



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:08 PM UTC

PDB ID : 4V5Z / pdb_00004v5z
EMDB ID : EMD-1480
Title : Structure of a mammalian 80S ribosome obtained by docking homology models of the RNA and proteins into an 8.7 Å cryo-EM map
Authors : Chandramouli, P.; Akey, C.W.
Deposited on : 2008-03-27
Resolution : 8.70 Å (reported)
Based on initial models : 1J5E, 1IGV, 1I6U, 1G1X, 1K7K, 1RQ6, 1FJG, 1VI6, 2AVY

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:

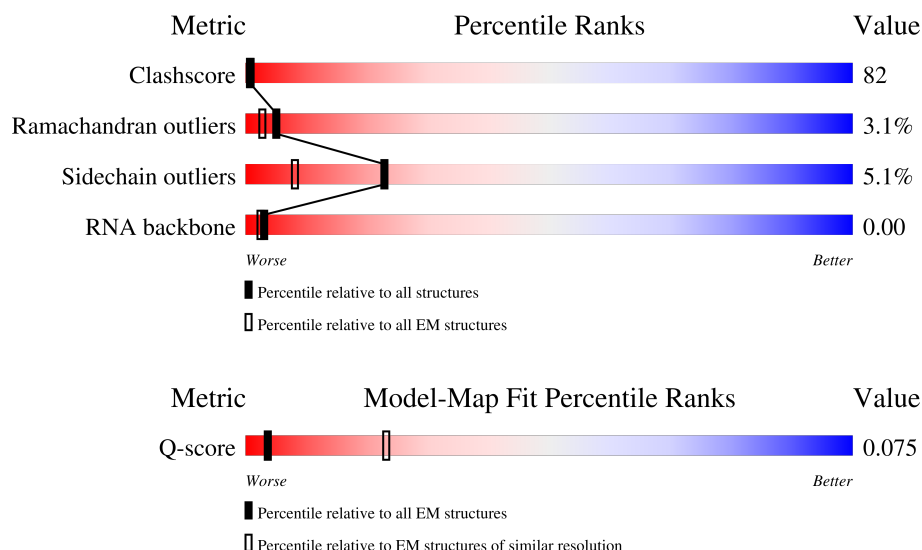
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 8.70 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	282 (8.20 - 9.20)

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	AA	1563	10% 88% 11%
2	AB	35	14% 91% 9%
3	AC	32	6% 91% 9%

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Mol	Chain	Length	Quality of chain
4	AD	42	
5	AE	32	
6	AF	31	
7	AG	14	
8	AH	41	
9	Aa	317	
10	Ab	295	
11	Ac	243	
12	Ad	209	
13	Ae	179	
14	Ag	204	
15	Ah	130	
16	Ai	146	
17	Aj	119	
18	Ak	151	
19	Al	143	
20	Am	152	
21	An	56	
22	Ao	89	
23	Aq	158	
24	As	145	
25	B1	123	
26	B0	2903	
27	BA	21	
28	BB	27	

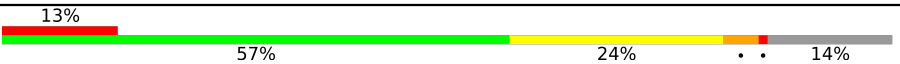
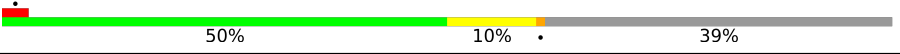
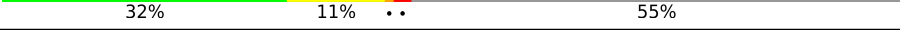
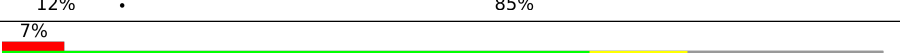
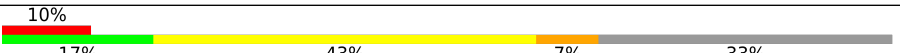
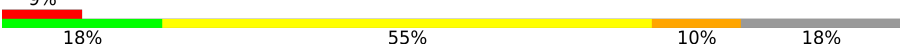
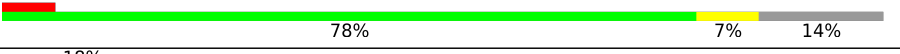
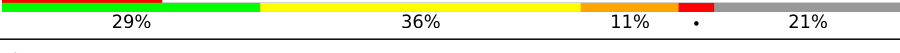
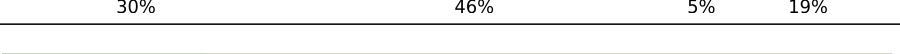
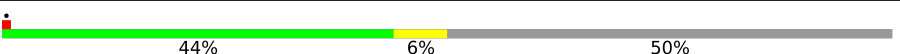
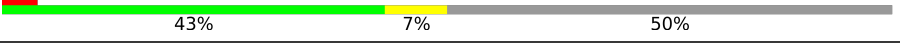
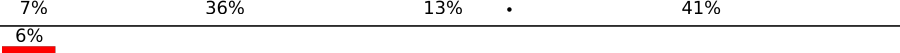
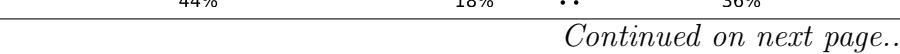
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Mol	Chain	Length	Quality of chain
29	BC	17	12% 100%
30	BD	16	12% 100%
31	BE	54	13% 100%
32	BF	120	8% 100%
33	BG	48	23% 100%
34	BH	25	24% 92% 8%
35	BI	72	10% 100%
36	BJ	30	17% 100%
37	BK	26	46% 96% .
38	BL	20	100%
39	BM	19	16% 89% 11%
40	BN	78	35% 100%
41	BO	20	5% 100%
42	BP	15	27% 100%
43	BQ	30	13% 100%
44	BR	30	17% 100%
45	BS	38	11% 100%
46	BT	30	13% 100%
47	BU	16	12% 100%
48	BV	22	27% 95% 5%
49	BW	16	44% 88% 12%
50	BX	113	10% 100%
51	BY	115	25% 92% 8%
52	BZ	72	14% 99% .
53	Ba	257	10% 83% 11% . 5%

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Mol	Chain	Length	Quality of chain
54	Bb	403	
55	Bc	421	
56	Bd	178	
57	Be	192	
58	Bf	266	
59	Bg	317	
60	Bh	214	
61	Bi	165	
62	Bj	203	
63	Bk	140	
64	Bl	148	
65	Bm	204	
66	Bn	297	
67	Bo	188	
68	Bp	196	
69	B7	13	
70	Bq	160	
71	Br	184	
72	Bs	156	
73	Bt	145	
74	Bu	157	
75	Bv	123	
76	B8	10	
77	Bw	270	
78	Bx	125	

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Mol	Chain	Length	Quality of chain
79	By	135	
80	B9	58	
81	Bz	92	
82	B2	97	
83	B3	51	
84	B4	106	
85	B5	212	
86	B6	115	

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 55531 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 RNA chain called 18S Ribosomal RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	AA	1391	Total	P	0	1391
			1391	1391		

- Molecule 2 is a RNA chain called RNA Expansion segment ES3.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	AB	32	Total	P	0	32
			32	32		

- Molecule 3 is a RNA chain called RNA Expansion segment ES4.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	AC	29	Total	P	0	29
			29	29		

- Molecule 4 is a RNA chain called RNA Expansion segment ES6 part I.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	AD	42	Total	P	0	42
			42	42		

- Molecule 5 is a RNA chain called RNA Expansion segment ES6 part II.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	AE	32	Total	P	0	32
			32	32		

- Molecule 6 is a RNA chain called RNA Expansion segment ES9.

Mol	Chain	Residues	Atoms		AltConf	Trace
6	AF	31	Total	P	0	31
			31	31		

- Molecule 7 is a RNA chain called RNA helix.

Mol	Chain	Residues	Atoms		AltConf	Trace
7	AG	14	Total	P	0	14
			14	14		

- Molecule 8 is a RNA chain called RNA helix.

Mol	Chain	Residues	Atoms		AltConf	Trace
8	AH	41	Total	P	0	41
			41	41		

- Molecule 9 is a protein called 40S Ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Aa	306	Total	C	N	O	S	0	0
			2380	1501	414	453	12		

- Molecule 10 is a protein called 40S Ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ab	192	Total	C	N	O	S	0	0
			1521	972	271	271	7		

- Molecule 11 is a protein called 40S Ribosomal protein S3e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ac	192	Total	C	N	O	S	0	0
			1498	953	274	264	7		

- Molecule 12 is a protein called 40S Ribosomal protein S9e.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Ad	103	Total	C	N	O	0	0
			845	527	172	146		

- Molecule 13 is a protein called 40S Ribosomal protein S2e.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Ae	148	Total	C	N	O	S	0	0
			1096	697	202	191	6		

- Molecule 14 is a protein called 40S Ribosomal protein S5e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Ag	163	Total	C	N	O	S	0	0
			1277	795	241	234	7		

- Molecule 15 is a protein called 40S Ribosomal protein S15ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ah	127	Total	C	N	O	S	0	0
			1016	648	188	174	6		

- Molecule 16 is a protein called 40S Ribosomal protein S16e.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ai	138	Total	C	N	O	S	0	0
			1102	699	209	191	3		

- Molecule 17 is a protein called 40S Ribosomal protein S20e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Aj	97	Total	C	N	O	S	0	0
			772	483	147	138	4		

- Molecule 18 is a protein called 40S Ribosomal protein S14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ak	125	Total	C	N	O	S	0	0
			935	572	181	176	6		

- Molecule 19 is a protein called 40S Ribosomal protein S23e.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Al	115	Total	C	N	O	S	0	0
			871	557	162	150	2		

- Molecule 20 is a protein called 40S Ribosomal protein S18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Am	140	Total	C	N	O	S	0	0
			1150	717	236	196	1		

- Molecule 21 is a protein called 40S Ribosomal protein S29e.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	An	49	Total	C	N	O	S	0	0
			410	258	84	63	5		

- Molecule 22 is a protein called 40S Ribosomal protein S13e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ao	85	Total	C	N	O	S	0	0
			710	445	141	122	2		

- Molecule 23 is a protein called 40S Ribosomal protein S11e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Aq	76	Total	C	N	O	S	0	0
			629	401	121	102	5		

- Molecule 24 is a protein called 40S Ribosomal protein S15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	As	88	Total	C	N	O	S	0	0
			721	459	139	118	5		

- Molecule 25 is a RNA chain called 5.8S Ribosomal RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
25	B1	97	Total	P	0	97
			97	97		

- Molecule 26 is a RNA chain called 28S Ribosomal RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
26	B0	2407	Total	P	0	2407
			2407	2407		

- Molecule 27 is a RNA chain called RNA Expansion segment ES3.

Mol	Chain	Residues	Atoms		AltConf	Trace
27	BA	21	Total	P	0	21
			21	21		

- Molecule 28 is a RNA chain called RNA Expansion segment ES4.

Mol	Chain	Residues	Atoms		AltConf	Trace
28	BB	27	Total	P	0	27
			27	27		

- Molecule 29 is a RNA chain called RNA Expansion segment ES5.

Mol	Chain	Residues	Atoms		AltConf	Trace
29	BC	17	Total	P	0	17
			17	17		

- Molecule 30 is a RNA chain called RNA Expansion segment ES7 part I.

Mol	Chain	Residues	Atoms		AltConf	Trace
30	BD	16	Total	P	0	16
			16	16		

- Molecule 31 is a RNA chain called RNA Expansion segment ES7 part II.

Mol	Chain	Residues	Atoms		AltConf	Trace
31	BE	54	Total	P	0	54
			54	54		

- Molecule 32 is a RNA chain called RNA Expansion segment ES7 part III.

Mol	Chain	Residues	Atoms		AltConf	Trace
32	BF	120	Total	P	0	120
			120	120		

- Molecule 33 is a RNA chain called RNA Expansion segment ES9.

Mol	Chain	Residues	Atoms		AltConf	Trace
33	BG	48	Total	P	0	48
			48	48		

- Molecule 34 is a RNA chain called RNA Expansion segment ES12.

Mol	Chain	Residues	Atoms		AltConf	Trace
34	BH	25	Total	P	0	25
			25	25		

- Molecule 35 is a RNA chain called RNA Expansion segment ES15 part I.

Mol	Chain	Residues	Atoms		AltConf	Trace
35	BI	72	Total	P	0	72
			72	72		

- Molecule 36 is a RNA chain called RNA Expansion segment ES15 part II.

Mol	Chain	Residues	Atoms		AltConf	Trace
36	BJ	30	Total	P	0	30
			30	30		

- Molecule 37 is a RNA chain called RNA Expansion segment ES19.

Mol	Chain	Residues	Atoms		AltConf	Trace
37	BK	25	Total	P	0	25
			25	25		

- Molecule 38 is a RNA chain called RNA Expansion segment ES20.

Mol	Chain	Residues	Atoms		AltConf	Trace
38	BL	20	Total	P	0	20
			20	20		

- Molecule 39 is a RNA chain called RNA Expansion segment ES24.

Mol	Chain	Residues	Atoms		AltConf	Trace
39	BM	19	Total	P	0	19
			19	19		

- Molecule 40 is a RNA chain called RNA Expansion segment ES27.

Mol	Chain	Residues	Atoms		AltConf	Trace
40	BN	78	Total	P	0	78
			78	78		

- Molecule 41 is a RNA chain called RNA Expansion segment ES30.

Mol	Chain	Residues	Atoms		AltConf	Trace
41	BO	20	Total	P	0	20
			20	20		

- Molecule 42 is a RNA chain called RNA Expansion segment ES31 part I.

Mol	Chain	Residues	Atoms		AltConf	Trace
42	BP	15	Total	P	0	15
			15	15		

- Molecule 43 is a RNA chain called RNA Expansion segment ES31 part II.

Mol	Chain	Residues	Atoms		AltConf	Trace
43	BQ	30	Total	P	0	30
			30	30		

- Molecule 44 is a RNA chain called RNA Expansion segment ES39 part I.

Mol	Chain	Residues	Atoms		AltConf	Trace
44	BR	30	Total	P	0	30
			30	30		

- Molecule 45 is a RNA chain called RNA Expansion segment ES39 part II.

Mol	Chain	Residues	Atoms		AltConf	Trace
45	BS	38	Total	P	0	38
			38	38		

- Molecule 46 is a RNA chain called RNA Expansion segment ES39 part III.

Mol	Chain	Residues	Atoms		AltConf	Trace
46	BT	30	Total	P	0	30
			30	30		

- Molecule 47 is a RNA chain called RNA Expansion segment ES41.

Mol	Chain	Residues	Atoms		AltConf	Trace
47	BU	16	Total	P	0	16
			16	16		

- Molecule 48 is a RNA chain called RNA Expansion segment ES9 part2.

Mol	Chain	Residues	Atoms		AltConf	Trace
48	BV	22	Total	P	0	22
			22	22		

- Molecule 49 is a RNA chain called RNA Expansion segment ES10.

Mol	Chain	Residues	Atoms		AltConf	Trace
49	BW	16	Total	P	0	16
			16	16		

- Molecule 50 is a RNA chain called RNA helices.

Mol	Chain	Residues	Atoms		AltConf	Trace
50	BX	113	Total	P	0	113
			113	113		

- Molecule 51 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
51	BY	115	Total	P	0	115
			115	115		

- Molecule 52 is a RNA chain called E site t-RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
52	BZ	72	Total	P	0	72
			72	72		

- Molecule 53 is a protein called 60S Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ba	244	Total	C	N	O	S	0	0
			1867	1172	382	307	6		

- Molecule 54 is a protein called 60S Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bb	345	Total	C	N	O	S	0	0
			2765	1758	521	474	12		

- Molecule 55 is a protein called 60S Ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bc	257	Total	C	N	O	S	0	0
			2035	1282	399	344	10		

- Molecule 56 is a protein called 60S Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bd	165	Total	C	N	O	S	0	0
			1325	837	248	234	6		

- Molecule 57 is a protein called 60S Ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Be	175	Total	C	N	O	S	0	0
			1407	889	264	249	5		

- Molecule 58 is a protein called 60S Ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bf	120	Total	C	N	O	S	0	0
			920	584	172	160	4		

- Molecule 59 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	Bg	48	Total	C	N	O	0	0
			327	206	52	69		

- Molecule 60 is a protein called 60S Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bh	166	Total	C	N	O	S	0	0
			1331	841	260	218	12		

- Molecule 61 is a protein called 60S Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bi	74	Total	C	N	O	S	0	0
			573	355	110	106	2		

- Molecule 62 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bj	136	Total	C	N	O	S	0	0
			1095	707	216	168	4		

- Molecule 63 is a protein called 60S Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bk	124	Total	C	N	O	S	0	0
			927	586	173	163	5		

- Molecule 64 is a protein called 60S Ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bl	122	Total	C	N	O	S	0	0
			951	601	193	154	3		

- Molecule 65 is a protein called 60S Ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Bm	175	Total	C	N	O	S	0	0
			1454	921	298	231	4		

- Molecule 66 is a protein called 60S Ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bn	236	Total	C	N	O	S	0	0
			1912	1209	340	350	13		

- Molecule 67 is a protein called 60S Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bo	120	Total	C	N	O	S	0	0
			956	607	185	160	4		

- Molecule 68 is a protein called 60S Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bp	159	Total	C	N	O	S	0	0
			1329	817	285	220	7		

- Molecule 69 is a protein called 60S Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	B7	13	Total	C	N	O	S	0	0
			129	80	34	14	1		

- Molecule 70 is a protein called 60S Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bq	96	Total	C	N	O	S	0	0
			773	492	155	121	5		

- Molecule 71 is a protein called 60S Ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Br	150	Total	C	N	O	S	0	0
			1217	760	237	211	9		

- Molecule 72 is a protein called 60S Ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bs	78	Total	C	N	O	S	0	0
			622	401	105	115	1		

- Molecule 73 is a protein called 60S Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bt	110	Total	C	N	O	S	0	0
			916	570	188	156	2		

- Molecule 74 is a protein called 60S Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bu	53	Total	C	N	O	S	0	0
			443	284	83	74	2		

- Molecule 75 is a protein called 60S Ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
75	Bv	61	Total	C	N	O	0	0
			477	300	93	84		

- Molecule 76 is a protein called 60S Ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	B8	10	Total	C	N	O	0	0
			78	48	15	15		

- Molecule 77 is a protein called 60S Ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bw	158	Total	C	N	O	S	0	0
			1281	823	240	213	5		

- Molecule 78 is a protein called 60S Ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bx	80	Total	C	N	O	S	0	0
			670	418	139	111	2		

- Molecule 79 is a protein called 60S Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	By	60	Total	C	N	O	S	0	0
			514	324	114	75	1		

- Molecule 80 is a protein called 60S Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	B9	58	Total	C	N	O	S	0	0
			460	290	87	79	4		

- Molecule 81 is a protein called 60S Ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bz	72	Total	C	N	O	S	0	0
			548	345	102	94	7		

- Molecule 82 is a protein called 60S Ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	B2	51	Total	C	N	O	S	0	0
			407	250	87	66	4		

- Molecule 83 is a protein called 60S Ribosomal protein L39e.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	B3	48	Total	C	N	O	S	0	0
			429	272	96	60	1		

- Molecule 84 is a protein called 60S Ribosomal protein L44e.

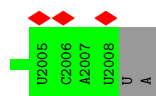
Mol	Chain	Residues	Atoms					AltConf	Trace
84	B4	92	Total	C	N	O	S	0	0
			760	478	154	122	6		

- Molecule 85 is a protein called 60S Ribosomal protein L10a.

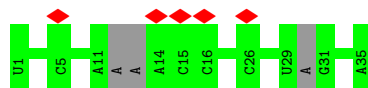
Mol	Chain	Residues	Atoms					AltConf	Trace
85	B5	210	Total	C	N	O	S	0	0
			1621	990	278	347	6		

- Molecule 86 is a protein called 60S Ribosomal protein L30e.

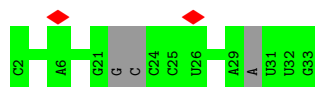
Mol	Chain	Residues	Atoms					AltConf	Trace
86	B6	113	Total	C	N	O	S	0	0
			874	552	154	161	7		



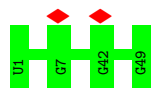
- Molecule 2: RNA Expansion segment ES3



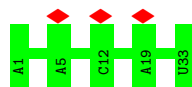
- Molecule 3: RNA Expansion segment ES4



- Molecule 4: RNA Expansion segment ES6 part I



- Molecule 5: RNA Expansion segment ES6 part II



- Molecule 6: RNA Expansion segment ES9

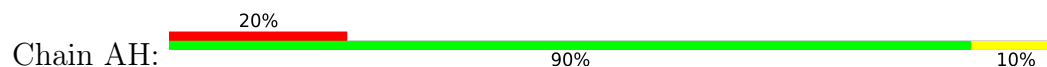


There are no outlier residues recorded for this chain.

- Molecule 7: RNA helix

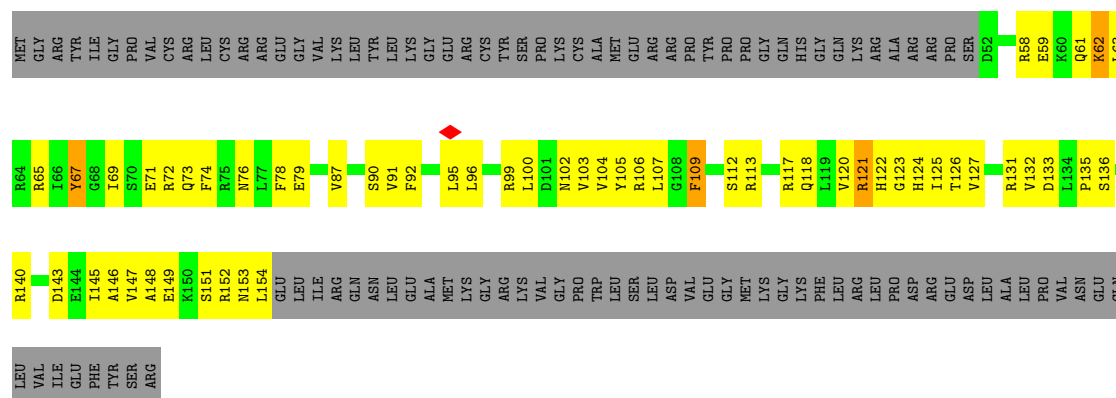


- Molecule 8: RNA helix



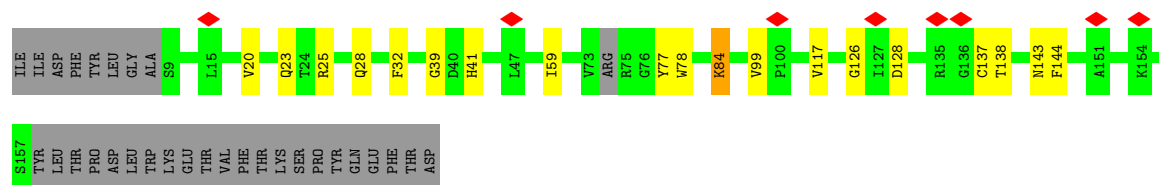
- Molecule 12: 40S Ribosomal protein S9e

Chain Ad:  22% 26% 51%



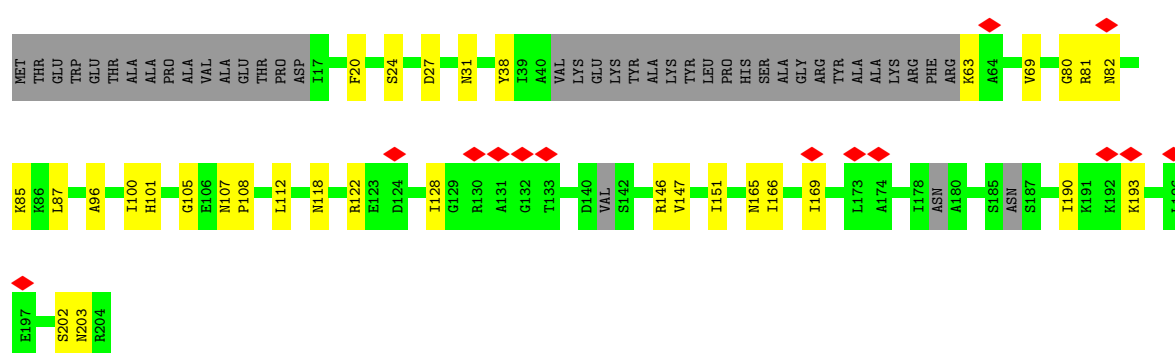
- Molecule 13: 40S Ribosomal protein S2e

Chain Ae:  72% 10% 17%



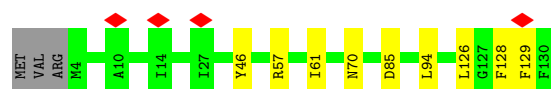
- Molecule 14: 40S Ribosomal protein S5e

Chain Ag:  7% 64% 20%



- Molecule 15: 40S Ribosomal protein S15ae

Chain Ah:  91% 7%



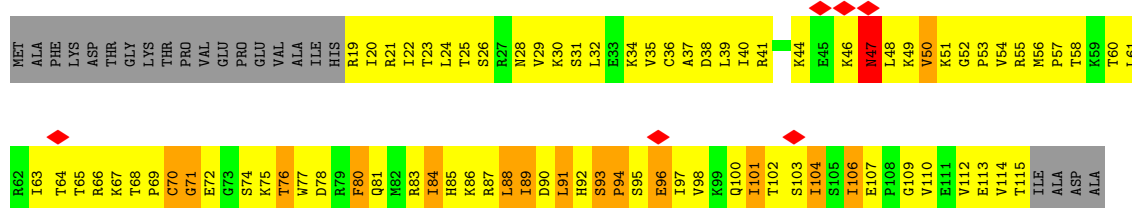
- Molecule 16: 40S Ribosomal protein S16e

Chain Ai:  80% 14% 5%



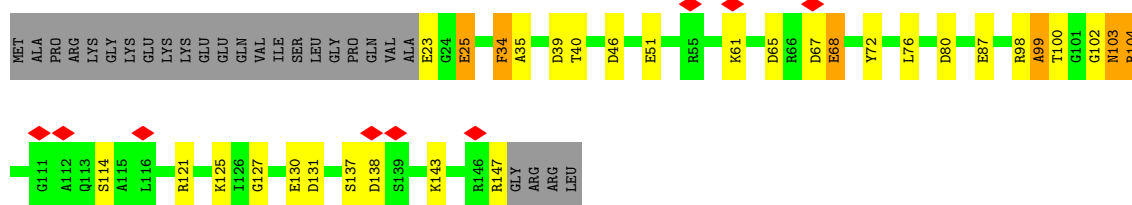
- Molecule 17: 40S Ribosomal protein S20e

Chain Aj:  5% 12% 56% 13% 18%



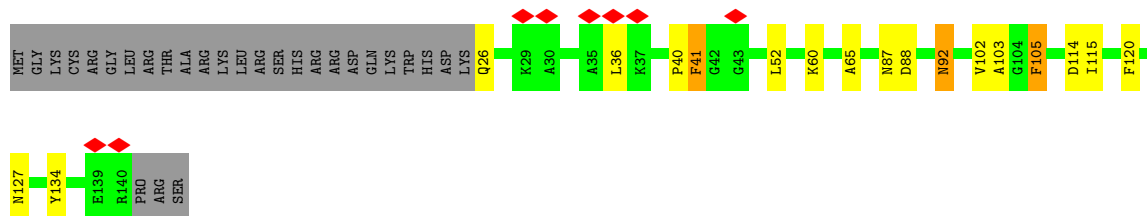
- Molecule 18: 40S Ribosomal protein S14e

Chain Ak:  6% 62% 17% 17%



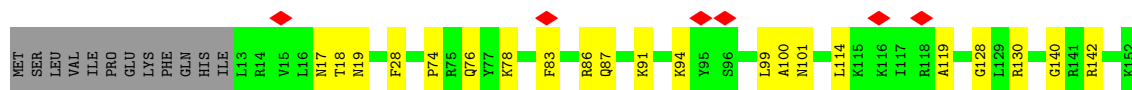
- Molecule 19: 40S Ribosomal protein S23e

Chain Al:  6% 68% 10% 20%

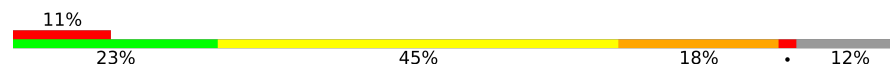


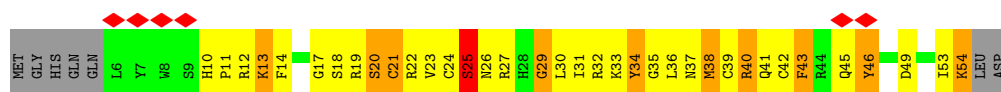
- Molecule 20: 40S Ribosomal protein S18e

Chain Am:  78% 14% 8%

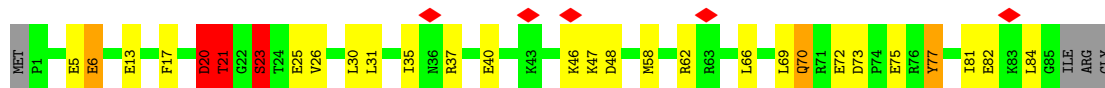


- Molecule 21: 40S Ribosomal protein S29e

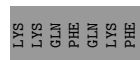
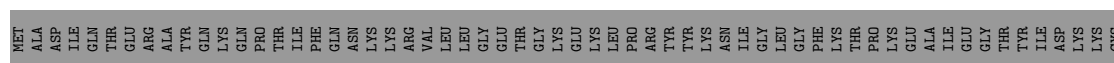
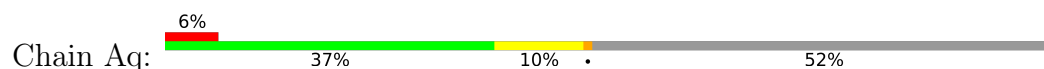
Chain An:  11% 23% 45% 18% 12%



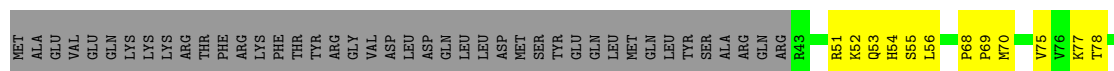
- Molecule 22: 40S Ribosomal protein S13e



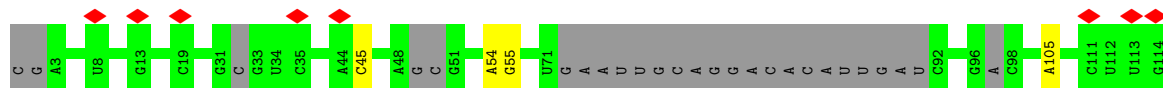
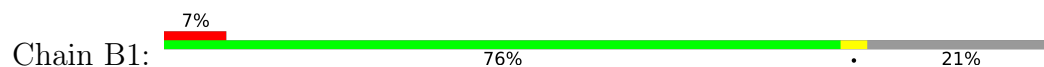
- Molecule 23: 40S Ribosomal protein S11e



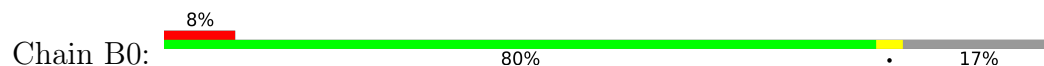
- Molecule 24: 40S Ribosomal protein S15e

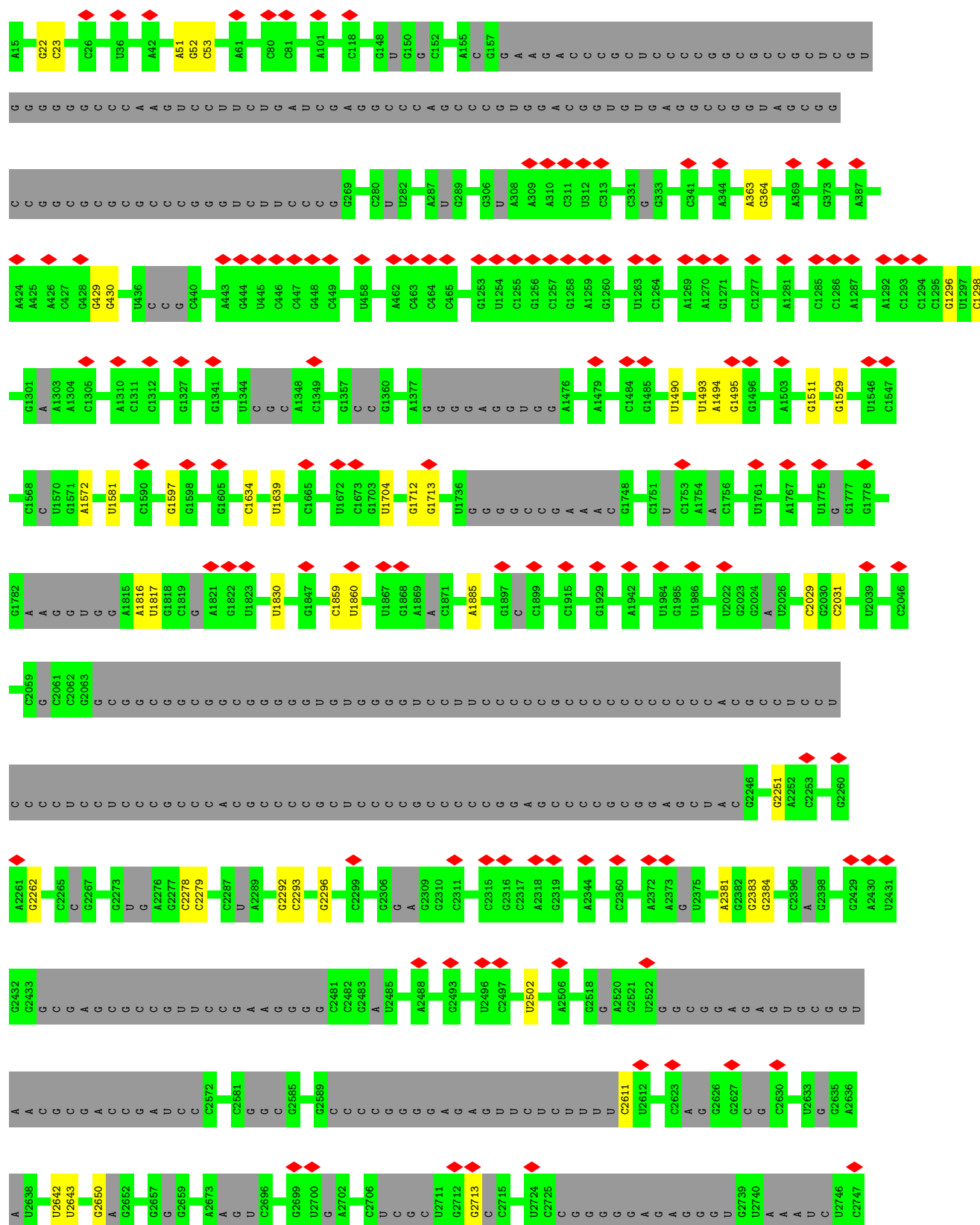


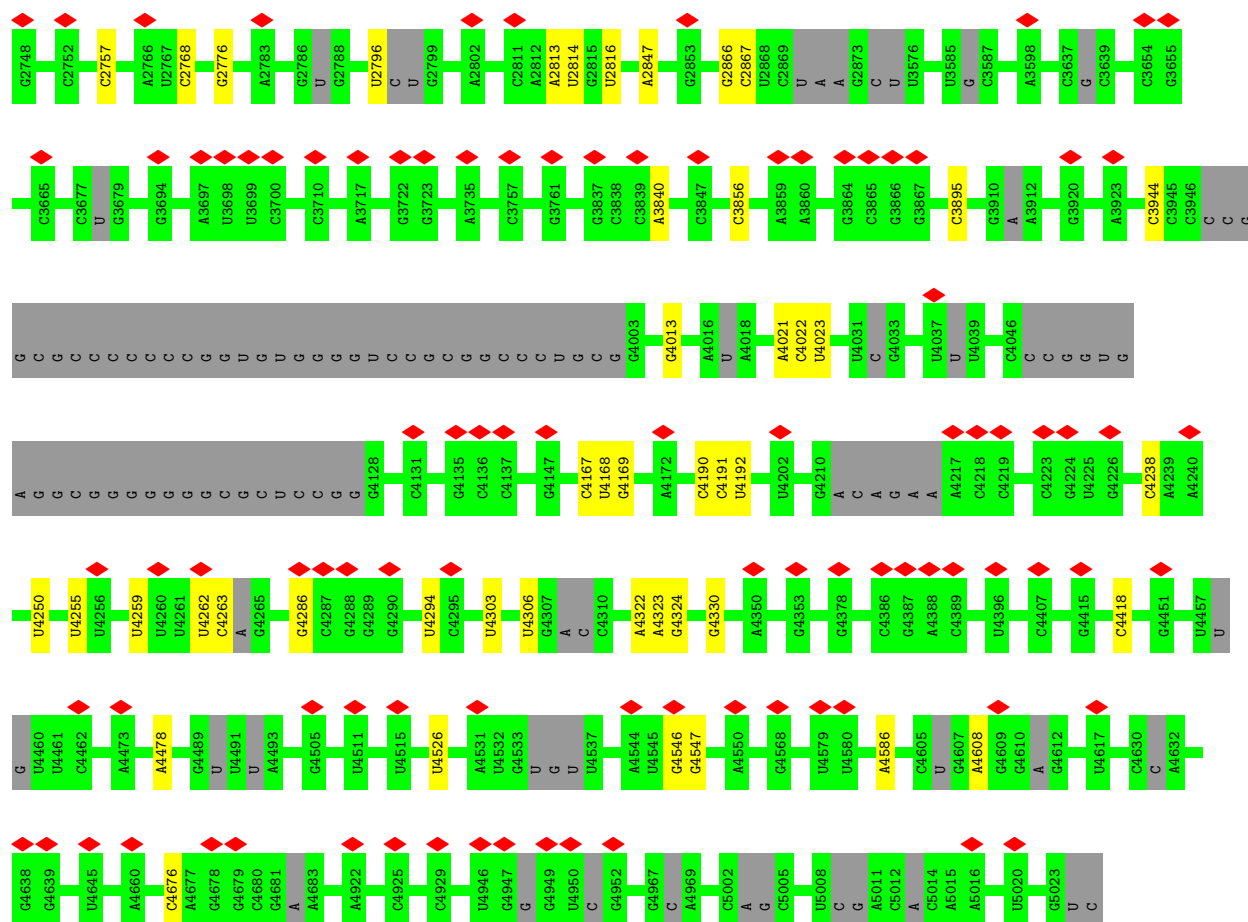
- Molecule 25: 5.8S Ribosomal RNA



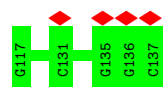
- Molecule 26: 28S Ribosomal RNA







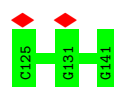
• Molecule 27: RNA Expansion segment ES3



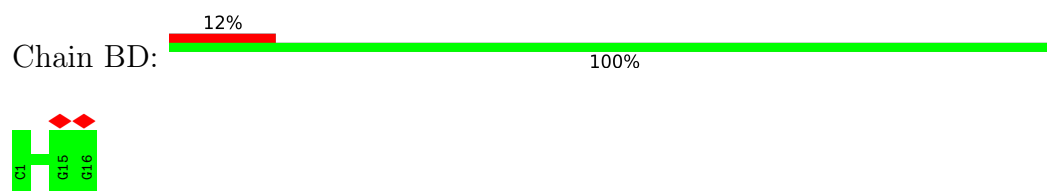
• Molecule 28: RNA Expansion segment ES4



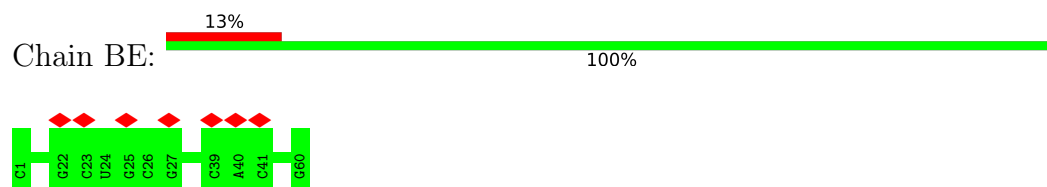
• Molecule 29: RNA Expansion segment ES5



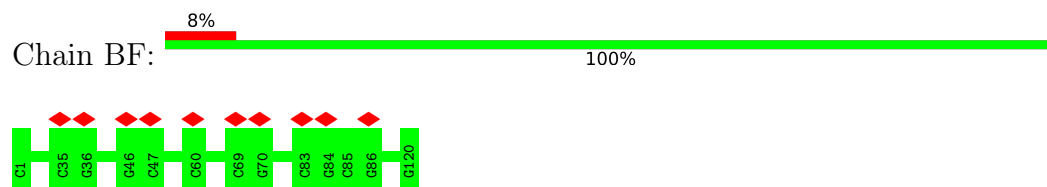
- Molecule 30: RNA Expansion segment ES7 part I



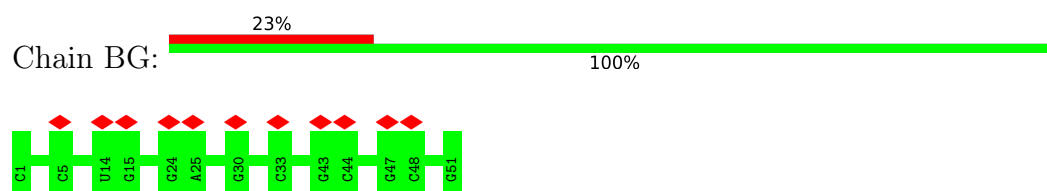
- Molecule 31: RNA Expansion segment ES7 part II



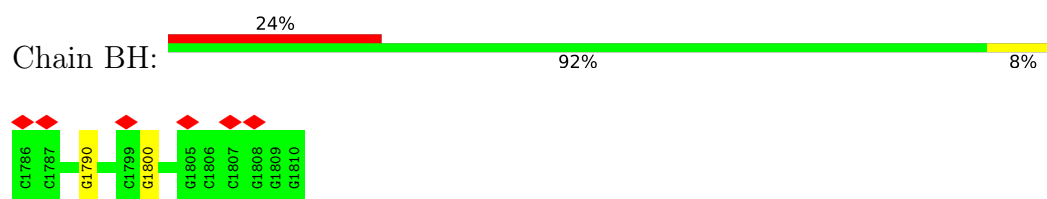
- Molecule 32: RNA Expansion segment ES7 part III



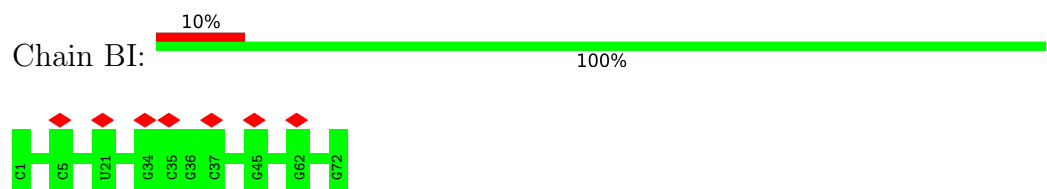
- Molecule 33: RNA Expansion segment ES9



- Molecule 34: RNA Expansion segment ES12

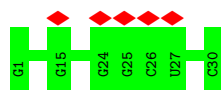


- Molecule 35: RNA Expansion segment ES15 part I

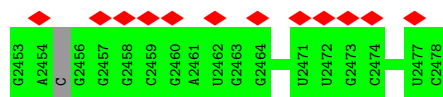


- Molecule 36: RNA Expansion segment ES15 part II





- Molecule 37: RNA Expansion segment ES19

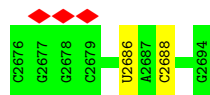


- Molecule 38: RNA Expansion segment ES20

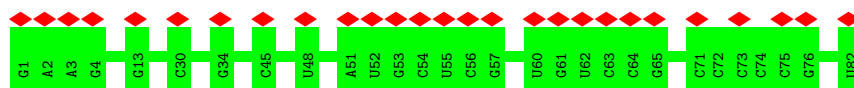


There are no outlier residues recorded for this chain.

