0.45
1:A:618:TYR:C	1:A:620:HIS:N	2.73	0.44
2:B:119:THR:HG23	2:B:187:ILE:HD13	1.99	0.44
2:B:132:VAL:CG2	2:B:141:GLN:OE1	2.62	0.44
2:B:867:ILE:O	2:B:893:SER:HB2	2.17	0.44
2:B:1005:ALA:C	2:B:1007:ASN:N	2.73	0.44
5:E:88:LYS:O	5:E:91:CYS:HB2	2.17	0.44
9:I:86:CYS:C	9:I:88:LYS:N	2.76	0.44
13:M:11:PRO:O	13:M:12:ARG:CB	2.63	0.44
15:O:3:TYR:HE2	15:O:99:ASP:HA	1.82	0.44
16:P:267:PRO:HG2	16:P:337:LYS:HB2	1.99	0.44
20:T:177:ARG:NH1	27:X:19:DG:H3'	2.31	0.44
24:1:4:VAL:HG22	24:1:5:LEU:N	2.32	0.44
24:1:22:TYR:CD1	24:1:23:LEU:HD23	2.48	0.44
24:1:54:GLN:O	24:1:57:VAL:HG12	2.16	0.44
25:2:56:VAL:HG23	25:2:57:MET:N	2.31	0.44
25:2:223:ALA:C	25:2:225:SER:H	2.24	0.44
26:3:33:THR:CG2	26:3:36:LYS:CB	2.95	0.44
26:3:71:TYR:CG	26:3:71:TYR:O	2.70	0.44
26:3:228:LEU:HD23	26:3:228:LEU:O	2.17	0.44
27:X:29:DC:H2''	27:X:30:DG:H5'	1.99	0.44
28:Y:56:DG:N2	28:Y:58:DC:OP1	2.51	0.44
28:Y:61:DA:H3'	28:Y:62:DC:H5''	1.98	0.44
1:A:393:ILE:CG2	6:F:74:ALA:HB1	2.47	0.44
1:A:574:VAL:O	8:H:74:GLU:HA	2.16	0.44
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.47	0.44
1:A:1308:TYR:O	1:A:1308:TYR:CG	2.70	0.44
2:B:133:ILE:HA	2:B:139:GLN:HA	1.98	0.44
2:B:402:PHE:C	2:B:402:PHE:CD1	2.95	0.44
2:B:632:LYS:HA	2:B:682:LEU:HD21	1.99	0.44
2:B:861:SER:O	2:B:896:LEU:HD23	2.17	0.44
8:H:38:ASP:OD1	8:H:39:LEU:N	2.51	0.44
8:H:65:TYR:HE1	8:H:84:ARG:HH21	1.66	0.44
9:I:58:ILE:C	9:I:60:HIS:N	2.74	0.44
9:I:65:LEU:HD23	9:I:122:ARG:NH2	2.32	0.44
13:M:52:TRP:O	13:M:54:THR:HG22	2.18	0.44
18:R:198:LYS:HG3	18:R:199:LYS:HG3	1.98	0.44
26:3:60:ILE:HG23	26:3:68:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:37:DT:H4'	27:X:38:DT:OP1	2.15	0.44
1:A:275:ASP:OD1	1:A:276:LEU:N	2.50	0.44
1:A:457:ILE:HG21	1:A:457:ILE:HD13	1.75	0.44
1:A:546:ARG:O	1:A:546:ARG:HG2	2.18	0.44
1:A:1210:TRP:CD1	1:A:1281:ASP:HB3	2.52	0.44
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.52	0.44
8:H:15:ILE:HD11	8:H:52:LEU:N	2.32	0.44
11:K:7:PHE:CD1	11:K:11:LEU:HD12	2.53	0.44
14:N:38:VAL:HG13	15:O:22:LEU:HD22	1.99	0.44
17:Q:17:LEU:HD11	17:Q:191:LEU:HB3	1.99	0.44
17:Q:105:TYR:HH	18:R:234:GLU:CD	2.07	0.44
17:Q:144:LEU:O	17:Q:153:ARG:N	2.44	0.44
20:T:202:LEU:O	20:T:206:THR:OG1	2.30	0.44
24:1:11:GLU:HG2	25:2:404:THR:OG1	2.17	0.44
25:2:243:SER:HB3	25:2:258:LEU:CD2	2.45	0.44
26:3:33:THR:HG22	26:3:36:LYS:CB	2.44	0.44
26:3:121:LYS:HD3	26:3:121:LYS:H	1.81	0.44
1:A:1298:LEU:O	1:A:1300:GLY:N	2.50	0.44
2:B:403:LEU:HD21	2:B:447:SER:HB2	2.00	0.44
2:B:760:THR:OG1	2:B:761:THR:N	2.51	0.44
2:B:853:LEU:HD13	2:B:907:VAL:HG11	1.97	0.44
4:D:118:LEU:HB2	4:D:122:PHE:CD2	2.52	0.44
7:G:96:GLY:O	7:G:128:TYR:HE2	2.00	0.44
8:H:11:ASP:OD2	8:H:55:LYS:HG2	2.17	0.44
18:R:206:LYS:HG3	18:R:207:SER:H	1.82	0.44
19:S:124:TYR:HE1	20:T:22:LYS:HG3	1.83	0.44
24:1:1:MET:SD	25:2:419:GLU:N	2.90	0.44
24:1:3:ASN:HB3	25:2:412:PHE:O	2.17	0.44
25:2:217:LEU:CD2	25:2:233:ILE:CD1	2.95	0.44
25:2:223:ALA:H	25:2:268:PHE:HE1	1.64	0.44
28:Y:70:DC:H2''	28:Y:71:DA:H8	1.83	0.44
1:A:811:ILE:HD12	1:A:811:ILE:HA	1.87	0.44
1:A:924:TYR:CE1	1:A:949:GLN:HG3	2.53	0.44
1:A:926:ASN:OD1	1:A:927:GLU:N	2.50	0.44
1:A:1057:GLU:O	1:A:1059:ARG:HG3	2.17	0.44
1:A:1176:TYR:HB2	1:A:1211:LEU:HD23	1.98	0.44
2:B:244:GLY:O	2:B:246:GLY:N	2.50	0.44
2:B:903:ILE:O	2:B:923:VAL:HG13	2.18	0.44
2:B:1021:HIS:HB2	3:C:203:TRP:CZ3	2.53	0.44
10:J:2:ILE:HD13	10:J:2:ILE:HG21	1.74	0.44
10:J:62:TYR:O	10:J:65:LEU:CD1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:114:ILE:CG1	18:R:218:LYS:HE3	2.47	0.44
18:R:206:LYS:O	18:R:207:SER:O	2.35	0.44
23:0:60:HIS:CE1	23:0:159:MET:SD	3.11	0.44
23:0:77:LYS:N	23:0:77:LYS:HD2	2.32	0.44
24:1:4:VAL:CG1	25:2:412:PHE:HD2	2.20	0.44
26:3:148:ASN:CG	26:3:157:MET:HE2	2.42	0.44
1:A:408:ARG:HD3	1:A:412:GLN:OE1	2.17	0.44
1:A:426:ARG:O	13:M:40:VAL:HG21	2.12	0.44
1:A:1127:LEU:HD11	1:A:1381:GLU:HB3	2.00	0.44
2:B:882:SER:CB	2:B:887:TYR:CE1	3.00	0.44
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.48	0.44
22:W:73:CYS:CB	22:W:209:TYR:CE2	3.00	0.44
25:2:61:PHE:CE1	25:2:99:GLN:NE2	2.85	0.44
26:3:184:ALA:C	26:3:187:GLN:HG2	2.43	0.44
1:A:601:ASN:ND2	1:A:632:ASN:H	2.15	0.44
1:A:800:PHE:HA	1:A:805:ARG:O	2.18	0.44
2:B:420:GLN:HA	2:B:423:ILE:HG12	1.99	0.44
2:B:536:SER:HB2	2:B:600:GLU:CD	2.43	0.44
2:B:818:GLU:OE2	2:B:828:VAL:HA	2.17	0.44
3:C:9:VAL:HG21	11:K:105:PHE:HA	2.00	0.44
9:I:11:PHE:HE1	9:I:54:TYR:HA	1.82	0.44
19:S:125:TYR:HD1	19:S:139:PRO:HA	1.82	0.44
20:T:146:ASP:O	20:T:147:LYS:CB	2.65	0.44
20:T:225:VAL:HA	20:T:231:ASN:HA	1.99	0.44
22:W:37:HIS:CD2	22:W:454:VAL:CG1	3.00	0.44
24:1:13:ASP:OD2	24:1:17:LYS:HB2	2.16	0.44
25:2:123:LEU:CD2	25:2:178:LEU:CD1	2.95	0.44
25:2:159:VAL:HG12	25:2:161:HIS:HB2	1.99	0.44
25:2:218:GLN:HE22	25:2:265:LEU:CA	2.28	0.44
25:2:270:LEU:HD23	25:2:270:LEU:C	2.42	0.44
1:A:931:ARG:C	1:A:933:THR:N	2.75	0.44
2:B:25:ALA:HA	2:B:28:ILE:HD12	2.00	0.44
2:B:132:VAL:O	2:B:139:GLN:HA	2.17	0.44
2:B:854:ILE:HD13	2:B:904:VAL:HG21	1.99	0.44
2:B:931:ILE:HD11	2:B:947:ILE:HA	1.99	0.44
7:G:1:MET:HB3	7:G:3:TYR:CZ	2.53	0.44
17:Q:113:ARG:HH12	18:R:218:LYS:HA	1.83	0.44
17:Q:115:GLU:O	17:Q:119:ARG:N	2.40	0.44
23:0:72:GLU:O	23:0:79:ASN:HB3	2.17	0.44
26:3:222:SER:HB3	26:3:225:GLN:CD	2.43	0.44
27:X:30:DG:H5''	27:X:31:DT:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:60:DA:H2''	28:Y:61:DA:C8	2.53	0.44
1:A:230:ASP:OD1	1:A:244:ARG:NH1	2.51	0.44
1:A:278:HIS:HB3	13:M:82:THR:HG23	2.00	0.44
1:A:1451:MET:HE2	1:A:1451:MET:HB3	1.56	0.44
1:A:1477:ALA:O	1:A:1480:CYS:HB2	2.18	0.44
2:B:128:ILE:HG21	2:B:431:LEU:HD21	2.00	0.44
2:B:882:SER:O	2:B:887:TYR:CD1	2.70	0.44
2:B:1080:ARG:HH21	13:M:50:SER:CB	2.27	0.44
10:J:35:LEU:HD13	10:J:46:ARG:HG2	1.99	0.44
12:L:16:ILE:HG21	12:L:47:LYS:CD	2.48	0.44
13:M:27:TYR:HD2	13:M:46:ILE:HB	1.82	0.44
17:Q:69:ASP:HB3	17:Q:71:PHE:HD2	1.83	0.44
18:R:223:VAL:O	18:R:224:THR:HG23	2.05	0.44
20:T:159:HIS:CG	20:T:160:GLN:N	2.85	0.44
21:V:282:LYS:HE3	21:V:482:PHE:CD1	2.53	0.44
23:O:106:ILE:HD11	23:O:127:HIS:HB3	2.00	0.44
25:2:35:TYR:CG	25:2:62:LEU:CD1	2.99	0.44
25:2:35:TYR:HB2	25:2:62:LEU:HD12	1.98	0.44
25:2:130:SER:HB2	25:2:179:LEU:HD23	1.99	0.44
26:3:178:MET:HA	26:3:181:ILE:HD12	1.99	0.44
27:X:77:DC:C2'	27:X:78:DT:H72	2.48	0.44
28:Y:88:DC:H2''	28:Y:89:DC:O4'	2.18	0.44
1:A:126:ILE:HD13	1:A:129:ILE:HD12	2.00	0.43
1:A:1116:ASN:O	1:A:1117:VAL:HB	2.18	0.43
2:B:32:SER:OG	2:B:643:LEU:HD22	2.17	0.43
2:B:203:ASN:O	2:B:571:GLY:HA3	2.18	0.43
2:B:754:PRO:HB2	2:B:773:PRO:HB2	1.99	0.43
7:G:104:MET:HE2	7:G:159:ALA:HB2	2.00	0.43
13:M:86:LYS:N	13:M:86:LYS:HD2	2.32	0.43
14:N:336:VAL:HG23	14:N:357:ILE:HB	2.00	0.43
16:P:165:LEU:HD21	16:P:258:MET:HE2	1.98	0.43
25:2:203:PHE:HD2	25:2:205:LEU:H	1.65	0.43
25:2:214:TYR:HB3	25:2:261:PHE:CE2	2.53	0.43
1:A:58:MET:HE3	1:A:58:MET:HB2	1.91	0.43
2:B:558:PRO:C	2:B:560:ALA:H	2.26	0.43
8:H:65:TYR:CD1	8:H:65:TYR:N	2.85	0.43
13:M:108:SER:HB3	13:M:112:ARG:NH1	2.30	0.43
14:N:372:GLY:HA3	15:O:58:PHE:CZ	2.53	0.43
25:2:81:LYS:CG	25:2:82:ALA:N	2.79	0.43
25:2:117:ASN:ND2	26:3:108:ASN:N	2.65	0.43
25:2:127:LYS:CA	25:2:178:LEU:HD23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:215:PHE:CE2	25:2:264:HIS:ND1	2.86	0.43
26:3:64:ILE:HB	26:3:123:ASP:CG	2.43	0.43
1:A:53:LYS:HE3	1:A:59:ASP:HB3	2.00	0.43
1:A:134:LYS:HA	1:A:140:ARG:NH2	2.33	0.43
1:A:285:LYS:HE3	1:A:285:LYS:HB3	1.83	0.43
1:A:485:ASN:O	1:A:486:LEU:C	2.62	0.43
2:B:333:GLU:HG2	2:B:337:LYS:HE3	2.00	0.43
3:C:44:ILE:O	3:C:167:LYS:HA	2.18	0.43
3:C:45:ILE:HG22	3:C:73:LEU:HD12	2.00	0.43
3:C:212:ASP:O	3:C:214:ASP:N	2.52	0.43
8:H:5:LEU:HD11	8:H:62:SER:HB3	2.00	0.43
14:N:356:GLY:HA3	14:N:367:PHE:CZ	2.54	0.43
17:Q:24:GLY:N	18:R:210:PHE:HD2	1.98	0.43
17:Q:108:ASP:CG	18:R:237:LEU:CD2	2.92	0.43
18:R:155:LEU:HA	18:R:161:ARG:HB2	2.00	0.43
21:V:405:VAL:HG12	21:V:406:ALA:H	1.82	0.43
21:V:517:GLU:CB	21:V:713:LEU:HD22	2.46	0.43
25:2:140:LYS:HD3	25:2:162:PHE:CE1	2.47	0.43
26:3:154:ASN:CG	26:3:155:GLN:H	2.26	0.43
26:3:160:ARG:CB	26:3:190:LEU:CD2	2.95	0.43
1:A:271:ARG:HG2	13:M:73:PRO:CD	2.47	0.43
1:A:426:ARG:C	13:M:40:VAL:HG21	2.43	0.43
1:A:931:ARG:C	1:A:933:THR:H	2.26	0.43
1:A:1192:TRP:O	1:A:1195:VAL:HB	2.19	0.43
2:B:625:LEU:CD1	2:B:675:LEU:HD11	2.49	0.43
2:B:993:LYS:HA	2:B:1018:TYR:OH	2.19	0.43
9:I:75:ASP:OD2	9:I:78:LEU:HG	2.18	0.43
13:M:48:VAL:HA	13:M:51:GLU:CD	2.43	0.43
22:W:73:CYS:HB3	22:W:209:TYR:CD2	2.52	0.43
25:2:117:ASN:ND2	26:3:104:LEU:O	2.52	0.43
25:2:206:LEU:CD2	25:2:206:LEU:H	2.30	0.43
26:3:229:TRP:CD1	26:3:229:TRP:C	2.96	0.43
1:A:275:ASP:HA	1:A:278:HIS:HD2	1.84	0.43
1:A:324:GLY:HA2	13:M:90:ALA:HB3	1.99	0.43
1:A:861:GLN:HE22	1:A:1093:GLN:HA	1.83	0.43
1:A:909:LEU:HA	1:A:909:LEU:HD23	1.68	0.43
1:A:1086:MET:SD	1:A:1466:ALA:HB1	2.58	0.43
2:B:281:ASP:H	9:I:22:ASN:HD22	1.66	0.43
2:B:329:GLY:C	2:B:331:THR:H	2.26	0.43
2:B:573:TRP:CZ3	2:B:575:GLY:HA2	2.54	0.43
2:B:651:TYR:HA	2:B:655:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:725:GLN:HG2	2:B:938:ARG:O	2.18	0.43
3:C:136:ASP:C	3:C:138:ASP:N	2.75	0.43
3:C:263:LEU:HD13	11:K:19:ILE:HD13	2.00	0.43
11:K:63:VAL:HG13	11:K:70:LYS:O	2.18	0.43
13:M:178:LYS:C	20:T:154:LYS:HB2	2.43	0.43
14:N:319:ASP:O	14:N:321:SER:O	2.36	0.43
21:V:514:MET:HE3	24:1:16:MET:CE	2.48	0.43
21:V:524:ALA:HB2	24:1:23:LEU:HD13	2.01	0.43
25:2:117:ASN:CA	26:3:104:LEU:HD21	2.47	0.43
25:2:118:LEU:CD1	26:3:43:VAL:HG22	2.39	0.43
25:2:166:SER:HB3	25:2:167:PRO:HD3	2.01	0.43
25:2:409:TYR:CD2	25:2:443:VAL:HG22	2.54	0.43
26:3:187:GLN:CD	26:3:189:ILE:HG13	2.43	0.43
27:X:41:DT:H2'	27:X:42:DT:O3'	2.19	0.43
1:A:413:TYR:CD1	1:A:414:PRO:HD3	2.54	0.43
2:B:779:ILE:HG23	2:B:779:ILE:HD12	1.76	0.43
5:E:111:THR:HG21	27:X:63:DC:O3'	2.19	0.43
15:O:64:THR:HA	16:P:189:ASN:OD1	2.18	0.43
17:Q:187:ILE:CD1	18:R:211:SER:HA	2.36	0.43
21:V:446:ILE:HD12	21:V:451:PHE:HB3	2.00	0.43
25:2:94:ARG:HD2	25:2:95:ILE:CD1	2.47	0.43
25:2:118:LEU:HD21	26:3:39:ASP:OD1	1.95	0.43
1:A:246:GLU:HG3	1:A:247:TRP:CD1	2.53	0.43
1:A:367:ILE:HG21	1:A:501:MET:HG3	1.99	0.43
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.43
3:C:45:ILE:O	3:C:73:LEU:HB2	2.18	0.43
17:Q:113:ARG:NH1	18:R:218:LYS:CA	2.82	0.43
20:T:30:GLN:NE2	20:T:62:LEU:O	2.48	0.43
21:V:428:GLU:CD	21:V:461:HIS:H	2.26	0.43
21:V:666:ASP:CB	24:1:17:LYS:HZ3	2.32	0.43
22:W:584:TYR:CB	22:W:591:GLY:HA3	2.49	0.43
25:2:34:LEU:N	25:2:34:LEU:HD22	2.33	0.43
25:2:87:THR:C	25:2:89:LEU:H	2.27	0.43
25:2:214:TYR:OH	25:2:265:LEU:HD13	2.18	0.43
26:3:65:GLN:O	26:3:132:LEU:HD11	2.18	0.43
26:3:69:PHE:HZ	26:3:139:LYS:HD2	1.80	0.43
28:Y:55:DG:H21	28:Y:56:DG:H1	1.67	0.43
1:A:364:ARG:HD3	1:A:500:GLU:OE1	2.19	0.43
1:A:914:LYS:O	1:A:918:LYS:HG2	2.19	0.43
2:B:549:SER:OG	2:B:577:HIS:NE2	2.25	0.43
9:I:14:ILE:CG1	9:I:16:PHE:CD1	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:58:ILE:O	9:I:60:HIS:N	2.51	0.43
12:L:19:CYS:HB3	12:L:23:HIS:N	2.33	0.43
16:P:305:PHE:CZ	28:Y:82:DT:H1'	2.54	0.43
17:Q:92:TYR:HE2	17:Q:94:ILE:HB	1.84	0.43
20:T:128:LYS:NZ	20:T:131:GLN:OE1	2.52	0.43
20:T:141:LEU:HB3	20:T:142:SER:H	1.57	0.43
20:T:159:HIS:O	20:T:162:ASN:HB3	2.19	0.43
21:V:519:TYR:HA	21:V:522:TYR:HB3	2.00	0.43
24:1:7:GLY:C	24:1:8:VAL:HG23	2.43	0.43
24:1:50:VAL:HG12	24:1:50:VAL:O	2.18	0.43
26:3:124:ILE:O	26:3:124:ILE:HG23	2.18	0.43
1:A:526:VAL:HA	1:A:533:PRO:HA	2.00	0.43
2:B:271:ILE:HG12	2:B:311:ILE:HD11	2.00	0.43
2:B:797:ASN:HB2	2:B:964:ASP:HA	2.00	0.43
5:E:49:SER:HB2	5:E:52:ARG:HH12	1.83	0.43
16:P:304:ILE:HD12	16:P:304:ILE:N	2.33	0.43
17:Q:26:TYR:OH	17:Q:69:ASP:OD2	2.25	0.43
18:R:195:PRO:HB2	18:R:199:LYS:CB	2.48	0.43
20:T:127:LEU:O	20:T:131:GLN:N	2.44	0.43
22:W:416:ILE:HA	22:W:434:HIS:O	2.19	0.43
25:2:171:VAL:HG13	25:2:216:MET:HB3	1.98	0.43
25:2:270:LEU:HA	25:2:273:GLN:HG3	2.00	0.43
26:3:11:LEU:CD1	26:3:48:HIS:NE2	2.82	0.43
26:3:133:LEU:CD2	26:3:134:ALA:N	2.82	0.43
2:B:758:LEU:HD11	10:J:47:ARG:HB3	2.01	0.43
5:E:52:ARG:HH21	5:E:54:ARG:HG3	1.79	0.43
17:Q:15:LYS:HE3	17:Q:38:ILE:HG23	2.01	0.43
24:1:8:VAL:CG1	24:1:9:LEU:N	2.80	0.43
25:2:44:VAL:CG1	25:2:45:PHE:N	2.82	0.43
25:2:171:VAL:CG1	25:2:216:MET:SD	3.06	0.43
25:2:236:PHE:CE1	25:2:239:GLN:NE2	2.87	0.43
25:2:236:PHE:HZ	25:2:258:LEU:HD11	1.83	0.43
1:A:117:LEU:HB2	1:A:232:GLU:CD	2.44	0.42
1:A:274:ASP:OD2	1:A:276:LEU:HB3	2.18	0.42
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.34	0.42
1:A:1254:LYS:HE3	9:I:3:PRO:HA	2.00	0.42
1:A:1405:MET:HE2	1:A:1405:MET:HB3	1.82	0.42
3:C:212:ASP:OD1	3:C:212:ASP:N	2.41	0.42
7:G:38:CYS:SG	7:G:156:ASP:HA	2.59	0.42
17:Q:58:GLN:HE22	18:R:194:ARG:HH11	1.65	0.42
17:Q:105:TYR:CZ	18:R:234:GLU:CD	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:86:GLN:O	20:T:112:GLN:NE2	2.52	0.42
25:2:35:TYR:CD1	25:2:62:LEU:HD12	2.52	0.42
25:2:201:PHE:CD1	25:2:201:PHE:C	2.96	0.42
25:2:258:LEU:HG	25:2:262:LEU:HD21	1.99	0.42
26:3:121:LYS:H	26:3:121:LYS:CD	2.32	0.42
26:3:137:LEU:HD12	26:3:177:PHE:CE1	2.54	0.42
27:X:2:DA:N6	28:Y:91:DT:O4	2.52	0.42
1:A:1301:ILE:O	1:A:1345:ARG:HD3	2.19	0.42
2:B:40:VAL:HG21	2:B:181:PRO:HB2	2.01	0.42
2:B:411:LEU:HD11	2:B:435:ILE:HG23	2.01	0.42
2:B:1069:ILE:HD12	2:B:1070:LEU:HD12	2.00	0.42
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.54	0.42
5:E:61:LEU:HD21	5:E:71:GLN:HB2	2.02	0.42
14:N:366:ILE:O	15:O:54:ASN:ND2	2.50	0.42
16:P:297:LYS:HD3	16:P:297:LYS:HA	1.39	0.42
17:Q:19:LYS:O	17:Q:23:ARG:HG3	2.19	0.42
17:Q:113:ARG:NH1	18:R:218:LYS:HA	2.33	0.42
19:S:135:PHE:HD1	19:S:135:PHE:HA	1.71	0.42
24:1:25:GLU:OE2	24:1:35:ILE:HG12	2.18	0.42
25:2:93:LEU:HA	25:2:93:LEU:HD23	1.76	0.42
25:2:117:ASN:HD21	26:3:108:ASN:N	2.16	0.42
25:2:159:VAL:HG11	25:2:161:HIS:CD2	2.49	0.42
25:2:230:LEU:C	25:2:230:LEU:HD13	2.44	0.42
1:A:959:MET:HE1	1:A:1046:ARG:O	2.19	0.42
1:A:1103:THR:HG21	1:A:1106:THR:OG1	2.18	0.42
1:A:1128:ILE:HG23	1:A:1414:ILE:HD11	2.01	0.42
2:B:570:ASN:OD1	2:B:616:THR:HG22	2.19	0.42
2:B:921:ILE:O	2:B:921:ILE:HG13	2.19	0.42
15:O:64:THR:HG22	15:O:75:VAL:HB	2.00	0.42
17:Q:114:ILE:HG12	18:R:218:LYS:HE3	2.00	0.42
21:V:514:MET:HB3	24:1:16:MET:SD	2.59	0.42
24:1:34:ILE:CG2	24:1:50:VAL:HG11	2.48	0.42
26:3:178:MET:O	26:3:182:PHE:HD2	2.01	0.42
1:A:567:LEU:HD22	1:A:570:TRP:HB2	2.00	0.42
1:A:1132:LYS:HE3	27:X:53:DA:H5'	2.01	0.42
2:B:33:TYR:CE1	2:B:37:LYS:HG3	2.54	0.42
2:B:499:ARG:CZ	2:B:522:LEU:HD11	2.49	0.42
2:B:894:THR:HG23	2:B:897:ARG:HH11	1.83	0.42
2:B:924:ARG:HH11	3:C:60:HIS:HB2	1.84	0.42
13:M:164:LEU:HD12	13:M:164:LEU:HA	1.80	0.42
22:W:107:LEU:HB2	22:W:175:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:10:ILE:HG22	25:2:407:VAL:CG2	2.49	0.42
25:2:28:PRO:HA	26:3:33:THR:CB	2.49	0.42
25:2:133:THR:CG2	25:2:134:SER:N	2.82	0.42
26:3:18:ASN:ND2	26:3:64:ILE:HD11	2.35	0.42
26:3:64:ILE:CB	26:3:123:ASP:HB3	2.50	0.42
26:3:128:HIS:NE2	26:3:130:GLU:CG	2.82	0.42
27:X:77:DC:H2"	27:X:78:DT:C7	2.50	0.42
1:A:94:VAL:HG21	1:A:314:VAL:HG21	2.01	0.42
1:A:1171:ALA:O	9:I:59:THR:CG2	2.67	0.42
1:A:1298:LEU:C	1:A:1300:GLY:N	2.77	0.42
2:B:711:ILE:O	2:B:714:PRO:HD3	2.19	0.42
4:D:110:GLU:HA	7:G:167:TYR:CE2	2.55	0.42
8:H:17:PRO:C	8:H:19:GLY:N	2.76	0.42
13:M:10:LEU:O	13:M:12:ARG:N	2.52	0.42
14:N:12:LYS:O	14:N:15:ARG:HB2	2.19	0.42
22:W:419:GLU:HB3	22:W:420:PRO:HD3	1.84	0.42
23:0:74:GLN:CA	23:0:78:PRO:O	2.66	0.42
24:1:18:GLN:HG3	24:1:19:PHE:N	2.34	0.42
25:2:188:THR:CG2	25:2:189:GLU:N	2.83	0.42
25:2:224:GLN:N	25:2:268:PHE:HZ	2.16	0.42
25:2:236:PHE:CE1	25:2:261:PHE:HB3	2.54	0.42
26:3:42:MET:SD	26:3:111:ILE:CD1	3.07	0.42
26:3:144:ILE:HG13	26:3:159:SER:OG	2.20	0.42
2:B:776:ILE:HD12	2:B:806:PHE:CD1	2.55	0.42
2:B:931:ILE:CD1	2:B:947:ILE:HA	2.48	0.42
5:E:52:ARG:HB2	5:E:53:PRO:HD2	1.13	0.42
8:H:34:SER:O	8:H:36:LYS:HG2	2.18	0.42
8:H:122:LEU:HA	8:H:122:LEU:HD23	1.82	0.42
8:H:135:PHE:O	8:H:137:VAL:HG22	2.19	0.42
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.84	0.42
17:Q:128:LYS:HB3	17:Q:164:ASP:HA	2.02	0.42
21:V:523:VAL:HG21	24:1:20:LEU:CD2	2.50	0.42
25:2:176:ALA:HB3	25:2:178:LEU:HD13	1.98	0.42
26:3:184:ALA:O	26:3:187:GLN:HG2	2.19	0.42
1:A:375:ILE:HD13	1:A:485:ASN:ND2	2.35	0.42
1:A:689:ILE:HD11	2:B:981:LEU:CB	2.50	0.42
1:A:878:THR:HA	1:A:889:LEU:O	2.20	0.42
2:B:1040:GLN:N	2:B:1040:GLN:CD	2.77	0.42
2:B:1089:MET:HA	2:B:1089:MET:HE3	2.01	0.42
3:C:220:TYR:CE2	3:C:222:PRO:HB3	2.55	0.42
3:C:263:LEU:O	3:C:266:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:ILE:O	5:E:125:TYR:HE1	2.03	0.42
9:I:14:ILE:HG12	9:I:16:PHE:CG	2.54	0.42
9:I:23:MET:HE3	9:I:25:TYR:CE1	2.55	0.42
18:R:223:VAL:HG23	18:R:224:THR:HG23	1.79	0.42
21:V:519:TYR:HB3	24:1:16:MET:HG3	2.00	0.42
23:0:72:GLU:O	23:0:79:ASN:HB2	2.20	0.42
24:1:1:MET:SD	25:2:413:LEU:CB	3.04	0.42
25:2:47:GLU:HG3	25:2:48:LEU:H	1.83	0.42
26:3:221:PRO:C	26:3:223:LEU:H	2.27	0.42
1:A:156:GLY:HA2	1:A:181:HIS:HD1	1.71	0.42
1:A:263:ALA:O	1:A:264:VAL:C	2.58	0.42
1:A:901:VAL:HB	1:A:978:VAL:HG13	2.02	0.42
1:A:942:VAL:HG21	1:A:1005:HIS:NE2	2.35	0.42
1:A:1141:VAL:HG13	1:A:1352:VAL:HG13	2.02	0.42
2:B:47:PHE:O	2:B:50:PHE:HB3	2.20	0.42
3:C:44:ILE:HG23	3:C:176:TRP:HD1	1.84	0.42
6:F:66:LEU:HD23	6:F:66:LEU:HA	1.92	0.42
13:M:62:LYS:HD3	29:Z:1:A:H4'	2.02	0.42
18:R:194:ARG:HA	18:R:194:ARG:HD3	1.49	0.42
20:T:151:THR:O	20:T:152:ASN:CG	2.62	0.42
22:W:584:TYR:CD1	22:W:594:ALA:CB	2.88	0.42
25:2:57:MET:CA	25:2:60:LEU:HG	2.49	0.42
26:3:105:THR:CG2	26:3:106:SER:N	2.83	0.42
26:3:160:ARG:CZ	26:3:190:LEU:CD1	2.97	0.42
27:X:1:DG:H2''	27:X:2:DA:C8	2.55	0.42
1:A:47:THR:O	1:A:48:GLU:HB2	2.20	0.42
1:A:375:ILE:HG13	1:A:666:ARG:NH1	2.34	0.42
1:A:672:ILE:HG23	1:A:673:GLN:N	2.35	0.42
2:B:180:ASP:OD1	2:B:181:PRO:HD2	2.20	0.42
2:B:246:GLY:HA3	19:S:169:LYS:HD2	2.02	0.42
13:M:79:ASP:OD1	13:M:79:ASP:N	2.53	0.42
15:O:9:THR:O	15:O:13:ASN:N	2.48	0.42
17:Q:70:LYS:NZ	18:R:226:ASP:HA	2.34	0.42
21:V:450:MET:HG3	27:X:75:DG:H3'	2.02	0.42
21:V:615:PHE:O	21:V:615:PHE:CG	2.71	0.42
21:V:689:VAL:CG2	25:2:391:ILE:HD13	2.50	0.42
24:1:1:MET:HE3	25:2:415:GLN:N	2.34	0.42
25:2:204:LEU:HD23	25:2:254:MET:HE3	2.02	0.42
26:3:9:ASN:OD1	26:3:158:LYS:HB3	2.19	0.42
26:3:202:LEU:N	26:3:202:LEU:CD2	2.82	0.42
1:A:365:THR:CG2	2:B:1059:ILE:HG22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:CYS:O	2:B:226:GLU:N	2.51	0.42
2:B:779:ILE:HD13	2:B:779:ILE:HA	1.86	0.42
5:E:187:ARG:HG3	5:E:210:GLN:HA	2.02	0.42
9:I:14:ILE:CG1	9:I:16:PHE:CD2	3.02	0.42
13:M:34:CYS:H	13:M:39:LEU:HB3	1.85	0.42
22:W:25:MET:SD	22:W:58:ALA:HB2	2.59	0.42
24:1:14:PRO:HG2	24:1:17:LYS:HB2	2.01	0.42
25:2:89:LEU:CD2	25:2:89:LEU:C	2.93	0.42
26:3:141:LEU:HA	26:3:144:ILE:HG22	2.01	0.42
1:A:368:THR:HB	1:A:369:PRO:HD2	2.01	0.41
1:A:532:ARG:HD2	1:A:647:THR:O	2.20	0.41
1:A:805:ARG:HG2	1:A:812:LYS:HA	2.01	0.41
1:A:904:GLN:HE22	1:A:982:ASN:HA	1.85	0.41
2:B:133:ILE:HG23	2:B:139:GLN:CD	2.45	0.41
2:B:479:LEU:HA	2:B:479:LEU:HD12	1.80	0.41
2:B:506:TRP:O	2:B:506:TRP:CD1	2.73	0.41
2:B:597:ILE:HB	2:B:600:GLU:HB2	2.02	0.41
2:B:953:ASP:OD1	3:C:36:ARG:NH1	2.51	0.41
21:V:315:VAL:HG13	22:W:500:ASP:HB2	0.42	0.41
23:0:79:ASN:C	23:0:81:LEU:N	2.77	0.41
24:1:29:LEU:C	24:1:29:LEU:CD2	2.93	0.41
26:3:197:ASP:O	26:3:198:SER:HB3	2.20	0.41
1:A:273:GLN:H	1:A:273:GLN:HG2	1.69	0.41
1:A:603:ILE:HG12	1:A:604:ARG:N	2.34	0.41
1:A:689:ILE:HG23	1:A:689:ILE:HD12	1.75	0.41
5:E:82:VAL:HB	5:E:110:MET:SD	2.60	0.41
7:G:90:THR:O	7:G:91:GLN:HG3	2.20	0.41
9:I:11:PHE:CE1	9:I:54:TYR:HA	2.55	0.41
13:M:69:ASP:OD1	13:M:70:SER:N	2.53	0.41
16:P:271:GLU:OE1	16:P:271:GLU:N	2.50	0.41
25:2:62:LEU:C	25:2:62:LEU:CD1	2.94	0.41
25:2:181:GLN:HA	25:2:181:GLN:NE2	2.34	0.41
28:Y:38:DT:H2''	28:Y:39:DG:O4'	2.20	0.41
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	2.02	0.41
1:A:1302:GLU:HG3	1:A:1304:ILE:HG12	2.02	0.41
4:D:90:LYS:HE3	4:D:130:ILE:HD11	2.01	0.41
4:D:92:LEU:HD23	4:D:122:PHE:CE2	2.56	0.41
4:D:94:LYS:HD3	4:D:94:LYS:HA	1.78	0.41
5:E:58:LEU:HD23	5:E:76:PHE:CE2	2.55	0.41
10:J:62:TYR:O	10:J:65:LEU:HD11	2.20	0.41
13:M:30:GLY:CA	13:M:44:ARG:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:24:GLY:O	18:R:215:GLU:OE2	2.38	0.41
19:S:147:THR:HA	19:S:148:PRO:HD3	1.89	0.41
24:1:31:LYS:C	24:1:33:PHE:H	2.28	0.41
26:3:14:VAL:HG22	26:3:162:LEU:O	2.21	0.41
26:3:109:GLU:HG3	26:3:110:VAL:N	2.35	0.41
26:3:217:VAL:HG12	26:3:218:PRO:O	2.20	0.41
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.53	0.41
2:B:1132:THR:HG23	2:B:1133:HIS:ND1	2.36	0.41
3:C:49:TRP:CE3	12:L:54:VAL:HG21	2.56	0.41
9:I:25:TYR:HD2	9:I:40:ARG:HG3	1.85	0.41
15:O:63:ASN:HB3	15:O:75:VAL:O	2.20	0.41
17:Q:23:ARG:NH2	18:R:206:LYS:C	2.77	0.41
19:S:166:ARG:HH11	19:S:166:ARG:CG	2.32	0.41
22:W:420:PRO:O	22:W:431:PRO:HB3	2.20	0.41
23:O:54:ARG:HA	26:3:209:ILE:HD13	1.06	0.41
24:1:43:VAL:CG1	24:1:44:PHE:N	2.83	0.41
26:3:33:THR:CG2	26:3:36:LYS:H	2.04	0.41
26:3:41:VAL:HG13	26:3:42:MET:N	2.34	0.41
1:A:388:MET:HE3	1:A:505:LEU:HD22	2.02	0.41
1:A:404:GLU:CD	1:A:407:ARG:HH12	2.22	0.41
1:A:602:CYS:H	1:A:630:VAL:CG1	2.33	0.41
1:A:889:LEU:HD23	1:A:889:LEU:HA	1.88	0.41
1:A:901:VAL:HB	1:A:978:VAL:CG1	2.51	0.41
2:B:767:LEU:C	2:B:769:PHE:N	2.78	0.41
2:B:831:LYS:HA	2:B:832:PRO:HD3	1.90	0.41
9:I:15:ARG:HD3	9:I:24:LEU:HD12	2.02	0.41
13:M:44:ARG:HD2	13:M:45:VAL:H	1.85	0.41