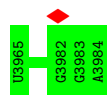
- Molecule 39: RNA Expansion segment ES24



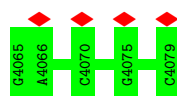
- Molecule 40: RNA Expansion segment ES27



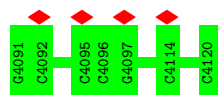
- Molecule 41: RNA Expansion segment ES30



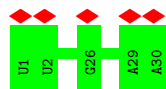
- Molecule 42: RNA Expansion segment ES31 part I



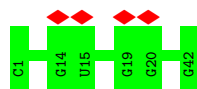
- Molecule 43: RNA Expansion segment ES31 part II



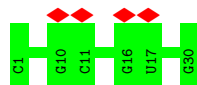
- Molecule 44: RNA Expansion segment ES39 part I



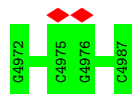
- Molecule 45: RNA Expansion segment ES39 part II



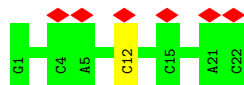
- Molecule 46: RNA Expansion segment ES39 part III



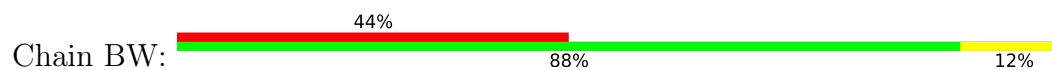
- Molecule 47: RNA Expansion segment ES41

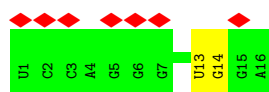


- Molecule 48: RNA Expansion segment ES9 part2

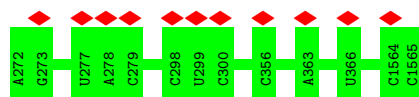


- Molecule 49: RNA Expansion segment ES10

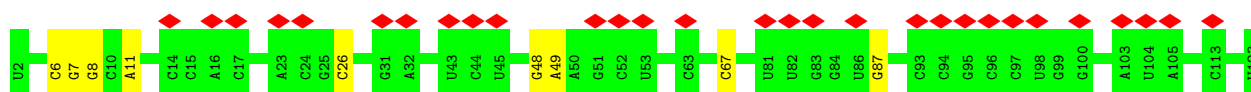




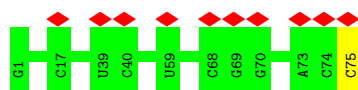
- Molecule 50: RNA helices



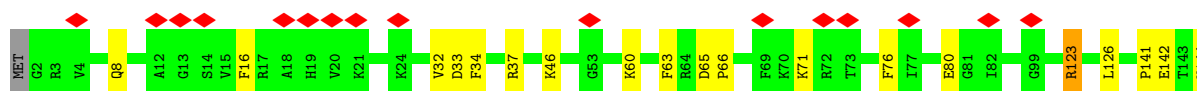
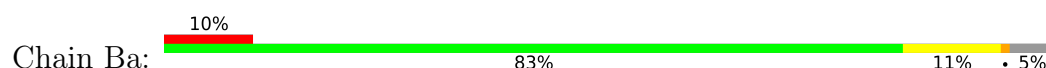
- Molecule 51: 5S Ribosomal RNA



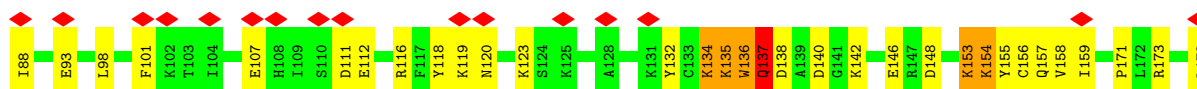
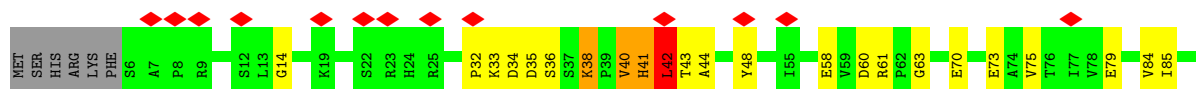
- Molecule 52: E site t-RNA



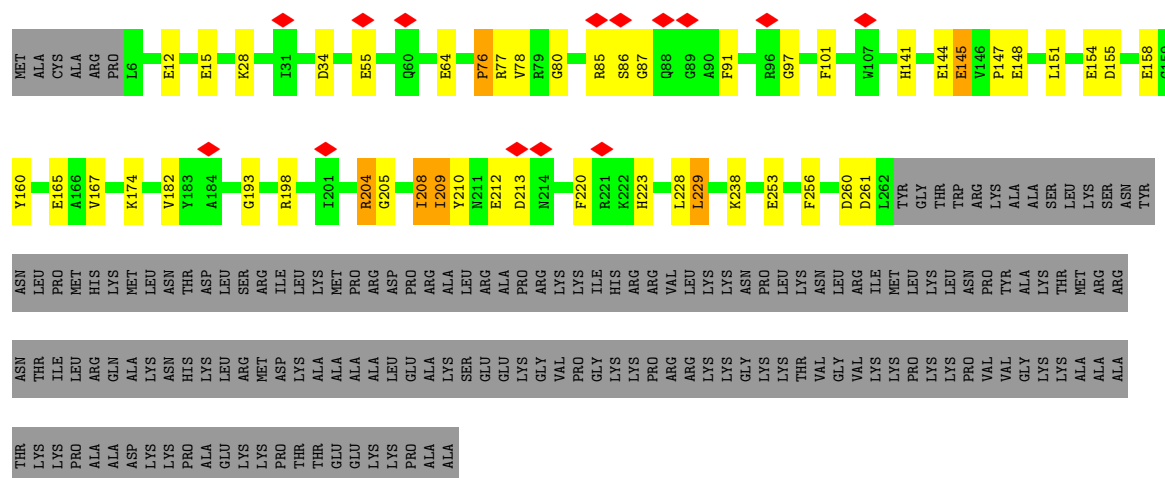
- Molecule 53: 60S Ribosomal protein L8



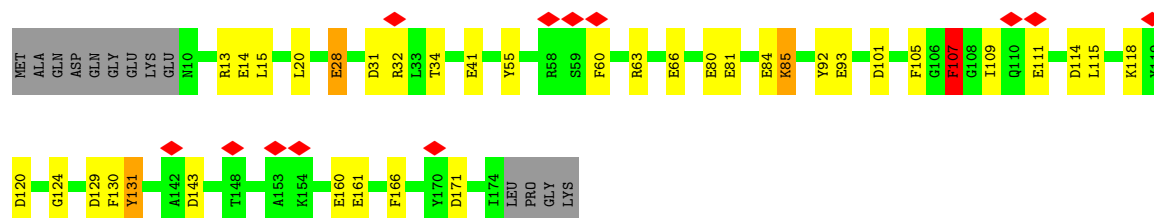
- Molecule 54: 60S Ribosomal protein L3



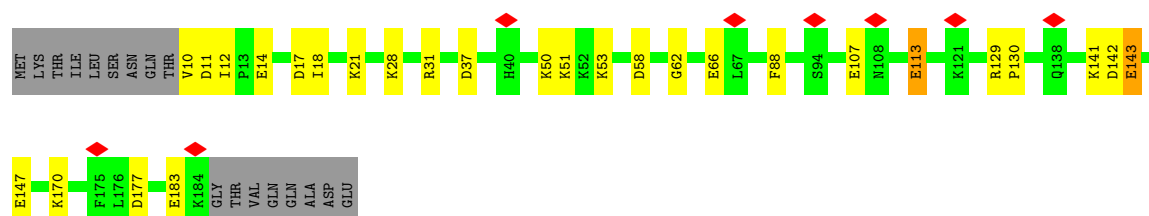
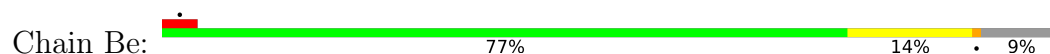
- Molecule 55: 60S Ribosomal protein L4



- Molecule 56: 60S Ribosomal protein L11

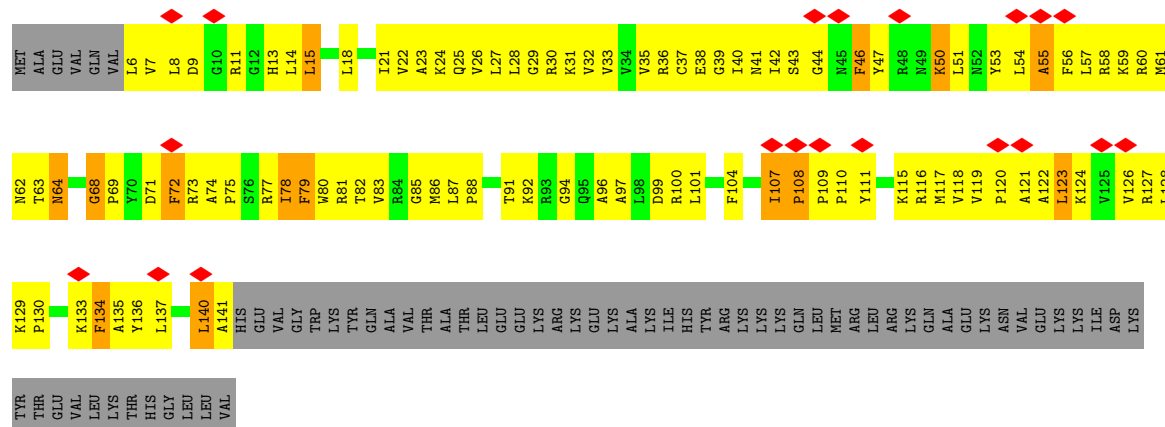
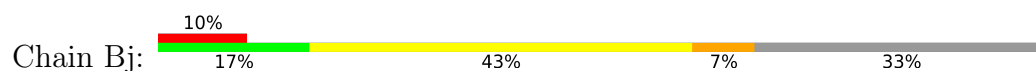


- Molecule 57: 60S Ribosomal protein L9

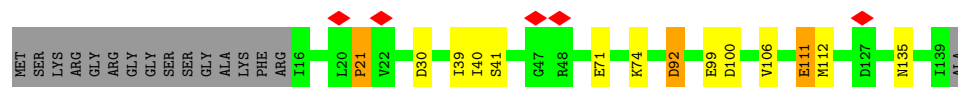
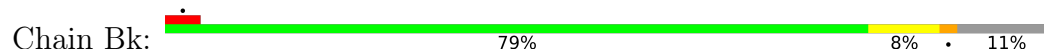




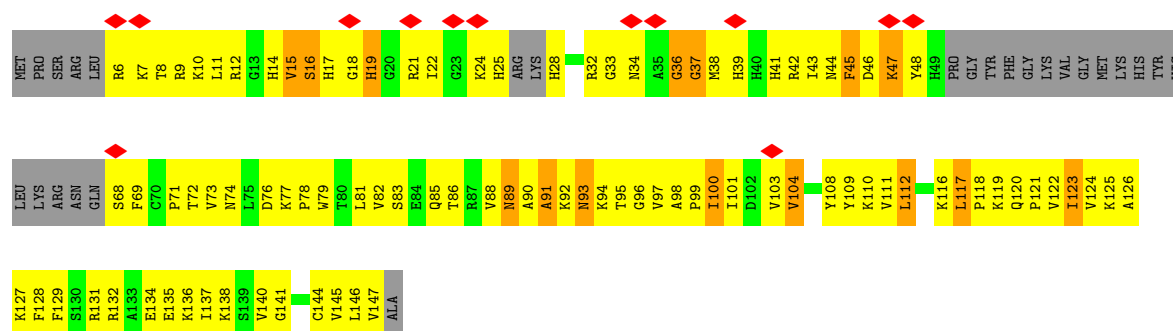
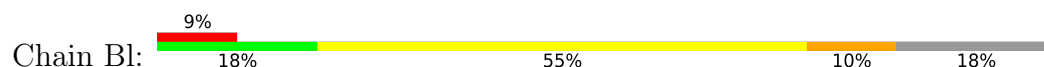
• Molecule 62: 60S ribosomal protein L13a



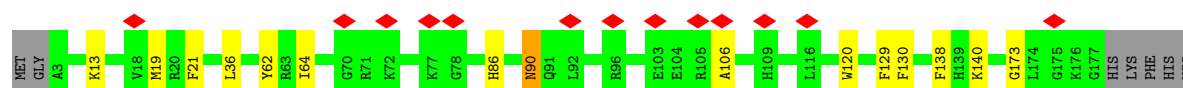
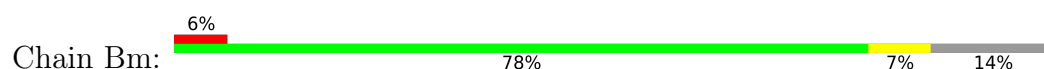
• Molecule 63: 60S Ribosomal protein L23



• Molecule 64: 60S Ribosomal protein L27a

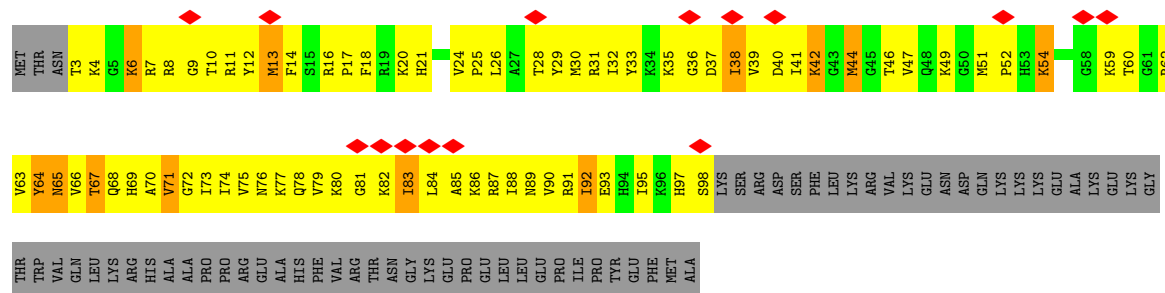


• Molecule 65: 60S Ribosomal protein L15e

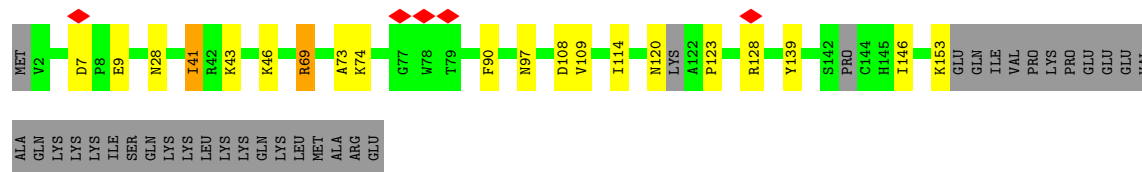


R192
M193
R194
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L196
R197
R198
L199
L200
R201
R202
Y203
R204

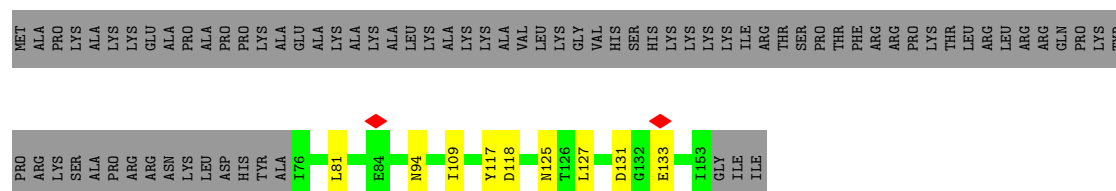
Chain Bq:



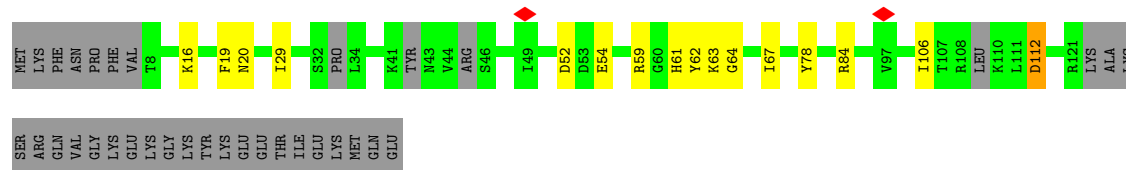
Chain Br:



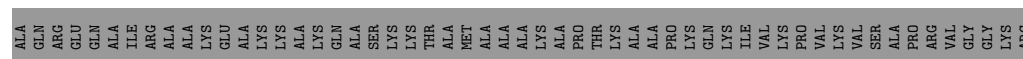
Chain Bs:



Chain Bt: 65% 10% 24%



WORLDWIDE
PDB
PROTEIN DATA BANK

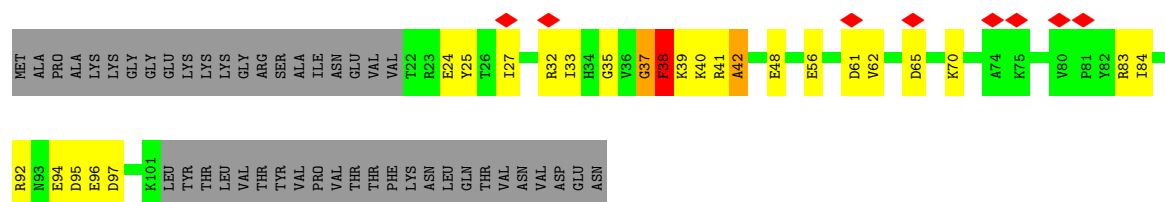


GLU	ASN	LEU	LYS	THR	LYS	LYS	GLN	GLN	ARG	LYS	GLU	ARG	LEU	PRO	PRO	ARG	LYS	ALA	VAL	LYS	ALA	MET	ALA	LYS	I4	R7	R10	G11	K12	K13	G38	A40	A41	S42	K43	L44	I47	G62	T64	GLN	LYS	GLU	ASN	LEU	ARG	LYS	PHE	THR	TYR	LYS	GLY	LYS	TYR	LYS	PRO	LEU	ASP	LEU	ARG	PRO	LYS	THR	ARG	ALA	MET	ARG	ARG	LEU	ASN	HIS
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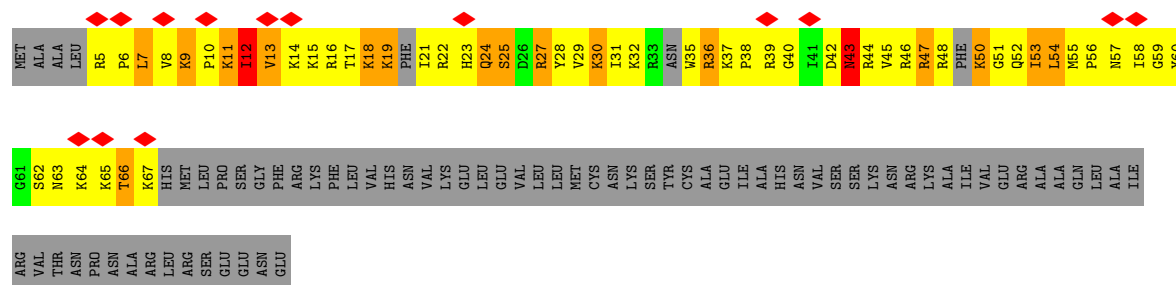
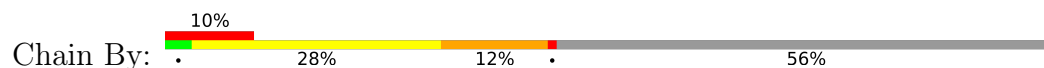
A55 N62 Q63 T64

[illegible]

Chain Bx:



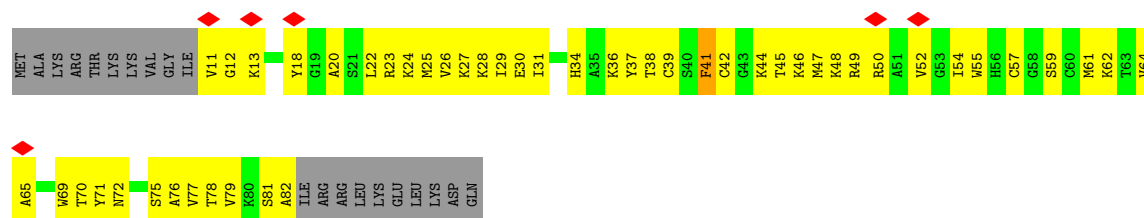
• Molecule 79: 60S Ribosomal protein L32



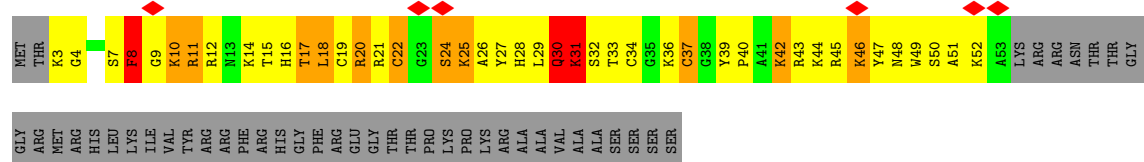
• Molecule 80: 60S Ribosomal protein L32



• Molecule 81: 60S Ribosomal protein L37a



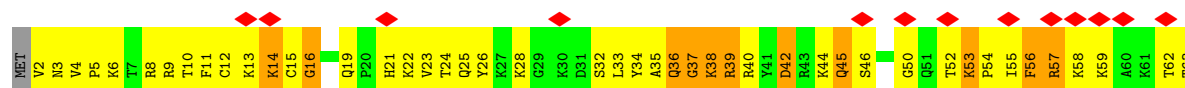
• Molecule 82: 60S Ribosomal protein L37e



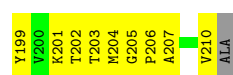
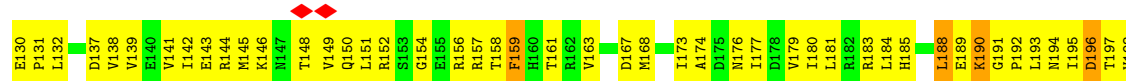
• Molecule 83: 60S Ribosomal protein L39e



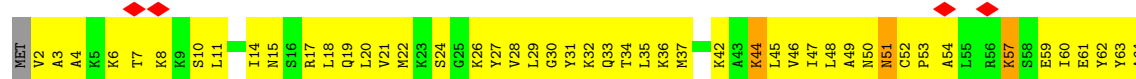
• Molecule 84: 60S Ribosomal protein L44e



• Molecule 85: 60S Ribosomal protein L10a



• Molecule 86: 60S Ribosomal protein L30e



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78800	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF correction using phase flipping and setsf in EMAN to correct the amplitudes	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	4400	Depositor
Magnification	51000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	23.447	Depositor
Minimum map value	-16.531	Depositor
Average map value	0.178	Depositor
Map value standard deviation	1.378	Depositor
Recommended contour level	1	Depositor
Map size (Å)	458.64, 458.64, 458.64	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.73, 2.73, 2.73	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	$\# Z > 5$
9	Aa	1.13	29/2434 (1.2%)	1.74	48/3309 (1.5%)
10	Ab	1.35	0/1556	1.58	17/2115 (0.8%)
11	Ac	0.97	17/1518 (1.1%)	1.29	3/2038 (0.1%)
12	Ad	1.43	0/856	1.44	3/1144 (0.3%)
13	Ae	1.43	0/1115	1.68	16/1505 (1.1%)
14	Ag	1.49	1/1288 (0.1%)	1.77	31/1725 (1.8%)
15	Ah	1.34	0/1033	1.63	5/1382 (0.4%)
16	Ai	1.52	1/1118 (0.1%)	1.72	23/1493 (1.5%)
17	Aj	1.47	0/781	1.76	14/1048 (1.3%)
18	Ak	1.27	17/947 (1.8%)	1.70	13/1271 (1.0%)
19	Al	1.44	0/884	1.65	8/1184 (0.7%)
20	Am	1.51	2/1165 (0.2%)	1.74	17/1555 (1.1%)
21	An	1.55	1/420 (0.2%)	1.88	16/557 (2.9%)
22	Ao	1.32	11/721 (1.5%)	1.71	6/962 (0.6%)
23	Aq	1.53	0/637	1.78	15/849 (1.8%)
24	As	1.46	0/735	1.80	14/980 (1.4%)
53	Ba	1.42	0/1904	1.65	21/2552 (0.8%)
54	Bb	1.29	37/2824 (1.3%)	1.78	42/3786 (1.1%)
55	Bc	1.07	17/2076 (0.8%)	1.51	13/2790 (0.5%)
56	Bd	1.17	22/1347 (1.6%)	1.65	18/1801 (1.0%)
57	Be	1.00	13/1426 (0.9%)	1.40	5/1916 (0.3%)
58	Bf	1.22	12/932 (1.3%)	1.85	17/1256 (1.4%)
59	Bg	1.17	8/332 (2.4%)	1.43	2/454 (0.4%)
60	Bh	1.00	11/1358 (0.8%)	1.58	5/1811 (0.3%)
61	Bi	1.43	0/578	1.62	5/775 (0.6%)
62	Bj	1.47	0/1118	1.66	20/1502 (1.3%)
63	Bk	0.92	6/940 (0.6%)	1.34	3/1264 (0.2%)
64	Bl	1.47	0/972	1.87	29/1299 (2.2%)
65	Bm	1.43	0/1491	1.63	14/1999 (0.7%)
66	Bn	1.31	28/1949 (1.4%)	1.84	50/2615 (1.9%)
67	Bo	1.52	1/965 (0.1%)	1.66	12/1292 (0.9%)
68	Bp	1.42	8/1338 (0.6%)	1.65	12/1766 (0.7%)
69	B7	1.70	0/129	1.44	1/167 (0.6%)
70	Bq	1.47	0/788	1.67	5/1049 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
71	Br	1.44	1/1240 (0.1%)	1.65	15/1660 (0.9%)
72	Bs	1.29	0/630	1.56	8/850 (0.9%)
73	Bt	1.43	0/924	1.68	15/1223 (1.2%)
74	Bu	0.91	2/455 (0.4%)	1.20	0/610
75	Bv	1.42	0/476	1.51	8/632 (1.3%)
76	B8	1.51	0/77	1.43	1/103 (1.0%)
77	Bw	1.49	0/1301	1.88	30/1737 (1.7%)
78	Bx	1.34	14/681 (2.1%)	1.89	9/908 (1.0%)
79	By	1.57	0/519	1.73	11/680 (1.6%)
80	B9	1.43	0/467	1.66	3/626 (0.5%)
81	Bz	1.34	0/558	1.59	4/745 (0.5%)
82	B2	1.57	0/415	2.07	15/547 (2.7%)
83	B3	1.48	0/439	1.56	4/580 (0.7%)
84	B4	1.48	0/773	1.69	14/1022 (1.4%)
85	B5	1.39	1/1638 (0.1%)	1.63	25/2222 (1.1%)
86	B6	1.39	0/885	1.63	7/1186 (0.6%)
All	All	1.34	260/51153 (0.5%)	1.67	692/68542 (1.0%)

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
9	Aa	0	17
11	Ac	0	1
18	Ak	1	5
22	Ao	0	4
23	Aq	0	1
54	Bb	1	19
55	Bc	0	9
56	Bd	0	6
57	Be	0	1
58	Bf	1	6
60	Bh	0	5
63	Bk	1	1
66	Bn	0	9
68	Bp	1	2
74	Bu	0	1
78	Bx	1	6
All	All	6	93