17:Q:154:CYS:SG	17:Q:155:THR:N	2.93	0.41
17:Q:184:ILE:CG1	18:R:213:ASP:OD1	2.68	0.41
20:T:213:LEU:HD23	20:T:213:LEU:HA	1.78	0.41
25:2:77:LYS:HD3	25:2:78:GLU:CG	2.50	0.41
25:2:172:SER:C	25:2:175:LEU:HD23	2.43	0.41
25:2:270:LEU:C	25:2:270:LEU:CD2	2.94	0.41
26:3:165:LYS:HZ1	26:3:200:SER:N	2.18	0.41
27:X:18:DG:OP2	27:X:18:DG:H2'	2.20	0.41
1:A:205:VAL:HB	1:A:206:ASN:H	1.63	0.41
1:A:265:VAL:HG21	13:M:48:VAL:CG2	2.51	0.41
1:A:457:ILE:HD11	2:B:1102:PHE:CE2	2.55	0.41
1:A:872:MET:HE3	1:A:872:MET:HB2	1.97	0.41
2:B:262:TYR:O	2:B:263:ILE:HD13	2.20	0.41
2:B:823:PHE:HA	13:M:140:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:856:PRO:HG2	12:L:46:LYS:O	2.20	0.41
2:B:1040:GLN:O	2:B:1041:ILE:HD13	2.21	0.41
3:C:67:ARG:NH1	3:C:67:ARG:HB3	2.36	0.41
5:E:41:LYS:HA	5:E:46:ASP:CB	2.40	0.41
6:F:104:ILE:O	6:F:120:VAL:HG23	2.21	0.41
7:G:18:PHE:HA	7:G:22:LEU:HD13	2.02	0.41
7:G:138:GLN:HG2	7:G:139:GLN:N	2.35	0.41
7:G:148:VAL:HG23	7:G:160:ILE:CD1	2.50	0.41
9:I:15:ARG:O	9:I:15:ARG:HG3	2.19	0.41
21:V:353:ALA:O	21:V:357:VAL:HG23	2.21	0.41
21:V:514:MET:HE2	21:V:667:THR:HG21	2.01	0.41
21:V:519:TYR:CE2	21:V:523:VAL:HG21	2.55	0.41
25:2:123:LEU:CD2	25:2:123:LEU:C	2.93	0.41
25:2:224:GLN:CB	25:2:268:PHE:CZ	2.94	0.41
26:3:146:ARG:HG3	26:3:147:MET:N	2.35	0.41
27:X:25:DG:N2	28:Y:70:DC:O2	2.53	0.41
1:A:378:VAL:HG23	1:A:484:LEU:HD23	2.02	0.41
1:A:679:TRP:CZ2	1:A:683:GLU:HG3	2.55	0.41
1:A:1201:ASP:O	1:A:1204:VAL:HG22	2.20	0.41
1:A:1308:TYR:CD1	1:A:1308:TYR:C	2.98	0.41
2:B:211:LYS:HE3	27:X:48:DT:H2'	2.02	0.41
2:B:215:TYR:CD1	2:B:238:SER:HB3	2.55	0.41
2:B:510:CYS:HB2	2:B:705:GLY:CA	2.49	0.41
2:B:554:GLU:OE1	19:S:115:LYS:HG3	2.20	0.41
2:B:704:LEU:HD23	2:B:704:LEU:HA	1.85	0.41
2:B:747:LEU:HD23	2:B:747:LEU:C	2.45	0.41
3:C:30:VAL:HG22	11:K:45:ILE:HD11	2.02	0.41
5:E:15:LYS:HA	5:E:15:LYS:HD3	1.80	0.41
10:J:2:ILE:HG12	10:J:3:ILE:N	2.36	0.41
17:Q:187:ILE:O	17:Q:191:LEU:HD13	2.21	0.41
20:T:34:ALA:C	20:T:35:SER:HG	2.26	0.41
24:1:1:MET:N	25:2:418:PHE:CB	2.83	0.41
24:1:52:VAL:CG2	24:1:53:LEU:N	2.83	0.41
25:2:211:GLN:HE21	25:2:257:SER:HB2	1.84	0.41
25:2:221:GLN:O	25:2:268:PHE:CE1	2.74	0.41
26:3:14:VAL:CG2	26:3:163:VAL:HG13	2.48	0.41
26:3:228:LEU:C	26:3:228:LEU:CD2	2.93	0.41
27:X:59:DC:H2''	27:X:60:DG:O5'	2.21	0.41
29:Z:3:U:H2'	29:Z:4:C:O4'	2.20	0.41
1:A:271:ARG:HG3	13:M:73:PRO:HG3	2.03	0.41
1:A:912:SER:HB3	1:A:915:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:VAL:CG2	2:B:141:GLN:CG	2.93	0.41
2:B:264:LYS:H	2:B:325:GLY:HA2	1.86	0.41
2:B:510:CYS:SG	2:B:511:PRO:HD2	2.61	0.41
2:B:847:LYS:O	2:B:854:ILE:HG22	2.21	0.41
6:F:64:ARG:NH1	7:G:61:PRO:HB3	2.35	0.41
7:G:17:TYR:HB3	7:G:25:THR:HG21	2.03	0.41
13:M:119:LYS:HD3	28:Y:60:DA:N6	2.34	0.41
13:M:178:LYS:HD3	13:M:279:GLY:HA3	2.01	0.41
22:W:15:ASP:HA	22:W:100:GLU:OE2	2.21	0.41
24:1:2:VAL:HG11	25:2:456:LYS:CB	2.44	0.41
25:2:28:PRO:C	26:3:25:GLN:C	2.88	0.41
26:3:24:LYS:CE	26:3:220:MET:SD	3.07	0.41
27:X:12:DA:C2	27:X:13:DT:C4	3.09	0.41
27:X:45:DT:H4'	27:X:46:DT:O4'	2.21	0.41
1:A:40:GLY:C	1:A:42:LYS:N	2.78	0.41
1:A:266:MET:HB3	13:M:52:TRP:CE3	2.56	0.41
1:A:499:ASP:OD1	29:Z:6:C:H4'	2.20	0.41
1:A:514:GLU:CD	2:B:1101:GLN:HE21	2.29	0.41
1:A:966:LEU:HA	1:A:969:ILE:HD12	2.03	0.41
1:A:1124:LEU:HD12	1:A:1124:LEU:HA	1.84	0.41
1:A:1324:GLU:H	1:A:1324:GLU:CD	2.28	0.41
8:H:113:SER:HA	8:H:125:LEU:O	2.20	0.41
8:H:137:VAL:HG21	8:H:140:ARG:HD2	2.01	0.41
8:H:147:LYS:C	8:H:149:ALA:H	2.29	0.41
10:J:56:ILE:HD12	10:J:56:ILE:HG23	1.76	0.41
16:P:159:SER:CB	16:P:329:TYR:CE2	2.93	0.41
17:Q:187:ILE:HD13	18:R:211:SER:CA	2.39	0.41
17:Q:188:TYR:CZ	18:R:210:PHE:HE1	2.34	0.41
18:R:223:VAL:C	18:R:224:THR:CG2	2.20	0.41
21:V:390:CYS:SG	21:V:399:LYS:HE3	2.61	0.41
21:V:518:PHE:CD1	21:V:713:LEU:HD13	2.55	0.41
22:W:233:PHE:HB2	22:W:456:ILE:HG22	2.02	0.41
24:1:1:MET:HG2	25:2:413:LEU:CB	2.47	0.41
24:1:10:ILE:C	24:1:10:ILE:CD1	2.93	0.41
24:1:38:ILE:CB	24:1:44:PHE:CD1	3.04	0.41
25:2:42:LEU:HA	25:2:42:LEU:HD23	1.78	0.41
25:2:93:LEU:HD23	25:2:96:TRP:HE1	1.85	0.41
25:2:93:LEU:O	25:2:96:TRP:CD1	2.74	0.41
26:3:34:LEU:C	26:3:34:LEU:CD1	2.94	0.41
26:3:100:LYS:HB2	26:3:100:LYS:HE2	1.89	0.41
26:3:165:LYS:C	26:3:165:LYS:CD	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:185:GLN:HA	26:3:185:GLN:NE2	2.26	0.41
28:Y:32:DC:H2''	28:Y:33:DT:C6	2.55	0.41
28:Y:56:DG:C4	28:Y:57:DA:H1'	2.56	0.41
1:A:367:ILE:HG22	1:A:482:PHE:HB2	2.02	0.41
1:A:520:MET:HG3	1:A:522:PRO:HD2	2.03	0.41
1:A:966:LEU:HD13	1:A:1043:ILE:HD11	2.03	0.41
2:B:497:LYS:HE2	2:B:497:LYS:HB3	1.77	0.41
2:B:502:HIS:CE1	2:B:504:THR:HG1	2.39	0.41
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.86	0.41
5:E:46:ASP:O	5:E:48:PRO:HD2	2.20	0.41
7:G:119:PHE:CE2	7:G:121:PRO:HB3	2.56	0.41
23:0:97:ASP:OD1	26:3:208:ASP:CG	2.61	0.41
25:2:140:LYS:CD	25:2:162:PHE:HE1	2.29	0.41
25:2:170:ALA:C	25:2:213:TRP:HZ3	2.27	0.41
25:2:236:PHE:HZ	25:2:258:LEU:CD1	2.34	0.41
26:3:100:LYS:CB	26:3:103:LEU:HD13	2.41	0.41
26:3:114:GLU:OE1	26:3:114:GLU:HA	2.21	0.41
26:3:172:LEU:C	26:3:172:LEU:CD1	2.94	0.41
1:A:466:LYS:HE3	1:A:466:LYS:HB2	1.88	0.40
1:A:1189:ASP:HA	1:A:1192:TRP:CZ3	2.56	0.40
1:A:1307:VAL:HG13	1:A:1308:TYR:H	1.86	0.40
2:B:51:ILE:HG22	20:T:141:LEU:CG	2.52	0.40
2:B:1030:ASN:N	2:B:1035:ARG:O	2.42	0.40
2:B:1112:ASP:OD2	2:B:1153:TYR:N	2.55	0.40
9:I:15:ARG:C	9:I:16:PHE:O	2.65	0.40
13:M:23:LEU:HD12	13:M:33:ILE:O	2.21	0.40
17:Q:71:PHE:CD1	17:Q:102:VAL:CG2	3.05	0.40
21:V:297:PHE:CG	21:V:298:ARG:N	2.89	0.40
21:V:518:PHE:HB2	24:1:16:MET:SD	2.61	0.40
22:W:535:ILE:HG12	22:W:617:ALA:HB3	2.04	0.40
25:2:34:LEU:CD2	25:2:34:LEU:N	2.84	0.40
25:2:89:LEU:O	25:2:93:LEU:HG	2.21	0.40
25:2:220:LEU:C	25:2:220:LEU:CD1	2.94	0.40
26:3:111:ILE:HG13	26:3:112:VAL:H	1.84	0.40
26:3:222:SER:HB3	26:3:225:GLN:CG	2.51	0.40
1:A:202:TRP:CB	1:A:212:LYS:CG	2.97	0.40
1:A:818:GLU:OE1	1:A:818:GLU:N	2.50	0.40
1:A:912:SER:HB3	1:A:915:ALA:CB	2.51	0.40
2:B:23:GLN:OE1	2:B:23:GLN:N	2.40	0.40
2:B:573:TRP:CH2	2:B:576:ILE:HG23	2.56	0.40
2:B:576:ILE:HD12	2:B:576:ILE:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:861:SER:O	2:B:896:LEU:CD2	2.69	0.40
11:K:7:PHE:CD1	11:K:7:PHE:C	3.00	0.40
14:N:14:TYR:CE1	15:O:11:LEU:HD22	2.56	0.40
19:S:24:LYS:HB2	20:T:99:SER:HA	2.04	0.40
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.57	0.40
19:S:169:LYS:HE3	19:S:169:LYS:HB3	1.83	0.40
22:W:492:PRO:HG2	22:W:678:VAL:HG22	2.03	0.40
24:1:18:GLN:OE1	24:1:19:PHE:CD1	2.74	0.40
25:2:60:LEU:CD1	25:2:95:ILE:CB	2.95	0.40
25:2:93:LEU:CA	25:2:96:TRP:HD1	2.31	0.40
25:2:202:GLN:HE21	25:2:202:GLN:N	2.15	0.40
26:3:59:VAL:CA	26:3:71:TYR:CD1	3.02	0.40
26:3:60:ILE:CG2	26:3:61:ALA:N	2.84	0.40
26:3:165:LYS:HE3	26:3:200:SER:N	2.36	0.40
26:3:174:TYR:CZ	26:3:178:MET:HG3	2.56	0.40
27:X:35:DT:H4'	27:X:36:DT:OP1	2.20	0.40
27:X:70:DG:N2	28:Y:25:DT:C2	2.90	0.40
1:A:202:TRP:CE3	1:A:212:LYS:C	2.98	0.40
1:A:672:ILE:HG21	1:A:672:ILE:HD13	1.79	0.40
2:B:781:ALA:HB1	2:B:1041:ILE:HG21	2.03	0.40
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.03	0.40
2:B:1118:VAL:HG12	2:B:1119:CYS:O	2.21	0.40
2:B:1127:ILE:HB	2:B:1128:ALA:H	1.75	0.40
8:H:5:LEU:HD22	8:H:133:HIS:HB3	2.02	0.40
14:N:341:LYS:H	14:N:352:HIS:HB2	1.86	0.40
16:P:329:TYR:N	16:P:330:PRO:HD2	2.36	0.40
17:Q:100:VAL:HG23	17:Q:101:ASN:N	2.37	0.40
18:R:195:PRO:HB2	18:R:199:LYS:HD2	2.04	0.40
20:T:51:ARG:NE	20:T:53:GLU:OE2	2.39	0.40
22:W:212:LEU:C	22:W:212:LEU:HD13	2.46	0.40
25:2:51:LEU:CD2	25:2:51:LEU:C	2.94	0.40
25:2:159:VAL:HG22	25:2:160:LEU:HD13	1.95	0.40
25:2:206:LEU:CD2	25:2:206:LEU:N	2.84	0.40
26:3:222:SER:O	26:3:226:TYR:CD2	2.75	0.40
26:3:222:SER:HB3	26:3:225:GLN:OE1	2.21	0.40
1:A:349:ARG:HG3	2:B:1161:GLU:OE1	2.22	0.40
1:A:360:ASP:HA	2:B:1062:ARG:HD3	2.04	0.40
1:A:623:PRO:HB2	8:H:27:ARG:NH2	2.37	0.40
1:A:733:LEU:HD12	1:A:733:LEU:HA	1.90	0.40
1:A:1192:TRP:NE1	1:A:1249:ASP:H	2.10	0.40
2:B:758:LEU:HD23	2:B:758:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:824:ASP:OD2	2:B:875:GLU:CG	2.70	0.40
4:D:32:LEU:HD11	7:G:4:HIS:HB2	2.02	0.40
7:G:44:PHE:CD2	7:G:103:PRO:HG2	2.57	0.40
9:I:14:ILE:HG13	9:I:16:PHE:CD1	2.56	0.40
16:P:207:PRO:O	16:P:208:ARG:O	2.39	0.40
21:V:593:LEU:HD11	21:V:615:PHE:CZ	2.55	0.40
24:1:52:VAL:O	24:1:56:ARG:HG2	2.21	0.40
25:2:94:ARG:HD2	25:2:95:ILE:HD13	2.02	0.40
25:2:174:ASP:OD2	25:2:213:TRP:CZ3	2.74	0.40
25:2:236:PHE:HZ	25:2:262:LEU:CD2	2.35	0.40
25:2:399:ASP:OD1	25:2:402:ARG:NH1	2.55	0.40
26:3:42:MET:HG2	26:3:111:ILE:CD1	2.52	0.40
1:A:265:VAL:HG21	13:M:48:VAL:CB	2.51	0.40
1:A:458:PHE:CZ	1:A:501:MET:HG3	2.57	0.40
1:A:496:PHE:C	1:A:498:GLY:H	2.29	0.40
1:A:1065:PHE:CZ	1:A:1069:LEU:HD21	2.57	0.40
1:A:1163:HIS:HA	1:A:1300:GLY:HA2	2.04	0.40
2:B:294:ASP:HA	2:B:295:PRO:HD3	1.79	0.40
16:P:173:ASN:OD1	16:P:175:GLY:N	2.40	0.40
19:S:144:TYR:CD2	20:T:96:PHE:HZ	2.39	0.40
20:T:160:GLN:HA	20:T:163:ILE:HD12	2.03	0.40
21:V:336:GLY:HA3	21:V:485:GLY:HA3	2.04	0.40
25:2:411:GLN:C	25:2:413:LEU:HD12	2.47	0.40
26:3:187:GLN:HE21	26:3:189:ILE:HB	1.87	0.40
26:3:229:TRP:O	26:3:229:TRP:HD1	2.04	0.40
28:Y:56:DG:H1'	28:Y:57:DA:H4'	2.03	0.40
28:Y:84:DG:C2	28:Y:85:DG:C4	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	1268 (87%)	120 (8%)	62 (4%)	2	17
2	B	1163/1174 (99%)	996 (86%)	116 (10%)	51 (4%)	2	17
3	C	273/275 (99%)	239 (88%)	25 (9%)	9 (3%)	3	21
4	D	127/142 (89%)	119 (94%)	8 (6%)	0	100	100
5	E	208/210 (99%)	191 (92%)	11 (5%)	6 (3%)	3	23
6	F	84/127 (66%)	82 (98%)	2 (2%)	0	100	100
7	G	169/172 (98%)	158 (94%)	10 (6%)	1 (1%)	21	59
8	H	148/150 (99%)	118 (80%)	20 (14%)	10 (7%)	1	11
9	I	123/125 (98%)	92 (75%)	16 (13%)	15 (12%)	0	4
10	J	65/67 (97%)	51 (78%)	9 (14%)	5 (8%)	1	9
11	K	115/117 (98%)	109 (95%)	4 (4%)	2 (2%)	7	36
12	L	44/58 (76%)	33 (75%)	9 (20%)	2 (4%)	2	16
13	M	308/316 (98%)	263 (85%)	32 (10%)	13 (4%)	2	17
14	N	109/376 (29%)	101 (93%)	6 (6%)	2 (2%)	6	34
15	O	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
16	P	183/339 (54%)	170 (93%)	6 (3%)	7 (4%)	2	19
17	Q	176/439 (40%)	158 (90%)	10 (6%)	8 (4%)	2	16
18	R	163/291 (56%)	140 (86%)	14 (9%)	9 (6%)	1	14
19	S	134/517 (26%)	120 (90%)	10 (8%)	4 (3%)	3	22
20	T	218/249 (88%)	190 (87%)	20 (9%)	8 (4%)	2	19
21	V	473/782 (60%)	398 (84%)	47 (10%)	28 (6%)	1	13
22	W	661/760 (87%)	570 (86%)	69 (10%)	22 (3%)	3	21
23	0	186/395 (47%)	168 (90%)	13 (7%)	5 (3%)	4	25
24	1	60/71 (84%)	53 (88%)	5 (8%)	2 (3%)	3	21
25	2	264/462 (57%)	246 (93%)	14 (5%)	4 (2%)	8	39
26	3	187/308 (61%)	176 (94%)	9 (5%)	2 (1%)	11	46
All	All	7188/10001 (72%)	6304 (88%)	607 (8%)	277 (4%)	4	18

All (277) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	153	ILE
1	A	204	HIS

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Mol	Chain	Res	Type
1	A	205	VAL
1	A	207	GLU
1	A	208	ASP
1	A	210	GLN
1	A	212	LYS
1	A	264	VAL
1	A	265	VAL
1	A	272	ASN
1	A	274	ASP
1	A	531	ASN
1	A	598	GLY
1	A	607	SER
1	A	610	PRO
1	A	623	PRO
1	A	911	PRO
1	A	930	LEU
1	A	931	ARG
1	A	1087	VAL
1	A	1101	GLN
1	A	1117	VAL
1	A	1118	THR
1	A	1200	PRO
1	A	1275	VAL
1	A	1299	GLN
1	A	1306	LYS
2	B	63	PRO
2	B	74	ALA
2	B	79	GLU
2	B	80	GLU
2	B	134	LYS
2	B	226	GLU
2	B	227	ASN
2	B	231	PRO
2	B	249	LYS
2	B	251	ALA
2	B	383	ASP
2	B	428	ASP
2	B	876	ASN
2	B	880	LEU
2	B	881	GLU
2	B	958	CYS
2	B	1007	ASN

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Mol	Chain	Res	Type
2	B	1136	GLU
3	C	7	PRO
5	E	47	LYS
5	E	52	ARG
5	E	53	PRO
8	H	67	ASP
8	H	86	ASP
8	H	108	ALA
9	I	15	ARG
9	I	16	PHE
9	I	60	HIS
9	I	62	VAL
9	I	85	PRO
9	I	103	ARG
9	I	104	ALA
9	I	106	ASP
9	I	119	CYS
11	K	112	LYS
13	M	12	ARG
13	M	42	GLY
13	M	43	ASP
13	M	47	ASP
13	M	95	GLU
13	M	101	TYR
14	N	320	VAL
16	P	160	GLY
16	P	162	VAL
16	P	206	GLU
16	P	208	ARG
17	Q	100	VAL
17	Q	102	VAL
17	Q	172	ASP
18	R	140	LYS
18	R	195	PRO
18	R	196	ASP
18	R	207	SER
20	T	124	TYR
20	T	145	LEU
20	T	146	ASP
21	V	385	ASP
21	V	461	HIS
21	V	491	ALA