All (260) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Ag	122	ARG	C-N	18.22	1.56	1.33
16	Ai	12	VAL	CA-CB	-14.34	1.40	1.55
66	Bn	198	ILE	N-CA	12.94	1.62	1.46
66	Bn	197	HIS	CA-C	12.85	1.70	1.52
56	Bd	115	LEU	CB-CG	11.62	1.76	1.53
67	Bo	52	MET	C-N	11.44	1.48	1.33
20	Am	99	LEU	CA-C	-9.78	1.42	1.53
56	Bd	115	LEU	CA-CB	8.49	1.68	1.53
66	Bn	197	HIS	C-N	7.77	1.44	1.33
54	Bb	316	LEU	CA-C	7.46	1.56	1.52
9	Aa	17	TRP	CA-C	7.28	1.62	1.53
66	Bn	197	HIS	N-CA	7.24	1.55	1.46
66	Bn	87	VAL	CA-C	7.11	1.61	1.52
66	Bn	198	ILE	CA-CB	7.06	1.64	1.54
66	Bn	196	LYS	CA-C	6.89	1.62	1.52
9	Aa	65	PHE	N-CA	6.79	1.54	1.46
54	Bb	211	GLY	CA-C	6.55	1.58	1.51
56	Bd	131	TYR	N-CA	6.45	1.54	1.46
54	Bb	280	ASN	CA-C	6.37	1.61	1.52
71	Br	109	VAL	CA-CB	-6.35	1.47	1.54
21	An	38	MET	CA-C	-6.31	1.44	1.52
18	Ak	99	ALA	N-CA	6.25	1.54	1.46
66	Bn	81	GLU	CD-OE2	6.21	1.37	1.25
54	Bb	211	GLY	N-CA	6.18	1.52	1.45
66	Bn	87	VAL	N-CA	6.04	1.52	1.46
54	Bb	210	PHE	CA-C	6.04	1.60	1.52
54	Bb	209	VAL	CA-C	6.03	1.58	1.52
9	Aa	283	PRO	CA-C	5.96	1.57	1.52
58	Bf	125	LYS	N-CA	5.93	1.53	1.46
54	Bb	135	LYS	CA-C	5.93	1.60	1.52
58	Bf	125	LYS	CA-C	5.84	1.60	1.52
85	B5	77	ASP	C-N	5.84	1.39	1.33
66	Bn	88	LYS	CA-C	5.76	1.60	1.53
56	Bd	115	LEU	N-CA	5.74	1.53	1.46
55	Bc	55	GLU	CD-OE2	5.73	1.36	1.25
57	Be	11	ASP	CG-OD2	5.66	1.36	1.25
54	Bb	213	ASP	CG-OD2	5.60	1.35	1.25
68	Bp	183	GLU	CD-OE2	5.59	1.35	1.25
9	Aa	282	GLU	CD-OE2	5.58	1.35	1.25
78	Bx	39	LYS	N-CA	5.57	1.52	1.46
18	Ak	34	PHE	CA-C	5.55	1.60	1.52
78	Bx	39	LYS	CA-C	5.51	1.59	1.52
9	Aa	304	ASP	CG-OD2	5.49	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Bb	35	ASP	CG-OD2	5.49	1.35	1.25
56	Bd	143	ASP	CG-OD2	5.47	1.35	1.25
54	Bb	198	GLU	CD-OE2	5.46	1.35	1.25
63	Bk	92	ASP	CG-OD2	5.45	1.35	1.25
54	Bb	34	ASP	CG-OD2	5.45	1.35	1.25
68	Bp	160	GLU	CD-OE2	5.45	1.35	1.25
78	Bx	94	GLU	CD-OE2	5.45	1.35	1.25
60	Bh	55	GLU	CD-OE2	5.44	1.35	1.25
54	Bb	58	GLU	CD-OE2	5.44	1.35	1.25
55	Bc	12	GLU	CD-OE2	5.43	1.35	1.25
22	Ao	5	GLU	CD-OE2	5.43	1.35	1.25
54	Bb	73	GLU	CD-OE2	5.43	1.35	1.25
54	Bb	140	ASP	CG-OD2	5.42	1.35	1.25
56	Bd	114	ASP	CG-OD2	5.42	1.35	1.25
57	Be	58	ASP	CG-OD2	5.41	1.35	1.25
22	Ao	82	GLU	CD-OE2	5.41	1.35	1.25
54	Bb	324	GLU	CD-OE2	5.41	1.35	1.25
54	Bb	112	GLU	CD-OE2	5.41	1.35	1.25
22	Ao	25	GLU	CD-OE2	5.40	1.35	1.25
54	Bb	194	ASP	CG-OD2	5.40	1.35	1.25
54	Bb	201	GLU	CD-OE2	5.39	1.35	1.25
54	Bb	310	ASP	CG-OD2	5.39	1.35	1.25
55	Bc	15	GLU	CD-OE2	5.39	1.35	1.25
54	Bb	60	ASP	CG-OD2	5.39	1.35	1.25
78	Bx	40	LYS	CA-C	5.39	1.59	1.52
18	Ak	138	ASP	CG-OD2	5.38	1.35	1.25
22	Ao	75	GLU	CD-OE2	5.38	1.35	1.25
54	Bb	93	GLU	CD-OE2	5.38	1.35	1.25
57	Be	147	GLU	CD-OE2	5.38	1.35	1.25
58	Bf	198	THR	N-CA	-5.38	1.39	1.46
22	Ao	13	GLU	CD-OE2	5.38	1.35	1.25
59	Bg	308	ASP	CG-OD2	5.37	1.35	1.25
11	Ac	85	GLU	CD-OE2	5.37	1.35	1.25
56	Bd	81	GLU	CD-OE2	5.37	1.35	1.25
54	Bb	148	ASP	CG-OD2	5.36	1.35	1.25
57	Be	183	GLU	CD-OE2	5.36	1.35	1.25
22	Ao	73	ASP	CG-OD2	5.36	1.35	1.25
18	Ak	25	GLU	CD-OE2	5.36	1.35	1.25
55	Bc	260	ASP	CG-OD2	5.36	1.35	1.25
55	Bc	148	GLU	CD-OE2	5.36	1.35	1.25
54	Bb	111	ASP	CG-OD2	5.35	1.35	1.25
78	Bx	56	GLU	CD-OE2	5.35	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Ak	68	GLU	CD-OE2	5.35	1.35	1.25
18	Ak	67	ASP	CG-OD2	5.35	1.35	1.25
54	Bb	79	GLU	CD-OE2	5.35	1.35	1.25
18	Ak	130	GLU	CD-OE2	5.34	1.35	1.25
22	Ao	48	ASP	CG-OD2	5.34	1.35	1.25
55	Bc	158	GLU	CD-OE2	5.34	1.35	1.25
66	Bn	135	ASP	CG-OD2	5.34	1.35	1.25
18	Ak	46	ASP	CG-OD2	5.34	1.35	1.25
54	Bb	305	ASP	CG-OD2	5.34	1.35	1.25
56	Bd	66	GLU	CD-OE2	5.34	1.35	1.25
9	Aa	171	ASP	CG-OD2	5.33	1.35	1.25
55	Bc	34	ASP	CG-OD2	5.33	1.35	1.25
78	Bx	61	ASP	CG-OD2	5.33	1.35	1.25
9	Aa	145	GLU	CD-OE2	5.33	1.35	1.25
11	Ac	28	GLU	CD-OE2	5.33	1.35	1.25
54	Bb	107	GLU	CD-OE2	5.33	1.35	1.25
63	Bk	100	ASP	CG-OD2	5.33	1.35	1.25
68	Bp	148	ASP	CG-OD2	5.32	1.35	1.25
9	Aa	126	ASP	CG-OD2	5.32	1.35	1.25
54	Bb	70	GLU	CD-OE2	5.32	1.35	1.25
68	Bp	174	GLU	CD-OE2	5.32	1.35	1.25
78	Bx	96	GLU	CD-OE2	5.31	1.35	1.25
60	Bh	57	GLU	CD-OE2	5.31	1.35	1.25
22	Ao	40	GLU	CD-OE2	5.31	1.35	1.25
57	Be	113	GLU	CD-OE2	5.31	1.35	1.25
66	Bn	127	ASP	CG-OD2	5.31	1.35	1.25
18	Ak	23	GLU	CD-OE2	5.31	1.35	1.25
54	Bb	191	GLU	CD-OE2	5.31	1.35	1.25
54	Bb	278	GLU	CD-OE2	5.31	1.35	1.25
55	Bc	253	GLU	CD-OE2	5.30	1.35	1.25
56	Bd	80	GLU	CD-OE2	5.30	1.35	1.25
11	Ac	89	GLU	CD-OE2	5.30	1.35	1.25
22	Ao	72	GLU	CD-OE2	5.30	1.35	1.25
58	Bf	105	GLU	CD-OE2	5.30	1.35	1.25
54	Bb	214	GLU	CD-OE2	5.30	1.35	1.25
54	Bb	294	ASP	CG-OD2	5.30	1.35	1.25
18	Ak	35	ALA	CA-C	5.30	1.59	1.52
18	Ak	51	GLU	CD-OE2	5.30	1.35	1.25
66	Bn	146	ASP	CG-OD2	5.30	1.35	1.25
78	Bx	48	GLU	CD-OE2	5.30	1.35	1.25
55	Bc	212	GLU	CD-OE2	5.29	1.35	1.25
59	Bg	299	GLU	CD-OE2	5.29	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	Bp	168	GLU	CD-OE2	5.29	1.35	1.25
54	Bb	328	ASP	CG-OD2	5.29	1.35	1.25
66	Bn	119	GLU	CD-OE2	5.29	1.35	1.25
59	Bg	306	GLU	CD-OE2	5.29	1.35	1.25
60	Bh	62	GLU	CD-OE2	5.29	1.35	1.25
66	Bn	213	GLU	CD-OE2	5.29	1.35	1.25
66	Bn	216	ASP	CG-OD2	5.29	1.35	1.25
68	Bp	175	GLU	CD-OE2	5.29	1.35	1.25
55	Bc	144	GLU	CD-OE2	5.28	1.35	1.25
66	Bn	69	GLU	CD-OE2	5.28	1.35	1.25
78	Bx	95	ASP	CG-OD2	5.28	1.35	1.25
9	Aa	149	GLU	CD-OE2	5.28	1.35	1.25
58	Bf	165	GLU	CD-OE2	5.28	1.35	1.25
63	Bk	30	ASP	CG-OD2	5.28	1.35	1.25
9	Aa	36	ARG	CA-C	5.27	1.59	1.52
18	Ak	87	GLU	CD-OE2	5.27	1.35	1.25
55	Bc	155	ASP	CG-OD2	5.27	1.35	1.25
56	Bd	14	GLU	CD-OE2	5.27	1.35	1.25
63	Bk	99	GLU	CD-OE2	5.27	1.35	1.25
18	Ak	65	ASP	CG-OD2	5.27	1.35	1.25
22	Ao	6	GLU	CD-OE2	5.27	1.35	1.25
54	Bb	307	ASP	CG-OD2	5.26	1.35	1.25
54	Bb	138	ASP	CG-OD2	5.26	1.35	1.25
59	Bg	263	GLU	CD-OE2	5.26	1.35	1.25
55	Bc	213	ASP	CG-OD2	5.25	1.35	1.25
58	Bf	162	ASP	CG-OD2	5.25	1.35	1.25
63	Bk	111	GLU	CD-OE2	5.25	1.35	1.25
78	Bx	24	GLU	CD-OE2	5.25	1.35	1.25
56	Bd	129	ASP	CG-OD2	5.25	1.35	1.25
60	Bh	27	ASP	CG-OD2	5.25	1.35	1.25
60	Bh	65	GLU	CD-OE2	5.25	1.35	1.25
9	Aa	294	ASP	CG-OD2	5.25	1.35	1.25
60	Bh	34	ASP	CG-OD2	5.25	1.35	1.25
9	Aa	84	ASP	CG-OD2	5.25	1.35	1.25
54	Bb	146	GLU	CD-OE2	5.25	1.35	1.25
9	Aa	48	ASP	CG-OD2	5.25	1.35	1.25
9	Aa	223	GLU	CD-OE2	5.25	1.35	1.25
56	Bd	28	GLU	CD-OE2	5.25	1.35	1.25
55	Bc	154	GLU	CD-OE2	5.24	1.35	1.25
22	Ao	20	ASP	CG-OD2	5.24	1.35	1.25
59	Bg	302	GLU	CD-OE2	5.24	1.35	1.25
54	Bb	217	ASP	CG-OD2	5.23	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Aa	37	ASP	CG-OD2	5.22	1.35	1.25
18	Ak	80	ASP	CG-OD2	5.22	1.35	1.25
56	Bd	41	GLU	CD-OE2	5.22	1.35	1.25
74	Bu	4	GLU	CD-OE2	5.22	1.35	1.25
11	Ac	38	GLU	CD-OE2	5.22	1.35	1.25
11	Ac	162	ASP	CG-OD2	5.22	1.35	1.25
9	Aa	116	ASP	CG-OD2	5.21	1.35	1.25
9	Aa	231	ASP	CG-OD2	5.21	1.35	1.25
11	Ac	61	GLU	CD-OE2	5.21	1.35	1.25
60	Bh	44	GLU	CD-OE2	5.21	1.35	1.25
18	Ak	34	PHE	CA-CB	5.21	1.59	1.52
57	Be	177	ASP	CG-OD2	5.21	1.35	1.25
58	Bf	160	ASP	CG-OD2	5.21	1.35	1.25
9	Aa	29	ASP	CG-OD2	5.21	1.35	1.25
56	Bd	111	GLU	CD-OE2	5.21	1.35	1.25
9	Aa	91	ASP	CG-OD2	5.20	1.35	1.25
66	Bn	215	GLU	CD-OE2	5.20	1.35	1.25
9	Aa	269	GLU	CD-OE2	5.20	1.35	1.25
57	Be	143	GLU	CD-OE2	5.20	1.35	1.25
11	Ac	103	GLU	CD-OE2	5.20	1.35	1.25
9	Aa	49	GLU	CD-OE2	5.20	1.35	1.25
57	Be	66	GLU	CD-OE2	5.19	1.35	1.25
66	Bn	28	ASP	CG-OD2	5.19	1.35	1.25
11	Ac	20	GLU	CD-OE2	5.19	1.35	1.25
55	Bc	145	GLU	CD-OE2	5.19	1.35	1.25
59	Bg	305	GLU	CD-OE2	5.19	1.35	1.25
78	Bx	65	ASP	CG-OD2	5.19	1.35	1.25
57	Be	14	GLU	CD-OE2	5.19	1.35	1.25
60	Bh	82	ASP	CG-OD2	5.19	1.35	1.25
58	Bf	220	GLU	CD-OE2	5.18	1.35	1.25
55	Bc	64	GLU	CD-OE2	5.18	1.35	1.25
57	Be	37	ASP	CG-OD2	5.18	1.35	1.25
66	Bn	24	GLU	CD-OE2	5.18	1.35	1.25
18	Ak	39	ASP	CG-OD2	5.18	1.35	1.25
9	Aa	213	ASP	CG-OD2	5.17	1.35	1.25
56	Bd	161	GLU	CD-OE2	5.17	1.35	1.25
58	Bf	210	GLU	CD-OE2	5.17	1.35	1.25
68	Bp	182	GLU	CD-OE2	5.17	1.35	1.25
58	Bf	109	GLU	CD-OE2	5.17	1.35	1.25
54	Bb	136	TRP	N-CA	5.16	1.52	1.46
60	Bh	149	GLU	CD-OE2	5.16	1.35	1.25
9	Aa	220	ASP	CG-OD2	5.16	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Aa	273	GLU	CD-OE2	5.16	1.35	1.25
56	Bd	160	GLU	CD-OE2	5.15	1.35	1.25
59	Bg	271	ASP	CG-OD2	5.15	1.35	1.25
11	Ac	23	GLU	CD-OE2	5.15	1.35	1.25
18	Ak	131	ASP	CG-OD2	5.15	1.35	1.25
56	Bd	93	GLU	CD-OE2	5.15	1.35	1.25
55	Bc	261	ASP	CG-OD2	5.14	1.35	1.25
58	Bf	148	GLU	CD-OE2	5.14	1.35	1.25
66	Bn	115	ASP	CG-OD2	5.14	1.35	1.25
66	Bn	123	GLU	CD-OE2	5.13	1.35	1.25
58	Bf	127	ASP	CG-OD2	5.13	1.35	1.25
57	Be	107	GLU	CD-OE2	5.12	1.35	1.25
56	Bd	101	ASP	CG-OD2	5.12	1.35	1.25
9	Aa	203	ASP	CG-OD2	5.12	1.35	1.25
11	Ac	47	GLU	CD-OE2	5.12	1.35	1.25
60	Bh	108	ASP	CG-OD2	5.12	1.35	1.25
78	Bx	40	LYS	N-CA	5.12	1.52	1.46
57	Be	17	ASP	CG-OD2	5.11	1.35	1.25
63	Bk	71	GLU	CD-OE2	5.11	1.35	1.25
9	Aa	144	ASP	CG-OD2	5.11	1.35	1.25
9	Aa	234	ASP	CG-OD2	5.10	1.35	1.25
57	Be	142	ASP	CG-OD2	5.10	1.35	1.25
11	Ac	68	GLU	CD-OE2	5.10	1.35	1.25
11	Ac	193	ASP	CG-OD2	5.10	1.35	1.25
66	Bn	212	GLU	CD-OE2	5.09	1.35	1.25
66	Bn	233	ASP	CG-OD2	5.09	1.35	1.25
9	Aa	74	ASP	CG-OD2	5.09	1.35	1.25
11	Ac	128	GLU	CD-OE2	5.08	1.35	1.25
60	Bh	43	ASP	CG-OD2	5.08	1.34	1.25
11	Ac	81	GLU	CD-OE2	5.08	1.34	1.25
66	Bn	132	GLU	CD-OE2	5.07	1.34	1.25
56	Bd	84	GLU	CD-OE2	5.07	1.34	1.25
56	Bd	171	ASP	CG-OD2	5.06	1.34	1.25
66	Bn	198	ILE	CA-C	5.06	1.59	1.52
11	Ac	14	ASP	CG-OD2	5.05	1.34	1.25
59	Bg	303	GLU	CD-OE2	5.04	1.34	1.25
78	Bx	38	PHE	CA-C	5.04	1.59	1.52
66	Bn	128	GLU	CD-OE2	5.04	1.34	1.25
68	Bp	157	ASP	CG-OD2	5.04	1.34	1.25
11	Ac	135	GLU	CD-OE2	5.03	1.34	1.25
20	Am	100	ALA	N-CA	-5.03	1.39	1.46
74	Bu	37	GLU	CD-OE2	5.03	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Bc	165	GLU	CD-OE2	5.03	1.34	1.25
9	Aa	18	VAL	N-CA	5.02	1.52	1.46
56	Bd	31	ASP	CG-OD2	5.02	1.34	1.25
56	Bd	120	ASP	CG-OD2	5.02	1.34	1.25
66	Bn	205	ASP	CG-OD2	5.02	1.34	1.25
11	Ac	169	ASP	CG-OD2	5.01	1.34	1.25
78	Bx	97	ASP	CG-OD2	5.01	1.34	1.25