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Mol	Chain	Res	Type
21	V	499	ASN
21	V	614	SER
21	V	615	PHE
21	V	616	ASP
21	V	632	SER
21	V	648	LYS
21	V	649	GLY
22	W	67	VAL
22	W	420	PRO
22	W	424	ARG
22	W	430	ASN
22	W	504	ILE
22	W	573	ASP
22	W	595	ILE
22	W	630	SER
23	0	78	PRO
23	0	80	ARG
24	1	48	GLU
25	2	49	PRO
26	3	120	THR
1	A	12	ALA
1	A	184	CYS
1	A	270	ALA
1	A	271	ARG
1	A	466	LYS
1	A	624	GLY
1	A	932	ARG
1	A	1119	LEU
1	A	1145	GLY
1	A	1435	THR
2	B	41	ARG
2	B	73	HIS
2	B	77	GLU
2	B	141	GLN
2	B	229	SER
2	B	253	GLY
2	B	491	ARG
2	B	785	TYR
2	B	875	GLU
2	B	879	GLU
2	B	884	ASN
2	B	900	GLU

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Mol	Chain	Res	Type
3	C	5	ASN
3	C	143	VAL
5	E	70	ASP
8	H	21	LYS
8	H	107	GLU
9	I	58	ILE
9	I	59	THR
9	I	67	GLN
9	I	99	SER
10	J	5	VAL
10	J	6	ARG
13	M	40	VAL
13	M	48	VAL
13	M	53	ARG
14	N	318	ASP
16	P	299	ARG
17	Q	126	SER
17	Q	158	HIS
18	R	164	GLY
18	R	194	ARG
18	R	223	VAL
18	R	224	THR
21	V	254	GLN
21	V	404	SER
21	V	460	ALA
21	V	613	THR
22	W	124	LEU
22	W	408	SER
22	W	646	ILE
25	2	223	ALA
25	2	231	VAL
1	A	48	GLU
1	A	61	ARG
1	A	70	ARG
1	A	134	LYS
1	A	599	HIS
1	A	612	ASP
1	A	1109	TYR
1	A	1116	ASN
1	A	1305	SER
2	B	61	ASP
2	B	233	SER

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Mol	Chain	Res	Type
2	B	245	GLN
2	B	458	LYS
2	B	549	SER
2	B	873	LEU
3	C	3	TYR
5	E	48	PRO
5	E	65	ASN
7	G	140	ASP
8	H	111	ARG
12	L	17	TYR
13	M	87	GLY
16	P	207	PRO
16	P	298	PRO
17	Q	125	ALA
17	Q	133	SER
19	S	160	ALA
20	T	147	LYS
21	V	343	GLY
22	W	147	GLN
22	W	155	CYS
22	W	509	GLU
26	3	198	SER
1	A	38	GLU
1	A	62	GLN
1	A	266	MET
1	A	611	ASP
1	A	1308	TYR
2	B	225	LEU
2	B	427	LYS
2	B	559	ALA
2	B	821	LYS
2	B	1032	PHE
8	H	100	GLU
8	H	128	ASP
9	I	73	SER
9	I	117	PRO
10	J	16	ASN
10	J	41	LYS
11	K	29	ASN
13	M	45	VAL
13	M	56	SER
18	R	228	MET

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Mol	Chain	Res	Type
19	S	156	THR
19	S	170	VAL
20	T	139	VAL
20	T	141	LEU
20	T	142	SER
21	V	310	LEU
21	V	436	GLY
21	V	470	LEU
21	V	475	ASP
21	V	502	ILE
21	V	629	HIS
1	A	51	ARG
1	A	981	CYS
1	A	1307	VAL
2	B	457	LYS
2	B	515	PRO
8	H	24	ARG
12	L	34	ILE
13	M	66	ARG
17	Q	25	PHE
20	T	152	ASN
21	V	427	MET
21	V	650	MET
22	W	152	LEU
22	W	551	SER
25	2	430	VAL
1	A	195	GLY
1	A	453	GLY
1	A	621	ILE
1	A	622	SER
3	C	2	PRO
3	C	6	GLN
19	S	154	THR
21	V	582	GLY
22	W	36	GLY
22	W	111	SER
22	W	345	ARG
23	0	77	LYS
1	A	1304	ILE
2	B	493	GLY
2	B	1006	VAL
2	B	1113	PRO

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Mol	Chain	Res	Type
21	V	311	LYS
21	V	651	VAL
22	W	174	ILE
23	0	216	GLY
3	C	58	VAL
3	C	78	ILE
21	V	457	ILE
22	W	495	ILE
2	B	561	ILE
2	B	931	ILE
3	C	151	VAL
8	H	49	PRO
21	V	405	VAL
24	1	2	VAL
1	A	56	GLY
2	B	289	ILE
2	B	1034	GLY
10	J	14	VAL
1	A	1312	PRO
2	B	489	ILE
22	W	45	GLY
23	0	56	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1279/1748 (73%)	1234 (96%)	45 (4%)	32	53
2	B	1020/1028 (99%)	979 (96%)	41 (4%)	28	49
3	C	252/252 (100%)	244 (97%)	8 (3%)	34	55
4	D	119/126 (94%)	118 (99%)	1 (1%)	73	80
5	E	192/192 (100%)	186 (97%)	6 (3%)	35	56
6	F	74/111 (67%)	74 (100%)	0	100	100
7	G	152/153 (99%)	151 (99%)	1 (1%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	131/131 (100%)	126 (96%)	5 (4%)	29	50
9	I	112/112 (100%)	106 (95%)	6 (5%)	20	41
10	J	56/56 (100%)	54 (96%)	2 (4%)	31	52
11	K	106/106 (100%)	105 (99%)	1 (1%)	70	79
12	L	43/55 (78%)	41 (95%)	2 (5%)	23	44
13	M	263/268 (98%)	256 (97%)	7 (3%)	39	60
14	N	105/324 (32%)	104 (99%)	1 (1%)	68	78
15	O	90/98 (92%)	89 (99%)	1 (1%)	65	76
16	P	159/293 (54%)	157 (99%)	2 (1%)	61	74
17	Q	164/373 (44%)	160 (98%)	4 (2%)	43	63
18	R	150/261 (58%)	138 (92%)	12 (8%)	11	31
19	S	121/448 (27%)	118 (98%)	3 (2%)	42	62
20	T	196/218 (90%)	190 (97%)	6 (3%)	35	56
21	V	422/688 (61%)	406 (96%)	16 (4%)	29	50
22	W	577/664 (87%)	545 (94%)	32 (6%)	19	41
23	0	171/352 (49%)	163 (95%)	8 (5%)	23	44
24	1	56/64 (88%)	52 (93%)	4 (7%)	13	35
25	2	238/399 (60%)	229 (96%)	9 (4%)	29	50
26	3	171/272 (63%)	161 (94%)	10 (6%)	18	39
All	All	6419/8792 (73%)	6186 (96%)	233 (4%)	32	52

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
1	A	132	LYS
1	A	203	LYS
1	A	204	HIS
1	A	205	VAL
1	A	226	LYS
1	A	259	SER
1	A	264	VAL
1	A	265	VAL
1	A	272	ASN
1	A	286	ILE

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Mol	Chain	Res	Type
1	A	303	ILE
1	A	305	GLU
1	A	463	THR
1	A	502	ASN
1	A	540	ASP
1	A	567	LEU
1	A	611	ASP
1	A	614	ASP
1	A	619	LYS
1	A	625	ASP
1	A	652	LEU
1	A	712	ASP
1	A	757	GLN
1	A	771	VAL
1	A	849	ASP
1	A	870	SER
1	A	873	VAL
1	A	908	THR
1	A	1036	ASN
1	A	1101	GLN
1	A	1102	MET
1	A	1119	LEU
1	A	1167	ARG
1	A	1279	MET
1	A	1282	ASP
1	A	1298	LEU
1	A	1306	LYS
1	A	1307	VAL
1	A	1308	TYR
1	A	1311	LEU
1	A	1337	GLU
1	A	1341	VAL
1	A	1385	VAL
1	A	1407	CYS
2	B	40	VAL
2	B	41	ARG
2	B	73	HIS
2	B	80	GLU
2	B	131	THR
2	B	132	VAL
2	B	140	LEU
2	B	156	LEU

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Mol	Chain	Res	Type
2	B	168	ASP
2	B	222	ARG
2	B	232	THR
2	B	250	SER
2	B	256	ILE
2	B	289	ILE
2	B	388	TYR
2	B	412	LEU
2	B	422	PHE
2	B	446	TYR
2	B	491	ARG
2	B	509	VAL
2	B	539	SER
2	B	573	TRP
2	B	606	ASP
2	B	641	ASP
2	B	666	ASP
2	B	667	THR
2	B	675	LEU
2	B	711	ILE
2	B	737	ILE
2	B	875	GLU
2	B	879	GLU
2	B	880	LEU
2	B	897	ARG
2	B	957	THR
2	B	959	GLU
2	B	961	ILE
2	B	1007	ASN
2	B	1056	ASP
2	B	1080	ARG
2	B	1090	GLU
2	B	1092	ASP
3	C	6	GLN
3	C	77	ASP
3	C	94	CYS
3	C	102	THR
3	C	137	ASN
3	C	177	ASN
3	C	212	ASP
3	C	242	GLU
4	D	135	GLN

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Mol	Chain	Res	Type
5	E	23	ASP
5	E	47	LYS
5	E	50	GLU
5	E	64	HIS
5	E	147	GLU
5	E	199	THR
7	G	128	TYR
8	H	11	ASP
8	H	65	TYR
8	H	84	ARG
8	H	107	GLU
8	H	116	VAL
9	I	14	ILE
9	I	15	ARG
9	I	58	ILE
9	I	84	HIS
9	I	95	VAL
9	I	105	GLU
10	J	47	ARG
10	J	65	LEU
11	K	48	SER
12	L	27	GLU
12	L	43	ILE
13	M	10	LEU
13	M	31	ASP
13	M	39	LEU
13	M	40	VAL
13	M	47	ASP
13	M	86	LYS
13	M	133	ASN
14	N	318	ASP
15	O	21	GLU
16	P	206	GLU
16	P	297	LYS
17	Q	38	ILE
17	Q	128	LYS
17	Q	135	THR
17	Q	191	LEU
18	R	100	ASP
18	R	105	GLU
18	R	152	LEU
18	R	163	LEU

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Mol	Chain	Res	Type
18	R	175	LEU
18	R	194	ARG
18	R	205	ASP
18	R	206	LYS
18	R	209	GLN
18	R	224	THR
18	R	225	VAL
18	R	228	MET
19	S	135	PHE
19	S	166	ARG
19	S	177	MET
20	T	140	ARG
20	T	141	LEU
20	T	145	LEU
20	T	154	LYS
20	T	160	GLN
20	T	206	THR
21	V	246	MET
21	V	271	GLU
21	V	332	ARG
21	V	362	LEU
21	V	371	VAL
21	V	429	TRP
21	V	458	VAL
21	V	471	VAL
21	V	479	ASP
21	V	482	PHE
21	V	492	ASN
21	V	517	GLU
21	V	568	LEU
21	V	581	TYR
21	V	590	MET
21	V	614	SER
22	W	37	HIS
22	W	64	PRO
22	W	87	LEU
22	W	95	GLU
22	W	101	LYS
22	W	112	ARG
22	W	122	THR
22	W	123	PRO
22	W	152	LEU

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Mol	Chain	Res	Type
22	W	166	ARG
22	W	196	ARG
22	W	263	LEU
22	W	283	ASP
22	W	288	LEU
22	W	307	ASN
22	W	309	VAL
22	W	327	GLU
22	W	333	LEU
22	W	346	VAL
22	W	425	THR
22	W	461	LEU
22	W	523	LEU
22	W	533	ASP
22	W	554	GLU
22	W	581	LEU
22	W	596	LEU
22	W	610	PHE
22	W	620	MET
22	W	647	ARG
22	W	664	VAL
22	W	669	ARG
22	W	676	LEU
23	0	77	LYS
23	0	103	GLN
23	0	125	ARG
23	0	174	LEU
23	0	202	SER
23	0	218	THR
23	0	222	ILE
23	0	223	LEU
24	1	10	ILE
24	1	16	MET
24	1	18	GLN
24	1	38	ILE
25	2	77	LYS
25	2	181	GLN
25	2	202	GLN
25	2	402	ARG
25	2	407	VAL
25	2	421	LEU
25	2	426	ARG

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Mol	Chain	Res	Type
25	2	430	VAL
25	2	452	LYS
26	3	24	LYS
26	3	25	GLN
26	3	56	LYS
26	3	109	GLU
26	3	124	ILE
26	3	133	LEU
26	3	144	ILE
26	3	185	GLN
26	3	190	LEU
26	3	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	188	GLN
1	A	278	HIS
1	A	403	GLN
1	A	410	ASN
1	A	449	HIS
1	A	465	HIS
1	A	516	GLN
1	A	711	GLN
1	A	740	GLN
1	A	757	GLN
1	A	790	GLN
1	A	947	HIS
1	A	1044	HIS
1	A	1077	ASN
1	A	1101	GLN
1	A	1105	ASN
1	A	1116	ASN
1	A	1190	GLN
1	A	1310	HIS
1	A	1313	GLN
1	A	1316	ASN
1	A	1445	HIS
2	B	203	ASN
2	B	654	GLN
2	B	695	HIS

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Mol	Chain	Res	Type
2	B	716	HIS
2	B	717	ASN
2	B	948	GLN
2	B	1053	HIS
2	B	1073	GLN
2	B	1097	HIS
2	B	1101	GLN
3	C	6	GLN
3	C	18	ASN
3	C	137	ASN
3	C	145	GLN
3	C	262	GLN
4	D	19	GLN
6	F	48	ASN
7	G	24	ASN
7	G	28	GLN
9	I	45	GLN
9	I	84	HIS
9	I	87	GLN
9	I	98	GLN
9	I	121	HIS
10	J	52	HIS
11	K	84	GLN
13	M	229	GLN
14	N	338	GLN
15	O	35	GLN
16	P	193	ASN
16	P	277	HIS
17	Q	95	ASN
17	Q	101	ASN
18	R	115	GLN
18	R	117	GLN
19	S	142	ASN
20	T	86	GLN
21	V	281	GLN
21	V	366	ASN
21	V	377	GLN
21	V	459	GLN
21	V	537	ASN
21	V	539	ASN
21	V	599	ASN
21	V	621	ASN

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Mol	Chain	Res	Type
21	V	665	GLN
21	V	677	GLN
22	W	187	GLN
22	W	203	ASN
22	W	316	GLN
22	W	328	HIS
22	W	430	ASN
23	0	60	HIS
24	1	27	ASN
24	1	42	HIS
24	1	51	ASN
25	2	97	HIS
25	2	161	HIS
25	2	181	GLN
25	2	202	GLN
25	2	221	GLN
25	2	239	GLN
25	2	263	GLN
25	2	273	GLN
25	2	411	GLN
25	2	458	GLN
26	3	25	GLN
26	3	52	ASN
26	3	63	HIS
26	3	148	ASN
26	3	155	GLN
26	3	185	GLN
26	3	187	GLN
26	3	225	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Z	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 12 ligands modelled in this entry, 12 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.

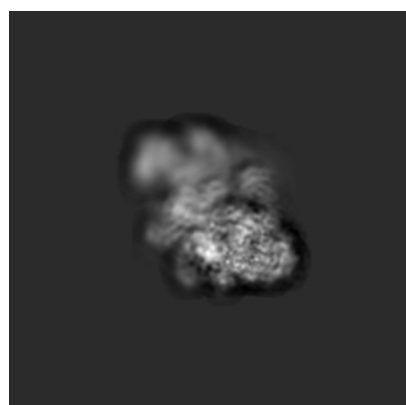
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8134. These allow visual inspection of the internal detail of the map and identification of artifacts.

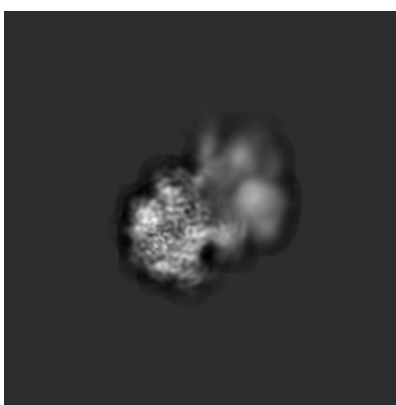
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

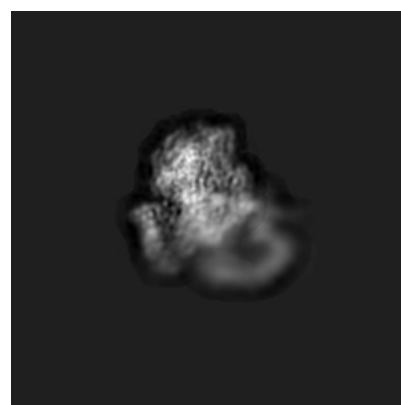
6.1.1 Primary map



X



Y

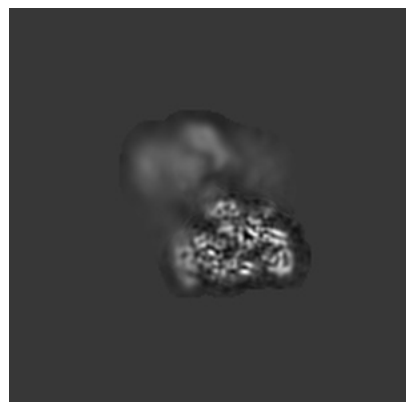


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 96



Y Index: 96

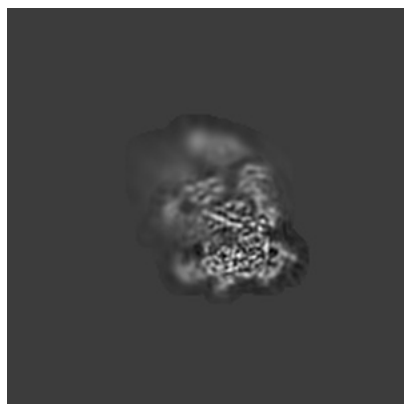


Z Index: 96

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

6.3 Largest variance slices [i](#)

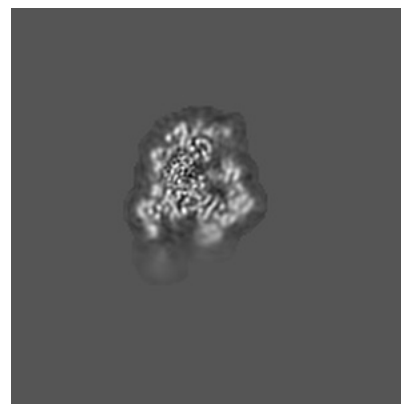
6.3.1 Primary map



X Index: 87



Y Index: 97



Z Index: 75

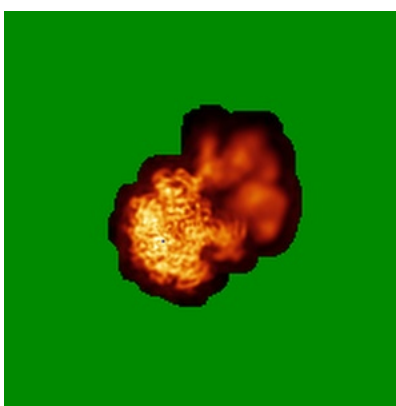
The images above show the largest variance slices of the map in three orthogonal directions.