All (692) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Bh	20	ARG	N-CA-C	-24.99	79.39	114.12
54	Bb	211	GLY	CA-C-N	19.31	156.47	121.70
54	Bb	211	GLY	C-N-CA	19.31	156.47	121.70
58	Bf	196	ARG	CA-CB-CG	17.78	149.66	114.10
9	Aa	14	HIS	CA-CB-CG	17.34	131.14	113.80
56	Bd	130	PHE	CA-C-O	-16.89	102.29	120.36
82	B2	17	THR	CA-C-N	-15.34	99.93	122.94
82	B2	17	THR	C-N-CA	-15.34	99.93	122.94
78	Bx	39	LYS	N-CA-C	14.37	126.98	111.03
60	Bh	20	ARG	CA-C-O	14.37	134.71	118.90
78	Bx	38	PHE	CA-CB-CG	13.97	127.77	113.80
78	Bx	38	PHE	CB-CA-C	13.91	138.10	110.42
56	Bd	115	LEU	CD1-CG-CD2	-12.93	82.36	110.80
54	Bb	211	GLY	O-C-N	-12.70	109.18	123.66
9	Aa	84	ASP	CA-CB-CG	-12.67	99.93	112.60
66	Bn	87	VAL	N-CA-C	12.55	127.89	108.44
64	Bl	69	PHE	CA-CB-CG	-11.38	102.42	113.80
58	Bf	197	LYS	CB-CA-C	11.21	132.73	110.42
60	Bh	20	ARG	O-C-N	11.08	135.13	122.27
66	Bn	236	GLU	CA-CB-CG	11.00	136.09	114.10
67	Bo	122	PHE	CA-CB-CG	-10.78	103.02	113.80
9	Aa	64	HIS	N-CA-CB	-10.77	94.08	110.45
14	Ag	107	ASN	CA-CB-CG	-10.74	101.86	112.60
9	Aa	65	PHE	CA-CB-CG	10.27	124.06	113.80
14	Ag	122	ARG	O-C-N	-10.24	108.33	122.46
18	Ak	99	ALA	N-CA-CB	10.22	129.09	112.63
53	Ba	34	PHE	N-CA-C	-10.01	100.37	111.28
68	Bp	90	PRO	N-CA-C	10.01	133.09	112.47
24	As	119	PHE	CA-CB-CG	-9.90	103.90	113.80
66	Bn	237	GLU	CA-CB-CG	9.87	133.85	114.10
9	Aa	63	SER	CA-C-N	9.84	141.99	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Aa	63	SER	C-N-CA	9.84	141.99	121.32
66	Bn	235	MET	CB-CA-C	9.81	123.49	110.94
66	Bn	198	ILE	N-CA-CB	9.80	127.41	111.23
20	Am	99	LEU	CB-CA-C	-9.80	102.16	114.40
19	Al	40	PRO	N-CA-C	-9.69	104.61	114.68
54	Bb	210	PHE	CA-CB-CG	9.63	123.43	113.80
13	Ae	144	PHE	CA-CB-CG	-9.61	104.19	113.80
77	Bw	262	ILE	N-CA-C	-9.60	101.51	110.53
85	B5	159	PHE	CA-CB-CG	-9.49	104.31	113.80
18	Ak	34	PHE	CA-CB-CG	9.44	123.24	113.80
18	Ak	98	ARG	CA-C-N	9.42	137.88	123.47
18	Ak	98	ARG	C-N-CA	9.42	137.88	123.47
62	Bj	72	PHE	CA-CB-CG	-9.37	104.43	113.80
67	Bo	95	PRO	N-CA-C	-9.34	101.33	113.57
77	Bw	156	ARG	N-CA-C	-9.23	100.90	112.72
9	Aa	82	SER	N-CA-C	9.23	120.10	107.73
73	Bt	59	ARG	N-CA-C	9.06	122.45	111.40
9	Aa	305	ASN	CA-CB-CG	-9.05	103.55	112.60
81	Bz	12	GLY	N-CA-C	-8.98	103.79	114.48
22	Ao	21	THR	N-CA-C	8.87	123.52	109.50
16	Ai	60	LYS	N-CA-C	-8.87	101.54	111.82
70	Bq	67	THR	N-CA-C	-8.86	99.10	110.53
17	Aj	94	PRO	N-CA-C	8.81	123.93	111.33
56	Bd	115	LEU	CB-CG-CD1	8.76	136.98	110.70
14	Ag	81	ARG	N-CA-C	-8.74	96.57	109.15
9	Aa	64	HIS	CA-C-N	8.61	137.98	121.54
9	Aa	64	HIS	C-N-CA	8.61	137.98	121.54
56	Bd	115	LEU	N-CA-CB	8.61	125.45	110.39
71	Br	109	VAL	CB-CA-C	-8.61	100.68	111.70
23	Aq	102	PHE	CA-CB-CG	-8.57	105.22	113.80
80	B9	88	LEU	N-CA-C	-8.56	101.95	111.28
14	Ag	203	ASN	CA-CB-CG	-8.56	104.04	112.60
68	Bp	191	GLU	CB-CA-C	8.52	126.28	110.10
66	Bn	198	ILE	CA-CB-CG2	8.51	124.97	110.50
9	Aa	34	ALA	N-CA-C	8.47	122.21	108.41
84	B4	76	ASN	N-CA-C	-8.42	102.95	113.23
71	Br	90	PHE	CA-CB-CG	-8.41	105.39	113.80
71	Br	9	GLU	N-CA-C	-8.38	102.15	111.28
9	Aa	64	HIS	N-CA-C	8.35	121.83	110.55
64	Bl	104	VAL	CB-CA-C	-8.35	100.87	112.14
9	Aa	62	HIS	CA-CB-CG	8.33	122.13	113.80
86	B6	51	ASN	CA-CB-CG	-8.26	104.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	As	98	ASN	CA-C-N	-8.25	109.94	120.34
24	As	98	ASN	C-N-CA	-8.25	109.94	120.34
56	Bd	171	ASP	CA-CB-CG	8.24	120.84	112.60
68	Bp	190	LYS	CA-C-O	-8.21	109.55	119.49
54	Bb	204	VAL	N-CA-C	8.19	115.91	109.19
84	B4	38	LYS	N-CA-C	-8.19	102.44	111.36
9	Aa	283	PRO	CA-C-N	8.12	129.99	119.84
9	Aa	283	PRO	C-N-CA	8.12	129.99	119.84
14	Ag	80	GLY	CA-C-N	-8.11	109.02	121.66
14	Ag	80	GLY	C-N-CA	-8.11	109.02	121.66
73	Bt	29	ILE	CA-C-N	8.05	134.16	120.72
73	Bt	29	ILE	C-N-CA	8.05	134.16	120.72
77	Bw	246	THR	CA-C-N	-8.04	108.14	122.45
77	Bw	246	THR	C-N-CA	-8.04	108.14	122.45
61	Bi	98	ILE	N-CA-C	-8.02	102.44	110.62
21	An	43	PHE	CA-CB-CG	-8.01	105.79	113.80
77	Bw	127	VAL	N-CA-C	-8.01	95.83	108.81
82	B2	18	LEU	CA-C-N	7.97	134.34	120.87
82	B2	18	LEU	C-N-CA	7.97	134.34	120.87
9	Aa	17	TRP	N-CA-C	7.96	122.56	107.75
78	Bx	41	ARG	CB-CG-CD	7.95	129.59	111.30
67	Bo	33	PHE	CA-CB-CG	-7.93	105.86	113.80
54	Bb	212	GLN	N-CA-CB	7.92	123.96	110.50
63	Bk	92	ASP	CA-CB-CG	7.92	120.52	112.60
13	Ae	128	ASP	CA-CB-CG	-7.84	104.76	112.60
53	Ba	210	PRO	CA-C-N	7.82	132.20	120.31
53	Ba	210	PRO	C-N-CA	7.82	132.20	120.31
21	An	21	CYS	N-CA-CB	7.82	121.43	110.17
65	Bm	138	PHE	CA-CB-CG	-7.80	106.00	113.80
53	Ba	16	PHE	CA-CB-CG	-7.77	106.03	113.80
17	Aj	103	SER	CA-C-N	-7.75	113.58	123.19
17	Aj	103	SER	C-N-CA	-7.75	113.58	123.19
13	Ae	32	PHE	CA-CB-CG	-7.75	106.05	113.80
14	Ag	20	PHE	CA-CB-CG	-7.74	106.06	113.80
20	Am	83	PHE	CA-CB-CG	-7.70	106.10	113.80
80	B9	77	PHE	CA-CB-CG	-7.67	106.13	113.80
67	Bo	51	PHE	CA-CB-CG	-7.63	106.17	113.80
54	Bb	210	PHE	N-CA-C	7.61	120.31	108.96
56	Bd	115	LEU	CA-CB-CG	7.59	142.88	116.30
56	Bd	131	TYR	N-CA-C	7.58	121.17	108.20
66	Bn	199	MET	CA-CB-CG	7.58	129.26	114.10
9	Aa	16	GLY	CA-C-N	7.57	133.37	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Aa	16	GLY	C-N-CA	7.57	133.37	122.85
64	Bl	34	ASN	CA-CB-CG	-7.56	105.04	112.60
13	Ae	99	VAL	CB-CA-C	-7.55	102.10	110.78
13	Ae	137	CYS	CA-C-N	-7.53	112.38	122.99
13	Ae	137	CYS	C-N-CA	-7.53	112.38	122.99
82	B2	31	LYS	N-CA-C	-7.53	101.15	110.41
20	Am	140	GLY	N-CA-C	-7.51	104.39	115.72
59	Bg	295	PRO	N-CA-CB	7.48	111.31	103.15
66	Bn	198	ILE	N-CA-C	7.47	124.88	109.34
16	Ai	17	LYS	CA-C-N	-7.43	112.83	122.79
16	Ai	17	LYS	C-N-CA	-7.43	112.83	122.79
65	Bm	106	ALA	CB-CA-C	-7.43	99.22	110.88
81	Bz	41	PHE	CA-CB-CG	-7.39	106.41	113.80
16	Ai	112	LEU	N-CA-C	-7.39	103.30	111.36
9	Aa	66	VAL	CB-CA-C	7.39	120.17	110.12
77	Bw	217	TYR	N-CA-C	-7.38	97.79	109.23
54	Bb	210	PHE	CA-C-N	7.37	134.68	121.05
54	Bb	210	PHE	C-N-CA	7.37	134.68	121.05
83	B3	7	PHE	CA-CB-CG	-7.33	106.47	113.80
24	As	68	PRO	N-CA-C	-7.30	101.79	110.70
64	Bl	91	ALA	N-CA-C	-7.29	95.28	110.80
78	Bx	38	PHE	O-C-N	-7.29	112.90	122.59
21	An	40	ARG	N-CA-C	-7.28	103.33	111.71
66	Bn	79	ALA	CA-C-N	7.27	130.02	120.28
66	Bn	79	ALA	C-N-CA	7.27	130.02	120.28
18	Ak	35	ALA	N-CA-C	7.27	121.64	107.98
77	Bw	154	MET	N-CA-C	-7.25	101.49	110.41
19	Al	120	PHE	CA-CB-CG	-7.25	106.55	113.80
15	Ah	128	PHE	CA-CB-CG	-7.24	106.56	113.80
85	B5	103	PHE	CA-CB-CG	-7.21	106.59	113.80
64	Bl	91	ALA	CA-C-N	-7.19	111.16	120.65
64	Bl	91	ALA	C-N-CA	-7.19	111.16	120.65
66	Bn	76	ALA	CA-C-N	7.18	133.11	122.99
66	Bn	76	ALA	C-N-CA	7.18	133.11	122.99
58	Bf	197	LYS	N-CA-CB	7.14	122.55	110.49
65	Bm	90	ASN	CA-C-N	7.13	132.02	120.60
65	Bm	90	ASN	C-N-CA	7.13	132.02	120.60
19	Al	41	PHE	CA-CB-CG	-7.13	106.67	113.80
72	Bs	131	ASP	CA-CB-CG	-7.12	105.48	112.60
65	Bm	86	HIS	CB-CA-C	-7.12	101.92	113.37
81	Bz	13	LYS	N-CA-C	-7.11	103.57	111.82
73	Bt	78	TYR	CA-CB-CG	-7.09	101.14	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	B5	21	PHE	CA-CB-CG	-7.09	106.71	113.80
64	Bl	44	ASN	CA-CB-CG	-7.09	105.51	112.60
20	Am	99	LEU	CA-C-N	-7.07	110.85	120.82
20	Am	99	LEU	C-N-CA	-7.07	110.85	120.82
85	B5	167	ASP	CA-CB-CG	-7.05	105.55	112.60
77	Bw	160	PRO	CA-C-N	-7.03	111.65	122.05
77	Bw	160	PRO	C-N-CA	-7.03	111.65	122.05
9	Aa	56	GLN	OE1-CD-NE2	-7.03	115.57	122.60
77	Bw	227	ASN	CA-CB-CG	-7.03	105.57	112.60
68	Bp	76	MET	N-CA-C	-7.02	103.71	111.36
56	Bd	130	PHE	CA-C-N	7.00	131.94	122.84
56	Bd	130	PHE	C-N-CA	7.00	131.94	122.84
62	Bj	46	PHE	CA-CB-CG	-7.00	106.81	113.80
21	An	20	SER	CA-C-N	-6.98	109.99	120.94
21	An	20	SER	C-N-CA	-6.98	109.99	120.94
66	Bn	81	GLU	CB-CA-C	6.97	124.89	110.31
71	Br	69	ARG	CA-C-N	-6.96	113.16	122.42
71	Br	69	ARG	C-N-CA	-6.96	113.16	122.42
20	Am	99	LEU	N-CA-C	-6.95	99.49	109.29
14	Ag	108	PRO	CB-CA-C	-6.92	101.51	113.20
9	Aa	17	TRP	CA-C-N	6.92	134.42	121.97
9	Aa	17	TRP	C-N-CA	6.92	134.42	121.97
62	Bj	104	PHE	CA-CB-CG	-6.90	106.90	113.80
54	Bb	280	ASN	CA-CB-CG	6.89	119.49	112.60
73	Bt	64	GLY	N-CA-C	-6.89	106.49	114.69
86	B6	97	ILE	CB-CA-C	-6.85	103.77	111.45
62	Bj	108	PRO	N-CA-C	-6.85	102.34	110.70
66	Bn	237	GLU	CB-CG-CD	6.85	124.24	112.60
9	Aa	64	HIS	CA-C-O	-6.84	113.73	121.81
65	Bm	173	GLY	N-CA-C	-6.82	105.82	115.43
58	Bf	204	PHE	CB-CA-C	6.79	120.44	110.26
22	Ao	23	SER	N-CA-C	6.78	119.83	110.35
54	Bb	253	ILE	CA-C-N	6.77	130.18	120.56
54	Bb	253	ILE	C-N-CA	6.77	130.18	120.56
56	Bd	85	LYS	CA-C-N	6.75	127.30	119.94
56	Bd	85	LYS	C-N-CA	6.75	127.30	119.94
14	Ag	112	LEU	CB-CA-C	-6.74	100.29	110.88
77	Bw	176	ILE	CA-C-N	6.74	129.31	120.28
77	Bw	176	ILE	C-N-CA	6.74	129.31	120.28
9	Aa	65	PHE	N-CA-CB	6.73	121.87	110.49
65	Bm	62	TYR	CA-CB-CG	-6.70	101.84	113.90
84	B4	73	VAL	N-CA-C	6.70	116.83	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	Bm	120	TRP	CA-C-N	6.68	131.14	121.52
65	Bm	120	TRP	C-N-CA	6.68	131.14	121.52
16	Ai	115	TYR	CA-C-N	6.67	135.27	121.94
16	Ai	115	TYR	C-N-CA	6.67	135.27	121.94
58	Bf	196	ARG	CB-CG-CD	6.66	126.62	111.30
10	Ab	72	ASP	CA-CB-CG	-6.65	105.95	112.60
71	Br	114	ILE	CB-CA-C	-6.65	105.10	112.68
10	Ab	30	ASP	CA-CB-CG	-6.64	105.96	112.60
16	Ai	104	SER	N-CA-C	-6.62	99.01	109.07
66	Bn	91	LEU	N-CA-CB	-6.61	100.14	110.44
75	Bv	11	GLY	N-CA-C	-6.59	107.23	115.08
66	Bn	197	HIS	CB-CA-C	6.59	123.53	110.42
24	As	102	PHE	CA-CB-CG	-6.59	107.21	113.80
66	Bn	203	VAL	N-CA-C	6.58	117.33	110.62
56	Bd	107	PHE	CA-CB-CG	6.58	120.38	113.80
9	Aa	18	VAL	CA-CB-CG2	6.57	121.57	110.40
85	B5	126	GLY	N-CA-C	-6.56	106.18	115.43
86	B6	68	LYS	N-CA-C	-6.56	104.58	112.58
53	Ba	76	PHE	CA-CB-CG	-6.54	107.26	113.80
54	Bb	281	LYS	CB-CA-C	-6.52	100.28	111.23
17	Aj	94	PRO	CA-C-N	6.50	129.88	120.38
17	Aj	94	PRO	C-N-CA	6.50	129.88	120.38
54	Bb	218	VAL	CB-CA-C	-6.50	102.10	111.34
66	Bn	88	LYS	N-CA-C	6.50	121.23	108.18
86	B6	99	PRO	N-CA-C	6.49	121.38	111.19
77	Bw	129	LYS	N-CA-C	-6.49	104.29	111.36
14	Ag	101	HIS	CB-CA-C	-6.48	100.70	110.88
54	Bb	213	ASP	N-CA-C	6.46	124.57	110.80
62	Bj	79	PHE	CA-CB-CG	-6.46	107.34	113.80
18	Ak	103	ASN	CA-CB-CG	6.46	119.06	112.60
9	Aa	35	SER	N-CA-C	6.46	119.22	109.41
20	Am	100	ALA	N-CA-C	-6.46	100.48	110.10
64	Bl	19	HIS	N-CA-C	-6.45	104.16	111.07
72	Bs	118	ASP	CA-CB-CG	-6.45	106.15	112.60
10	Ab	129	ASP	CA-CB-CG	-6.44	106.16	112.60
10	Ab	31	PHE	CA-CB-CG	-6.44	107.36	113.80
54	Bb	279	ILE	CB-CA-C	6.43	122.13	111.51
64	Bl	119	LYS	N-CA-C	-6.42	104.33	111.71
62	Bj	107	ILE	CA-C-N	-6.40	113.78	120.38
62	Bj	107	ILE	C-N-CA	-6.40	113.78	120.38
16	Ai	64	ALA	N-CA-C	-6.40	104.35	111.71
13	Ae	84	LYS	CA-C-N	6.39	127.83	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Ae	84	LYS	C-N-CA	6.39	127.83	119.84
20	Am	19	ASN	CA-CB-CG	-6.39	106.21	112.60
23	Aq	113	LEU	N-CA-C	-6.39	104.32	111.28
67	Bo	31	TYR	CB-CA-C	-6.38	100.20	110.79
66	Bn	196	LYS	CB-CA-C	6.38	119.82	110.26
66	Bn	197	HIS	N-CA-C	6.37	124.37	110.80
21	An	35	GLY	N-CA-C	-6.37	106.53	115.32
21	An	38	MET	N-CA-C	-6.37	104.34	111.28
24	As	118	GLU	CA-C-N	6.37	132.87	121.66
24	As	118	GLU	C-N-CA	6.37	132.87	121.66
23	Aq	137	THR	CA-C-N	-6.35	115.30	122.48
23	Aq	137	THR	C-N-CA	-6.35	115.30	122.48
86	B6	111	GLN	CA-C-N	-6.34	112.67	122.87
86	B6	111	GLN	C-N-CA	-6.34	112.67	122.87
14	Ag	38	TYR	CA-CB-CG	-6.34	102.49	113.90
54	Bb	41	HIS	CA-CB-CG	6.32	120.12	113.80
9	Aa	262	GLU	N-CA-C	6.31	116.57	108.24
16	Ai	17	LYS	CB-CA-C	-6.31	109.28	116.54
24	As	53	GLN	N-CA-C	-6.30	104.33	111.07
54	Bb	209	VAL	N-CA-C	6.29	117.00	111.90
82	B2	31	LYS	CA-C-N	-6.29	113.81	122.87
82	B2	31	LYS	C-N-CA	-6.29	113.81	122.87
23	Aq	83	GLN	N-CA-C	-6.29	101.63	110.50
73	Bt	19	PHE	CA-CB-CG	-6.28	107.52	113.80
9	Aa	18	VAL	N-CA-C	6.28	122.40	109.34
18	Ak	34	PHE	CA-C-N	6.28	132.38	122.34
18	Ak	34	PHE	C-N-CA	6.28	132.38	122.34
71	Br	139	TYR	CA-CB-CG	-6.27	102.62	113.90
64	Bl	117	LEU	O-C-N	6.26	128.99	121.60
15	Ah	129	PHE	CA-CB-CG	-6.26	107.54	113.80
77	Bw	225	GLU	N-CA-C	-6.25	104.47	111.28
14	Ag	169	ILE	CB-CA-C	-6.25	103.70	112.14
62	Bj	56	PHE	N-CA-C	-6.23	104.40	111.07
53	Ba	123	ARG	CB-CA-C	-6.22	98.04	110.42
20	Am	28	PHE	CA-CB-CG	-6.21	107.59	113.80
54	Bb	135	LYS	N-CA-C	6.20	124.00	110.80
65	Bm	129	PHE	CA-CB-CG	-6.19	107.61	113.80
22	Ao	70	GLN	CB-CA-C	-6.19	100.56	110.84
66	Bn	189	PHE	CA-CB-CG	-6.19	107.61	113.80
13	Ae	77	TYR	CB-CA-C	-6.17	100.60	111.22
58	Bf	196	ARG	CD-NE-CZ	6.17	133.03	124.40
64	Bl	92	LYS	N-CA-C	-6.16	104.25	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Ae	138	THR	CA-C-N	6.15	130.98	120.72
13	Ae	138	THR	C-N-CA	6.15	130.98	120.72
83	B3	12	PHE	CA-CB-CG	-6.14	107.66	113.80
77	Bw	263	ASN	N-CA-C	-6.13	102.44	110.53
24	As	55	SER	N-CA-C	-6.13	104.68	111.36
20	Am	87	GLN	CB-CA-C	-6.12	105.64	114.87
84	B4	36	GLN	CA-C-N	-6.12	112.95	122.86
84	B4	36	GLN	C-N-CA	-6.12	112.95	122.86
84	B4	56	PHE	CA-CB-CG	-6.11	107.69	113.80
54	Bb	202	GLN	N-CA-C	6.11	118.58	108.99
19	Al	88	ASP	N-CA-C	-6.10	104.43	112.72
53	Ba	144	LYS	CA-C-N	-6.09	112.24	122.29
53	Ba	144	LYS	C-N-CA	-6.09	112.24	122.29
14	Ag	24	SER	CA-C-N	6.09	130.88	120.72
14	Ag	24	SER	C-N-CA	6.09	130.88	120.72
14	Ag	146	ARG	CA-C-N	6.09	128.23	120.56
14	Ag	146	ARG	C-N-CA	6.09	128.23	120.56
77	Bw	188	ARG	N-CA-C	-6.09	102.50	110.53
54	Bb	120	ASN	OD1-CG-ND2	-6.08	116.52	122.60
77	Bw	133	LEU	N-CA-C	-6.07	104.73	111.71
82	B2	42	LYS	CB-CA-C	-6.07	105.70	114.87
66	Bn	197	HIS	CA-C-N	6.07	132.89	121.97
66	Bn	197	HIS	C-N-CA	6.07	132.89	121.97
57	Be	10	VAL	O-C-N	-6.06	113.30	123.00
85	B5	77	ASP	CA-C-O	-6.06	115.65	122.01
53	Ba	32	VAL	N-CA-C	-6.06	98.48	107.51
66	Bn	107	ARG	NH1-CZ-NH2	6.05	127.17	119.30
68	Bp	188	LEU	N-CA-CB	6.05	119.14	110.06
23	Aq	100	ASN	CA-CB-CG	-6.05	106.55	112.60
67	Bo	58	PRO	N-CA-C	6.04	118.07	110.70
14	Ag	105	GLY	N-CA-C	-6.04	106.90	115.30
54	Bb	208	GLN	CA-C-N	6.04	128.52	122.66
54	Bb	208	GLN	C-N-CA	6.04	128.52	122.66
14	Ag	151	ILE	CB-CA-C	-6.03	103.90	112.22
54	Bb	211	GLY	CA-C-O	-6.02	115.12	121.56
77	Bw	169	LEU	N-CA-C	-6.02	102.58	110.53
14	Ag	202	SER	CA-C-N	-6.00	113.95	122.41
14	Ag	202	SER	C-N-CA	-6.00	113.95	122.41
55	Bc	204	ARG	CA-C-N	6.00	131.28	121.87
55	Bc	204	ARG	C-N-CA	6.00	131.28	121.87
77	Bw	246	THR	N-CA-C	-5.99	101.17	110.10
75	Bv	10	ARG	N-CA-C	-5.98	102.63	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Ag	100	ILE	N-CA-CB	5.98	120.87	110.65
53	Ba	63	PHE	CA-CB-CG	-5.97	107.83	113.80
82	B2	8	PHE	CB-CA-C	-5.97	98.54	110.42
58	Bf	125	LYS	N-CA-C	5.96	123.50	110.80
71	Br	73	ALA	N-CA-C	-5.96	105.27	112.54
24	As	117	GLY	N-CA-C	-5.96	99.30	112.17
64	Bl	112	LEU	CA-C-N	5.96	131.40	120.79
64	Bl	112	LEU	C-N-CA	5.96	131.40	120.79
21	An	13	LYS	N-CA-C	-5.95	104.70	111.07
66	Bn	198	ILE	CB-CA-C	-5.95	101.53	111.29
12	Ad	67	TYR	CA-CB-CG	-5.94	103.20	113.90
10	Ab	199	ASP	CA-CB-CG	-5.94	106.66	112.60
63	Bk	21	PRO	CA-N-CD	-5.94	103.69	112.00
54	Bb	281	LYS	N-CA-C	5.93	119.60	107.69
10	Ab	187	THR	N-CA-C	-5.92	104.82	111.28
15	Ah	85	ASP	CA-CB-CG	-5.92	106.67	112.60
70	Bq	64	TYR	CA-CB-CG	-5.92	103.25	113.90
16	Ai	12	VAL	CA-CB-CG1	-5.92	100.34	110.40
9	Aa	306	LEU	CD1-CG-CD2	-5.92	97.79	110.80
56	Bd	131	TYR	N-CA-CB	5.91	120.13	110.37
58	Bf	124	GLY	N-CA-C	5.91	120.24	110.55
58	Bf	129	PRO	CA-C-N	5.90	130.42	120.81
58	Bf	129	PRO	C-N-CA	5.90	130.42	120.81
15	Ah	46	TYR	CA-CB-CG	-5.89	103.30	113.90
64	Bl	45	PHE	CA-CB-CG	-5.88	107.92	113.80
72	Bs	117	TYR	CA-CB-CG	-5.88	103.31	113.90
14	Ag	165	ASN	CA-C-N	5.88	128.76	120.42
14	Ag	165	ASN	C-N-CA	5.88	128.76	120.42
84	B4	76	ASN	CA-CB-CG	-5.87	106.73	112.60
18	Ak	34	PHE	CB-CA-C	5.87	121.10	111.41
66	Bn	237	GLU	CA-C-O	5.87	126.72	119.97
9	Aa	14	HIS	CB-CG-CD2	-5.87	123.57	131.20
66	Bn	237	GLU	CA-C-N	5.87	128.07	120.44
66	Bn	237	GLU	C-N-CA	5.87	128.07	120.44
14	Ag	87	LEU	N-CA-C	-5.86	105.02	111.82
58	Bf	128	VAL	N-CA-C	5.86	113.67	108.63
17	Aj	88	LEU	N-CA-C	5.86	120.47	112.04
57	Be	31	ARG	CA-CB-CG	5.85	125.80	114.10
56	Bd	105	PHE	O-C-N	5.84	130.74	123.15
9	Aa	302	TYR	N-CA-C	5.83	117.71	108.79
54	Bb	233	ARG	CA-C-N	5.83	131.53	122.26
54	Bb	233	ARG	C-N-CA	5.83	131.53	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	Bn	203	VAL	CB-CA-C	-5.83	104.28	112.14
75	Bv	38	GLY	N-CA-C	-5.82	106.70	115.32
54	Bb	280	ASN	N-CA-C	5.82	123.19	110.80
10	Ab	28	ASN	CA-CB-CG	-5.79	106.81	112.60
66	Bn	197	HIS	CA-C-O	-5.79	112.23	120.51
55	Bc	208	ILE	CA-CB-CG1	5.79	120.24	110.40
54	Bb	137	GLN	N-CA-C	5.79	117.87	109.71
76	B8	62	ASN	CA-CB-CG	-5.78	106.82	112.60
85	B5	188	LEU	N-CA-C	5.78	117.39	111.14
68	Bp	191	GLU	N-CA-CB	5.78	120.33	110.50
17	Aj	70	CYS	N-CA-C	-5.78	104.88	111.07
53	Ba	142	GLU	CB-CA-C	-5.78	108.10	116.54
79	By	47	ARG	CA-C-N	-5.78	111.30	121.70
79	By	47	ARG	C-N-CA	-5.78	111.30	121.70
16	Ai	132	PHE	CA-CB-CG	-5.78	108.02	113.80
66	Bn	223	SER	CA-C-N	5.77	132.13	122.20
66	Bn	223	SER	C-N-CA	5.77	132.13	122.20
71	Br	120	ASN	CA-CB-CG	-5.77	106.83	112.60
13	Ae	126	GLY	N-CA-C	-5.77	107.22	115.64
86	B6	101	ASP	CA-CB-CG	-5.76	106.84	112.60
73	Bt	84	ARG	CA-C-N	-5.75	116.27	122.59
73	Bt	84	ARG	C-N-CA	-5.75	116.27	122.59
75	Bv	62	ASN	CA-CB-CG	-5.75	106.86	112.60
16	Ai	29	ASN	CA-CB-CG	-5.74	106.86	112.60
9	Aa	253	GLY	CA-C-N	5.74	127.02	119.84
9	Aa	253	GLY	C-N-CA	5.74	127.02	119.84
82	B2	30	GLN	N-CA-C	-5.73	98.60	110.80
23	Aq	117	PHE	CA-CB-CG	-5.72	108.08	113.80
85	B5	45	GLU	N-CA-C	5.72	118.52	110.23
23	Aq	112	HIS	N-CA-C	-5.71	100.93	109.15
70	Bq	65	ASN	CA-C-N	-5.71	114.31	121.96
70	Bq	65	ASN	C-N-CA	-5.71	114.31	121.96
79	By	47	ARG	N-CA-C	-5.70	102.46	110.50
9	Aa	304	ASP	N-CA-CB	5.70	118.43	110.56
58	Bf	203	ALA	N-CA-C	5.68	117.62	107.80
54	Bb	282	LYS	N-CA-CB	-5.67	100.69	109.48
64	Bl	46	ASP	CA-CB-CG	-5.67	106.93	112.60
20	Am	74	PRO	CA-C-N	-5.67	113.29	122.82
20	Am	74	PRO	C-N-CA	-5.67	113.29	122.82
71	Br	28	ASN	CA-CB-CG	-5.67	106.93	112.60
67	Bo	112	ILE	CB-CA-C	-5.66	104.72	111.97
84	B4	46	SER	N-CA-C	-5.66	102.14	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	Bw	223	PHE	CA-CB-CG	-5.66	108.14	113.80
53	Ba	33	ASP	CA-CB-CG	-5.66	106.94	112.60
71	Br	41	ILE	N-CA-CB	5.65	118.23	110.54
22	Ao	17	PHE	N-CA-C	5.65	113.30	108.22
10	Ab	36	TYR	CA-CB-CG	-5.65	103.73	113.90
79	By	54	LEU	CA-C-N	-5.65	113.94	122.07
79	By	54	LEU	C-N-CA	-5.65	113.94	122.07
9	Aa	35	SER	N-CA-CB	-5.64	102.46	111.43
54	Bb	134	LYS	N-CA-C	5.64	118.41	109.50
79	By	25	SER	N-CA-C	-5.63	105.22	111.36
23	Aq	131	CYS	O-C-N	-5.63	116.36	123.17
24	As	98	ASN	N-CA-C	-5.63	98.81	110.80
84	B4	53	LYS	N-CA-C	-5.62	105.17	113.16
14	Ag	118	ASN	CA-CB-CG	-5.62	106.98	112.60
19	Al	127	ASN	CA-CB-CG	-5.62	106.98	112.60
23	Aq	98	LYS	N-CA-C	-5.62	104.46	113.28
65	Bm	21	PHE	CA-CB-CG	-5.62	108.18	113.80
75	Bv	39	GLY	CA-C-N	5.61	128.84	120.31
75	Bv	39	GLY	C-N-CA	5.61	128.84	120.31
65	Bm	130	PHE	CA-CB-CG	-5.61	108.19	113.80
9	Aa	283	PRO	CB-CA-C	5.61	117.76	110.92
62	Bj	68	GLY	CA-C-N	5.60	126.09	120.04
62	Bj	68	GLY	C-N-CA	5.60	126.09	120.04
20	Am	99	LEU	N-CA-CB	5.59	115.84	108.96
58	Bf	202	VAL	O-C-N	-5.59	116.85	123.00
66	Bn	238	MET	N-CA-CB	-5.59	101.90	110.01
73	Bt	61	HIS	N-CA-C	-5.59	105.33	111.82
75	Bv	10	ARG	CA-C-N	-5.59	114.30	122.46
75	Bv	10	ARG	C-N-CA	-5.59	114.30	122.46
66	Bn	80	HIS	CB-CA-C	-5.58	101.53	110.79
14	Ag	96	ALA	CA-C-N	5.58	127.75	120.28
14	Ag	96	ALA	C-N-CA	5.58	127.75	120.28
10	Ab	69	ASN	CA-C-O	5.57	122.91	119.29
24	As	99	GLY	N-CA-C	-5.57	105.50	113.86
23	Aq	111	VAL	CA-C-N	-5.57	112.97	121.66
23	Aq	111	VAL	C-N-CA	-5.57	112.97	121.66
54	Bb	218	VAL	N-CA-CB	5.57	117.88	110.26
24	As	56	LEU	N-CA-C	5.56	117.03	110.97
85	B5	104	PHE	CA-CB-CG	-5.56	108.24	113.80
10	Ab	69	ASN	CA-CB-CG	-5.56	107.04	112.60
85	B5	102	ASP	CA-CB-CG	-5.56	107.04	112.60
54	Bb	154	LYS	CA-C-N	5.55	132.15	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Bb	154	LYS	C-N-CA	5.55	132.15	121.54
79	By	12	ILE	CA-C-N	5.55	131.97	121.97
79	By	12	ILE	C-N-CA	5.55	131.97	121.97
78	Bx	42	ALA	N-CA-C	5.55	122.08	109.81
66	Bn	238	MET	CG-SD-CE	5.55	113.10	100.90
19	Al	92	ASN	CA-CB-CG	-5.54	107.06	112.60
13	Ae	143	ASN	CA-CB-CG	-5.54	107.06	112.60
60	Bh	85	HIS	N-CA-C	5.53	118.47	109.06
16	Ai	133	GLY	N-CA-C	-5.53	108.02	115.21
56	Bd	32	ARG	CA-C-N	5.53	130.60	121.86
56	Bd	32	ARG	C-N-CA	5.53	130.60	121.86
61	Bi	120	SER	CA-C-N	5.53	130.08	120.68
61	Bi	120	SER	C-N-CA	5.53	130.08	120.68
85	B5	77	ASP	N-CA-C	-5.53	103.34	110.19
66	Bn	37	ILE	CB-CA-C	5.52	120.34	111.29
12	Ad	109	PHE	CA-CB-CG	-5.51	108.28	113.80
64	Bl	47	LYS	N-CA-C	-5.51	105.37	111.71
54	Bb	212	GLN	OE1-CD-NE2	-5.51	117.09	122.60
57	Be	12	ILE	N-CA-CB	5.51	118.92	111.21
11	Ac	151	LYS	CA-C-N	5.50	132.05	121.54
11	Ac	151	LYS	C-N-CA	5.50	132.05	121.54
66	Bn	156	ASN	N-CA-C	5.50	117.42	110.33
53	Ba	176	ASP	CA-CB-CG	-5.50	107.10	112.60
16	Ai	67	ASP	CA-C-N	-5.49	115.31	122.94
16	Ai	67	ASP	C-N-CA	-5.49	115.31	122.94
62	Bj	62	ASN	CA-CB-CG	-5.47	107.12	112.60
72	Bs	81	LEU	CA-C-N	-5.47	115.28	123.00
72	Bs	81	LEU	C-N-CA	-5.47	115.28	123.00
53	Ba	71	LYS	N-CA-C	-5.47	105.21	111.07
62	Bj	110	PRO	N-CA-C	-5.47	107.03	113.86
64	Bl	18	GLY	N-CA-C	-5.47	105.41	114.48
9	Aa	188	HIS	CA-CB-CG	-5.46	108.34	113.80
85	B5	2	ASP	CA-CB-CG	-5.46	107.14	112.60
78	Bx	40	LYS	N-CA-C	5.46	119.51	112.41
9	Aa	65	PHE	CA-C-N	-5.46	114.35	122.70
9	Aa	65	PHE	C-N-CA	-5.46	114.35	122.70
72	Bs	109	ILE	CB-CA-C	-5.46	104.69	112.22
69	B7	203	TYR	CA-CB-CG	-5.45	104.08	113.90
77	Bw	218	THR	N-CA-C	-5.45	103.48	111.17
16	Ai	63	PHE	N-CA-C	-5.45	99.19	110.80
62	Bj	107	ILE	N-CA-C	-5.44	105.82	112.35
53	Ba	231	ALA	CA-C-N	5.44	126.94	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	Ba	231	ALA	C-N-CA	5.44	126.94	120.14
68	Bp	109	TYR	CA-CB-CG	-5.43	104.12	113.90
66	Bn	107	ARG	NE-CZ-NH1	-5.43	116.07	121.50
54	Bb	214	GLU	N-CA-C	5.43	117.84	110.35
55	Bc	87	GLY	N-CA-C	5.43	117.76	110.43
64	Bl	90	ALA	CA-C-N	5.43	131.91	121.54
64	Bl	90	ALA	C-N-CA	5.43	131.91	121.54
72	Bs	133	GLU	N-CA-C	5.42	117.53	110.53
21	An	45	GLN	CA-C-N	-5.42	115.53	122.79
21	An	45	GLN	C-N-CA	-5.42	115.53	122.79
58	Bf	186	GLY	CA-C-N	5.42	127.80	120.38
58	Bf	186	GLY	C-N-CA	5.42	127.80	120.38
77	Bw	126	LYS	CA-C-N	5.42	130.60	122.58
77	Bw	126	LYS	C-N-CA	5.42	130.60	122.58
78	Bx	38	PHE	CA-C-O	-5.42	112.76	120.51
85	B5	41	ASN	CA-C-N	-5.42	115.46	123.05
85	B5	41	ASN	C-N-CA	-5.42	115.46	123.05
54	Bb	88	ILE	CB-CA-C	-5.42	104.74	111.08
64	Bl	100	ILE	N-CA-C	5.42	116.90	111.00
58	Bf	200	THR	N-CA-CB	-5.41	102.13	110.20
21	An	46	TYR	CA-CB-CG	-5.41	104.17	113.90
84	B4	37	GLY	N-CA-C	-5.41	107.05	114.67
18	Ak	40	THR	CA-C-N	5.40	131.48	122.73
18	Ak	40	THR	C-N-CA	5.40	131.48	122.73
68	Bp	190	LYS	CA-C-N	5.38	131.39	121.70
68	Bp	190	LYS	C-N-CA	5.38	131.39	121.70
82	B2	25	LYS	CA-C-N	-5.38	114.94	123.12
82	B2	25	LYS	C-N-CA	-5.38	114.94	123.12
85	B5	15	ASP	CA-CB-CG	-5.38	107.22	112.60
55	Bc	141	HIS	ND1-CE1-NE2	5.38	113.78	108.40
84	B4	16	GLY	N-CA-C	-5.38	107.85	115.43
16	Ai	63	PHE	CA-CB-CG	-5.37	108.43	113.80
10	Ab	46	TYR	CA-CB-CG	-5.36	104.25	113.90
77	Bw	113	PHE	CA-C-N	-5.36	116.12	123.14
77	Bw	113	PHE	C-N-CA	-5.36	116.12	123.14
54	Bb	316	LEU	N-CA-C	5.36	116.64	108.12
71	Br	7	ASP	CA-CB-CG	-5.36	107.24	112.60
14	Ag	27	ASP	CA-CB-CG	-5.35	107.25	112.60
9	Aa	178	ASN	CA-C-N	5.35	127.90	120.63
9	Aa	178	ASN	C-N-CA	5.35	127.90	120.63
59	Bg	281	VAL	N-CA-CB	5.35	116.81	110.55
71	Br	74	LYS	CA-C-N	-5.34	113.55	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	Br	74	LYS	C-N-CA	-5.34	113.55	121.24
55	Bc	223	HIS	ND1-CE1-NE2	5.34	113.74	108.40
66	Bn	199	MET	N-CA-CB	5.34	119.38	110.41
53	Ba	194	ASN	CA-CB-CG	-5.34	107.26	112.60
84	B4	42	ASP	CA-CB-CG	-5.34	107.26	112.60
13	Ae	39	GLY	CA-C-N	5.33	129.74	120.68
13	Ae	39	GLY	C-N-CA	5.33	129.74	120.68
16	Ai	104	SER	CA-C-N	-5.33	112.72	120.29
16	Ai	104	SER	C-N-CA	-5.33	112.72	120.29
79	By	59	GLY	N-CA-C	-5.32	100.57	113.18
66	Bn	203	VAL	CG1-CB-CG2	5.32	122.50	110.80
20	Am	128	GLY	N-CA-C	-5.31	107.46	115.32
62	Bj	15	LEU	CB-CA-C	-5.31	102.54	110.88
55	Bc	209	ILE	CB-CA-C	5.31	118.71	110.96
15	Ah	70	ASN	CA-CB-CG	-5.31	107.29	112.60
10	Ab	86	VAL	CB-CA-C	-5.29	105.19	111.97
60	Bh	118	PHE	CA-CB-CG	-5.29	108.51	113.80
66	Bn	198	ILE	CB-CG1-CD1	5.29	124.90	113.80
67	Bo	52	MET	O-C-N	5.29	129.62	122.59
12	Ad	153	ASN	CA-CB-CG	-5.28	107.32	112.60
64	Bl	141	GLY	N-CA-C	-5.28	107.51	115.32
66	Bn	191	ALA	CA-C-N	-5.27	113.30	122.37
66	Bn	191	ALA	C-N-CA	-5.27	113.30	122.37
20	Am	101	ASN	CA-CB-CG	-5.27	107.33	112.60
9	Aa	304	ASP	CB-CA-C	-5.27	101.70	110.81
53	Ba	141	PRO	N-CA-C	5.27	123.32	112.47
79	By	66	THR	N-CA-C	-5.26	104.66	111.71
85	B5	78	VAL	CB-CA-C	-5.26	103.69	111.80
55	Bc	167	VAL	CA-CB-CG2	5.26	119.35	110.40
9	Aa	178	ASN	CA-CB-CG	5.26	117.86	112.60
64	Bl	89	ASN	CA-CB-CG	-5.25	107.36	112.60
56	Bd	171	ASP	N-CA-C	5.24	116.11	108.14
55	Bc	174	LYS	CA-C-N	5.24	128.27	120.31
55	Bc	174	LYS	C-N-CA	5.24	128.27	120.31
62	Bj	123	LEU	N-CA-C	-5.23	102.31	110.42
64	Bl	68	SER	CA-C-N	-5.23	115.61	122.99
64	Bl	68	SER	C-N-CA	-5.23	115.61	122.99
10	Ab	68	GLU	CA-C-N	-5.23	114.84	121.74
10	Ab	68	GLU	C-N-CA	-5.23	114.84	121.74
18	Ak	114	SER	N-CA-C	5.22	116.66	111.07
64	Bl	16	SER	N-CA-C	-5.22	105.50	111.14
16	Ai	101	ASP	CA-CB-CG	-5.22	107.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Am	18	THR	N-CA-C	-5.22	104.07	110.65
66	Bn	199	MET	CB-CA-C	-5.21	99.58	109.95
81	Bz	18	TYR	CA-CB-CG	-5.21	104.52	113.90
85	B5	104	PHE	CA-C-N	-5.21	116.34	123.12
85	B5	104	PHE	C-N-CA	-5.21	116.34	123.12
17	Aj	93	SER	CA-C-N	5.21	125.95	120.11
17	Aj	93	SER	C-N-CA	5.21	125.95	120.11
11	Ac	163	PRO	N-CA-CB	5.21	107.80	103.17
19	Al	114	ASP	CA-CB-CG	-5.21	107.39	112.60
66	Bn	197	HIS	O-C-N	-5.21	115.67	122.59
9	Aa	64	HIS	ND1-CG-CD2	5.20	111.30	106.10
83	B3	20	ASN	CA-CB-CG	-5.19	107.41	112.60
57	Be	129	ARG	CB-CA-C	5.19	118.84	109.61
54	Bb	202	GLN	CA-C-N	5.18	131.43	121.54
54	Bb	202	GLN	C-N-CA	5.18	131.43	121.54
64	Bl	128	PHE	CA-CB-CG	-5.18	108.62	113.80
78	Bx	32	ARG	N-CA-CB	5.18	117.68	110.07
62	Bj	38	GLU	CA-C-N	5.17	126.79	120.22
62	Bj	38	GLU	C-N-CA	5.17	126.79	120.22
55	Bc	229	LEU	N-CA-C	5.17	116.66	108.96
20	Am	87	GLN	N-CA-CB	5.17	114.78	109.51
66	Bn	32	ARG	CB-CA-C	5.16	120.22	109.95
9	Aa	64	HIS	CB-CG-CD2	-5.16	124.49	131.20
21	An	29	GLY	N-CA-C	-5.16	107.93	115.72
53	Ba	162	ASN	CA-CB-CG	-5.16	107.44	112.60
77	Bw	224	LYS	N-CA-C	-5.16	99.82	110.80
73	Bt	52	ASP	CA-CB-CG	-5.15	107.45	112.60
21	An	20	SER	N-CA-C	-5.15	100.31	108.14
79	By	43	ASN	CA-CB-CG	-5.15	107.45	112.60
58	Bf	204	PHE	CA-CB-CG	5.14	118.94	113.80
82	B2	18	LEU	N-CA-CB	5.14	119.78	110.83
66	Bn	211	MET	CA-C-N	5.14	130.82	122.39
66	Bn	211	MET	C-N-CA	5.14	130.82	122.39
72	Bs	125	ASN	CA-CB-CG	-5.14	107.46	112.60
17	Aj	96	GLU	N-CA-C	-5.14	105.80	111.71
85	B5	113	ASP	CA-CB-CG	-5.13	107.47	112.60
56	Bd	107	PHE	N-CA-C	5.13	117.78	109.06
13	Ae	41	HIS	N-CA-C	-5.13	106.97	113.23
85	B5	96	ASP	CA-CB-CG	-5.13	107.47	112.60
23	Aq	88	ILE	N-CA-CB	5.12	116.31	110.72
57	Be	147	GLU	N-CA-C	5.12	117.17	109.23
67	Bo	128	GLU	CA-C-N	-5.12	116.86	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	Bo	128	GLU	C-N-CA	-5.12	116.86	123.16
66	Bn	44	ASN	OD1-CG-ND2	-5.12	117.48	122.60
61	Bi	97	ASN	CA-CB-CG	-5.12	107.48	112.60
19	Al	105	PHE	CA-CB-CG	-5.12	108.69	113.80
66	Bn	89	VAL	N-CA-C	5.11	115.06	108.82
17	Aj	28	ASN	CA-CB-CG	-5.11	107.49	112.60
55	Bc	55	GLU	CB-CA-C	5.11	120.43	110.57
67	Bo	73	GLY	N-CA-C	-5.11	104.57	113.76
70	Bq	71	VAL	N-CA-C	-5.11	98.72	109.34
68	Bp	180	LYS	CA-C-O	-5.10	113.63	119.60
71	Br	108	ASP	CA-CB-CG	-5.10	107.50	112.60
64	Bl	36	GLY	N-CA-C	-5.10	108.22	115.30
14	Ag	147	VAL	N-CA-CB	-5.10	104.59	110.55
14	Ag	31	ASN	CA-CB-CG	-5.09	107.51	112.60
73	Bt	62	TYR	CA-CB-CG	-5.09	104.73	113.90
85	B5	3	GLN	N-CA-C	-5.09	106.17	112.38
65	Bm	90	ASN	CA-CB-CG	-5.09	107.51	112.60
17	Aj	76	THR	N-CA-C	-5.09	105.98	113.61
17	Aj	80	PHE	CA-CB-CG	-5.09	108.71	113.80
65	Bm	140	LYS	N-CA-C	-5.09	104.15	110.41
73	Bt	112	ASP	CA-CB-CG	-5.09	107.51	112.60
53	Ba	205	ASN	CA-CB-CG	-5.08	107.52	112.60
55	Bc	260	ASP	CA-CB-CG	5.08	117.68	112.60
77	Bw	182	GLY	N-CA-C	-5.08	103.92	112.77
9	Aa	306	LEU	CB-CA-C	5.08	120.20	109.79
73	Bt	20	ASN	CA-CB-CG	-5.08	107.52	112.60
62	Bj	85	GLY	CA-C-N	5.08	128.03	120.31
62	Bj	85	GLY	C-N-CA	5.08	128.03	120.31
18	Ak	99	ALA	CA-C-O	5.07	125.95	120.12
23	Aq	124	ASP	CA-CB-CG	-5.07	107.53	112.60
67	Bo	105	SER	N-CA-C	-5.07	103.84	110.53
82	B2	37	CYS	CA-C-N	-5.07	117.41	123.44
82	B2	37	CYS	C-N-CA	-5.07	117.41	123.44
21	An	34	TYR	CA-CB-CG	-5.07	104.78	113.90
83	B3	39	SER	N-CA-C	-5.07	107.05	113.18
85	B5	196	ASP	CA-CB-CG	-5.07	107.53	112.60
61	Bi	129	ILE	CB-CA-C	-5.06	105.31	112.14
16	Ai	123	ASP	CA-C-N	5.06	124.75	119.64
16	Ai	123	ASP	C-N-CA	5.06	124.75	119.64
80	B9	92	ASN	CA-CB-CG	-5.06	107.54	112.60
24	As	119	PHE	N-CA-C	-5.06	106.96	113.23
73	Bt	54	GLU	CA-C-N	-5.06	115.89	122.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	Bt	54	GLU	C-N-CA	-5.06	115.89	122.51
53	Ba	222	PRO	N-CA-C	5.05	120.47	113.65
9	Aa	68	ASP	N-CA-C	5.05	116.86	109.24
14	Ag	69	VAL	CB-CA-C	-5.05	105.32	112.14
22	Ao	46	LYS	CA-C-N	5.05	127.55	120.28
22	Ao	46	LYS	C-N-CA	5.05	127.55	120.28
63	Bk	135	ASN	CA-CB-CG	-5.04	107.56	112.60
21	An	25	SER	CA-C-N	-5.04	113.71	120.87
21	An	25	SER	C-N-CA	-5.04	113.71	120.87
84	B4	28	LYS	CA-C-N	-5.04	117.69	122.17
84	B4	28	LYS	C-N-CA	-5.04	117.69	122.17
10	Ab	107	PHE	CA-CB-CG	-5.03	108.77	113.80
54	Bb	216	ILE	O-C-N	-5.03	117.33	122.82
10	Ab	182	LEU	CA-C-N	5.03	129.12	120.72
10	Ab	182	LEU	C-N-CA	5.03	129.12	120.72
9	Aa	56	GLN	CB-CA-C	5.03	120.43	110.42
68	Bp	10	LEU	N-CA-CB	5.03	117.60	110.16
23	Aq	118	ARG	N-CA-C	-5.03	104.70	111.54
62	Bj	134	PHE	CA-CB-CG	-5.03	108.77	113.80
77	Bw	226	ALA	N-CA-C	-5.02	102.95	110.23
64	Bl	93	ASN	CA-CB-CG	-5.02	107.58	112.60
16	Ai	95	TYR	N-CA-C	-5.02	105.70	111.07
77	Bw	185	ASN	CA-C-N	-5.02	115.41	122.94
77	Bw	185	ASN	C-N-CA	-5.02	115.41	122.94
64	Bl	37	GLY	N-CA-C	-5.01	106.67	113.24
17	Aj	38	ASP	CA-CB-CG	-5.01	107.59	112.60
54	Bb	63	GLY	N-CA-C	5.01	119.96	114.40
85	B5	43	VAL	CA-C-N	5.01	130.22	122.26
85	B5	43	VAL	C-N-CA	5.01	130.22	122.26
68	Bp	190	LYS	CG-CD-CE	5.00	122.80	111.30
85	B5	20	ASN	CA-CB-CG	-5.00	107.60	112.60

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	Ak	99	ALA	CA
54	Bb	137	GLN	CA
58	Bf	197	LYS	CA
63	Bk	21	PRO	CA
68	Bp	191	GLU	CA
78	Bx	38	PHE	CA

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	Aa	104	HIS	Sidechain
9	Aa	14	HIS	Sidechain
9	Aa	140	TYR	Sidechain
9	Aa	156	PHE	Sidechain
9	Aa	191	HIS	Sidechain
9	Aa	194	TYR	Sidechain
9	Aa	251	ALA	Peptide
9	Aa	253	GLY	Peptide
9	Aa	269	GLU	Peptide
9	Aa	302	TYR	Sidechain
9	Aa	304	ASP	Peptide
9	Aa	34	ALA	Peptide
9	Aa	64	HIS	Sidechain
9	Aa	65	PHE	Sidechain
9	Aa	77	PHE	Sidechain
9	Aa	81	GLY	Peptide
9	Aa	99	ARG	Sidechain
11	Ac	152	PHE	Sidechain
18	Ak	100	THR	Peptide
18	Ak	102	GLY	Peptide
18	Ak	34	PHE	Sidechain
18	Ak	72	TYR	Sidechain
18	Ak	99	ALA	Peptide
22	Ao	20	ASP	Peptide
22	Ao	21	THR	Peptide,Mainchain
22	Ao	77	TYR	Sidechain
23	Aq	131	CYS	Mainchain
54	Bb	101	PHE	Sidechain
54	Bb	118	TYR	Sidechain
54	Bb	132	TYR	Sidechain
54	Bb	137	GLN	Peptide
54	Bb	153	LYS	Peptide,Mainchain
54	Bb	155	TYR	Sidechain
54	Bb	219	ILE	Peptide
54	Bb	263	PHE	Sidechain
54	Bb	284	TYR	Sidechain
54	Bb	290	TYR	Sidechain
54	Bb	304	THR	Peptide
54	Bb	322	TYR	Sidechain
54	Bb	40	VAL	Peptide
54	Bb	41	HIS	Sidechain
54	Bb	42	LEU	Peptide

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Mol	Chain	Res	Type	Group
54	Bb	48	TYR	Sidechain
54	Bb	61	ARG	Sidechain
54	Bb	84	VAL	Peptide
55	Bc	101	PHE	Sidechain
55	Bc	160	TYR	Sidechain
55	Bc	204	ARG	Peptide
55	Bc	210	TYR	Sidechain
55	Bc	220	PHE	Sidechain
55	Bc	256	PHE	Sidechain
55	Bc	76	PRO	Peptide
55	Bc	85	ARG	Peptide
55	Bc	91	PHE	Sidechain
56	Bd	107	PHE	Sidechain
56	Bd	13	ARG	Sidechain
56	Bd	131	TYR	Sidechain
56	Bd	166	PHE	Sidechain
56	Bd	60	PHE	Peptide
56	Bd	92	TYR	Peptide
57	Be	88	PHE	Sidechain
58	Bf	135	VAL	Peptide
58	Bf	136	LEU	Peptide
58	Bf	162	ASP	Peptide
58	Bf	195	HIS	Peptide
58	Bf	196	ARG	Peptide
58	Bf	204	PHE	Sidechain
60	Bh	19	SER	Peptide
60	Bh	45	PHE	Sidechain
60	Bh	74	TYR	Sidechain
60	Bh	8	TYR	Sidechain
60	Bh	84	PHE	Sidechain
63	Bk	40	ILE	Peptide
66	Bn	107	ARG	Sidechain
66	Bn	15	TYR	Sidechain
66	Bn	225	TYR	Sidechain
66	Bn	239	TYR	Sidechain
66	Bn	29	TYR	Sidechain
66	Bn	32	ARG	Peptide
66	Bn	43	TYR	Sidechain
66	Bn	44	ASN	Peptide
66	Bn	85	TYR	Sidechain
68	Bp	181	LYS	Peptide
68	Bp	190	LYS	Peptide

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Mol	Chain	Res	Type	Group
74	Bu	8	PHE	Sidechain
78	Bx	25	TYR	Sidechain
78	Bx	35	GLY	Peptide
78	Bx	37	GLY	Peptide
78	Bx	38	PHE	Peptide,Sidechain,Mainchain

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	AA	1391	0	0	40	0
2	AB	32	0	0	0	0
3	AC	29	0	0	0	0
4	AD	42	0	0	0	0
5	AE	32	0	0	0	0
6	AF	31	0	0	0	0
7	AG	14	0	0	0	0
8	AH	41	0	0	13	0
9	Aa	2380	0	2337	221	0
10	Ab	1521	0	1531	0	0
11	Ac	1498	0	1575	0	0
12	Ad	845	0	879	76	0
13	Ae	1096	0	1160	0	0
14	Ag	1277	0	1325	0	0
15	Ah	1016	0	1057	0	0
16	Ai	1102	0	1160	0	0
17	Aj	772	0	839	175	0
18	Ak	935	0	951	0	0
19	Al	871	0	927	0	0
20	Am	1150	0	1202	0	0
21	An	410	0	408	120	0
22	Ao	710	0	743	24	0
23	Aq	629	0	674	0	0
24	As	721	0	759	0	0
25	B1	97	0	0	12	0
26	B0	2407	0	0	238	0
27	BA	21	0	0	0	0
28	BB	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BC	17	0	0	0	0
30	BD	16	0	0	0	0
31	BE	54	0	0	0	0
32	BF	120	0	0	0	0
33	BG	48	0	0	0	0
34	BH	25	0	0	3	0
35	BI	72	0	0	0	0
36	BJ	30	0	0	0	0
37	BK	25	0	0	0	0
38	BL	20	0	0	0	0
39	BM	19	0	0	4	0
40	BN	78	0	0	0	0
41	BO	20	0	0	0	0
42	BP	15	0	0	0	0
43	BQ	30	0	0	0	0
44	BR	30	0	0	0	0
45	BS	38	0	0	0	0
46	BT	30	0	0	0	0
47	BU	16	0	0	0	0
48	BV	22	0	0	4	0
49	BW	16	0	0	3	0
50	BX	113	0	0	0	0
51	BY	115	0	0	29	0
52	BZ	72	0	0	4	0
53	Ba	1867	0	1961	0	0
54	Bb	2765	0	2878	24	0
55	Bc	2035	0	2119	0	0
56	Bd	1325	0	1358	0	0
57	Be	1407	0	1481	0	0
58	Bf	920	0	1003	0	0
59	Bg	327	0	323	0	0
60	Bh	1331	0	1384	0	0
61	Bi	573	0	608	0	0
62	Bj	1095	0	1188	283	0
63	Bk	927	0	986	0	0
64	Bl	951	0	985	177	0
65	Bm	1454	0	1498	0	0
66	Bn	1912	0	1887	364	0
67	Bo	956	0	1057	0	0
68	Bp	1329	0	1449	143	0
69	B7	129	0	152	11	0
70	Bq	773	0	829	291	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	Br	1217	0	1241	0	0
72	Bs	622	0	661	0	0
73	Bt	916	0	977	0	0
74	Bu	443	0	435	0	0
75	Bv	477	0	546	0	0
76	B8	78	0	84	0	0
77	Bw	1281	0	1362	371	0
78	Bx	670	0	710	0	0
79	By	514	0	578	209	0
80	B9	460	0	481	99	0
81	Bz	548	0	567	88	0
82	B2	407	0	423	151	0
83	B3	429	0	466	85	0
84	B4	760	0	820	147	0
85	B5	1621	0	1559	339	0
86	B6	874	0	920	215	0
All	All	55531	0	52503	3488	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 82.

All (3488) 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:B0:1572:A:P	54:Bb:245:ARG:HD2	1.21	1.75
51:BY:11:A:P	66:Bn:17:VAL:HG23	1.29	1.71
49:BW:13:U:P	64:Bl:131:ARG:HG2	1.18	1.70
26:B0:2251:G:P	77:Bw:186:LYS:HB3	1.25	1.69
8:AH:9:G:P	21:An:13:LYS:HD3	1.31	1.64
1:AA:1435:G:P	21:An:13:LYS:HD3	1.36	1.64
26:B0:4255:U:P	84:B4:13:LYS:HE2	1.35	1.64
25:B1:54:A:P	83:B3:21:ARG:HG2	1.40	1.61
79:By:11:LYS:HE2	80:B9:69:MET:CE	1.16	1.61
66:Bn:40:LYS:HE2	70:Bq:67:THR:CA	1.25	1.60
51:BY:67:C:P	66:Bn:12:PHE:HA	1.36	1.58
1:AA:1653:C:P	21:An:38:MET:HE3	1.46	1.54
26:B0:4168:U:P	70:Bq:8:ARG:HG2	1.48	1.52
34:BH:1800:G:P	66:Bn:46:PRO:HG3	1.48	1.50
17:Aj:72:GLU:HG2	21:An:54:LYS:CG	1.39	1.49
26:B0:4192:U:P	84:B4:2:VAL:HG21	1.53	1.48
66:Bn:40:LYS:CE	70:Bq:67:THR:C	1.81	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BZ:75:C:P	84:B4:54:PRO:HG2	1.51	1.47
26:B0:2757:C:P	83:B3:7:PHE:CD1	2.08	1.47
26:B0:4021:A:P	85:B5:199:TYR:CE2	2.09	1.46
79:By:11:LYS:CE	80:B9:69:MET:HE2	0.99	1.45
66:Bn:14:ARG:NE	70:Bq:18:PHE:HD2	0.95	1.42
51:BY:11:A:P	66:Bn:17:VAL:CG2	2.08	1.41
66:Bn:14:ARG:NE	70:Bq:18:PHE:CD2	1.87	1.41
66:Bn:40:LYS:HZ1	70:Bq:67:THR:CB	1.34	1.39
1:AA:1444:C:P	21:An:30:LEU:HB2	1.62	1.39
66:Bn:40:LYS:HE2	70:Bq:67:THR:C	0.99	1.39
8:AH:16:G:P	21:An:30:LEU:HB2	1.60	1.38
1:AA:1435:G:P	21:An:13:LYS:CD	2.11	1.38
26:B0:1572:A:P	54:Bb:245:ARG:CD	2.09	1.38
26:B0:4322:A:P	84:B4:34:TYR:CG	2.14	1.37
81:Bz:42:CYS:CA	86:B6:53:PRO:HB3	1.55	1.36
8:AH:9:G:P	21:An:13:LYS:CD	2.11	1.36
26:B0:1298:C:P	64:Bl:25:HIS:HB2	1.61	1.36
26:B0:430:G:P	79:By:16:ARG:CZ	2.12	1.35
66:Bn:40:LYS:NZ	70:Bq:67:THR:CB	1.85	1.35
26:B0:4250:U:P	84:B4:9:ARG:NH1	2.00	1.34
26:B0:4322:A:P	84:B4:34:TYR:CA	2.15	1.34
49:BW:13:U:P	64:Bl:131:ARG:CG	2.12	1.34
26:B0:429:G:P	79:By:19:LYS:NZ	2.00	1.33
26:B0:430:G:P	79:By:16:ARG:HH11	0.72	1.33
26:B0:430:G:P	79:By:16:ARG:NH1	1.09	1.33
26:B0:2866:G:P	68:Bp:75:HIS:NE2	2.02	1.33
25:B1:54:A:P	83:B3:21:ARG:CG	2.16	1.33
26:B0:2251:G:P	77:Bw:186:LYS:CB	2.16	1.33
26:B0:4323:A:P	84:B4:36:GLN:N	2.01	1.33
66:Bn:40:LYS:CE	70:Bq:67:THR:O	1.67	1.32
26:B0:1493:U:P	64:Bl:33:GLY:HA2	1.69	1.32
26:B0:1859:C:P	79:By:46:ARG:NH1	2.02	1.32
26:B0:2611:C:P	68:Bp:60:ARG:HG2	1.68	1.30
66:Bn:40:LYS:NZ	70:Bq:67:THR:HB	1.00	1.30
26:B0:2768:C:P	82:B2:11:ARG:HH22	1.53	1.30
26:B0:2296:G:P	79:By:35:TRP:CE3	2.23	1.30
26:B0:364:G:P	82:B2:36:LYS:HE2	1.72	1.29
26:B0:4168:U:P	70:Bq:8:ARG:CG	2.21	1.29
26:B0:4021:A:P	85:B5:199:TYR:CZ	2.25	1.28
66:Bn:40:LYS:CE	70:Bq:67:THR:HB	1.63	1.28
17:Aj:72:GLU:CG	21:An:54:LYS:HG2	1.63	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B0:2296:G:P	79:By:35:TRP:HE3	1.55	1.28
26:B0:4255:U:P	84:B4:13:LYS:CE	2.20	1.27
1:AA:1800:U:P	17:Aj:77:TRP:HH2	1.58	1.27
1:AA:1800:U:P	17:Aj:77:TRP:CH2	2.27	1.26
17:Aj:72:GLU:CG	21:An:54:LYS:CG	2.13	1.26
26:B0:2757:C:P	83:B3:7:PHE:HD1	1.49	1.26
26:B0:4250:U:P	84:B4:9:ARG:CZ	2.25	1.24
1:AA:1444:C:P	21:An:30:LEU:HD22	1.75	1.24
17:Aj:72:GLU:HG2	21:An:54:LYS:CD	1.67	1.23
1:AA:1444:C:P	21:An:30:LEU:CB	2.26	1.22
51:BY:67:C:P	66:Bn:12:PHE:CA	2.13	1.22
1:AA:1444:C:P	21:An:30:LEU:CG	2.27	1.22
66:Bn:14:ARG:CZ	70:Bq:18:PHE:CD2	2.21	1.21
66:Bn:40:LYS:CE	70:Bq:67:THR:CA	2.10	1.21
66:Bn:40:LYS:CE	70:Bq:67:THR:CB	2.19	1.21
26:B0:4023:U:P	85:B5:31:LEU:O	1.98	1.20
81:Bz:42:CYS:HA	86:B6:53:PRO:CB	1.72	1.20
66:Bn:38:GLN:HG2	70:Bq:29:TYR:CE2	1.77	1.19
51:BY:26:C:P	66:Bn:57:ARG:HG3	1.82	1.19
66:Bn:40:LYS:CG	70:Bq:67:THR:O	1.91	1.18
51:BY:26:C:P	66:Bn:57:ARG:CG	2.32	1.18
81:Bz:42:CYS:SG	86:B6:53:PRO:CB	2.32	1.17
70:Bq:63:VAL:HG13	70:Bq:74:ILE:HD13	1.25	1.17
25:B1:45:C:P	83:B3:15:LYS:HE2	1.84	1.16
52:BZ:75:C:P	84:B4:54:PRO:CG	2.31	1.16
21:An:21:CYS:HB3	21:An:38:MET:H	1.04	1.16
21:An:30:LEU:HA	21:An:37:ASN:HA	1.22	1.16
85:B5:143:GLU:HA	85:B5:146:LYS:HE2	1.27	1.16
26:B0:363:A:P	82:B2:24:SER:OG	2.03	1.15
79:By:27:ARG:HD3	79:By:28:TYR:HD1	1.08	1.15
26:B0:4608:A:P	68:Bp:62:ARG:HH12	1.68	1.15
66:Bn:38:GLN:CD	70:Bq:29:TYR:CD2	2.25	1.15
26:B0:1581:U:P	82:B2:3:LYS:HG2	1.87	1.14
34:BH:1800:G:P	66:Bn:46:PRO:CG	2.36	1.14
77:Bw:223:PHE:HB3	77:Bw:226:ALA:HB3	1.28	1.14
51:BY:7:G:P	66:Bn:27:THR:HG21	1.88	1.14
77:Bw:130:VAL:HG23	77:Bw:154:MET:HE3	1.21	1.14
1:AA:1444:C:P	21:An:30:LEU:CD2	2.35	1.13
26:B0:1511:G:P	82:B2:16:HIS:CE1	2.41	1.13
26:B0:1713:G:P	70:Bq:12:TYR:HB3	1.88	1.13
86:B6:96:ILE:HD13	86:B6:105:ILE:HD11	1.26	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1444:C:P	21:An:30:LEU:HD13	1.88	1.12
79:By:8:VAL:HG23	79:By:11:LYS:HE3	1.12	1.11
70:Bq:17:PRO:HB2	70:Bq:20:LYS:HD3	1.23	1.11
70:Bq:66:VAL:HG23	70:Bq:71:VAL:HA	1.32	1.11
26:B0:4294:U:P	70:Bq:7:ARG:NH2	2.23	1.11
77:Bw:238:PRO:HG3	77:Bw:269:MET:HE2	1.32	1.11
86:B6:81:LEU:HD22	86:B6:91:VAL:HB	1.33	1.11
51:BY:26:C:P	66:Bn:57:ARG:HH11	1.74	1.10
17:Aj:67:LYS:HE2	17:Aj:78:ASP:HB2	1.30	1.10
26:B0:1817:U:P	77:Bw:135:ARG:NH1	2.24	1.10
79:By:19:LYS:HD2	79:By:21:ILE:HD13	1.30	1.10
66:Bn:14:ARG:CZ	70:Bq:18:PHE:CB	2.28	1.10
84:B4:70:LEU:HD11	84:B4:83:LEU:HD11	1.28	1.10
62:Bj:54:LEU:HD12	62:Bj:58:ARG:HG2	1.19	1.09
66:Bn:40:LYS:HE2	70:Bq:67:THR:CB	1.80	1.09
66:Bn:193:VAL:HG23	66:Bn:235:MET:O	1.51	1.09
8:AH:16:G:P	21:An:30:LEU:CB	2.28	1.08
68:Bp:32:ILE:HD12	68:Bp:50:ILE:HD11	1.33	1.08
79:By:11:LYS:CG	80:B9:69:MET:HE1	1.82	1.08
79:By:8:VAL:HA	79:By:11:LYS:HD2	1.30	1.08
79:By:22:ARG:HG3	79:By:36:ARG:HD3	1.35	1.08
80:B9:87:VAL:HG12	80:B9:89:LEU:H	1.17	1.08
62:Bj:11:ARG:HB2	62:Bj:36:ARG:HD3	1.30	1.08
26:B0:4330:G:P	84:B4:85:ILE:HD13	1.93	1.08
66:Bn:14:ARG:NH2	70:Bq:18:PHE:CG	2.07	1.08
77:Bw:173:ASN:HB3	77:Bw:213:ILE:HD13	1.32	1.08
85:B5:106:ALA:HB1	85:B5:110:LEU:HD12	1.35	1.08
1:AA:1653:C:P	21:An:38:MET:CE	2.42	1.07
85:B5:74:VAL:HG21	85:B5:142:ILE:HD12	1.36	1.07
62:Bj:36:ARG:HB2	62:Bj:107:ILE:HA	1.30	1.07
84:B4:34:TYR:HA	84:B4:38:LYS:HD2	1.32	1.07
81:Bz:42:CYS:SG	86:B6:53:PRO:HB2	1.94	1.07
8:AH:16:G:P	21:An:30:LEU:HD13	1.90	1.07
77:Bw:115:ILE:HD12	77:Bw:235:LEU:HD11	1.07	1.07
1:AA:660:A:P	12:Ad:72:ARG:NH1	2.28	1.06
26:B0:2292:G:P	80:B9:71:PRO:HG3	1.96	1.06
62:Bj:40:ILE:HG23	62:Bj:137:LEU:HD13	1.36	1.06
83:B3:23:ILE:HG21	83:B3:35:ILE:HG22	1.32	1.06
66:Bn:14:ARG:NH2	70:Bq:18:PHE:CD2	2.23	1.06
79:By:11:LYS:CE	80:B9:69:MET:CE	1.91	1.06
79:By:37:LYS:HD2	79:By:38:PRO:HD2	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:B9:79:VAL:HG23	80:B9:84:GLU:HB2	1.36	1.06
84:B4:65:LYS:HB3	84:B4:85:ILE:HG12	1.37	1.06
77:Bw:117:ILE:HG13	77:Bw:245:LYS:HE3	1.31	1.06
79:By:45:VAL:HA	79:By:53:ILE:HD13	1.37	1.06
66:Bn:14:ARG:CZ	70:Bq:18:PHE:HB3	1.81	1.06
66:Bn:42:LYS:HE2	70:Bq:33:TYR:N	1.69	1.05
66:Bn:192:GLU:HA	66:Bn:238:MET:HB3	1.37	1.05
70:Bq:38:ILE:HD12	70:Bq:98:SER:HB3	1.30	1.05
26:B0:4323:A:P	84:B4:36:GLN:CA	2.44	1.05
66:Bn:40:LYS:CE	70:Bq:67:THR:N	2.19	1.05
62:Bj:91:THR:HG23	62:Bj:94:GLY:H	1.19	1.05
1:AA:1444:C:P	21:An:30:LEU:CD1	2.44	1.05
51:BY:11:A:P	66:Bn:16:GLN:O	2.14	1.05
68:Bp:9:ARG:HD2	68:Bp:10:LEU:HD12	1.07	1.05
64:Bl:101:ILE:HG13	64:Bl:104:VAL:HG22	1.37	1.05
79:By:11:LYS:HG3	80:B9:69:MET:HE1	1.09	1.05
82:B2:18:LEU:HB2	82:B2:25:LYS:HA	1.34	1.04
1:AA:1149:A:P	22:Ao:37:ARG:HH12	1.79	1.04
64:Bl:117:LEU:HD21	64:Bl:136:LYS:HD2	1.40	1.04
66:Bn:14:ARG:CZ	70:Bq:18:PHE:HD2	1.59	1.04
17:Aj:46:LYS:HD2	17:Aj:96:GLU:HG2	1.38	1.04
26:B0:2650:G:P	86:B6:92:CYS:H	1.80	1.04
26:B0:4192:U:P	84:B4:2:VAL:CG2	2.45	1.04
64:Bl:73:VAL:HG21	64:Bl:101:ILE:HG22	1.40	1.03
66:Bn:38:GLN:CD	70:Bq:29:TYR:HD2	1.60	1.03
26:B0:4330:G:P	84:B4:85:ILE:CD1	2.47	1.03
84:B4:40:ARG:HA	84:B4:44:LYS:HB3	1.38	1.03
26:B0:4478:A:P	54:Bb:257:HIS:H	1.82	1.03
62:Bj:7:VAL:HG23	62:Bj:115:LYS:HA	1.41	1.03
26:B0:4263:C:P	70:Bq:80:LYS:O	2.17	1.02
8:AH:17:C:P	21:An:19:ARG:O	2.17	1.02
64:Bl:117:LEU:HD22	64:Bl:136:LYS:HB3	1.41	1.02
70:Bq:79:VAL:HG12	70:Bq:82:LYS:HB2	1.39	1.01
77:Bw:193:ASP:HA	77:Bw:196:LEU:HD21	1.42	1.01
26:B0:4262:U:P	70:Bq:81:GLY:HA3	1.98	1.01
68:Bp:24:LEU:HD23	68:Bp:32:ILE:HD13	1.41	1.01
26:B0:1298:C:P	64:Bl:25:HIS:CB	2.47	1.01
26:B0:2611:C:P	68:Bp:60:ARG:CG	2.47	1.01
62:Bj:40:ILE:HD13	62:Bj:79:PHE:HE2	1.23	1.01
66:Bn:85:TYR:CG	66:Bn:246:ILE:HG22	1.96	1.01
17:Aj:50:VAL:HG11	17:Aj:89:ILE:HG12	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:202:THR:HG23	85:B5:205:GLY:H	1.24	1.00
62:Bj:36:ARG:HD2	62:Bj:107:ILE:HB	1.40	1.00
77:Bw:118:ARG:HD2	77:Bw:161:TYR:HB3	1.44	1.00
17:Aj:72:GLU:HG2	21:An:54:LYS:HD3	1.41	1.00
26:B0:1816:A:P	77:Bw:135:ARG:HG3	2.00	1.00
62:Bj:21:ILE:HD12	62:Bj:24:LYS:HD2	1.43	1.00
79:By:19:LYS:HB2	79:By:21:ILE:HD11	1.44	1.00
62:Bj:15:LEU:HA	62:Bj:40:ILE:HD11	1.43	0.99
62:Bj:58:ARG:HB2	62:Bj:61:MET:HB3	1.44	0.99
77:Bw:127:VAL:HG22	77:Bw:157:ILE:HD11	1.44	0.99
26:B0:2867:C:P	68:Bp:74:ARG:CZ	2.51	0.99
66:Bn:40:LYS:HE2	70:Bq:67:THR:N	1.78	0.99
66:Bn:40:LYS:HE3	70:Bq:67:THR:O	1.59	0.99
85:B5:84:LEU:HD23	85:B5:110:LEU:HD21	1.42	0.99
17:Aj:72:GLU:HG2	21:An:54:LYS:HG3	1.39	0.99
26:B0:1713:G:P	70:Bq:12:TYR:CD2	2.56	0.99
79:By:11:LYS:HG3	80:B9:69:MET:CE	1.92	0.99
26:B0:1830:U:P	64:Bl:21:ARG:HH22	1.85	0.98
66:Bn:38:GLN:O	70:Bq:29:TYR:CE2	2.16	0.98
70:Bq:79:VAL:HG13	70:Bq:82:LYS:H	1.24	0.98
86:B6:22:MET:HA	86:B6:27:TYR:CD2	1.99	0.98
26:B0:4322:A:P	84:B4:34:TYR:O	2.20	0.98
66:Bn:40:LYS:CD	70:Bq:67:THR:O	2.11	0.98
62:Bj:36:ARG:HH11	62:Bj:107:ILE:HB	1.27	0.98
62:Bj:61:MET:HA	62:Bj:61:MET:HE3	1.45	0.98
66:Bn:38:GLN:CG	70:Bq:29:TYR:CE2	2.46	0.98
81:Bz:46:LYS:HD2	81:Bz:59:SER:HB2	1.45	0.98
86:B6:31:TYR:HA	86:B6:93:THR:HG21	1.46	0.98
26:B0:23:C:P	82:B2:44:LYS:HE3	2.03	0.97
86:B6:71:VAL:HG23	86:B6:109:PRO:HA	1.45	0.97
62:Bj:64:ASN:HA	62:Bj:69:PRO:HB3	1.44	0.97
26:B0:4478:A:P	54:Bb:257:HIS:HB2	2.04	0.97
83:B3:27:ILE:HG12	83:B3:35:ILE:HD12	1.43	0.96
62:Bj:26:VAL:HB	62:Bj:101:LEU:HD21	1.43	0.96
64:Bl:14:HIS:CD2	79:By:39:ARG:HH12	1.84	0.96
66:Bn:40:LYS:HG2	70:Bq:67:THR:O	1.58	0.96
79:By:11:LYS:CD	80:B9:69:MET:CE	2.42	0.96
79:By:66:THR:O	80:B9:69:MET:SD	2.23	0.96
82:B2:31:LYS:HD2	82:B2:33:THR:H	1.26	0.96
26:B0:2768:C:P	82:B2:11:ARG:NH2	2.38	0.96
66:Bn:52:VAL:HG21	66:Bn:158:VAL:HG23	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Bz:11:VAL:HG22	81:Bz:27:LYS:HD3	1.44	0.96
64:Bl:97:VAL:HG11	64:Bl:109:TYR:CZ	2.00	0.96
26:B0:1830:U:P	64:Bl:21:ARG:NH2	2.39	0.96
77:Bw:131:LEU:HD21	77:Bw:136:LEU:HB2	1.47	0.96
86:B6:51:ASN:HB3	86:B6:78:ASN:HD21	1.30	0.96
62:Bj:72:PHE:HB2	62:Bj:77:ARG:HG3	1.47	0.96
81:Bz:42:CYS:SG	86:B6:53:PRO:CG	2.54	0.96
77:Bw:135:ARG:HG3	77:Bw:231:TRP:CZ2	2.01	0.96
62:Bj:15:LEU:HD21	62:Bj:137:LEU:HD11	1.45	0.95
1:AA:1800:U:P	17:Aj:77:TRP:CZ2	2.58	0.95
62:Bj:72:PHE:CE1	62:Bj:78:ILE:HG12	2.01	0.95
79:By:11:LYS:NZ	80:B9:69:MET:HE2	1.80	0.95
85:B5:159:PHE:CZ	85:B5:161:THR:HB	2.00	0.95
81:Bz:11:VAL:HB	81:Bz:23:ARG:HG3	1.48	0.95
21:An:26:ASN:H	21:An:38:MET:HB2	1.31	0.95
26:B0:4324:G:P	84:B4:36:GLN:OE1	2.25	0.95
66:Bn:185:GLU:HG2	66:Bn:201:GLN:HB2	1.49	0.95
77:Bw:215:GLU:HG2	77:Bw:223:PHE:CE2	2.01	0.95
79:By:27:ARG:HD3	79:By:28:TYR:CD1	2.01	0.95
62:Bj:15:LEU:HD12	62:Bj:40:ILE:HG12	1.46	0.95
17:Aj:40:ILE:HB	17:Aj:89:ILE:HD11	1.49	0.95
66:Bn:40:LYS:CD	70:Bq:67:THR:C	2.40	0.95
66:Bn:187:LYS:HE2	66:Bn:188:GLU:HG2	1.48	0.95
85:B5:151:LEU:HD12	85:B5:159:PHE:CE1	2.01	0.95
26:B0:4021:A:P	85:B5:199:TYR:CD2	2.59	0.94
62:Bj:15:LEU:HD21	62:Bj:137:LEU:HD21	1.50	0.94
17:Aj:72:GLU:CG	21:An:54:LYS:HD3	1.96	0.94
85:B5:103:PHE:CD1	85:B5:145:MET:HE3	2.02	0.94
26:B0:4322:A:P	84:B4:34:TYR:C	2.49	0.94
85:B5:84:LEU:HD11	85:B5:118:LEU:HD21	1.48	0.94
26:B0:4022:C:P	85:B5:197:THR:N	2.41	0.94
51:BY:49:A:P	66:Bn:219:LYS:HG3	2.08	0.94
62:Bj:54:LEU:HD12	62:Bj:58:ARG:CG	1.98	0.94
66:Bn:41:ASN:OD1	70:Bq:71:VAL:HG13	1.67	0.94
77:Bw:219:VAL:HB	77:Bw:222:ARG:HB3	1.47	0.94
86:B6:79:ILE:HG22	86:B6:90:ARG:HG2	1.50	0.94
68:Bp:9:ARG:HD2	68:Bp:10:LEU:CD1	1.98	0.94
26:B0:1713:G:P	70:Bq:12:TYR:CB	2.56	0.94
62:Bj:9:ASP:HB2	62:Bj:115:LYS:HB2	1.45	0.94
62:Bj:35:VAL:HB	62:Bj:115:LYS:HG2	1.48	0.94
81:Bz:42:CYS:HA	86:B6:53:PRO:HB3	0.93	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Aj:67:LYS:H	17:Aj:76:THR:HG23	1.32	0.93
17:Aj:72:GLU:CG	21:An:54:LYS:CD	2.44	0.93
1:AA:1653:C:P	21:An:42:CYS:HB2	2.08	0.93
79:By:11:LYS:CD	80:B9:69:MET:HE2	1.98	0.93
66:Bn:40:LYS:HE3	70:Bq:66:VAL:HG22	1.47	0.93
26:B0:4608:A:P	68:Bp:62:ARG:NH1	2.41	0.93
26:B0:2650:G:P	86:B6:91:VAL:HA	2.09	0.93
68:Bp:119:MET:HA	68:Bp:119:MET:HE2	1.50	0.93
77:Bw:115:ILE:CD1	77:Bw:235:LEU:HD11	1.98	0.93
82:B2:45:ARG:HD3	82:B2:47:TYR:CE2	2.03	0.93
85:B5:62:PHE:CG	85:B5:110:LEU:HG	2.03	0.93
86:B6:37:MET:HE1	86:B6:97:ILE:HA	1.48	0.93
70:Bq:44:MET:HE2	70:Bq:44:MET:HA	1.48	0.93
85:B5:151:LEU:HD12	85:B5:159:PHE:CD1	2.04	0.93
86:B6:6:LYS:HE3	86:B6:73:HIS:HB2	1.49	0.93
77:Bw:131:LEU:CD2	77:Bw:136:LEU:HB2	1.99	0.92
12:Ad:100:LEU:HD23	12:Ad:120:VAL:HG21	1.50	0.92
64:Bl:101:ILE:CG1	64:Bl:104:VAL:HG22	1.98	0.92
77:Bw:239:ARG:HG2	77:Bw:268:ARG:CB	2.00	0.92
21:An:26:ASN:HB2	21:An:38:MET:HA	1.50	0.92
77:Bw:118:ARG:HB2	77:Bw:161:TYR:HB2	1.48	0.92
85:B5:84:LEU:CD2	85:B5:110:LEU:HD21	1.98	0.92
79:By:22:ARG:HG3	79:By:36:ARG:CD	2.00	0.92
82:B2:18:LEU:HB2	82:B2:25:LYS:CA	1.99	0.92
84:B4:53:LYS:HB2	84:B4:54:PRO:HD3	1.52	0.92
62:Bj:7:VAL:HG12	62:Bj:33:VAL:CG1	2.00	0.92
66:Bn:184:SER:HB3	66:Bn:199:MET:N	1.83	0.92
70:Bq:24:VAL:HB	70:Bq:46:THR:HG21	1.49	0.92
17:Aj:66:ARG:HG3	17:Aj:77:TRP:CD1	2.05	0.92
62:Bj:124:LYS:HB2	62:Bj:130:PRO:HD3	1.52	0.92
82:B2:37:CYS:HG	82:B2:39:TYR:HD1	1.07	0.92
86:B6:20:LEU:HD13	86:B6:104:ILE:HD13	1.50	0.92
86:B6:96:ILE:CD1	86:B6:105:ILE:HD11	2.00	0.92
85:B5:110:LEU:CD1	85:B5:114:ILE:HB	2.00	0.92
84:B4:37:GLY:HA2	84:B4:40:ARG:HB3	1.52	0.91
17:Aj:67:LYS:HE2	17:Aj:78:ASP:CB	2.01	0.91
26:B0:1572:A:P	54:Bb:245:ARG:HH11	1.92	0.91
66:Bn:38:GLN:CG	70:Bq:29:TYR:CD2	2.53	0.91
85:B5:5:ILE:CD1	85:B5:177:ILE:HG21	1.99	0.91
79:By:11:LYS:CG	80:B9:69:MET:CE	2.49	0.91
85:B5:159:PHE:CE2	85:B5:161:THR:HB	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bj:54:LEU:HD23	62:Bj:141:ALA:HA	1.51	0.91
1:AA:660:A:P	12:Ad:72:ARG:CZ	2.59	0.91
39:BM:2686:U:P	68:Bp:43:LYS:HE2	2.10	0.91
82:B2:18:LEU:HD23	82:B2:24:SER:H	1.34	0.91
62:Bj:32:VAL:HB	62:Bj:101:LEU:HD12	1.52	0.91
82:B2:28:HIS:HB3	82:B2:31:LYS:CG	1.99	0.91
85:B5:110:LEU:HD11	85:B5:114:ILE:HB	1.52	0.91
26:B0:2643:U:P	68:Bp:103:ARG:HH22	1.94	0.91
66:Bn:40:LYS:HE2	70:Bq:67:THR:O	1.45	0.91
85:B5:62:PHE:CE1	85:B5:81:GLU:HG2	2.05	0.91
86:B6:98:ASP:HB3	86:B6:99:PRO:HD3	1.51	0.91
62:Bj:8:LEU:HD12	62:Bj:18:LEU:HD11	1.52	0.90
79:By:9:LYS:HB3	79:By:10:PRO:HD3	1.51	0.90
82:B2:18:LEU:HD12	82:B2:19:CYS:H	1.33	0.90
82:B2:28:HIS:C	82:B2:31:LYS:HE2	1.96	0.90
86:B6:26:LYS:HB3	86:B6:97:ILE:HG12	1.53	0.90
26:B0:1493:U:P	64:Bl:33:GLY:CA	2.58	0.90
68:Bp:25:ASP:HB3	68:Bp:28:GLU:HG2	1.54	0.90
77:Bw:127:VAL:HG22	77:Bw:157:ILE:CD1	2.01	0.90
66:Bn:185:GLU:HG3	66:Bn:237:GLU:OE1	1.69	0.90
84:B4:70:LEU:HD11	84:B4:83:LEU:CD1	2.01	0.90
85:B5:60:VAL:HG13	85:B5:101:THR:HG21	1.52	0.90
62:Bj:40:ILE:HD13	62:Bj:79:PHE:CE2	2.05	0.90
70:Bq:71:VAL:HB	70:Bq:74:ILE:CD1	2.02	0.90
85:B5:59:ILE:CD1	85:B5:145:MET:HB3	2.00	0.90
86:B6:77:ASN:HB3	86:B6:79:ILE:CD1	2.01	0.90
82:B2:27:TYR:HD1	82:B2:29:LEU:HD22	1.37	0.90
85:B5:58:THR:CG2	85:B5:101:THR:HA	2.01	0.90
68:Bp:32:ILE:CD1	68:Bp:50:ILE:HD11	2.02	0.90
84:B4:69:ARG:CG	84:B4:80:LYS:HD3	2.02	0.90
62:Bj:15:LEU:CD1	62:Bj:40:ILE:HG12	2.01	0.90
82:B2:18:LEU:HD23	82:B2:24:SER:N	1.84	0.90
85:B5:105:ILE:HG22	85:B5:132:LEU:HG	1.54	0.90
79:By:7:LEU:HD11	79:By:63:ASN:CB	2.02	0.89
85:B5:87:LEU:HB3	85:B5:117:TYR:CZ	2.05	0.89
21:An:10:HIS:HB2	21:An:11:PRO:HD3	1.53	0.89
64:Bl:125:LYS:HG2	64:Bl:145:VAL:HG11	1.50	0.89
25:B1:105:A:P	82:B2:39:TYR:HE2	1.94	0.89
26:B0:2296:G:P	79:By:35:TRP:CZ3	2.65	0.89
62:Bj:25:GLN:HG2	62:Bj:30:ARG:HB2	1.52	0.89
85:B5:62:PHE:CZ	85:B5:81:GLU:HA	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:74:VAL:CG2	85:B5:139:VAL:HA	2.03	0.89
26:B0:2867:C:P	68:Bp:74:ARG:NH2	2.46	0.89
79:By:28:TYR:CD2	79:By:30:LYS:HG3	2.07	0.89
82:B2:18:LEU:HD12	82:B2:27:TYR:HB2	1.52	0.89
26:B0:2814:U:P	54:Bb:248:ARG:HG2	2.12	0.89
68:Bp:44:LEU:HD22	68:Bp:49:LEU:HD22	1.52	0.89
86:B6:14:ILE:CG2	86:B6:108:MET:HE2	2.03	0.89
26:B0:1572:A:P	54:Bb:245:ARG:NH1	2.47	0.88
62:Bj:54:LEU:HB3	62:Bj:140:LEU:CD2	2.02	0.88
77:Bw:115:ILE:HD12	77:Bw:235:LEU:CD1	2.01	0.88
21:An:21:CYS:HB3	21:An:38:MET:N	1.87	0.88
26:B0:1581:U:P	82:B2:3:LYS:CG	2.62	0.88
26:B0:4294:U:P	70:Bq:7:ARG:HH22	1.96	0.88
62:Bj:40:ILE:HG23	62:Bj:137:LEU:CD1	2.04	0.88
9:Aa:17:TRP:HA	9:Aa:305:ASN:HB3	1.55	0.88
64:Bl:76:ASP:HA	64:Bl:79:TRP:CD1	2.08	0.88
77:Bw:216:ILE:HA	77:Bw:219:VAL:HG12	1.56	0.88
85:B5:74:VAL:HG11	85:B5:142:ILE:CG2	2.03	0.88
1:AA:1655:G:P	21:An:40:ARG:NH1	2.47	0.88
79:By:8:VAL:CG2	79:By:11:LYS:HE3	2.02	0.88
17:Aj:72:GLU:HG3	21:An:54:LYS:HG2	1.54	0.88
66:Bn:102:LEU:HD22	66:Bn:246:ILE:HD11	1.52	0.88
66:Bn:38:GLN:HG2	70:Bq:29:TYR:HE2	1.37	0.88
85:B5:5:ILE:HD13	85:B5:177:ILE:HG21	1.54	0.88
86:B6:71:VAL:CG2	86:B6:109:PRO:HA	2.04	0.88
26:B0:4676:C:P	54:Bb:275:HIS:CE1	2.67	0.88
62:Bj:50:LYS:HB2	62:Bj:55:ALA:CB	2.04	0.88
77:Bw:113:PHE:HE2	77:Bw:115:ILE:HD11	1.37	0.87
51:BY:26:C:P	66:Bn:57:ARG:CD	2.63	0.87
64:Bl:101:ILE:HG21	64:Bl:109:TYR:CD1	2.09	0.87
85:B5:74:VAL:HG11	85:B5:142:ILE:HB	1.56	0.87
70:Bq:36:GLY:HA2	70:Bq:62:ARG:HD3	1.57	0.87
66:Bn:40:LYS:HZ3	70:Bq:67:THR:HB	1.12	0.87
79:By:28:TYR:HE2	79:By:30:LYS:HD2	1.38	0.87
85:B5:151:LEU:HA	85:B5:159:PHE:CE1	2.10	0.87
17:Aj:107:GLU:HG3	17:Aj:109:GLY:H	1.40	0.87
21:An:39:CYS:SG	21:An:41:GLN:HB3	2.14	0.87
66:Bn:184:SER:HB3	66:Bn:199:MET:H	1.33	0.87
26:B0:4322:A:P	84:B4:34:TYR:CB	0.97	0.87
66:Bn:38:GLN:OE1	70:Bq:29:TYR:HD2	1.57	0.87
80:B9:82:VAL:HG23	80:B9:83:LYS:HD2	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B0:2867:C:P	68:Bp:74:ARG:NH1	2.48	0.87
66:Bn:85:TYR:CD1	66:Bn:246:ILE:HG22	2.10	0.87
1:AA:1655:G:P	21:An:40:ARG:HH12	1.98	0.87
77:Bw:117:ILE:HG13	77:Bw:245:LYS:CE	2.05	0.87
62:Bj:32:VAL:HB	62:Bj:101:LEU:CD1	2.04	0.86
86:B6:77:ASN:HB3	86:B6:79:ILE:HD13	1.55	0.86
62:Bj:26:VAL:CB	62:Bj:101:LEU:HD21	2.04	0.86
17:Aj:25:THR:HG22	17:Aj:86:LYS:HD2	1.54	0.86
77:Bw:239:ARG:HG2	77:Bw:268:ARG:HB2	1.57	0.86
86:B6:96:ILE:HD13	86:B6:105:ILE:CD1	2.05	0.86
70:Bq:64:TYR:CE1	70:Bq:76:ASN:HB2	2.10	0.86
79:By:48:ARG:HE	79:By:53:ILE:HG21	1.39	0.86
21:An:30:LEU:CA	21:An:37:ASN:HA	2.03	0.86
21:An:34:TYR:HB3	21:An:36:LEU:HD23	1.57	0.86
85:B5:59:ILE:HD11	85:B5:146:LYS:N	1.89	0.86
86:B6:45:LEU:HD12	86:B6:71:VAL:HB	1.57	0.86
79:By:28:TYR:HD2	79:By:30:LYS:HG3	1.37	0.86
85:B5:60:VAL:HG21	85:B5:104:PHE:CD2	2.10	0.86
77:Bw:196:LEU:HD11	77:Bw:209:MET:HA	1.58	0.86
79:By:37:LYS:CD	79:By:38:PRO:HD2	2.06	0.86
85:B5:117:TYR:HD2	85:B5:118:LEU:HD22	1.40	0.86
85:B5:74:VAL:HG22	85:B5:139:VAL:HA	1.58	0.86
85:B5:143:GLU:HA	85:B5:146:LYS:CE	2.05	0.85
1:AA:1435:G:P	21:An:13:LYS:HD2	2.14	0.85
17:Aj:24:LEU:HB3	17:Aj:32:LEU:HD11	1.57	0.85
68:Bp:28:GLU:HG3	68:Bp:49:LEU:HG	1.55	0.85
77:Bw:239:ARG:H	77:Bw:268:ARG:HB2	1.40	0.85
81:Bz:11:VAL:CB	81:Bz:23:ARG:HG3	2.05	0.85
17:Aj:24:LEU:CB	17:Aj:32:LEU:HD11	2.07	0.85
51:BY:26:C:P	66:Bn:57:ARG:CB	2.64	0.85
66:Bn:42:LYS:N	70:Bq:32:ILE:HG12	1.91	0.85
69:B7:198:ARG:HA	69:B7:201:ARG:HE	1.42	0.85
85:B5:34:LEU:HD21	85:B5:40:SER:HB3	1.58	0.85
86:B6:44:LYS:HD3	86:B6:98:ASP:HA	1.58	0.85
1:AA:1540:C:P	9:Aa:60:ARG:HA	2.17	0.85
66:Bn:108:LEU:HD22	66:Bn:170:LEU:HD11	1.58	0.85
70:Bq:66:VAL:HA	70:Bq:74:ILE:HG21	1.57	0.85
62:Bj:27:LEU:HD21	62:Bj:87:LEU:HD22	1.55	0.85
70:Bq:38:ILE:CD1	70:Bq:98:SER:HB3	2.06	0.85
70:Bq:82:LYS:HG3	70:Bq:86:LYS:HB2	1.58	0.85
85:B5:59:ILE:HD13	85:B5:145:MET:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bj:36:ARG:CB	62:Bj:107:ILE:HA	2.07	0.85
85:B5:78:VAL:C	85:B5:79:LEU:HD12	2.02	0.85
85:B5:94:ALA:HB2	85:B5:117:TYR:CZ	2.11	0.85
26:B0:1597:G:P	82:B2:10:LYS:HG2	2.15	0.85
62:Bj:8:LEU:HD13	62:Bj:9:ASP:N	1.92	0.85
77:Bw:230:LEU:HD12	77:Bw:232:PRO:HD3	1.60	0.84
86:B6:50:ASN:HD22	86:B6:76:GLY:HA2	1.42	0.84
17:Aj:40:ILE:HB	17:Aj:89:ILE:CD1	2.06	0.84
26:B0:1885:A:P	77:Bw:244:LYS:NZ	2.51	0.84
64:Bl:11:LEU:HD23	64:Bl:12:ARG:H	1.40	0.84
66:Bn:14:ARG:NH1	70:Bq:18:PHE:HB3	1.91	0.84
70:Bq:72:GLY:O	70:Bq:89:ASN:HA	1.76	0.84