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

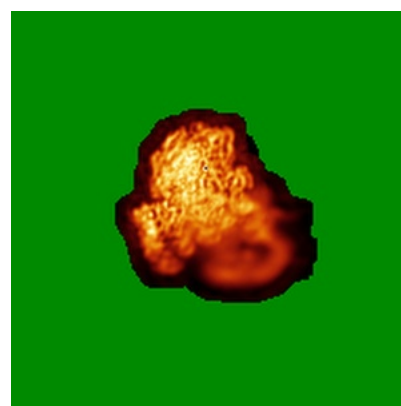
6.4.1 Primary map



X



Y

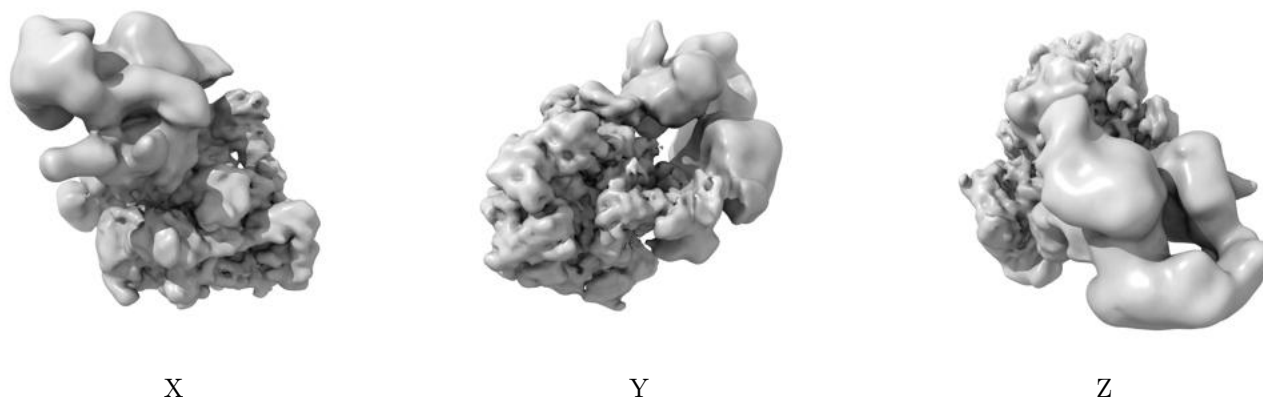


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

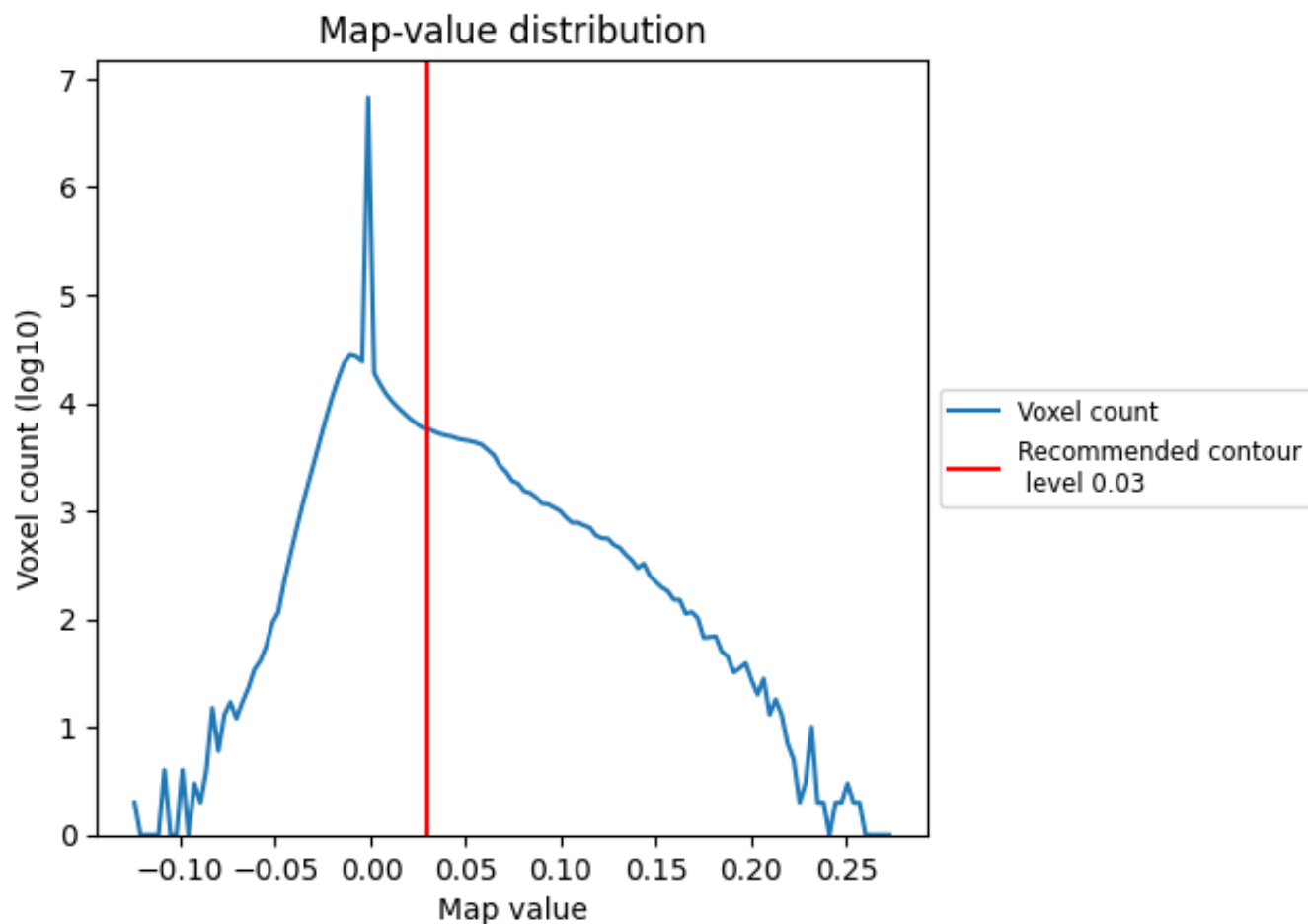
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

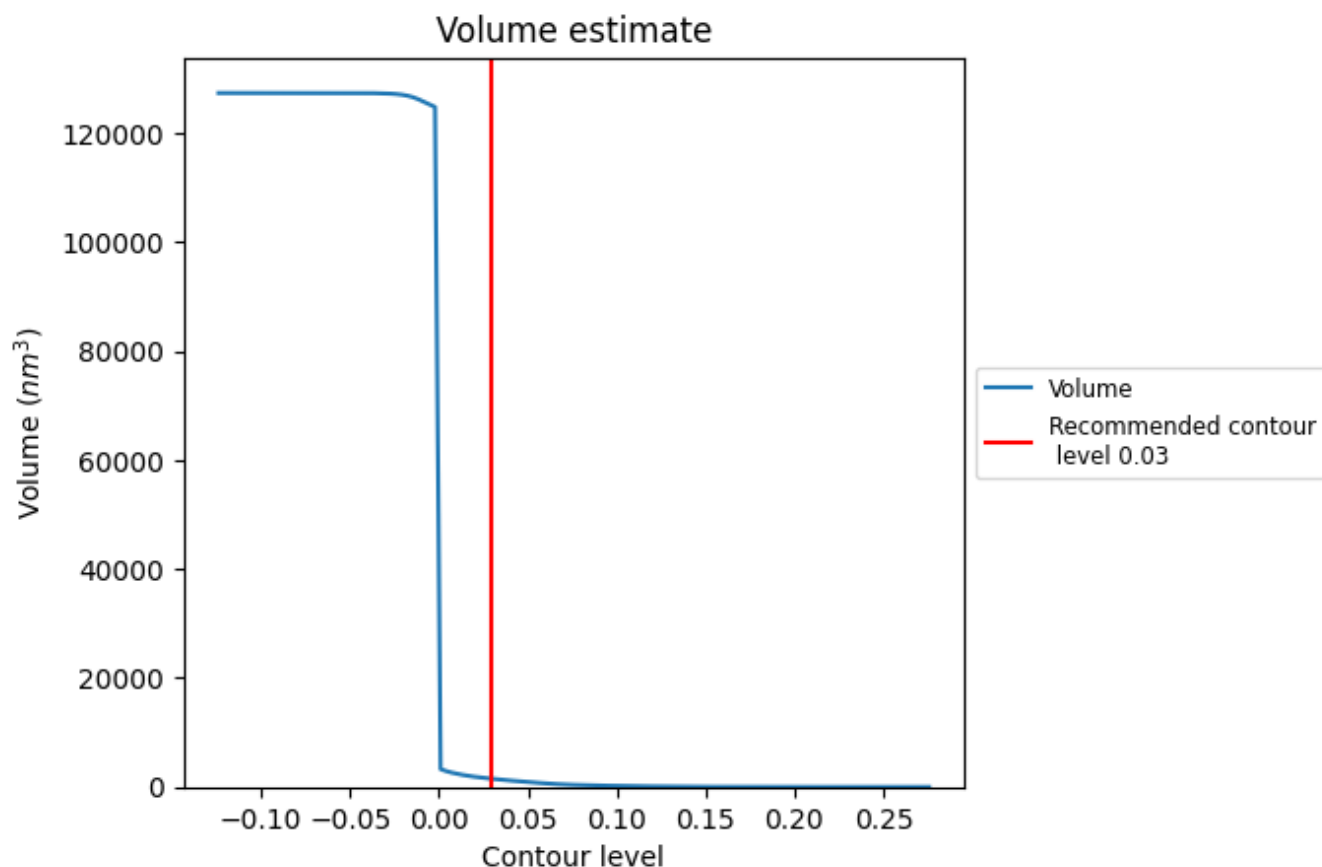
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

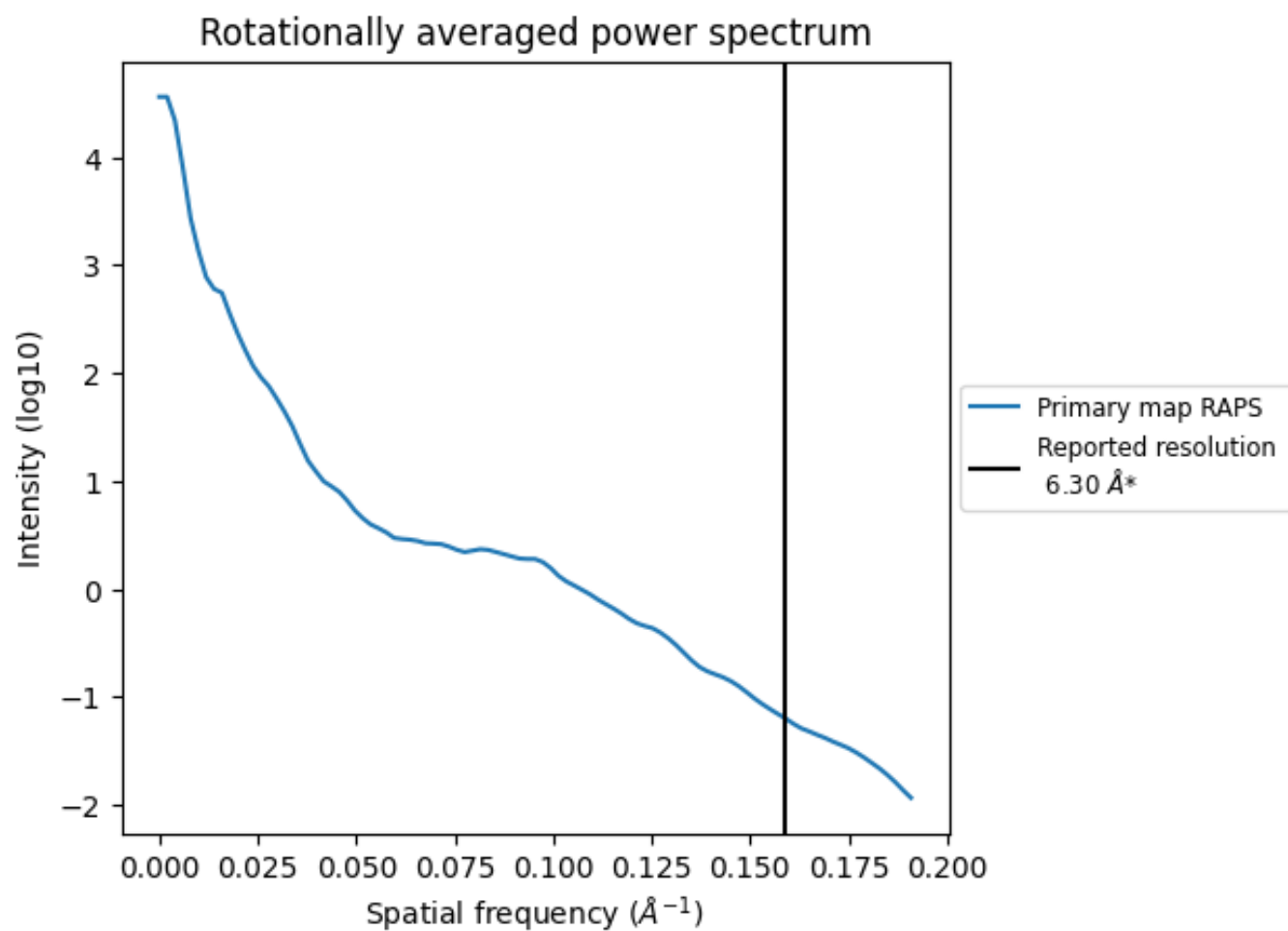
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1495 nm^3 ; this corresponds to an approximate mass of 1350 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 ⓘ