62:Bj:79:PHE:O	62:Bj:82:THR:HG22	1.77	0.84
70:Bq:82:LYS:HD3	70:Bq:85:ALA:CA	2.08	0.84
79:By:15:LYS:HD3	79:By:16:ARG:N	1.92	0.84
85:B5:62:PHE:CD1	85:B5:110:LEU:HG	2.12	0.84
12:Ad:73:GLN:HA	12:Ad:76:ASN:ND2	1.93	0.84
62:Bj:15:LEU:HA	62:Bj:40:ILE:CD1	2.08	0.84
62:Bj:15:LEU:CD2	62:Bj:137:LEU:HD11	2.08	0.84
85:B5:103:PHE:CZ	85:B5:148:THR:HG23	2.12	0.84
21:An:26:ASN:HB2	21:An:38:MET:CA	2.07	0.84
51:BY:7:G:P	66:Bn:27:THR:CG2	2.65	0.84
80:B9:92:ASN:HB3	80:B9:119:ALA:O	1.78	0.84
77:Bw:214:HIS:HA	77:Bw:217:TYR:HD2	1.42	0.84
82:B2:27:TYR:CE1	82:B2:29:LEU:HD13	2.13	0.84
9:Aa:14:HIS:CE1	9:Aa:18:VAL:HG13	2.13	0.84
26:B0:4250:U:P	84:B4:9:ARG:HH12	2.00	0.84
26:B0:4323:A:P	84:B4:35:ALA:C	2.60	0.84
64:Bl:76:ASP:HA	64:Bl:79:TRP:HD1	1.40	0.84
77:Bw:219:VAL:HB	77:Bw:222:ARG:CB	2.07	0.84
79:By:5:ARG:HB2	79:By:6:PRO:HD3	1.58	0.84
85:B5:62:PHE:CZ	85:B5:81:GLU:HG2	2.12	0.84
26:B0:1296:G:P	79:By:43:ASN:HD21	2.01	0.84
86:B6:81:LEU:HD21	86:B6:94:LEU:HG	1.59	0.84
77:Bw:214:HIS:HA	77:Bw:217:TYR:CD2	2.13	0.83
79:By:11:LYS:HE2	80:B9:69:MET:HE3	1.52	0.83
85:B5:84:LEU:HD11	85:B5:118:LEU:CD2	2.07	0.83
77:Bw:244:LYS:HD3	77:Bw:245:LYS:N	1.93	0.83
77:Bw:224:LYS:HB3	77:Bw:231:TRP:HB3	1.58	0.83
17:Aj:47:ASN:CG	17:Aj:93:SER:HB2	2.04	0.83
77:Bw:196:LEU:HD23	77:Bw:196:LEU:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bj:37:CYS:O	62:Bj:40:ILE:HG22	1.78	0.83
66:Bn:14:ARG:CZ	70:Bq:18:PHE:CG	2.52	0.83
66:Bn:189:PHE:O	66:Bn:238:MET:HE1	1.79	0.83
68:Bp:104:ARG:HA	68:Bp:107:ARG:HE	1.41	0.83
85:B5:74:VAL:HG11	85:B5:142:ILE:CB	2.09	0.83
62:Bj:74:ALA:HB1	62:Bj:75:PRO:HD2	1.59	0.83
26:B0:4322:A:P	84:B4:34:TYR:HB2	0.29	0.83
64:Bl:8:THR:O	64:Bl:11:LEU:HD22	1.78	0.83
64:Bl:79:TRP:HB2	64:Bl:118:PRO:HB3	1.59	0.83
77:Bw:224:LYS:O	77:Bw:229:PHE:HB3	1.79	0.83
86:B6:4:ALA:HB3	86:B6:73:HIS:CD2	2.13	0.83
64:Bl:14:HIS:CD2	79:By:39:ARG:NH1	2.46	0.83
70:Bq:39:VAL:CG2	70:Bq:95:ILE:HD11	2.08	0.83
77:Bw:215:GLU:HG2	77:Bw:223:PHE:HE2	1.40	0.83
81:Bz:11:VAL:HG11	81:Bz:23:ARG:O	1.78	0.83
85:B5:34:LEU:HB3	85:B5:157:ARG:CD	2.08	0.83
85:B5:106:ALA:CB	85:B5:110:LEU:HD12	2.09	0.82
66:Bn:77:ARG:HG3	66:Bn:100:THR:HG23	1.61	0.82
84:B4:23:VAL:HG23	84:B4:70:LEU:HD23	1.61	0.82
62:Bj:35:VAL:HG11	62:Bj:115:LYS:HD2	1.61	0.82
64:Bl:117:LEU:HD13	64:Bl:136:LYS:CA	2.09	0.82
77:Bw:113:PHE:CE2	77:Bw:115:ILE:HD11	2.14	0.82
85:B5:110:LEU:HD22	85:B5:113:ASP:HB2	1.61	0.82
86:B6:21:VAL:HG11	86:B6:96:ILE:HG13	1.58	0.82
79:By:45:VAL:HA	79:By:53:ILE:CD1	2.09	0.82
26:B0:2384:G:P	83:B3:44:TRP:HB3	2.20	0.82
77:Bw:133:LEU:HD13	77:Bw:134:LEU:N	1.93	0.82
80:B9:114:ARG:O	80:B9:118:LEU:HD13	1.78	0.82
86:B6:45:LEU:HD12	86:B6:71:VAL:CB	2.09	0.82
62:Bj:54:LEU:HA	62:Bj:58:ARG:CG	2.10	0.82
81:Bz:25:MET:HA	81:Bz:28:LYS:CE	2.09	0.82
62:Bj:88:PRO:O	62:Bj:94:GLY:HA3	1.79	0.82
83:B3:24:PRO:O	83:B3:27:ILE:HG22	1.78	0.82
62:Bj:36:ARG:HD2	62:Bj:107:ILE:CB	2.10	0.82
62:Bj:118:VAL:HG22	62:Bj:120:PRO:HD2	1.62	0.82
84:B4:69:ARG:HD2	84:B4:80:LYS:HD3	1.62	0.82
85:B5:43:VAL:HG13	85:B5:188:LEU:CD1	2.10	0.82
21:An:21:CYS:N	21:An:37:ASN:HB2	1.95	0.81
77:Bw:174:GLU:O	77:Bw:177:TYR:HB3	1.80	0.81
62:Bj:73:ARG:H	62:Bj:77:ARG:HE	1.28	0.81
84:B4:69:ARG:CD	84:B4:80:LYS:HD3	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B0:4168:U:P	70:Bq:8:ARG:HG3	2.17	0.81
62:Bj:26:VAL:HG11	62:Bj:87:LEU:HD11	1.63	0.81
62:Bj:26:VAL:HG21	62:Bj:97:ALA:O	1.80	0.81
83:B3:23:ILE:CG2	83:B3:35:ILE:HG22	2.10	0.81
85:B5:74:VAL:CG2	85:B5:142:ILE:HD12	2.10	0.81
25:B1:54:A:P	83:B3:21:ARG:CD	2.69	0.81
62:Bj:72:PHE:CD2	62:Bj:81:ARG:HG3	2.15	0.81
70:Bq:17:PRO:CB	70:Bq:20:LYS:HD3	2.08	0.81
77:Bw:129:LYS:O	77:Bw:132:GLN:HB3	1.81	0.81
83:B3:8:ARG:O	83:B3:11:ARG:HG2	1.80	0.81
85:B5:34:LEU:CD2	85:B5:40:SER:HB3	2.10	0.81
8:AH:9:G:P	21:An:13:LYS:HD2	2.20	0.81
62:Bj:96:ALA:O	62:Bj:100:ARG:HG3	1.81	0.81
66:Bn:77:ARG:HD3	66:Bn:81:GLU:CG	2.11	0.81
66:Bn:191:ALA:HB3	66:Bn:238:MET:SD	2.21	0.81
85:B5:5:ILE:CD1	85:B5:177:ILE:HD13	2.09	0.81
64:Bl:73:VAL:CG2	64:Bl:101:ILE:HG22	2.10	0.81
70:Bq:35:LYS:HD2	70:Bq:65:ASN:HA	1.62	0.81
77:Bw:158:VAL:HG13	77:Bw:162:ILE:HG12	1.60	0.81
85:B5:62:PHE:CD2	85:B5:110:LEU:HG	2.14	0.81
64:Bl:117:LEU:CD2	64:Bl:136:LYS:HB3	2.11	0.81
79:By:8:VAL:HG23	79:By:11:LYS:CE	2.05	0.81
80:B9:87:VAL:HG12	80:B9:89:LEU:N	1.96	0.81
51:BY:26:C:P	66:Bn:57:ARG:NH1	2.52	0.80
64:Bl:16:SER:CA	64:Bl:19:HIS:HB2	2.11	0.80
77:Bw:210:GLU:HA	77:Bw:213:ILE:HG12	1.61	0.80
85:B5:143:GLU:CA	85:B5:146:LYS:HE2	2.10	0.80
26:B0:1713:G:P	70:Bq:12:TYR:CG	2.74	0.80
79:By:7:LEU:HD11	79:By:63:ASN:CG	2.06	0.80
81:Bz:46:LYS:HD3	81:Bz:59:SER:N	1.96	0.80
85:B5:117:TYR:CD2	85:B5:118:LEU:HD22	2.16	0.80
21:An:30:LEU:HD13	21:An:37:ASN:CG	2.06	0.80
26:B0:1816:A:P	77:Bw:135:ARG:CG	2.69	0.80
70:Bq:71:VAL:HB	70:Bq:74:ILE:HG12	1.63	0.80
86:B6:17:ARG:HH12	86:B6:108:MET:HB2	1.45	0.80
70:Bq:66:VAL:HG23	70:Bq:71:VAL:CA	2.09	0.80
26:B0:430:G:P	79:By:16:ARG:CD	2.69	0.80
26:B0:4323:A:P	84:B4:36:GLN:HA	2.20	0.80
62:Bj:129:LYS:HB3	62:Bj:130:PRO:HD3	1.64	0.80
83:B3:43:HIS:HD2	83:B3:46:ARG:H	1.28	0.80
85:B5:60:VAL:CG2	85:B5:104:PHE:HA	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Aj:66:ARG:HG3	17:Aj:77:TRP:NE1	1.95	0.80
26:B0:430:G:P	79:By:16:ARG:HH12	1.56	0.80
62:Bj:21:ILE:HD12	62:Bj:24:LYS:CD	2.10	0.80
66:Bn:224:GLN:HG3	66:Bn:231:THR:HB	1.64	0.80
25:B1:105:A:P	82:B2:39:TYR:CE2	2.74	0.80
26:B0:364:G:P	82:B2:36:LYS:CE	2.66	0.80
77:Bw:118:ARG:HD2	77:Bw:161:TYR:CB	2.12	0.80
85:B5:58:THR:HG23	85:B5:101:THR:HA	1.64	0.80
26:B0:1296:G:P	79:By:43:ASN:ND2	2.55	0.80
69:B7:195:ILE:O	69:B7:199:LEU:HD13	1.82	0.80
77:Bw:148:ASN:O	77:Bw:152:ILE:HG23	1.80	0.80
82:B2:27:TYR:HE1	82:B2:29:LEU:HD13	1.46	0.80
84:B4:14:LYS:HA	84:B4:14:LYS:HE3	1.63	0.80
85:B5:111:MET:CE	85:B5:131:PRO:HG3	2.12	0.80
17:Aj:46:LYS:HD2	17:Aj:96:GLU:CG	2.12	0.80
62:Bj:55:ALA:N	62:Bj:58:ARG:HG3	1.96	0.80
64:Bl:134:GLU:O	64:Bl:138:LYS:HG2	1.82	0.80
62:Bj:50:LYS:HB2	62:Bj:55:ALA:HB1	1.65	0.79
85:B5:105:ILE:HG21	85:B5:132:LEU:HD23	1.62	0.79
26:B0:4286:G:P	66:Bn:37:ILE:CD1	2.70	0.79
62:Bj:72:PHE:CD1	62:Bj:78:ILE:HA	2.16	0.79
81:Bz:42:CYS:CB	86:B6:53:PRO:HB3	2.12	0.79
12:Ad:149:GLU:HG3	12:Ad:152:ARG:HH21	1.47	0.79
66:Bn:41:ASN:CG	70:Bq:71:VAL:HG13	2.07	0.79
66:Bn:203:VAL:HG21	66:Bn:234:MET:HB2	1.65	0.79
70:Bq:10:THR:HA	70:Bq:13:MET:SD	2.22	0.79
70:Bq:28:THR:O	70:Bq:92:ILE:HD12	1.80	0.79
12:Ad:117:ARG:O	12:Ad:120:VAL:HG12	1.83	0.79
26:B0:1597:G:P	82:B2:10:LYS:CG	2.71	0.79
62:Bj:21:ILE:CD1	62:Bj:24:LYS:HD2	2.11	0.79
84:B4:68:LEU:HD11	84:B4:91:PHE:CZ	2.17	0.79
52:BZ:75:C:P	84:B4:54:PRO:CD	2.70	0.79
26:B0:22:G:P	82:B2:44:LYS:HZ3	2.06	0.79
62:Bj:64:ASN:CG	62:Bj:69:PRO:HG3	2.08	0.79
77:Bw:216:ILE:CA	77:Bw:219:VAL:HG12	2.12	0.79
66:Bn:203:VAL:CG2	66:Bn:234:MET:HB2	2.13	0.79
17:Aj:32:LEU:HD21	17:Aj:87:ARG:HG2	1.65	0.79
82:B2:24:SER:C	82:B2:25:LYS:HD2	2.08	0.79
70:Bq:71:VAL:HB	70:Bq:74:ILE:CG1	2.13	0.78
77:Bw:173:ASN:HA	77:Bw:213:ILE:HG21	1.65	0.78
85:B5:45:GLU:OE2	85:B5:188:LEU:HD11	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bj:8:LEU:HD22	62:Bj:116:ARG:O	1.83	0.78
62:Bj:15:LEU:HD11	62:Bj:137:LEU:CD1	2.13	0.78
66:Bn:38:GLN:C	70:Bq:29:TYR:HE2	1.90	0.78
77:Bw:223:PHE:CB	77:Bw:226:ALA:HB3	2.12	0.78
83:B3:13:LEU:HD23	83:B3:49:LEU:HD21	1.64	0.78
86:B6:91:VAL:HG11	86:B6:94:LEU:HD21	1.65	0.78
79:By:28:TYR:CE2	79:By:31:ILE:HG12	2.18	0.78
85:B5:138:VAL:O	85:B5:141:VAL:HG22	1.83	0.78
62:Bj:35:VAL:CG2	62:Bj:109:PRO:HB3	2.13	0.78
68:Bp:101:ILE:O	68:Bp:105:LEU:HD13	1.82	0.78
80:B9:78:LEU:HD23	80:B9:79:VAL:N	1.97	0.78
84:B4:65:LYS:CB	84:B4:85:ILE:HG12	2.12	0.78
26:B0:1511:G:P	82:B2:16:HIS:HE1	2.01	0.78
64:Bl:125:LYS:HG2	64:Bl:145:VAL:CG1	2.13	0.78
79:By:55:MET:HA	79:By:60:TYR:OH	1.83	0.78
86:B6:31:TYR:O	86:B6:34:THR:HG22	1.83	0.78
68:Bp:25:ASP:HB3	68:Bp:28:GLU:CG	2.14	0.78
48:BV:12:C:P	64:Bl:136:LYS:NZ	2.57	0.78
68:Bp:121:HIS:O	68:Bp:125:LEU:HD13	1.84	0.78
70:Bq:82:LYS:HD3	70:Bq:85:ALA:N	1.98	0.78
85:B5:48:VAL:HG21	85:B5:144:ARG:HE	1.49	0.78
17:Aj:39:LEU:O	17:Aj:39:LEU:HD13	1.84	0.78
51:BY:48:G:P	66:Bn:218:TYR:CE2	2.76	0.78
77:Bw:238:PRO:HB3	77:Bw:268:ARG:HD2	1.65	0.78
85:B5:190:LYS:H	85:B5:190:LYS:HD3	1.49	0.78
86:B6:44:LYS:HB2	86:B6:96:ILE:HG23	1.64	0.78
86:B6:45:LEU:HB2	86:B6:71:VAL:HB	1.64	0.78
51:BY:26:C:P	66:Bn:57:ARG:HD2	2.22	0.78
79:By:50:LYS:HE2	79:By:50:LYS:HA	1.66	0.78
85:B5:192:PRO:O	85:B5:195:ILE:HG22	1.83	0.78
17:Aj:23:THR:OG1	17:Aj:113:GLU:HB2	1.84	0.78
21:An:26:ASN:HB2	21:An:38:MET:HG3	1.65	0.78
26:B0:1885:A:P	77:Bw:244:LYS:HZ1	2.06	0.78
26:B0:2381:A:P	82:B2:14:LYS:HE3	2.24	0.78
86:B6:28:VAL:CG1	86:B6:33:GLN:HB3	2.14	0.78
64:Bl:37:GLY:HA3	64:Bl:47:LYS:HD3	1.66	0.77
81:Bz:47:MET:SD	81:Bz:55:TRP:HB3	2.24	0.77
85:B5:5:ILE:HD13	85:B5:177:ILE:HD13	1.67	0.77
85:B5:95:LYS:HA	85:B5:121:VAL:HG11	1.66	0.77
17:Aj:107:GLU:HG3	17:Aj:109:GLY:N	1.99	0.77
26:B0:2251:G:P	77:Bw:186:LYS:CA	2.73	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B0:2383:G:P	83:B3:48:LYS:HD2	2.23	0.77
26:B0:4167:C:P	70:Bq:4:LYS:HB2	2.24	0.77
79:By:8:VAL:HA	79:By:11:LYS:CD	2.12	0.77
79:By:11:LYS:HE2	79:By:66:THR:CG2	2.13	0.77
82:B2:31:LYS:CD	82:B2:33:THR:H	1.96	0.77
8:AH:16:G:P	21:An:30:LEU:CD1	2.49	0.77
9:Aa:17:TRP:HA	9:Aa:305:ASN:CB	2.12	0.77
26:B0:4322:A:P	84:B4:34:TYR:HB3	1.37	0.77
62:Bj:15:LEU:HD21	62:Bj:137:LEU:CD1	2.15	0.77
66:Bn:185:GLU:CG	66:Bn:201:GLN:HB2	2.14	0.77
77:Bw:242:MET:HE3	77:Bw:268:ARG:NH2	1.99	0.77
86:B6:21:VAL:HG21	86:B6:96:ILE:CD1	2.14	0.77
77:Bw:238:PRO:CG	77:Bw:269:MET:HE2	2.12	0.77
85:B5:58:THR:HG21	85:B5:100:ASP:O	1.84	0.77
64:Bl:137:ILE:O	64:Bl:140:VAL:HG12	1.83	0.77
77:Bw:230:LEU:HD12	77:Bw:232:PRO:CD	2.15	0.77
80:B9:75:ARG:HB3	80:B9:95:TYR:CD2	2.18	0.77
81:Bz:11:VAL:HG22	81:Bz:27:LYS:CD	2.15	0.77
21:An:30:LEU:C	21:An:31:ILE:HD12	2.10	0.77
70:Bq:92:ILE:O	70:Bq:95:ILE:HG22	1.85	0.77
84:B4:2:VAL:HA	84:B4:90:HIS:CE1	2.18	0.77
85:B5:111:MET:HE1	85:B5:131:PRO:HG3	1.65	0.77
26:B0:1639:U:P	64:Bl:15:VAL:HB	2.24	0.77
51:BY:11:A:P	66:Bn:17:VAL:HG22	2.23	0.77
62:Bj:54:LEU:CD1	62:Bj:58:ARG:HG2	2.10	0.77
64:Bl:137:ILE:HD11	64:Bl:144:CYS:HB2	1.66	0.77
66:Bn:38:GLN:O	70:Bq:29:TYR:HE2	1.64	0.77
77:Bw:118:ARG:O	77:Bw:139:ILE:HD12	1.85	0.77
85:B5:62:PHE:CE2	85:B5:81:GLU:HA	2.19	0.77
86:B6:48:LEU:HD21	86:B6:60:ILE:HD13	1.67	0.77
26:B0:4286:G:P	66:Bn:37:ILE:HD12	2.24	0.77
70:Bq:73:ILE:HD11	70:Bq:87:ARG:CD	2.15	0.77
77:Bw:125:PRO:HB3	77:Bw:129:LYS:HZ3	1.50	0.77
80:B9:87:VAL:CG1	80:B9:89:LEU:HD23	2.15	0.77
81:Bz:29:ILE:HD12	81:Bz:30:GLU:N	2.00	0.77
17:Aj:58:THR:HG23	17:Aj:84:ILE:O	1.86	0.77
62:Bj:80:TRP:O	62:Bj:83:VAL:HG22	1.84	0.77
70:Bq:71:VAL:HB	70:Bq:74:ILE:HD11	1.67	0.77
79:By:19:LYS:CD	79:By:21:ILE:HD13	2.14	0.77
79:By:55:MET:HE3	79:By:56:PRO:HA	1.66	0.77
81:Bz:27:LYS:O	81:Bz:31:ILE:HG12	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:58:THR:HG21	85:B5:101:THR:HA	1.67	0.77
17:Aj:40:ILE:O	17:Aj:44:LYS:HG2	1.85	0.76
17:Aj:40:ILE:CD1	17:Aj:50:VAL:HB	2.15	0.76
85:B5:104:PHE:CZ	85:B5:122:LEU:HD21	2.20	0.76
66:Bn:182:TYR:CE2	66:Bn:198:ILE:HG21	2.19	0.76
70:Bq:8:ARG:HB3	70:Bq:8:ARG:NH1	1.99	0.76
77:Bw:242:MET:CE	77:Bw:243:LYS:H	1.98	0.76
82:B2:18:LEU:CD1	82:B2:19:CYS:H	1.97	0.76
86:B6:51:ASN:HB3	86:B6:78:ASN:ND2	2.00	0.76
26:B0:4323:A:P	84:B4:36:GLN:H	2.06	0.76
62:Bj:55:ALA:H	62:Bj:58:ARG:HG3	1.47	0.76
68:Bp:91:GLU:O	68:Bp:94:THR:HG22	1.84	0.76
82:B2:18:LEU:HD22	82:B2:26:ALA:H	1.48	0.76
12:Ad:121:ARG:O	12:Ad:121:ARG:HD3	1.86	0.76
70:Bq:66:VAL:HG22	70:Bq:67:THR:O	1.84	0.76
77:Bw:242:MET:HE2	77:Bw:243:LYS:H	1.48	0.76
62:Bj:15:LEU:HD11	62:Bj:137:LEU:HD11	1.68	0.76
64:Bl:77:LYS:O	64:Bl:81:LEU:HG	1.85	0.76
66:Bn:85:TYR:CE1	66:Bn:103:LEU:HD12	2.19	0.76
86:B6:50:ASN:ND2	86:B6:76:GLY:HA2	1.99	0.76
86:B6:81:LEU:HD21	86:B6:94:LEU:CD1	2.16	0.76
12:Ad:103:VAL:HG11	12:Ad:145:ILE:HD12	1.68	0.76
17:Aj:98:VAL:O	17:Aj:101:ILE:HG22	1.84	0.76
79:By:18:LYS:HA	79:By:18:LYS:NZ	2.00	0.76
70:Bq:65:ASN:H	70:Bq:74:ILE:HB	1.51	0.76
77:Bw:216:ILE:HD12	77:Bw:223:PHE:H	1.50	0.76
85:B5:62:PHE:CE1	85:B5:110:LEU:HB2	2.20	0.76
86:B6:17:ARG:O	86:B6:21:VAL:HG23	1.85	0.76
70:Bq:83:ILE:HG13	70:Bq:84:LEU:H	1.49	0.76
77:Bw:155:LEU:HA	77:Bw:158:VAL:CG1	2.16	0.76
79:By:23:HIS:O	79:By:24:GLN:HG3	1.86	0.76
80:B9:100:ALA:O	80:B9:103:VAL:HG22	1.86	0.76
84:B4:91:PHE:HE2	84:B4:93:LEU:HD21	1.50	0.76
85:B5:43:VAL:HG11	85:B5:151:LEU:HG	1.67	0.76
26:B0:429:G:P	79:By:19:LYS:HZ2	2.05	0.76
26:B0:2384:G:P	83:B3:44:TRP:CB	2.73	0.76
64:Bl:45:PHE:O	64:Bl:48:TYR:HB3	1.86	0.76
66:Bn:184:SER:HB3	66:Bn:198:ILE:C	2.11	0.76
81:Bz:20:ALA:HB1	81:Bz:24:LYS:NZ	2.01	0.76
9:Aa:262:GLU:HA	9:Aa:270:LEU:HD23	1.67	0.76
62:Bj:6:LEU:HG	62:Bj:30:ARG:HH21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bj:107:ILE:HG23	62:Bj:108:PRO:CD	2.15	0.76
64:Bl:117:LEU:HD13	64:Bl:136:LYS:HA	1.67	0.76
79:By:22:ARG:HG3	79:By:36:ARG:CG	2.15	0.76
79:By:28:TYR:CE2	79:By:30:LYS:HD2	2.21	0.76
85:B5:198:VAL:HG22	85:B5:210:VAL:HG22	1.68	0.76
70:Bq:78:GLN:HA	70:Bq:82:LYS:HE2	1.66	0.75
77:Bw:186:LYS:H	77:Bw:186:LYS:HD3	1.50	0.75
85:B5:34:LEU:CD1	85:B5:40:SER:HB2	2.15	0.75
26:B0:4191:C:P	84:B4:2:VAL:CG1	2.75	0.75
66:Bn:40:LYS:HE3	70:Bq:67:THR:N	2.01	0.75
79:By:12:ILE:O	79:By:13:VAL:HG13	1.86	0.75
79:By:19:LYS:HD2	79:By:21:ILE:CD1	2.14	0.75
84:B4:66:ILE:CG2	84:B4:68:LEU:HG	2.15	0.75
85:B5:50:PRO:HG3	85:B5:179:VAL:HG21	1.66	0.75
79:By:19:LYS:HB2	79:By:21:ILE:CD1	2.15	0.75
85:B5:163:VAL:CG1	85:B5:173:ILE:HG23	2.15	0.75
17:Aj:31:SER:O	17:Aj:35:VAL:HG23	1.85	0.75
17:Aj:68:THR:HG22	17:Aj:70:CYS:H	1.51	0.75
21:An:21:CYS:CB	21:An:38:MET:H	1.92	0.75
70:Bq:82:LYS:HD2	70:Bq:83:ILE:N	2.01	0.75
79:By:22:ARG:HD3	79:By:23:HIS:O	1.86	0.75
86:B6:21:VAL:HG21	86:B6:96:ILE:HD12	1.68	0.75
17:Aj:46:LYS:HB2	17:Aj:97:ILE:HA	1.68	0.75
77:Bw:223:PHE:O	77:Bw:224:LYS:HG3	1.87	0.75
79:By:18:LYS:HG3	79:By:19:LYS:HE2	1.67	0.75
79:By:24:GLN:HE22	79:By:28:TYR:HE1	1.32	0.75
21:An:30:LEU:HD13	21:An:37:ASN:OD1	1.86	0.75
26:B0:2278:C:P	80:B9:103:VAL:HA	2.26	0.75
77:Bw:193:ASP:HA	77:Bw:196:LEU:CD2	2.16	0.75
82:B2:28:HIS:O	82:B2:31:LYS:HG3	1.87	0.75
21:An:20:SER:C	21:An:37:ASN:HB2	2.10	0.75
22:Ao:77:TYR:CE2	22:Ao:81:ILE:HB	2.22	0.75
48:BV:12:C:P	64:Bl:136:LYS:HZ1	2.10	0.75
82:B2:15:THR:HG22	82:B2:16:HIS:H	1.51	0.75
82:B2:18:LEU:HD13	82:B2:26:ALA:C	2.12	0.75
82:B2:31:LYS:HE3	82:B2:32:SER:HA	1.68	0.75
77:Bw:130:VAL:CG2	77:Bw:154:MET:HE3	2.11	0.75
80:B9:79:VAL:HG23	80:B9:84:GLU:CB	2.17	0.75
1:AA:1149:A:P	22:Ao:37:ARG:NH1	2.57	0.74
17:Aj:22:ILE:HG12	17:Aj:91:LEU:HD23	1.67	0.74
68:Bp:47:ASP:CB	68:Bp:49:LEU:HD13	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Bw:266:ILE:HD12	77:Bw:267:ARG:N	2.02	0.74
79:By:28:TYR:OH	79:By:31:ILE:HD11	1.87	0.74
17:Aj:46:LYS:CD	17:Aj:96:GLU:HG2	2.16	0.74
62:Bj:36:ARG:CD	62:Bj:107:ILE:HB	2.17	0.74
85:B5:19:ARG:HG3	85:B5:204:MET:HG3	1.69	0.74
26:B0:2278:C:P	80:B9:104:SER:H	2.11	0.74
68:Bp:9:ARG:CD	68:Bp:10:LEU:HD12	2.03	0.74
77:Bw:216:ILE:CD1	77:Bw:223:PHE:H	1.99	0.74
77:Bw:244:LYS:CD	77:Bw:246:THR:H	1.99	0.74
77:Bw:247:THR:HG23	77:Bw:255:ALA:HB2	1.69	0.74
64:Bl:101:ILE:HD13	64:Bl:109:TYR:HB2	1.69	0.74
79:By:7:LEU:HD23	79:By:66:THR:OG1	1.88	0.74
80:B9:81:ASN:HD22	80:B9:83:LYS:H	1.34	0.74
85:B5:202:THR:HG23	85:B5:205:GLY:N	2.00	0.74
62:Bj:15:LEU:HD21	62:Bj:137:LEU:CD2	2.17	0.74
62:Bj:47:TYR:O	62:Bj:50:LYS:HG3	1.88	0.74
62:Bj:127:ARG:HD3	62:Bj:136:TYR:OH	1.87	0.74
66:Bn:40:LYS:HG2	70:Bq:67:THR:C	2.07	0.74
26:B0:2757:C:P	83:B3:7:PHE:CE1	2.77	0.74
26:B0:4250:U:P	84:B4:9:ARG:NH2	2.60	0.74
62:Bj:7:VAL:CG2	62:Bj:115:LYS:HA	2.17	0.74
64:Bl:14:HIS:O	64:Bl:15:VAL:HG12	1.88	0.74
66:Bn:85:TYR:CD2	66:Bn:246:ILE:HG22	2.23	0.74
70:Bq:67:THR:OG1	70:Bq:72:GLY:HA3	1.87	0.74
83:B3:27:ILE:HD12	83:B3:30:LYS:HD2	1.69	0.74
17:Aj:67:LYS:N	17:Aj:76:THR:HG23	2.03	0.74
70:Bq:29:TYR:HD1	70:Bq:93:GLU:HG2	1.52	0.74
77:Bw:157:ILE:O	77:Bw:157:ILE:HD13	1.86	0.74
86:B6:44:LYS:HB2	86:B6:96:ILE:CG2	2.18	0.74
62:Bj:72:PHE:HE1	62:Bj:78:ILE:HG12	1.50	0.74
66:Bn:184:SER:HB3	66:Bn:198:ILE:CA	2.18	0.74
77:Bw:170:LYS:HA	77:Bw:173:ASN:HD21	1.53	0.74
86:B6:79:ILE:HD13	86:B6:79:ILE:H	1.52	0.74
12:Ad:73:GLN:HA	12:Ad:76:ASN:HD21	1.53	0.74
62:Bj:6:LEU:HD12	62:Bj:25:GLN:NE2	2.02	0.74
62:Bj:15:LEU:HD13	62:Bj:42:ILE:HG13	1.69	0.74
70:Bq:33:TYR:HE1	70:Bq:92:ILE:HG12	1.53	0.74
77:Bw:166:TYR:CE1	77:Bw:259:GLU:HB2	2.23	0.74
81:Bz:42:CYS:CB	86:B6:53:PRO:CB	2.65	0.74
82:B2:33:THR:HA	82:B2:40:PRO:HD2	1.69	0.74
85:B5:145:MET:O	85:B5:148:THR:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Ad:149:GLU:O	12:Ad:152:ARG:HG2	1.87	0.73
26:B0:4238:C:P	70:Bq:21:HIS:NE2	2.61	0.73
62:Bj:54:LEU:HA	62:Bj:58:ARG:HG2	1.69	0.73
64:Bl:16:SER:C	64:Bl:19:HIS:HB2	2.13	0.73
17:Aj:56:MET:HG3	17:Aj:57:PRO:HD2	1.69	0.73
26:B0:4013:G:P	85:B5:124:PRO:HB3	2.28	0.73
26:B0:4322:A:P	84:B4:34:TYR:CD1	2.81	0.73
70:Bq:73:ILE:HD11	70:Bq:87:ARG:HD2	1.68	0.73
84:B4:12:CYS:SG	84:B4:15:CYS:HB2	2.28	0.73
85:B5:163:VAL:HG11	85:B5:173:ILE:HG23	1.70	0.73
68:Bp:62:ARG:NH1	68:Bp:62:ARG:HB2	2.02	0.73
84:B4:34:TYR:CA	84:B4:38:LYS:HD2	2.16	0.73
26:B0:4255:U:P	84:B4:13:LYS:NZ	2.61	0.73
86:B6:45:LEU:HD12	86:B6:71:VAL:CG1	2.18	0.73
77:Bw:238:PRO:HG3	77:Bw:269:MET:CE	2.16	0.73
80:B9:81:ASN:HD21	80:B9:83:LYS:HB2	1.54	0.73
81:Bz:25:MET:HA	81:Bz:28:LYS:HE2	1.70	0.73
17:Aj:50:VAL:HG11	17:Aj:89:ILE:CG1	2.17	0.73
26:B0:4191:C:P	84:B4:2:VAL:HG12	2.29	0.73
77:Bw:118:ARG:HG2	77:Bw:119:GLY:H	1.54	0.73
25:B1:54:A:P	83:B3:21:ARG:CB	2.76	0.73
26:B0:22:G:P	82:B2:44:LYS:NZ	2.61	0.73
64:Bl:11:LEU:HD23	64:Bl:12:ARG:N	2.03	0.73
80:B9:99:ILE:CG2	80:B9:103:VAL:HG21	2.18	0.73
82:B2:18:LEU:CD2	82:B2:24:SER:HB3	2.19	0.73
82:B2:27:TYR:CD1	82:B2:29:LEU:HD22	2.23	0.73
85:B5:87:LEU:HB3	85:B5:117:TYR:CE2	2.23	0.73
17:Aj:50:VAL:HG22	17:Aj:91:LEU:HD13	1.69	0.73
17:Aj:72:GLU:CD	21:An:54:LYS:HD3	2.14	0.73
86:B6:29:LEU:HD21	86:B6:87:LYS:HE3	1.68	0.73
26:B0:1572:A:P	54:Bb:245:ARG:NE	2.61	0.73
39:BM:2688:C:P	68:Bp:39:GLN:OE1	2.47	0.73
77:Bw:118:ARG:CB	77:Bw:161:TYR:HB2	2.19	0.73
81:Bz:46:LYS:CD	81:Bz:59:SER:HB2	2.16	0.73
86:B6:81:LEU:O	86:B6:81:LEU:HD23	1.88	0.73
26:B0:2031:C:P	62:Bj:14:LEU:HD23	2.29	0.73
70:Bq:77:LYS:O	70:Bq:86:LYS:HB3	1.88	0.73
81:Bz:25:MET:HA	81:Bz:28:LYS:HE3	1.70	0.73
83:B3:41:ARG:NH1	83:B3:41:ARG:HB3	2.03	0.73
85:B5:36:LEU:HD23	85:B5:36:LEU:O	1.89	0.73
86:B6:18:LEU:O	86:B6:18:LEU:HD13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B6:26:LYS:HB3	86:B6:97:ILE:CG1	2.19	0.73
86:B6:81:LEU:HD21	86:B6:94:LEU:CG	2.18	0.73
17:Aj:67:LYS:HB2	17:Aj:76:THR:OG1	1.89	0.72
68:Bp:24:LEU:HD23	68:Bp:32:ILE:CD1	2.16	0.72
68:Bp:64:ARG:O	68:Bp:68:LEU:HG	1.89	0.72
77:Bw:178:LYS:HD3	77:Bw:270:ASN:O	1.89	0.72
86:B6:6:LYS:HD2	86:B6:14:ILE:HD13	1.71	0.72
86:B6:49:ALA:HB3	86:B6:52:CYS:SG	2.29	0.72
26:B0:53:C:P	82:B2:47:TYR:HE1	2.11	0.72
66:Bn:81:GLU:HG3	66:Bn:84:LYS:HD2	1.71	0.72
85:B5:27:LEU:CD1	85:B5:29:VAL:HG23	2.19	0.72
85:B5:60:VAL:HG13	85:B5:101:THR:CG2	2.19	0.72
21:An:26:ASN:CG	21:An:38:MET:HG3	2.13	0.72
26:B0:1494:A:P	64:Bl:32:ARG:CB	2.78	0.72
80:B9:70:LEU:HD11	80:B9:76:LYS:HB3	1.71	0.72
82:B2:28:HIS:HB3	82:B2:31:LYS:HG3	1.69	0.72
85:B5:11:ARG:HA	85:B5:11:ARG:HE	1.54	0.72
64:Bl:74:ASN:O	64:Bl:78:PRO:HD2	1.88	0.72
64:Bl:120:GLN:HG3	64:Bl:121:PRO:HD2	1.70	0.72
64:Bl:125:LYS:HA	64:Bl:145:VAL:HG13	1.71	0.72
85:B5:60:VAL:HG22	85:B5:103:PHE:O	1.89	0.72
62:Bj:37:CYS:SG	62:Bj:79:PHE:HB2	2.29	0.72
66:Bn:42:LYS:CA	70:Bq:32:ILE:HG12	2.19	0.72
66:Bn:48:TYR:HB2	66:Bn:63:ILE:HD11	1.71	0.72
85:B5:27:LEU:HD11	85:B5:29:VAL:HG23	1.71	0.72
83:B3:13:LEU:CD2	83:B3:49:LEU:HD21	2.19	0.72
83:B3:23:ILE:HG21	83:B3:35:ILE:CG2	2.16	0.72
9:Aa:18:VAL:HB	9:Aa:305:ASN:C	2.15	0.72
9:Aa:83:TRP:HA	9:Aa:108:VAL:HG22	1.71	0.72
84:B4:14:LYS:HA	84:B4:14:LYS:CE	2.19	0.72
64:Bl:101:ILE:HG21	64:Bl:109:TYR:CE1	2.24	0.72
68:Bp:89:MET:HB3	68:Bp:90:PRO:HD3	1.72	0.72
77:Bw:239:ARG:HG2	77:Bw:268:ARG:HB3	1.70	0.72
82:B2:4:GLY:HA3	82:B2:8:PHE:CZ	2.23	0.72
9:Aa:21:ILE:CD1	9:Aa:307:VAL:HG11	2.20	0.72
21:An:26:ASN:CB	21:An:38:MET:HA	2.18	0.72
22:Ao:70:GLN:HG2	22:Ao:77:TYR:CD2	2.25	0.72
26:B0:2650:G:P	86:B6:92:CYS:N	2.60	0.72
77:Bw:146:LYS:HE3	77:Bw:220:GLY:HA2	1.71	0.72
77:Bw:166:TYR:CZ	77:Bw:259:GLU:HB2	2.25	0.72
85:B5:43:VAL:HG12	85:B5:151:LEU:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Aa:206:LEU:HD13	9:Aa:218:LEU:HD11	1.72	0.71
17:Aj:47:ASN:HB3	17:Aj:93:SER:OG	1.89	0.71
66:Bn:184:SER:CB	66:Bn:199:MET:N	2.53	0.71
66:Bn:192:GLU:HA	66:Bn:238:MET:CB	2.20	0.71
77:Bw:155:LEU:O	77:Bw:155:LEU:HD13	1.90	0.71
86:B6:91:VAL:HG11	86:B6:94:LEU:CD2	2.20	0.71
26:B0:4478:A:P	54:Bb:257:HIS:N	2.61	0.71
85:B5:60:VAL:HG23	85:B5:104:PHE:HA	1.72	0.71
62:Bj:96:ALA:HA	62:Bj:99:ASP:OD2	1.90	0.71
64:Bl:89:ASN:CB	64:Bl:94:LYS:HE2	2.20	0.71
70:Bq:39:VAL:HB	70:Bq:95:ILE:CG1	2.20	0.71
26:B0:4330:G:P	84:B4:85:ILE:HD11	2.27	0.71
64:Bl:132:ARG:O	64:Bl:136:LYS:HG2	1.91	0.71
66:Bn:192:GLU:O	66:Bn:193:VAL:HG13	1.90	0.71
68:Bp:24:LEU:HG	68:Bp:50:ILE:CD1	2.20	0.71
68:Bp:64:ARG:O	68:Bp:67:THR:HG22	1.89	0.71
83:B3:5:LYS:HB2	83:B3:9:ILE:CG2	2.20	0.71
51:BY:67:C:P	66:Bn:13:LYS:H	2.13	0.71
66:Bn:85:TYR:CD1	66:Bn:103:LEU:HD12	2.25	0.71
79:By:22:ARG:NH1	79:By:31:ILE:HD12	2.06	0.71
85:B5:29:VAL:HG22	85:B5:198:VAL:HG12	1.73	0.71
17:Aj:20:ILE:HG23	17:Aj:115:THR:O	1.91	0.71
83:B3:38:ASN:ND2	83:B3:41:ARG:HD3	2.05	0.71
86:B6:6:LYS:HD3	86:B6:14:ILE:HG21	1.72	0.71
9:Aa:62:HIS:HB3	9:Aa:84:ASP:CG	2.16	0.71
9:Aa:216:ALA:HB1	9:Aa:247:TRP:CH2	2.26	0.71
62:Bj:73:ARG:H	62:Bj:77:ARG:NE	1.89	0.71
83:B3:21:ARG:HD2	83:B3:21:ARG:O	1.91	0.71
85:B5:63:ALA:HB1	85:B5:67:THR:HB	1.71	0.71
12:Ad:118:GLN:HG2	12:Ad:122:HIS:CD2	2.26	0.71
77:Bw:242:MET:HE1	77:Bw:243:LYS:HG2	1.71	0.71
84:B4:35:ALA:O	84:B4:38:LYS:HG2	1.91	0.71
84:B4:69:ARG:HB3	84:B4:80:LYS:CD	2.21	0.71
84:B4:75:PRO:HG2	84:B4:77:CYS:H	1.55	0.71
86:B6:48:LEU:HD12	86:B6:74:TYR:CZ	2.25	0.71
21:An:21:CYS:HA	21:An:37:ASN:H	1.56	0.71
66:Bn:85:TYR:CZ	66:Bn:103:LEU:HG	2.26	0.71
66:Bn:217:ALA:HA	66:Bn:234:MET:CE	2.20	0.71
84:B4:91:PHE:CE2	84:B4:93:LEU:HD21	2.26	0.71
21:An:26:ASN:HB2	21:An:38:MET:CB	2.20	0.71
70:Bq:66:VAL:CA	70:Bq:74:ILE:HG21	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:84:LEU:CD1	85:B5:118:LEU:HD21	2.20	0.71
85:B5:150:GLN:HE21	85:B5:152:ARG:HD3	1.55	0.71
85:B5:151:LEU:HD12	85:B5:159:PHE:CZ	2.26	0.71
21:An:26:ASN:CB	21:An:38:MET:HG3	2.21	0.70
66:Bn:40:LYS:CE	70:Bq:67:THR:H	2.01	0.70
66:Bn:77:ARG:HE	66:Bn:103:LEU:CB	2.03	0.70
70:Bq:79:VAL:HG13	70:Bq:82:LYS:N	2.02	0.70
79:By:25:SER:HA	79:By:31:ILE:HG21	1.73	0.70
82:B2:18:LEU:HD23	82:B2:24:SER:CA	2.21	0.70
62:Bj:7:VAL:HG12	62:Bj:33:VAL:HG11	1.73	0.70
85:B5:195:ILE:HD11	85:B5:198:VAL:CG1	2.21	0.70
22:Ao:70:GLN:CG	22:Ao:77:TYR:CD2	2.75	0.70
51:BY:26:C:P	66:Bn:57:ARG:HB3	2.30	0.70
66:Bn:108:LEU:HD21	66:Bn:140:ALA:HB3	1.74	0.70
86:B6:32:LYS:HG2	86:B6:36:LYS:HE3	1.73	0.70
9:Aa:14:HIS:CA	9:Aa:35:SER:HB3	2.21	0.70
17:Aj:24:LEU:HD22	17:Aj:112:VAL:HG22	1.74	0.70
26:B0:430:G:P	79:By:16:ARG:HD3	2.32	0.70
77:Bw:242:MET:HG2	77:Bw:268:ARG:HH21	1.56	0.70
85:B5:59:ILE:HD11	85:B5:145:MET:C	2.16	0.70
77:Bw:244:LYS:HD2	77:Bw:246:THR:H	1.55	0.70
85:B5:34:LEU:HD13	85:B5:35:ASP:N	2.06	0.70
9:Aa:18:VAL:HG23	9:Aa:305:ASN:O	1.92	0.70
80:B9:70:LEU:HD11	80:B9:76:LYS:CB	2.22	0.70
1:AA:1540:C:P	9:Aa:61:GLY:N	2.65	0.70
77:Bw:173:ASN:CA	77:Bw:213:ILE:HG21	2.22	0.70
9:Aa:56:GLN:HE21	9:Aa:66:VAL:HG21	1.55	0.70
66:Bn:89:VAL:HB	66:Bn:193:VAL:HA	1.73	0.70
70:Bq:33:TYR:HB3	70:Bq:37:ASP:OD2	1.91	0.70
82:B2:45:ARG:HD3	82:B2:47:TYR:HE2	1.55	0.70
85:B5:50:PRO:HG3	85:B5:179:VAL:CG2	2.22	0.70
85:B5:74:VAL:HG21	85:B5:142:ILE:CD1	2.20	0.70
25:B1:55:G:P	83:B3:21:ARG:NH2	2.65	0.70
62:Bj:35:VAL:HG21	62:Bj:109:PRO:HB3	1.72	0.70
66:Bn:187:LYS:CE	66:Bn:188:GLU:H	2.04	0.70
85:B5:27:LEU:HG	85:B5:180:ILE:HD11	1.74	0.70
85:B5:151:LEU:HA	85:B5:159:PHE:CZ	2.25	0.70
17:Aj:63:ILE:HD11	17:Aj:80:PHE:HB2	1.74	0.70
62:Bj:18:LEU:HD23	62:Bj:22:VAL:HG23	1.73	0.70
26:B0:4022:C:P	85:B5:197:THR:H	2.15	0.69
70:Bq:39:VAL:HG23	70:Bq:95:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Bq:92:ILE:O	70:Bq:92:ILE:HD13	1.92	0.69
77:Bw:247:THR:CG2	77:Bw:255:ALA:HB2	2.22	0.69
81:Bz:64:VAL:HG11	81:Bz:71:TYR:OH	1.91	0.69
85:B5:43:VAL:HG13	85:B5:188:LEU:HD12	1.72	0.69
26:B0:4021:A:P	85:B5:199:TYR:CE1	2.84	0.69
62:Bj:15:LEU:CD2	62:Bj:137:LEU:HD21	2.22	0.69
83:B3:13:LEU:HD23	83:B3:49:LEU:CD2	2.22	0.69
12:Ad:133:ASP:O	12:Ad:135:PRO:HD3	1.92	0.69
26:B0:2292:G:P	80:B9:71:PRO:CG	2.78	0.69
62:Bj:109:PRO:HD3	62:Bj:115:LYS:NZ	2.07	0.69
77:Bw:219:VAL:HB	77:Bw:222:ARG:CG	2.22	0.69
82:B2:4:GLY:HA3	82:B2:8:PHE:CE2	2.27	0.69
85:B5:34:LEU:HD11	85:B5:40:SER:HB2	1.74	0.69
26:B0:53:C:P	82:B2:47:TYR:CE1	2.85	0.69
9:Aa:21:ILE:HD13	9:Aa:307:VAL:HG11	1.73	0.69
26:B0:4259:U:P	70:Bq:87:ARG:CZ	2.80	0.69
62:Bj:18:LEU:O	62:Bj:21:ILE:HG22	1.91	0.69
77:Bw:216:ILE:CD1	77:Bw:222:ARG:HB2	2.22	0.69
86:B6:22:MET:HE3	86:B6:86:GLY:HA3	1.74	0.69
17:Aj:21:ARG:HA	17:Aj:90:ASP:OD1	1.93	0.69
66:Bn:108:LEU:C	66:Bn:108:LEU:HD23	2.17	0.69
17:Aj:72:GLU:CD	21:An:54:LYS:CD	2.65	0.69
21:An:36:LEU:HD12	21:An:42:CYS:HB3	1.72	0.69
62:Bj:23:ALA:O	62:Bj:26:VAL:HG12	1.93	0.69
66:Bn:77:ARG:HD3	66:Bn:81:GLU:HG2	1.75	0.69
66:Bn:184:SER:CB	66:Bn:199:MET:H	2.04	0.69
77:Bw:216:ILE:HD12	77:Bw:222:ARG:HB2	1.74	0.69
80:B9:76:LYS:HD2	80:B9:76:LYS:O	1.91	0.69
86:B6:71:VAL:HG22	86:B6:112:THR:OG1	1.92	0.69
9:Aa:208:ALA:HB1	9:Aa:247:TRP:CZ2	2.28	0.69
34:BH:1790:G:P	66:Bn:121:GLN:H	2.15	0.69
9:Aa:87:LEU:HD21	9:Aa:120:ILE:HG12	1.73	0.69
12:Ad:126:THR:HG22	12:Ad:146:ALA:O	1.92	0.69
17:Aj:40:ILE:CB	17:Aj:89:ILE:HD11	2.21	0.69
64:Bl:109:TYR:OH	64:Bl:111:VAL:HG22	1.92	0.69
69:B7:196:LEU:O	69:B7:200:LEU:HG	1.93	0.69
70:Bq:29:TYR:HD1	70:Bq:93:GLU:CG	2.06	0.69
82:B2:10:LYS:HE3	82:B2:12:ARG:N	2.07	0.69
17:Aj:40:ILE:HD13	17:Aj:89:ILE:HD11	1.75	0.68
26:B0:1494:A:P	64:Bl:32:ARG:HB2	2.33	0.68
12:Ad:122:HIS:HB2	12:Ad:124:HIS:CD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:77:ARG:CG	66:Bn:100:THR:HG23	2.22	0.68
77:Bw:155:LEU:HA	77:Bw:158:VAL:HG12	1.73	0.68
84:B4:12:CYS:HB3	84:B4:21:HIS:CE1	2.28	0.68
85:B5:45:GLU:HG3	85:B5:183:ARG:HG3	1.76	0.68
26:B0:1529:G:P	68:Bp:84:THR:HG21	2.33	0.68
70:Bq:31:ARG:HB2	70:Bq:92:ILE:CD1	2.23	0.68
70:Bq:41:ILE:HD13	70:Bq:77:LYS:HE2	1.73	0.68
9:Aa:14:HIS:HB3	9:Aa:35:SER:HB3	1.75	0.68
17:Aj:19:ARG:HG3	17:Aj:92:HIS:CD2	2.27	0.68
26:B0:2031:C:P	62:Bj:14:LEU:CD2	2.81	0.68
62:Bj:26:VAL:HG13	62:Bj:97:ALA:HB1	1.75	0.68
77:Bw:238:PRO:HB3	77:Bw:268:ARG:CD	2.23	0.68
84:B4:66:ILE:O	84:B4:85:ILE:HG13	1.92	0.68
85:B5:94:ALA:HB2	85:B5:117:TYR:OH	1.93	0.68
62:Bj:8:LEU:HD13	62:Bj:9:ASP:C	2.18	0.68
66:Bn:85:TYR:CE1	66:Bn:246:ILE:HG22	2.28	0.68
68:Bp:24:LEU:HG	68:Bp:50:ILE:HD12	1.76	0.68
84:B4:19:GLN:OE1	84:B4:74:GLU:HB3	1.92	0.68
85:B5:34:LEU:CD2	85:B5:41:ASN:HD22	2.06	0.68
9:Aa:87:LEU:HD13	9:Aa:109:LEU:HD21	1.75	0.68
68:Bp:102:LEU:O	68:Bp:106:LEU:HG	1.93	0.68
70:Bq:29:TYR:CD1	70:Bq:93:GLU:HG2	2.29	0.68
26:B0:1572:A:P	54:Bb:245:ARG:CZ	2.81	0.68
79:By:22:ARG:HD2	79:By:31:ILE:CG2	2.23	0.68
79:By:24:GLN:OE1	79:By:31:ILE:HG13	1.94	0.68
80:B9:88:LEU:O	80:B9:88:LEU:HD13	1.93	0.68
85:B5:38:ASP:HB3	85:B5:39:PRO:HD2	1.76	0.68
17:Aj:37:ALA:O	17:Aj:40:ILE:HG22	1.94	0.68
17:Aj:65:THR:O	17:Aj:77:TRP:HA	1.93	0.68
26:B0:4303:U:P	84:B4:36:GLN:O	2.52	0.68
80:B9:108:ARG:O	80:B9:112:VAL:HG23	1.93	0.68
81:Bz:42:CYS:SG	86:B6:53:PRO:HG3	2.31	0.68
62:Bj:72:PHE:CB	62:Bj:77:ARG:HG3	2.23	0.68
70:Bq:33:TYR:HE1	70:Bq:92:ILE:CG1	2.07	0.68
83:B3:15:LYS:HD2	83:B3:15:LYS:C	2.19	0.68
84:B4:38:LYS:HG2	84:B4:39:ARG:HD3	1.76	0.68
84:B4:70:LEU:O	84:B4:80:LYS:HA	1.93	0.68
86:B6:105:ILE:O	86:B6:109:PRO:HD2	1.94	0.68
62:Bj:78:ILE:O	62:Bj:78:ILE:HD13	1.94	0.68
64:Bl:85:GLN:O	64:Bl:88:VAL:HG12	1.93	0.68
82:B2:28:HIS:O	82:B2:31:LYS:HE2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Bp:47:ASP:HB3	68:Bp:49:LEU:HD13	1.76	0.67
80:B9:92:ASN:HD22	80:B9:120:ILE:HG12	1.59	0.67
86:B6:44:LYS:HD3	86:B6:98:ASP:OD1	1.94	0.67
62:Bj:91:THR:CG2	62:Bj:94:GLY:H	2.03	0.67
68:Bp:10:LEU:HB2	68:Bp:41:ILE:CD1	2.24	0.67
68:Bp:97:ARG:O	68:Bp:101:ILE:HG13	1.93	0.67
86:B6:77:ASN:HB3	86:B6:79:ILE:HD11	1.76	0.67
17:Aj:32:LEU:CD2	17:Aj:87:ARG:HG2	2.25	0.67
77:Bw:130:VAL:HG23	77:Bw:154:MET:CE	2.13	0.67
85:B5:34:LEU:HB3	85:B5:157:ARG:HD3	1.76	0.67
9:Aa:14:HIS:CB	9:Aa:35:SER:HB3	2.24	0.67
17:Aj:25:THR:HB	17:Aj:84:ILE:HD11	1.74	0.67
17:Aj:50:VAL:HG22	17:Aj:91:LEU:CD1	2.25	0.67
21:An:26:ASN:HB2	21:An:38:MET:CG	2.25	0.67
77:Bw:196:LEU:HD11	77:Bw:209:MET:CA	2.24	0.67
84:B4:68:LEU:HD11	84:B4:91:PHE:CE1	2.30	0.67
85:B5:103:PHE:HB3	85:B5:145:MET:HE3	1.76	0.67
85:B5:161:THR:HG21	85:B5:180:ILE:HD13	1.76	0.67
9:Aa:79:LEU:HD23	9:Aa:89:LEU:HA	1.75	0.67
17:Aj:47:ASN:HB3	17:Aj:93:SER:CB	2.24	0.67
21:An:26:ASN:N	21:An:38:MET:HB2	2.09	0.67
66:Bn:38:GLN:CG	70:Bq:29:TYR:HE2	2.00	0.67
77:Bw:193:ASP:O	77:Bw:197:ILE:HG23	1.93	0.67
82:B2:18:LEU:HD21	82:B2:22:CYS:HB3	1.76	0.67
86:B6:6:LYS:HB3	86:B6:10:SER:CB	2.25	0.67
68:Bp:12:SER:OG	68:Bp:19:LYS:HA	1.94	0.67
77:Bw:116:ARG:NH1	77:Bw:131:LEU:HB2	2.08	0.67
81:Bz:11:VAL:CG1	81:Bz:27:LYS:HG2	2.24	0.67
82:B2:31:LYS:HE3	82:B2:32:SER:CA	2.24	0.67
86:B6:46:VAL:CG1	86:B6:72:HIS:HA	2.24	0.67
51:BY:7:G:P	66:Bn:27:THR:OG1	2.53	0.67
62:Bj:124:LYS:HB2	62:Bj:130:PRO:CD	2.24	0.67
66:Bn:187:LYS:HE3	66:Bn:187:LYS:HA	1.77	0.67
66:Bn:217:ALA:HA	66:Bn:234:MET:HE2	1.77	0.67
70:Bq:39:VAL:HB	70:Bq:95:ILE:HG13	1.75	0.67
70:Bq:51:MET:SD	70:Bq:54:LYS:HE2	2.34	0.67
79:By:8:VAL:CA	79:By:11:LYS:HD2	2.18	0.67
51:BY:67:C:P	66:Bn:13:LYS:N	2.68	0.67
62:Bj:11:ARG:HD2	62:Bj:107:ILE:HD12	1.77	0.67
62:Bj:15:LEU:CD1	62:Bj:137:LEU:HD11	2.24	0.67
62:Bj:61:MET:HE3	62:Bj:61:MET:CA	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:79:ALA:HB3	66:Bn:91:LEU:HD11	1.76	0.67
70:Bq:6:LYS:H	70:Bq:6:LYS:HD2	1.60	0.67
79:By:45:VAL:HG13	79:By:52:GLN:NE2	2.09	0.67
62:Bj:72:PHE:HD2	62:Bj:81:ARG:HG3	1.60	0.67
77:Bw:223:PHE:HB3	77:Bw:226:ALA:CB	2.17	0.67
9:Aa:282:GLU:CG	9:Aa:308:ARG:HH22	2.08	0.66
25:B1:55:G:P	83:B3:21:ARG:CZ	2.82	0.66
51:BY:6:C:P	66:Bn:53:ARG:NH2	2.67	0.66
66:Bn:38:GLN:O	70:Bq:29:TYR:CZ	2.49	0.66
77:Bw:116:ARG:HD2	77:Bw:161:TYR:CE2	2.29	0.66
26:B0:1860:U:P	79:By:47:ARG:NH1	2.68	0.66
68:Bp:106:LEU:HB3	68:Bp:120:TYR:CE1	2.31	0.66
1:AA:1436:A:P	21:An:13:LYS:NZ	2.68	0.66
17:Aj:26:SER:OG	17:Aj:110:VAL:HG22	1.95	0.66
62:Bj:64:ASN:OD1	62:Bj:69:PRO:HG3	1.95	0.66
70:Bq:33:TYR:CE1	70:Bq:92:ILE:HG12	2.30	0.66
70:Bq:79:VAL:HG12	70:Bq:82:LYS:CB	2.19	0.66
77:Bw:123:VAL:HG21	77:Bw:127:VAL:CG1	2.26	0.66
12:Ad:69:ILE:HD11	12:Ad:73:GLN:OE1	1.95	0.66
64:Bl:97:VAL:HG12	64:Bl:101:ILE:HG23	1.78	0.66
64:Bl:101:ILE:CD1	64:Bl:109:TYR:HB2	2.25	0.66
82:B2:31:LYS:HE3	82:B2:31:LYS:C	2.21	0.66
85:B5:62:PHE:CE2	85:B5:110:LEU:HG	2.31	0.66
26:B0:2816:U:P	54:Bb:245:ARG:HE	2.19	0.66
80:B9:83:LYS:HD2	80:B9:83:LYS:H	1.60	0.66
85:B5:43:VAL:HG11	85:B5:151:LEU:CD2	2.25	0.66
12:Ad:103:VAL:HG11	12:Ad:145:ILE:CD1	2.25	0.66
70:Bq:38:ILE:HD11	70:Bq:60:THR:CG2	2.25	0.66
70:Bq:38:ILE:HD11	70:Bq:60:THR:HG23	1.78	0.66
85:B5:23:GLU:OE1	85:B5:204:MET:HB2	1.96	0.66
86:B6:17:ARG:HD3	86:B6:105:ILE:CD1	2.25	0.66
17:Aj:53:PRO:HA	17:Aj:89:ILE:HB	1.78	0.66
66:Bn:105:ALA:HB1	66:Bn:170:LEU:HD23	1.77	0.66
85:B5:151:LEU:HD12	85:B5:159:PHE:CG	2.31	0.66
17:Aj:36:CYS:SG	17:Aj:53:PRO:HB3	2.36	0.66
62:Bj:13:HIS:O	62:Bj:40:ILE:HG13	1.95	0.66
79:By:14:LYS:HD2	79:By:14:LYS:C	2.21	0.66
84:B4:66:ILE:HG22	84:B4:68:LEU:HG	1.76	0.66
1:AA:1540:C:P	9:Aa:60:ARG:C	2.79	0.66
26:B0:4022:C:P	85:B5:30:ASN:HB3	2.36	0.66
62:Bj:59:LYS:HG3	62:Bj:60:ARG:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bj:107:ILE:HG23	62:Bj:108:PRO:HD3	1.78	0.66
81:Bz:20:ALA:HB1	81:Bz:24:LYS:HZ2	1.60	0.66
82:B2:52:LYS:HD3	82:B2:52:LYS:H	1.60	0.66
85:B5:59:ILE:HD11	85:B5:145:MET:HB3	1.77	0.66
12:Ad:105:TYR:HE1	12:Ad:112:SER:HA	1.59	0.66
66:Bn:82:LEU:HG	66:Bn:87:VAL:HG21	1.78	0.66
66:Bn:193:VAL:CG2	66:Bn:235:MET:O	2.36	0.66
85:B5:88:GLY:HA2	85:B5:117:TYR:CD1	2.30	0.66
86:B6:44:LYS:CD	86:B6:98:ASP:HA	2.24	0.66
17:Aj:24:LEU:HB3	17:Aj:32:LEU:CD1	2.26	0.65
66:Bn:89:VAL:HG22	66:Bn:90:GLY:N	2.11	0.65
79:By:22:ARG:HD2	79:By:31:ILE:HG23	1.78	0.65
79:By:43:ASN:HB3	79:By:46:ARG:CB	2.26	0.65
81:Bz:37:TYR:HB2	81:Bz:47:MET:HB3	1.77	0.65
52:BZ:75:C:P	84:B4:54:PRO:HD2	2.37	0.65
77:Bw:248:HIS:C	77:Bw:255:ALA:HB3	2.21	0.65
85:B5:105:ILE:HG21	85:B5:132:LEU:CD2	2.25	0.65
9:Aa:164:ILE:HD12	9:Aa:178:ASN:HA	1.77	0.65
17:Aj:72:GLU:CD	21:An:54:LYS:HG2	2.19	0.65
26:B0:1859:C:P	79:By:46:ARG:CZ	2.84	0.65
62:Bj:53:TYR:CE2	62:Bj:78:ILE:HD11	2.31	0.65
64:Bl:79:TRP:HB2	64:Bl:118:PRO:CB	2.25	0.65
66:Bn:199:MET:O	66:Bn:237:GLU:HA	1.96	0.65
79:By:30:LYS:C	79:By:30:LYS:HD3	2.21	0.65
83:B3:6:THR:O	83:B3:9:ILE:HG22	1.96	0.65
84:B4:14:LYS:HG2	84:B4:77:CYS:SG	2.37	0.65
86:B6:45:LEU:HD12	86:B6:71:VAL:HG11	1.77	0.65
62:Bj:23:ALA:HB1	62:Bj:87:LEU:HD21	1.77	0.65
85:B5:105:ILE:CG2	85:B5:132:LEU:HG	2.25	0.65
85:B5:117:TYR:HD2	85:B5:118:LEU:CD2	2.07	0.65
85:B5:198:VAL:HG22	85:B5:210:VAL:CG2	2.26	0.65
86:B6:6:LYS:HB3	86:B6:10:SER:HB2	1.79	0.65
66:Bn:105:ALA:HB2	66:Bn:165:ALA:HA	1.77	0.65
81:Bz:69:TRP:CD1	81:Bz:70:THR:HG1	2.15	0.65
84:B4:69:ARG:CB	84:B4:80:LYS:HD3	2.26	0.65
9:Aa:262:GLU:HG2	9:Aa:270:LEU:CD2	2.26	0.65
21:An:20:SER:HB3	21:An:25:SER:O	1.96	0.65
68:Bp:23:TRP:CE3	68:Bp:51:ILE:HG22	2.31	0.65
77:Bw:168:ASN:O	77:Bw:171:SER:HB3	1.97	0.65
85:B5:62:PHE:CE1	85:B5:110:LEU:HG	2.31	0.65
17:Aj:47:ASN:OD1	17:Aj:94:PRO:HD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:An:36:LEU:HD12	21:An:42:CYS:SG	2.36	0.65
26:B0:4306:U:P	84:B4:80:LYS:NZ	2.70	0.65
51:BY:6:C:P	66:Bn:53:ARG:HH21	2.19	0.65
84:B4:34:TYR:HA	84:B4:38:LYS:CD	2.19	0.65
85:B5:103:PHE:CG	85:B5:145:MET:HE3	2.32	0.65
12:Ad:118:GLN:HG2	12:Ad:122:HIS:HD2	1.61	0.65
70:Bq:16:ARG:HD3	70:Bq:20:LYS:HB3	1.78	0.65
77:Bw:179:ARG:HD3	77:Bw:234:LYS:O	1.97	0.65
84:B4:65:LYS:HB3	84:B4:85:ILE:CG1	2.20	0.65
85:B5:57:THR:HG22	85:B5:146:LYS:C	2.22	0.65
85:B5:58:THR:HG23	85:B5:102:ASP:H	1.62	0.65
86:B6:31:TYR:OH	86:B6:59:GLU:HB2	1.96	0.65
66:Bn:207:MET:HG2	66:Bn:233:ASP:HA	1.79	0.65
86:B6:6:LYS:NZ	86:B6:14:ILE:HG21	2.12	0.65
86:B6:17:ARG:NH2	86:B6:45:LEU:HD11	2.11	0.65
1:AA:1406:A:P	21:An:41:GLN:NE2	2.69	0.65
17:Aj:63:ILE:O	17:Aj:63:ILE:HG13	1.97	0.65
22:Ao:70:GLN:CG	22:Ao:77:TYR:CE2	2.80	0.65
70:Bq:83:ILE:HG13	70:Bq:84:LEU:N	2.12	0.65
82:B2:18:LEU:CD1	82:B2:27:TYR:HB2	2.25	0.65
85:B5:43:VAL:HG13	85:B5:45:GLU:HG2	1.79	0.65
85:B5:57:THR:HG22	85:B5:146:LYS:O	1.97	0.65
9:Aa:14:HIS:HB2	9:Aa:18:VAL:CA	2.27	0.64
17:Aj:46:LYS:CB	17:Aj:97:ILE:HA	2.27	0.64
62:Bj:40:ILE:CG2	62:Bj:137:LEU:HD13	2.23	0.64
68:Bp:25:ASP:CB	68:Bp:28:GLU:HG2	2.26	0.64
68:Bp:29:THR:O	68:Bp:32:ILE:HG22	1.97	0.64
84:B4:12:CYS:HB3	84:B4:21:HIS:NE2	2.11	0.64
84:B4:15:CYS:SG	84:B4:75:PRO:HG3	2.36	0.64
84:B4:69:ARG:HB3	84:B4:80:LYS:HD3	1.76	0.64
85:B5:56:GLU:OE1	85:B5:146:LYS:HD2	1.95	0.64
86:B6:45:LEU:CD1	86:B6:71:VAL:HB	2.26	0.64
26:B0:4262:U:P	70:Bq:81:GLY:CA	2.79	0.64
62:Bj:59:LYS:O	62:Bj:63:THR:HG23	1.97	0.64
66:Bn:199:MET:O	66:Bn:237:GLU:CA	2.45	0.64
77:Bw:149:LYS:O	77:Bw:152:ILE:HG12	1.97	0.64
77:Bw:238:PRO:CB	77:Bw:268:ARG:HD2	2.26	0.64
79:By:55:MET:HA	79:By:60:TYR:HH	1.60	0.64
9:Aa:14:HIS:HB2	9:Aa:18:VAL:HA	1.77	0.64
62:Bj:35:VAL:CG1	62:Bj:109:PRO:HB3	2.26	0.64
66:Bn:187:LYS:HE2	66:Bn:188:GLU:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:B7:193:MET:HE3	69:B7:197:ARG:NH2	2.12	0.64
77:Bw:140:PHE:HB2	77:Bw:235:LEU:HB2	1.79	0.64
77:Bw:162:ILE:CD1	77:Bw:164:TRP:HD1	2.11	0.64
79:By:30:LYS:O	79:By:32:LYS:HD2	1.97	0.64
9:Aa:14:HIS:HA	9:Aa:35:SER:HB3	1.78	0.64
68:Bp:99:MET:HE3	68:Bp:103:ARG:NH2	2.12	0.64
70:Bq:82:LYS:HD2	70:Bq:82:LYS:C	2.21	0.64
82:B2:18:LEU:CD2	82:B2:22:CYS:HB3	2.27	0.64
85:B5:69:LEU:H	85:B5:69:LEU:HD22	1.62	0.64
85:B5:110:LEU:O	85:B5:110:LEU:HD13	1.97	0.64
62:Bj:50:LYS:CE	62:Bj:51:LEU:HD23	2.26	0.64
70:Bq:72:GLY:C	70:Bq:89:ASN:HA	2.23	0.64
82:B2:19:CYS:SG	82:B2:20:ARG:HD3	2.38	0.64
9:Aa:282:GLU:HG3	9:Aa:308:ARG:HH22	1.61	0.64
12:Ad:120:VAL:CG1	12:Ad:135:PRO:HG3	2.28	0.64
64:Bl:79:TRP:CB	64:Bl:118:PRO:HB3	2.27	0.64
77:Bw:159:GLU:HG3	77:Bw:162:ILE:HD11	1.79	0.64
81:Bz:75:SER:O	81:Bz:78:THR:HG22	1.98	0.64
83:B3:23:ILE:HB	83:B3:24:PRO:HD2	1.79	0.64
84:B4:37:GLY:HA2	84:B4:40:ARG:CB	2.26	0.64
17:Aj:47:ASN:CG	17:Aj:94:PRO:HD2	2.23	0.64
51:BY:67:C:P	66:Bn:12:PHE:C	2.81	0.64
62:Bj:29:GLY:HA2	62:Bj:100:ARG:NH1	2.12	0.64
77:Bw:243:LYS:HG3	77:Bw:253:GLY:HA3	1.78	0.64
86:B6:79:ILE:HG22	86:B6:90:ARG:CG	2.25	0.64
66:Bn:77:ARG:HE	66:Bn:103:LEU:HB3	1.61	0.64
66:Bn:85:TYR:CE1	66:Bn:103:LEU:HG	2.33	0.64
84:B4:67:VAL:HG22	84:B4:85:ILE:HD12	1.80	0.64
85:B5:110:LEU:CD2	85:B5:113:ASP:HB2	2.28	0.64
77:Bw:172:VAL:CG2	77:Bw:213:ILE:HB	2.27	0.64
80:B9:83:LYS:HD2	80:B9:83:LYS:N	2.13	0.64
9:Aa:217:MET:HE2	9:Aa:226:HIS:CG	2.33	0.64
17:Aj:107:GLU:HG2	17:Aj:110:VAL:HG23	1.80	0.64
64:Bl:71:PRO:HB2	64:Bl:101:ILE:HD12	1.80	0.64
68:Bp:47:ASP:HB3	68:Bp:49:LEU:CD1	2.28	0.64
70:Bq:52:PRO:HB3	70:Bq:88:ILE:HG21	1.79	0.64
80:B9:87:VAL:HG11	80:B9:89:LEU:HB2	1.79	0.64
85:B5:98:ALA:O	85:B5:127:LYS:HE3	1.98	0.64
26:B0:4286:G:P	66:Bn:37:ILE:HD13	2.38	0.63
66:Bn:89:VAL:HG23	66:Bn:193:VAL:HG12	1.81	0.63
86:B6:7:THR:HG22	86:B6:8:LYS:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Aj:31:SER:HB3	17:Aj:107:GLU:HG2	1.80	0.63
26:B0:1713:G:P	70:Bq:12:TYR:HD2	2.17	0.63
62:Bj:26:VAL:CG1	62:Bj:97:ALA:HB1	2.28	0.63
64:Bl:19:HIS:CD2	64:Bl:22:ILE:HG22	2.34	0.63
68:Bp:115:ILE:HG23	68:Bp:119:MET:HB2	1.79	0.63
70:Bq:41:ILE:HG12	70:Bq:77:LYS:HZ1	1.63	0.63
85:B5:43:VAL:HG22	85:B5:188:LEU:CD1	2.28	0.63
85:B5:150:GLN:NE2	85:B5:152:ARG:HD3	2.12	0.63
48:BV:12:C:P	64:Bl:135:GLU:OE2	2.56	0.63
77:Bw:172:VAL:HA	77:Bw:175:LEU:HD23	1.79	0.63
83:B3:5:LYS:HB2	83:B3:9:ILE:HG21	1.80	0.63
85:B5:163:VAL:HG11	85:B5:173:ILE:CG2	2.28	0.63
17:Aj:67:LYS:CE	17:Aj:78:ASP:HB2	2.20	0.63
68:Bp:47:ASP:HB2	68:Bp:49:LEU:HD13	1.78	0.63
70:Bq:71:VAL:CB	70:Bq:74:ILE:HG12	2.28	0.63
77:Bw:136:LEU:N	77:Bw:136:LEU:HD12	2.14	0.63
79:By:40:GLY:HA3	79:By:43:ASN:ND2	2.14	0.63
86:B6:14:ILE:HG22	86:B6:108:MET:HE2	1.81	0.63
86:B6:29:LEU:O	86:B6:29:LEU:HD12	1.99	0.63
62:Bj:46:PHE:CD1	62:Bj:135:ALA:HB2	2.33	0.63
77:Bw:243:LYS:HB2	77:Bw:253:GLY:C	2.24	0.63
84:B4:75:PRO:HG2	84:B4:77:CYS:HB3	1.81	0.63
66:Bn:191:ALA:C	66:Bn:238:MET:SD	2.82	0.63
68:Bp:122:SER:O	68:Bp:126:LYS:HG2	1.99	0.63
77:Bw:188:ARG:NH1	77:Bw:188:ARG:HB2	2.14	0.63
77:Bw:244:LYS:HD3	77:Bw:245:LYS:H	1.63	0.63
83:B3:35:ILE:HG23	83:B3:37:TYR:N	2.13	0.63
1:AA:1540:C:P	9:Aa:60:ARG:CA	2.87	0.63
26:B0:2713:G:P	81:Bz:34:HIS:CE1	2.92	0.63
66:Bn:98:TYR:CE2	66:Bn:102:LEU:HD11	2.33	0.63
86:B6:79:ILE:CG2	86:B6:90:ARG:HG2	2.27	0.63
21:An:21:CYS:HB2	21:An:36:LEU:HA	1.81	0.63
62:Bj:50:LYS:HD2	62:Bj:51:LEU:N	2.14	0.63
70:Bq:6:LYS:HD3	70:Bq:7:ARG:HG3	1.80	0.63
84:B4:38:LYS:CG	84:B4:39:ARG:HD3	2.28	0.63
26:B0:51:A:P	82:B2:49:TRP:CD1	2.92	0.63
62:Bj:11:ARG:HB2	62:Bj:36:ARG:CD	2.19	0.63
62:Bj:55:ALA:O	62:Bj:58:ARG:HD2	1.99	0.63
77:Bw:116:ARG:NH2	77:Bw:158:VAL:HG21	2.14	0.63
77:Bw:216:ILE:C	77:Bw:219:VAL:HG12	2.23	0.63
82:B2:18:LEU:HD22	82:B2:24:SER:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:143:GLU:HG2	85:B5:146:LYS:HE2	1.81	0.63
12:Ad:78:PHE:HA	12:Ad:92:PHE:CD1	2.34	0.62
39:BM:2686:U:P	68:Bp:43:LYS:CE	2.86	0.62
62:Bj:36:ARG:HH11	62:Bj:107:ILE:CB	2.07	0.62
85:B5:45:GLU:HG2	85:B5:188:LEU:HD11	1.81	0.62
86:B6:82:GLY:HA2	86:B6:91:VAL:HG23	1.79	0.62
9:Aa:191:HIS:CG	9:Aa:195:LEU:HD21	2.33	0.62
62:Bj:54:LEU:HB3	62:Bj:140:LEU:HD21	1.77	0.62
77:Bw:194:ASN:HA	77:Bw:197:ILE:HG12	1.81	0.62
79:By:55:MET:HE3	79:By:56:PRO:HB3	1.81	0.62
85:B5:195:ILE:HD11	85:B5:198:VAL:HG13	1.79	0.62
22:Ao:70:GLN:HG3	22:Ao:77:TYR:CE2	2.34	0.62
64:Bl:16:SER:O	64:Bl:19:HIS:HB2	1.98	0.62
79:By:11:LYS:O	79:By:13:VAL:HG22	2.00	0.62
81:Bz:69:TRP:HD1	81:Bz:70:THR:HG1	1.47	0.62
86:B6:104:ILE:HG13	86:B6:105:ILE:N	2.13	0.62
64:Bl:101:ILE:HD13	64:Bl:109:TYR:CD1	2.34	0.62
64:Bl:108:TYR:HD2	64:Bl:127:LYS:HB3	1.64	0.62
70:Bq:40:ASP:O	70:Bq:95:ILE:HD12	2.00	0.62
86:B6:11:LEU:HD12	86:B6:14:ILE:HD11	1.81	0.62
9:Aa:217:MET:HE3	9:Aa:229:THR:HG22	1.81	0.62
85:B5:110:LEU:HD22	85:B5:110:LEU:O	1.99	0.62
86:B6:20:LEU:O	86:B6:20:LEU:HD23	1.98	0.62
9:Aa:18:VAL:N	9:Aa:305:ASN:HB3	2.15	0.62
9:Aa:284:PRO:CD	9:Aa:304:ASP:HB2	2.30	0.62
17:Aj:56:MET:CG	17:Aj:57:PRO:HD2	2.28	0.62