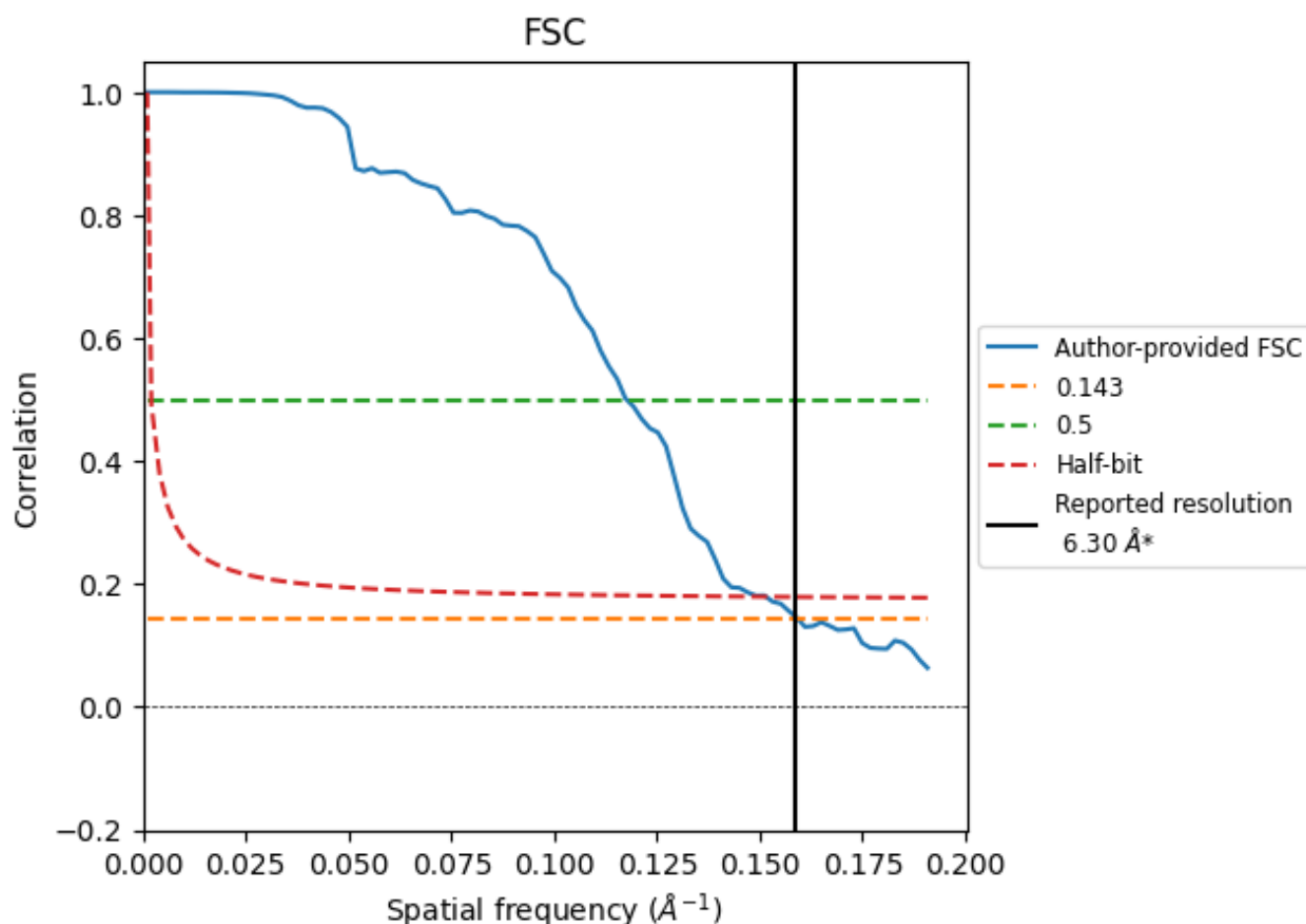


*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

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 0.159 Å⁻¹

8.2 Resolution estimates [i](#)

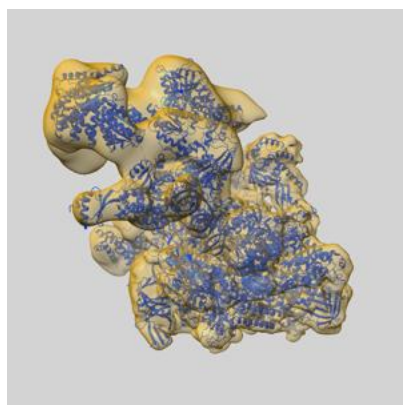
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.28	8.50	6.60
Unmasked-calculated*	-	-	-

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

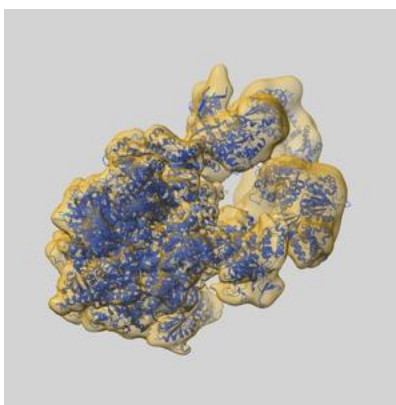
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8134 and PDB model 5IY9. Per-residue inclusion information can be found in section 3 on page 10.

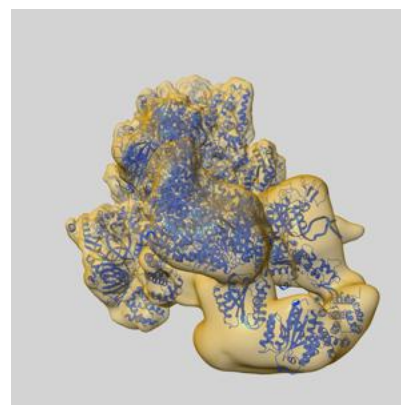
9.1 Map-model overlay [i](#)



X



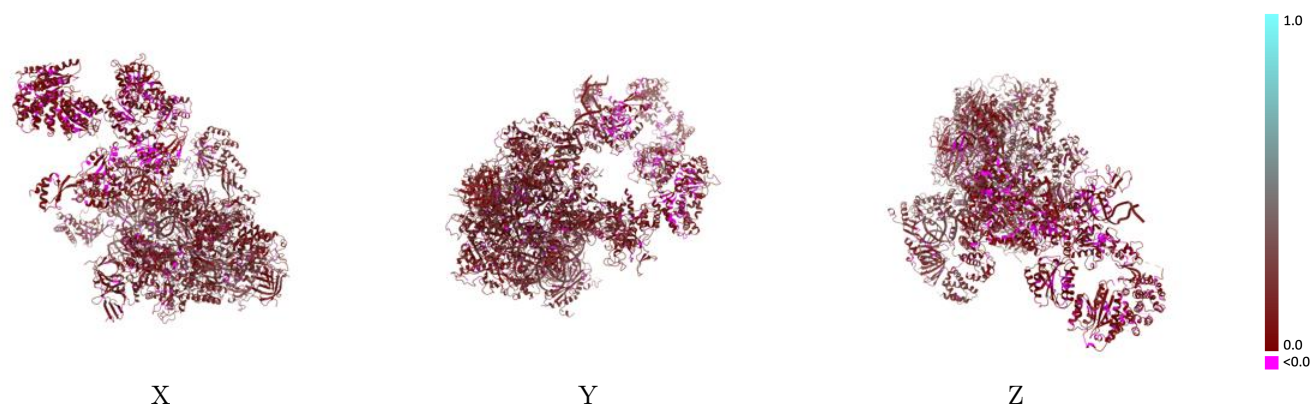
Y



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](#)

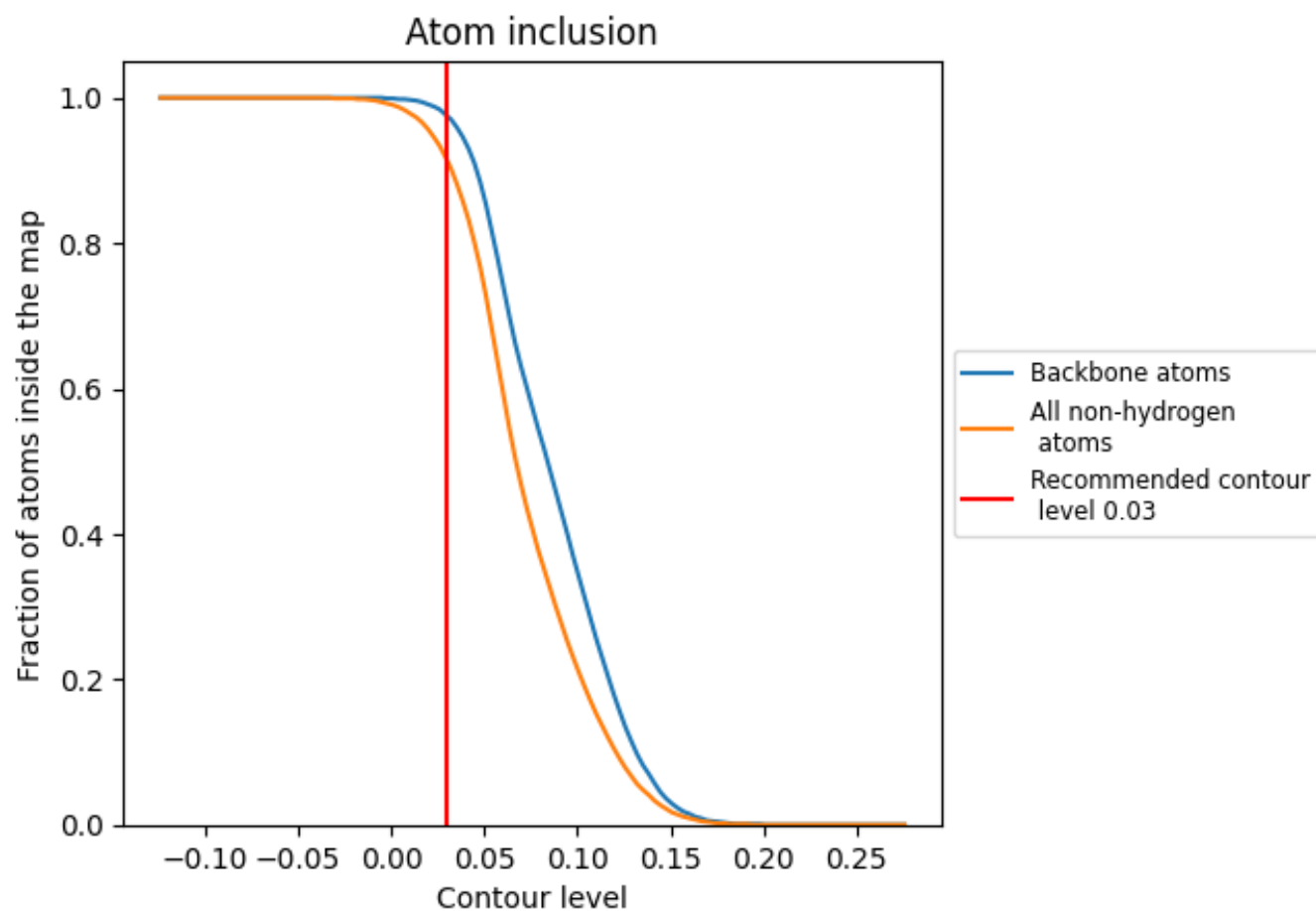


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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	 0.9140	 0.1320
0	 0.9530	 0.0630
1	 0.9530	 0.0690
2	 0.9090	 0.0740
3	 0.9440	 0.0530
A	 0.8890	 0.1560
B	 0.8800	 0.1570
C	 0.9470	 0.1600
D	 0.9500	 0.1400
E	 0.9290	 0.1510
F	 0.8650	 0.1620
G	 0.9560	 0.1330
H	 0.9510	 0.1530
I	 0.9160	 0.1470
J	 0.9330	 0.1560
K	 0.9320	 0.1680
L	 0.9620	 0.1770
M	 0.8790	 0.1520
N	 0.9660	 0.1470
O	 0.9750	 0.1370
P	 0.9660	 0.1480
Q	 0.9300	 0.1300
R	 0.8940	 0.1250
S	 0.9080	 0.1190
T	 0.9250	 0.1440
V	 0.9290	 0.0650
W	 0.9180	 0.0590
X	 0.9010	 0.1710
Y	 0.9650	 0.1910
Z	 0.9360	 0.2190