26:B0:2384:G:P	83:B3:44:TRP:HB2	2.39	0.62
64:Bl:109:TYR:CD2	64:Bl:126:ALA:HB1	2.34	0.62
70:Bq:73:ILE:HG13	70:Bq:87:ARG:HG3	1.81	0.62
77:Bw:127:VAL:HG12	77:Bw:161:TYR:OH	1.99	0.62
77:Bw:191:LEU:HG	77:Bw:192:THR:HG23	1.80	0.62
79:By:11:LYS:O	79:By:15:LYS:HB2	1.99	0.62
82:B2:31:LYS:HE3	82:B2:31:LYS:O	1.99	0.62
85:B5:103:PHE:HB3	85:B5:145:MET:CE	2.28	0.62
85:B5:122:LEU:HD12	85:B5:129:PRO:HD3	1.81	0.62
1:AA:1654:C:P	21:An:29:GLY:HA3	2.40	0.62
12:Ad:91:VAL:O	12:Ad:95:LEU:HD13	1.99	0.62
26:B0:2502:U:P	68:Bp:37:SER:HB2	2.40	0.62
64:Bl:82:VAL:HA	64:Bl:85:GLN:HE21	1.65	0.62
66:Bn:39:ASP:O	70:Bq:29:TYR:OH	2.17	0.62
62:Bj:119:VAL:HG13	62:Bj:120:PRO:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Bq:3:THR:HG22	70:Bq:4:LYS:N	2.15	0.62
82:B2:3:LYS:C	82:B2:8:PHE:HZ	2.07	0.62
25:B1:45:C:P	83:B3:15:LYS:CE	2.75	0.62
64:Bl:42:ARG:HD2	64:Bl:42:ARG:O	2.00	0.62
70:Bq:92:ILE:HA	70:Bq:95:ILE:HG22	1.81	0.62
17:Aj:84:ILE:HD13	17:Aj:85:HIS:O	1.99	0.62
17:Aj:93:SER:OG	17:Aj:97:ILE:HG21	1.99	0.62
26:B0:4478:A:P	54:Bb:257:HIS:CB	2.84	0.62
68:Bp:106:LEU:HD11	68:Bp:127:VAL:HG21	1.81	0.62
77:Bw:201:LEU:H	77:Bw:201:LEU:HD12	1.65	0.62
84:B4:39:ARG:HD3	84:B4:39:ARG:H	1.65	0.62
85:B5:43:VAL:HG11	85:B5:151:LEU:CG	2.29	0.62
26:B0:1494:A:P	64:Bl:32:ARG:HB3	2.40	0.61
62:Bj:36:ARG:HD2	62:Bj:107:ILE:CG1	2.30	0.61
83:B3:17:GLN:O	83:B3:20:ASN:HB2	1.99	0.61
9:Aa:247:TRP:HB2	9:Aa:261:LEU:HB2	1.82	0.61
64:Bl:137:ILE:HG13	64:Bl:138:LYS:N	2.14	0.61
68:Bp:17:CYS:SG	68:Bp:52:ARG:HG3	2.40	0.61
68:Bp:112:SER:OG	68:Bp:114:LYS:HD3	2.00	0.61
70:Bq:66:VAL:CG2	70:Bq:71:VAL:HA	2.21	0.61
80:B9:96:CYS:SG	80:B9:121:ARG:HB3	2.39	0.61
82:B2:20:ARG:HG2	82:B2:21:ARG:N	2.15	0.61
85:B5:103:PHE:HD1	85:B5:145:MET:HE3	1.65	0.61
86:B6:66:LEU:C	86:B6:66:LEU:HD13	2.25	0.61
9:Aa:79:LEU:HD12	9:Aa:120:ILE:HD13	1.82	0.61
17:Aj:24:LEU:HB2	17:Aj:32:LEU:HD11	1.81	0.61
17:Aj:47:ASN:CB	17:Aj:93:SER:HB2	2.30	0.61
17:Aj:50:VAL:HG12	17:Aj:52:GLY:H	1.66	0.61
26:B0:1639:U:P	64:Bl:15:VAL:CB	2.88	0.61
79:By:28:TYR:CZ	79:By:31:ILE:HD11	2.33	0.61
86:B6:14:ILE:HG23	86:B6:108:MET:HE2	1.82	0.61
9:Aa:10:THR:HG21	9:Aa:306:LEU:HD23	1.82	0.61
9:Aa:89:LEU:HB3	9:Aa:100:ARG:HG2	1.82	0.61
26:B0:1634:C:P	64:Bl:28:HIS:CE1	2.94	0.61
62:Bj:36:ARG:NH1	62:Bj:107:ILE:HB	2.08	0.61
66:Bn:38:GLN:CB	70:Bq:29:TYR:CE2	2.84	0.61
82:B2:31:LYS:HD2	82:B2:33:THR:N	2.09	0.61
9:Aa:254:PRO:HG3	9:Aa:284:PRO:C	2.26	0.61
17:Aj:97:ILE:HD12	17:Aj:98:VAL:N	2.14	0.61
80:B9:75:ARG:HB3	80:B9:95:TYR:HD2	1.65	0.61
85:B5:34:LEU:HD21	85:B5:41:ASN:HD22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Bp:19:LYS:O	68:Bp:22:VAL:HG22	2.01	0.61
86:B6:44:LYS:HG2	86:B6:98:ASP:HA	1.82	0.61
86:B6:45:LEU:O	86:B6:45:LEU:HD23	1.99	0.61
9:Aa:14:HIS:HA	9:Aa:35:SER:CB	2.31	0.61
17:Aj:104:ILE:H	17:Aj:104:ILE:HD13	1.65	0.61
26:B0:1885:A:P	77:Bw:244:LYS:HZ3	2.24	0.61
68:Bp:23:TRP:HE3	68:Bp:51:ILE:HG22	1.65	0.61
70:Bq:78:GLN:HG2	70:Bq:78:GLN:O	2.00	0.61
86:B6:6:LYS:CD	86:B6:14:ILE:HG21	2.31	0.61
26:B0:2611:C:P	68:Bp:60:ARG:H	2.23	0.61
26:B0:4286:G:P	66:Bn:37:ILE:HG21	2.41	0.61
70:Bq:38:ILE:C	70:Bq:38:ILE:HD13	2.26	0.61
85:B5:62:PHE:CZ	85:B5:110:LEU:HG	2.36	0.61
9:Aa:11:LEU:HD11	9:Aa:31:ILE:HD13	1.81	0.61
51:BY:87:G:P	77:Bw:246:THR:HG23	2.40	0.61
77:Bw:172:VAL:HG23	77:Bw:213:ILE:HB	1.82	0.61
77:Bw:211:ASP:HA	77:Bw:214:HIS:HD2	1.66	0.61
77:Bw:231:TRP:HE3	77:Bw:231:TRP:H	1.49	0.61
79:By:48:ARG:NE	79:By:53:ILE:HG21	2.11	0.61
84:B4:65:LYS:HA	84:B4:87:ARG:HA	1.83	0.61
84:B4:89:LYS:HG3	84:B4:90:HIS:N	2.16	0.61
85:B5:191:GLY:HA2	85:B5:194:ASN:OD1	2.01	0.61
86:B6:17:ARG:HD3	86:B6:105:ILE:HD11	1.82	0.61
9:Aa:18:VAL:H	9:Aa:305:ASN:HB3	1.65	0.61
9:Aa:79:LEU:CD1	9:Aa:120:ILE:HD13	2.31	0.61
62:Bj:73:ARG:HB2	62:Bj:77:ARG:HH21	1.65	0.61
66:Bn:81:GLU:CG	66:Bn:103:LEU:HD22	2.30	0.61
66:Bn:84:LYS:HZ2	66:Bn:107:ARG:HH12	1.47	0.61
77:Bw:116:ARG:HH22	77:Bw:158:VAL:HG21	1.65	0.61
77:Bw:127:VAL:CG1	77:Bw:161:TYR:HE1	2.14	0.61
85:B5:5:ILE:O	85:B5:9:VAL:HG23	2.01	0.61
85:B5:190:LYS:HG2	85:B5:191:GLY:H	1.66	0.61
86:B6:29:LEU:HD12	86:B6:29:LEU:C	2.26	0.61
86:B6:45:LEU:CD2	86:B6:96:ILE:HG22	2.31	0.61
86:B6:48:LEU:HD21	86:B6:60:ILE:CD1	2.31	0.61
9:Aa:14:HIS:CB	9:Aa:18:VAL:HA	2.31	0.60
66:Bn:185:GLU:CD	66:Bn:201:GLN:HB2	2.25	0.60
77:Bw:130:VAL:HG13	77:Bw:131:LEU:N	2.16	0.60
77:Bw:242:MET:SD	77:Bw:254:ASP:HB3	2.41	0.60
77:Bw:258:ARG:HG3	77:Bw:260:ASP:OD1	2.01	0.60
9:Aa:217:MET:HE3	9:Aa:229:THR:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B0:2293:C:P	79:By:67:LYS:O	2.59	0.60
77:Bw:131:LEU:O	77:Bw:131:LEU:HD13	2.00	0.60
77:Bw:135:ARG:HA	77:Bw:135:ARG:HE	1.65	0.60
77:Bw:176:ILE:HD13	77:Bw:233:PHE:HE2	1.66	0.60
86:B6:45:LEU:HD23	86:B6:96:ILE:HG22	1.82	0.60
9:Aa:248:LEU:CD2	9:Aa:298:LEU:CD1	2.78	0.60
64:Bl:97:VAL:HG23	64:Bl:124:VAL:HG13	1.83	0.60
79:By:64:LYS:HA	79:By:67:LYS:HE3	1.82	0.60
80:B9:82:VAL:HG12	80:B9:111:ILE:HA	1.83	0.60
82:B2:45:ARG:HD2	82:B2:45:ARG:C	2.27	0.60
85:B5:70:ARG:HG3	85:B5:137:ASP:HA	1.82	0.60
85:B5:180:ILE:HG13	85:B5:181:LEU:N	2.15	0.60
1:AA:1948:C:P	26:B0:2847:A:P	2.99	0.60
9:Aa:98:THR:HG21	9:Aa:101:PHE:CZ	2.36	0.60
62:Bj:50:LYS:HB2	62:Bj:55:ALA:HB2	1.80	0.60
62:Bj:57:LEU:HD23	62:Bj:58:ARG:N	2.16	0.60
62:Bj:58:ARG:CB	62:Bj:61:MET:HB3	2.26	0.60
64:Bl:124:VAL:O	64:Bl:145:VAL:HG12	2.01	0.60
66:Bn:77:ARG:HD3	66:Bn:81:GLU:CB	2.31	0.60
66:Bn:89:VAL:CB	66:Bn:193:VAL:HA	2.30	0.60
66:Bn:195:ARG:CG	66:Bn:203:VAL:HG11	2.31	0.60
70:Bq:73:ILE:CD1	70:Bq:87:ARG:HD2	2.30	0.60
77:Bw:210:GLU:CA	77:Bw:213:ILE:HG12	2.30	0.60
12:Ad:107:LEU:HD12	12:Ad:109:PHE:HE2	1.65	0.60
62:Bj:72:PHE:CD1	62:Bj:78:ILE:HG12	2.36	0.60
66:Bn:16:GLN:OE1	70:Bq:21:HIS:O	2.19	0.60
66:Bn:184:SER:HB3	66:Bn:198:ILE:CG2	2.32	0.60
79:By:30:LYS:HD3	79:By:31:ILE:N	2.16	0.60
84:B4:38:LYS:HG3	84:B4:39:ARG:N	2.16	0.60
64:Bl:97:VAL:CG2	64:Bl:124:VAL:HG13	2.31	0.60
77:Bw:133:LEU:C	77:Bw:133:LEU:HD22	2.26	0.60
77:Bw:164:TRP:O	77:Bw:262:ILE:HD11	2.02	0.60
85:B5:58:THR:O	85:B5:101:THR:HG23	2.02	0.60
86:B6:59:GLU:O	86:B6:63:TYR:HD1	1.84	0.60
62:Bj:107:ILE:HG23	62:Bj:108:PRO:HD2	1.82	0.60
79:By:25:SER:HA	79:By:31:ILE:CG2	2.31	0.60
79:By:48:ARG:HE	79:By:53:ILE:CG2	2.14	0.60
79:By:58:ILE:HG13	79:By:58:ILE:O	2.01	0.60
82:B2:15:THR:HG22	82:B2:16:HIS:N	2.16	0.60
83:B3:13:LEU:HD13	83:B3:13:LEU:O	2.01	0.60
86:B6:44:LYS:CG	86:B6:98:ASP:HA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Bl:82:VAL:HG23	64:Bl:83:SER:N	2.16	0.60
64:Bl:101:ILE:HG13	64:Bl:104:VAL:CG2	2.24	0.60
64:Bl:123:ILE:HD12	64:Bl:123:ILE:N	2.16	0.60
70:Bq:68:GLN:HG2	70:Bq:69:HIS:N	2.15	0.60
70:Bq:77:LYS:HD2	70:Bq:88:ILE:HD12	1.84	0.60
77:Bw:156:ARG:HA	77:Bw:156:ARG:NE	2.17	0.60
77:Bw:196:LEU:HD11	77:Bw:208:CYS:C	2.27	0.60
77:Bw:219:VAL:HG23	77:Bw:220:GLY:N	2.15	0.60
77:Bw:261:GLN:O	77:Bw:265:LEU:HB2	2.01	0.60
79:By:64:LYS:HD2	79:By:64:LYS:C	2.27	0.60
80:B9:82:VAL:CG2	80:B9:83:LYS:HD2	2.29	0.60
82:B2:48:ASN:O	82:B2:51:ALA:HB3	2.01	0.60
85:B5:27:LEU:HD11	85:B5:29:VAL:CG2	2.32	0.60
85:B5:84:LEU:HD12	85:B5:87:LEU:HD12	1.83	0.60
26:B0:2642:U:P	68:Bp:124:TYR:OH	2.60	0.60
64:Bl:118:PRO:O	64:Bl:140:VAL:HG21	2.01	0.60
68:Bp:115:ILE:HG22	68:Bp:116:ASP:O	2.01	0.60
77:Bw:153:ASN:O	77:Bw:156:ARG:HB3	2.01	0.60
9:Aa:305:ASN:C	9:Aa:306:LEU:HD12	2.27	0.60
17:Aj:40:ILE:CD1	17:Aj:89:ILE:HD11	2.31	0.60
51:BY:8:G:P	70:Bq:26:LEU:HD21	2.42	0.60
66:Bn:37:ILE:HG22	66:Bn:45:THR:H	1.67	0.60
66:Bn:187:LYS:HB2	66:Bn:237:GLU:OE2	2.02	0.60
70:Bq:71:VAL:CA	70:Bq:74:ILE:HG12	2.32	0.60
70:Bq:82:LYS:HD3	70:Bq:85:ALA:C	2.27	0.60
77:Bw:213:ILE:HG13	77:Bw:214:HIS:N	2.17	0.60
79:By:7:LEU:HD11	79:By:63:ASN:HB3	1.82	0.60
85:B5:50:PRO:CG	85:B5:179:VAL:HG21	2.31	0.60
85:B5:74:VAL:CG1	85:B5:142:ILE:HB	2.31	0.60
86:B6:4:ALA:HB3	86:B6:73:HIS:NE2	2.17	0.60
26:B0:3944:C:P	85:B5:204:MET:HE1	2.42	0.59
64:Bl:97:VAL:HG11	64:Bl:109:TYR:CE2	2.37	0.59
66:Bn:198:ILE:HG23	66:Bn:199:MET:N	2.17	0.59
85:B5:27:LEU:HD13	85:B5:28:ALA:N	2.17	0.59
85:B5:43:VAL:HG22	85:B5:188:LEU:HD12	1.83	0.59
86:B6:50:ASN:OD1	86:B6:74:TYR:HB3	2.02	0.59
26:B0:430:G:P	79:By:16:ARG:NE	2.73	0.59
64:Bl:117:LEU:HD21	64:Bl:136:LYS:CD	2.25	0.59
68:Bp:42:ARG:O	68:Bp:45:ILE:HG12	2.01	0.59
77:Bw:134:LEU:HB3	77:Bw:136:LEU:CD1	2.32	0.59
12:Ad:100:LEU:HD23	12:Ad:120:VAL:CG2	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Ad:123:GLY:O	12:Ad:131:ARG:HD3	2.03	0.59
17:Aj:47:ASN:HD22	17:Aj:48:LEU:N	2.00	0.59
17:Aj:94:PRO:O	17:Aj:97:ILE:HG13	2.02	0.59
51:By:87:G:P	77:Bw:246:THR:CG2	2.90	0.59
62:Bj:8:LEU:C	62:Bj:115:LYS:HB3	2.26	0.59
79:By:66:THR:O	80:B9:69:MET:CE	2.50	0.59
81:Bz:11:VAL:HG21	81:Bz:23:ARG:CG	2.32	0.59
81:Bz:57:CYS:O	81:Bz:61:MET:HA	2.02	0.59
17:Aj:40:ILE:HD12	17:Aj:50:VAL:HG21	1.84	0.59
21:An:36:LEU:HD12	21:An:42:CYS:CB	2.32	0.59
62:Bj:26:VAL:CG1	62:Bj:87:LEU:HD11	2.32	0.59
68:Bp:24:LEU:N	68:Bp:24:LEU:HD12	2.18	0.59
79:By:8:VAL:O	79:By:11:LYS:HD3	2.02	0.59
26:B0:2262:G:P	64:Bl:6:ARG:NH1	2.75	0.59
62:Bj:6:LEU:HD12	62:Bj:25:GLN:HE22	1.67	0.59
64:Bl:98:ALA:O	64:Bl:104:VAL:HG21	2.01	0.59
17:Aj:47:ASN:ND2	17:Aj:93:SER:HB2	2.17	0.59
26:B0:2279:C:P	80:B9:104:SER:HB3	2.43	0.59
77:Bw:260:ASP:O	77:Bw:261:GLN:HG2	2.02	0.59
84:B4:55:ILE:HG22	84:B4:56:PHE:O	2.02	0.59
66:Bn:38:GLN:CB	70:Bq:29:TYR:HE2	2.16	0.59
70:Bq:41:ILE:HD12	70:Bq:41:ILE:N	2.18	0.59
79:By:55:MET:HE3	79:By:56:PRO:CA	2.30	0.59
85:B5:47:VAL:CG1	85:B5:179:VAL:HG12	2.32	0.59
85:B5:69:LEU:HD22	85:B5:69:LEU:N	2.16	0.59
64:Bl:117:LEU:HD11	64:Bl:136:LYS:HD3	1.83	0.59
77:Bw:180:GLY:O	77:Bw:181:TYR:HB2	2.01	0.59
77:Bw:242:MET:HE2	77:Bw:243:LYS:N	2.18	0.59
85:B5:61:VAL:HG23	85:B5:76:ASP:OD2	2.03	0.59
86:B6:31:TYR:CE1	86:B6:57:LYS:HA	2.38	0.59
9:Aa:256:ILE:HD11	9:Aa:300:ALA:HB1	1.84	0.59
26:B0:1597:G:P	82:B2:10:LYS:HG3	2.41	0.59
62:Bj:46:PHE:CE1	62:Bj:135:ALA:HB1	2.38	0.59
68:Bp:69:ALA:HB1	68:Bp:75:HIS:HD1	1.66	0.59
77:Bw:247:THR:OG1	77:Bw:255:ALA:HB2	2.03	0.59
77:Bw:258:ARG:O	77:Bw:262:ILE:HG12	2.03	0.59
77:Bw:262:ILE:O	77:Bw:265:LEU:HB3	2.03	0.59
85:B5:34:LEU:O	85:B5:157:ARG:HD3	2.03	0.59
85:B5:60:VAL:HG13	85:B5:101:THR:CB	2.32	0.59
21:An:17:GLY:O	21:An:19:ARG:HD2	2.03	0.59
26:B0:3856:C:P	62:Bj:81:ARG:HH22	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:By:13:VAL:HG23	79:By:14:LYS:N	2.17	0.59
82:B2:31:LYS:CE	82:B2:33:THR:H	2.16	0.59
85:B5:62:PHE:CZ	85:B5:110:LEU:HD23	2.37	0.59
85:B5:149:VAL:HG21	85:B5:161:THR:OG1	2.03	0.59
62:Bj:54:LEU:HB3	62:Bj:140:LEU:HD23	1.80	0.58
62:Bj:58:ARG:HB2	62:Bj:61:MET:CB	2.28	0.58
64:Bl:22:ILE:O	64:Bl:22:ILE:HG23	2.03	0.58
70:Bq:70:ALA:HB2	70:Bq:91:ARG:HG2	1.84	0.58
77:Bw:212:LEU:O	77:Bw:216:ILE:HG12	2.03	0.58
83:B3:13:LEU:HD13	83:B3:13:LEU:C	2.27	0.58
9:Aa:168:CYS:SG	9:Aa:174:VAL:HG22	2.43	0.58
62:Bj:109:PRO:HD3	62:Bj:115:LYS:HZ2	1.68	0.58
79:By:18:LYS:HA	79:By:18:LYS:CE	2.32	0.58
85:B5:43:VAL:HG13	85:B5:188:LEU:HD11	1.83	0.58
86:B6:2:VAL:HG23	86:B6:2:VAL:O	2.03	0.58
1:AA:1436:A:P	21:An:13:LYS:HZ2	2.26	0.58
9:Aa:241:PHE:CD1	9:Aa:246:TYR:HB2	2.37	0.58
9:Aa:248:LEU:CD2	9:Aa:298:LEU:HD11	2.33	0.58
12:Ad:59:GLU:OE1	12:Ad:59:GLU:HA	2.02	0.58
17:Aj:46:LYS:HE3	17:Aj:100:GLN:HE22	1.67	0.58
62:Bj:9:ASP:CB	62:Bj:115:LYS:HB2	2.29	0.58
64:Bl:117:LEU:HD22	64:Bl:136:LYS:CB	2.25	0.58
66:Bn:38:GLN:C	70:Bq:29:TYR:CE2	2.74	0.58
70:Bq:79:VAL:HG22	70:Bq:80:LYS:N	2.17	0.58
77:Bw:158:VAL:HG22	77:Bw:162:ILE:HG23	1.84	0.58
77:Bw:171:SER:O	77:Bw:174:GLU:HB3	2.03	0.58
82:B2:46:LYS:H	82:B2:46:LYS:HD3	1.68	0.58
82:B2:46:LYS:HD3	82:B2:46:LYS:N	2.18	0.58
85:B5:24:THR:HG22	85:B5:203:THR:OG1	2.03	0.58
85:B5:156:ARG:HG2	85:B5:157:ARG:N	2.16	0.58
12:Ad:63:LEU:HD11	12:Ad:96:LEU:CD1	2.33	0.58
12:Ad:121:ARG:HD3	12:Ad:121:ARG:C	2.26	0.58
17:Aj:101:ILE:O	17:Aj:101:ILE:HD13	2.03	0.58
66:Bn:184:SER:CB	66:Bn:198:ILE:CA	2.80	0.58
82:B2:45:ARG:HD3	82:B2:47:TYR:CD2	2.38	0.58
85:B5:190:LYS:HG2	85:B5:191:GLY:N	2.18	0.58
66:Bn:79:ALA:HB1	66:Bn:91:LEU:CD2	2.33	0.58
70:Bq:28:THR:O	70:Bq:92:ILE:HG23	2.04	0.58
77:Bw:208:CYS:SG	77:Bw:210:GLU:HB3	2.43	0.58
80:B9:109:LYS:HA	80:B9:109:LYS:HE3	1.86	0.58
82:B2:43:ARG:HG2	82:B2:44:LYS:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B6:15:ASN:ND2	86:B6:80:GLU:HG3	2.18	0.58
17:Aj:19:ARG:HD3	17:Aj:19:ARG:N	2.18	0.58
21:An:46:TYR:HB3	21:An:49:ASP:HB2	1.85	0.58
62:Bj:134:PHE:HE1	62:Bj:136:TYR:HH	1.51	0.58
77:Bw:162:ILE:HD11	77:Bw:164:TRP:HD1	1.68	0.58
79:By:11:LYS:HG2	79:By:12:ILE:N	2.18	0.58
79:By:21:ILE:N	79:By:21:ILE:HD12	2.17	0.58
79:By:44:ARG:HA	79:By:44:ARG:HE	1.68	0.58
82:B2:19:CYS:HB2	82:B2:27:TYR:HD2	1.68	0.58
9:Aa:201:SER:HB2	9:Aa:206:LEU:HD11	1.86	0.58
17:Aj:97:ILE:HD12	17:Aj:97:ILE:C	2.29	0.58
62:Bj:25:GLN:HG2	62:Bj:30:ARG:CB	2.31	0.58
66:Bn:39:ASP:HA	70:Bq:29:TYR:OH	2.04	0.58
66:Bn:42:LYS:CA	70:Bq:32:ILE:CG1	2.80	0.58
66:Bn:235:MET:HG3	66:Bn:237:GLU:HG2	1.86	0.58
70:Bq:92:ILE:HD13	70:Bq:95:ILE:HG22	1.86	0.58
77:Bw:127:VAL:HG11	77:Bw:161:TYR:HE1	1.68	0.58
82:B2:18:LEU:HD13	82:B2:27:TYR:N	2.17	0.58
9:Aa:64:HIS:CE1	9:Aa:65:PHE:HB2	2.38	0.58
21:An:21:CYS:SG	21:An:38:MET:HB3	2.43	0.58
26:B0:4259:U:P	70:Bq:87:ARG:NH2	2.76	0.58
66:Bn:63:ILE:HG23	66:Bn:74:VAL:HG13	1.85	0.58
77:Bw:196:LEU:HD23	77:Bw:196:LEU:N	2.17	0.58
77:Bw:266:ILE:HD12	77:Bw:266:ILE:C	2.28	0.58
85:B5:110:LEU:HD13	85:B5:114:ILE:HB	1.81	0.58
85:B5:163:VAL:HG12	85:B5:173:ILE:HG23	1.85	0.58
12:Ad:63:LEU:HD13	12:Ad:63:LEU:C	2.28	0.58
17:Aj:48:LEU:HD12	17:Aj:92:HIS:O	2.04	0.58
17:Aj:50:VAL:CG2	17:Aj:91:LEU:HD13	2.34	0.58
77:Bw:123:VAL:HG22	77:Bw:124:SER:N	2.19	0.58
77:Bw:190:ALA:HA	77:Bw:195:SER:OG	2.02	0.58
84:B4:45:GLN:HA	84:B4:45:GLN:HE21	1.69	0.58
85:B5:74:VAL:HG22	85:B5:139:VAL:CA	2.32	0.58
9:Aa:21:ILE:HG23	9:Aa:307:VAL:HG21	1.86	0.58
70:Bq:74:ILE:HD12	70:Bq:75:VAL:N	2.19	0.58
79:By:22:ARG:CZ	79:By:31:ILE:HD12	2.33	0.58
81:Bz:70:THR:HG22	81:Bz:71:TYR:N	2.19	0.58
83:B3:41:ARG:HB3	83:B3:41:ARG:HH11	1.69	0.58
83:B3:42:ARG:HG3	83:B3:47:THR:OG1	2.03	0.58
86:B6:46:VAL:HG13	86:B6:72:HIS:HA	1.86	0.58
9:Aa:201:SER:CB	9:Aa:206:LEU:HD11	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Bl:140:VAL:O	64:Bl:140:VAL:HG22	2.04	0.57
66:Bn:85:TYR:CE1	66:Bn:103:LEU:CD1	2.87	0.57
66:Bn:187:LYS:HA	66:Bn:199:MET:HE2	1.78	0.57
70:Bq:74:ILE:HD12	70:Bq:74:ILE:C	2.28	0.57
77:Bw:183:LYS:HG3	77:Bw:184:ILE:N	2.19	0.57
82:B2:28:HIS:HB3	82:B2:31:LYS:CD	2.33	0.57
82:B2:52:LYS:HD3	82:B2:52:LYS:N	2.18	0.57
17:Aj:39:LEU:HD13	17:Aj:39:LEU:C	2.29	0.57
66:Bn:77:ARG:HD2	66:Bn:78:TYR:O	2.03	0.57
66:Bn:195:ARG:HG3	66:Bn:203:VAL:HG11	1.86	0.57
77:Bw:149:LYS:N	77:Bw:149:LYS:HD2	2.20	0.57
79:By:8:VAL:HG13	79:By:9:LYS:N	2.19	0.57
79:By:46:ARG:HD2	79:By:46:ARG:C	2.29	0.57
80:B9:81:ASN:HA	80:B9:111:ILE:HD11	1.86	0.57
83:B3:27:ILE:CG1	83:B3:35:ILE:HD12	2.26	0.57
85:B5:30:ASN:HD22	85:B5:31:LEU:H	1.53	0.57
86:B6:17:ARG:HG2	86:B6:104:ILE:HD12	1.86	0.57
86:B6:79:ILE:HD13	86:B6:79:ILE:N	2.17	0.57
64:Bl:77:LYS:HB2	64:Bl:78:PRO:CD	2.34	0.57
66:Bn:193:VAL:HG22	66:Bn:238:MET:HG3	1.86	0.57
68:Bp:106:LEU:HB3	68:Bp:120:TYR:HE1	1.68	0.57
70:Bq:44:MET:HA	70:Bq:44:MET:CE	2.31	0.57
77:Bw:158:VAL:CG1	77:Bw:162:ILE:HG12	2.34	0.57
77:Bw:188:ARG:HB2	77:Bw:188:ARG:CZ	2.34	0.57
80:B9:87:VAL:CG1	80:B9:89:LEU:HB2	2.34	0.57
85:B5:5:ILE:HD13	85:B5:177:ILE:CD1	2.33	0.57
85:B5:122:LEU:CD1	85:B5:129:PRO:HD3	2.34	0.57
86:B6:22:MET:HA	86:B6:27:TYR:HD2	1.65	0.57
62:Bj:8:LEU:HD13	62:Bj:8:LEU:C	2.29	0.57
62:Bj:26:VAL:HG21	62:Bj:97:ALA:C	2.29	0.57
66:Bn:81:GLU:OE2	66:Bn:103:LEU:HD22	2.05	0.57
77:Bw:175:LEU:HD11	77:Bw:266:ILE:HB	1.84	0.57
77:Bw:193:ASP:O	77:Bw:197:ILE:HG12	2.05	0.57
79:By:45:VAL:HG23	79:By:46:ARG:N	2.17	0.57
17:Aj:50:VAL:HG12	17:Aj:51:LYS:N	2.19	0.57
62:Bj:36:ARG:HG2	62:Bj:36:ARG:O	2.03	0.57
68:Bp:99:MET:O	68:Bp:103:ARG:HG3	2.04	0.57
77:Bw:221:LYS:HD2	77:Bw:221:LYS:C	2.30	0.57
85:B5:15:ASP:O	85:B5:206:PRO:HD2	2.04	0.57
85:B5:98:ALA:CB	85:B5:121:VAL:HG12	2.35	0.57
9:Aa:201:SER:CB	9:Aa:206:LEU:CD1	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Ad:149:GLU:HA	12:Ad:152:ARG:CZ	2.34	0.57
12:Ad:149:GLU:HA	12:Ad:152:ARG:NH2	2.18	0.57
66:Bn:191:ALA:N	66:Bn:238:MET:SD	2.77	0.57
68:Bp:102:LEU:HD22	68:Bp:127:VAL:HG13	1.87	0.57
81:Bz:42:CYS:CB	86:B6:53:PRO:HB2	2.33	0.57
82:B2:18:LEU:HD11	82:B2:34:CYS:SG	2.45	0.57
82:B2:28:HIS:ND1	82:B2:30:GLN:HB3	2.20	0.57
84:B4:75:PRO:HG2	84:B4:77:CYS:CB	2.33	0.57
85:B5:106:ALA:HB1	85:B5:110:LEU:CD1	2.21	0.57
86:B6:26:LYS:HG2	86:B6:97:ILE:HD11	1.87	0.57
9:Aa:17:TRP:CG	9:Aa:305:ASN:ND2	2.72	0.57
12:Ad:105:TYR:CE1	12:Ad:112:SER:HA	2.39	0.57
26:B0:2796:U:P	68:Bp:57:VAL:HG22	2.43	0.57
62:Bj:29:GLY:HA2	62:Bj:100:ARG:HH11	1.69	0.57
66:Bn:59:ILE:HD12	66:Bn:97:ALA:HA	1.85	0.57
70:Bq:92:ILE:HA	70:Bq:95:ILE:CG2	2.34	0.57
79:By:22:ARG:NH1	79:By:36:ARG:HD3	2.19	0.57
79:By:22:ARG:CG	79:By:36:ARG:HD3	2.24	0.57
80:B9:87:VAL:HG12	80:B9:88:LEU:N	2.20	0.57
80:B9:123:THR:HG23	80:B9:124:ASN:N	2.20	0.57
9:Aa:100:ARG:HH21	9:Aa:102:VAL:CG2	2.17	0.57
17:Aj:91:LEU:HD22	17:Aj:91:LEU:N	2.19	0.57
66:Bn:85:TYR:CE1	66:Bn:103:LEU:CG	2.87	0.57
70:Bq:79:VAL:CG1	70:Bq:82:LYS:HB2	2.25	0.57
77:Bw:113:PHE:O	77:Bw:164:TRP:HA	2.05	0.57
77:Bw:189:ILE:HG23	77:Bw:189:ILE:O	2.05	0.57
79:By:18:LYS:HE3	79:By:19:LYS:H	1.69	0.57
85:B5:45:GLU:HB3	85:B5:183:ARG:HE	1.69	0.57
85:B5:53:THR:HG23	85:B5:55:GLN:O	2.05	0.57
66:Bn:85:TYR:CD1	66:Bn:246:ILE:CG2	2.87	0.57
77:Bw:242:MET:CE	77:Bw:243:LYS:HG2	2.35	0.57
79:By:54:LEU:N	79:By:54:LEU:HD22	2.19	0.57
81:Bz:36:LYS:HB3	81:Bz:45:THR:HB	1.87	0.57
82:B2:27:TYR:HD2	82:B2:34:CYS:HG	1.52	0.57
83:B3:24:PRO:HB2	83:B3:26:TRP:CD1	2.40	0.57
85:B5:27:LEU:HD13	85:B5:27:LEU:C	2.28	0.57
86:B6:31:TYR:CA	86:B6:93:THR:HG21	2.28	0.57
12:Ad:107:LEU:HD12	12:Ad:109:PHE:CE2	2.40	0.57
17:Aj:84:ILE:HD13	17:Aj:84:ILE:C	2.30	0.57
21:An:23:VAL:CG2	21:An:36:LEU:HD11	2.35	0.57
64:Bl:38:MET:HG3	64:Bl:39:HIS:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:81:GLU:HG2	66:Bn:103:LEU:HD22	1.85	0.57
69:B7:193:MET:O	69:B7:197:ARG:HG3	2.04	0.57
77:Bw:170:LYS:CA	77:Bw:173:ASN:HD21	2.16	0.57
77:Bw:172:VAL:HG23	77:Bw:173:ASN:N	2.19	0.57
77:Bw:207:ILE:O	77:Bw:207:ILE:HG23	2.05	0.57
82:B2:19:CYS:HB2	82:B2:27:TYR:CD2	2.39	0.57
85:B5:70:ARG:HD2	85:B5:137:ASP:CG	2.30	0.57
9:Aa:65:PHE:O	9:Aa:82:SER:CB	2.53	0.56
66:Bn:89:VAL:HG21	66:Bn:194:HIS:H	1.70	0.56
79:By:11:LYS:HG2	79:By:12:ILE:H	1.70	0.56
79:By:66:THR:O	79:By:66:THR:HG22	2.04	0.56
83:B3:23:ILE:HD13	83:B3:23:ILE:H	1.69	0.56
17:Aj:40:ILE:HG23	17:Aj:41:ARG:N	2.19	0.56
17:Aj:40:ILE:HD11	17:Aj:50:VAL:HB	1.87	0.56
64:Bl:14:HIS:HD2	79:By:39:ARG:HH12	1.50	0.56
66:Bn:187:LYS:HG3	66:Bn:189:PHE:H	1.68	0.56
70:Bq:24:VAL:HG22	70:Bq:25:PRO:N	2.20	0.56
70:Bq:40:ASP:C	70:Bq:41:ILE:HD12	2.30	0.56
77:Bw:117:ILE:O	77:Bw:245:LYS:HD2	2.05	0.56
77:Bw:173:ASN:HD22	77:Bw:173:ASN:H	1.53	0.56
80:B9:70:LEU:H	80:B9:70:LEU:HD12	1.69	0.56
84:B4:85:ILE:HG23	84:B4:85:ILE:O	2.05	0.56
85:B5:57:THR:HG22	85:B5:146:LYS:HA	1.87	0.56
1:AA:1406:A:P	21:An:41:GLN:HE22	2.27	0.56
26:B0:1634:C:P	64:Bl:24:LYS:NZ	2.78	0.56
64:Bl:16:SER:HA	64:Bl:19:HIS:HB2	1.86	0.56
68:Bp:93:VAL:HG23	68:Bp:94:THR:N	2.20	0.56
70:Bq:33:TYR:HE2	70:Bq:97:HIS:HB3	1.70	0.56
77:Bw:133:LEU:HD13	77:Bw:134:LEU:H	1.70	0.56
77:Bw:139:ILE:HG22	77:Bw:140:PHE:HD1	1.71	0.56
77:Bw:197:ILE:HG22	77:Bw:207:ILE:HA	1.87	0.56
77:Bw:216:ILE:HD11	77:Bw:223:PHE:CD2	2.40	0.56
77:Bw:228:ASN:HD22	77:Bw:228:ASN:H	1.52	0.56
81:Bz:11:VAL:HG13	81:Bz:27:LYS:HG2	1.87	0.56
9:Aa:162:ASN:CB	9:Aa:163:PRO:HD2	2.36	0.56
17:Aj:54:VAL:HB	17:Aj:88:LEU:HB2	1.87	0.56
17:Aj:101:ILE:HG23	17:Aj:102:THR:N	2.20	0.56
62:Bj:119:VAL:CG1	62:Bj:120:PRO:HD3	2.35	0.56
66:Bn:42:LYS:HE2	70:Bq:33:TYR:H	1.68	0.56
77:Bw:117:ILE:O	77:Bw:117:ILE:HG23	2.04	0.56
77:Bw:137:ARG:O	77:Bw:138:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:B2:11:ARG:HG3	82:B2:12:ARG:N	2.19	0.56
82:B2:27:TYR:HD2	82:B2:34:CYS:SG	2.28	0.56
83:B3:23:ILE:HD13	83:B3:23:ILE:N	2.21	0.56
86:B6:11:LEU:CD1	86:B6:75:SER:HB3	2.35	0.56
86:B6:45:LEU:CB	86:B6:71:VAL:HB	2.33	0.56
9:Aa:64:HIS:NE2	9:Aa:65:PHE:CD1	2.73	0.56
64:Bl:117:LEU:HD23	64:Bl:117:LEU:N	2.20	0.56
66:Bn:77:ARG:HD3	66:Bn:81:GLU:HB3	1.88	0.56
81:Bz:37:TYR:CE2	81:Bz:70:THR:HG23	2.40	0.56
83:B3:27:ILE:HG13	83:B3:31:THR:CG2	2.36	0.56
84:B4:52:THR:O	84:B4:52:THR:HG23	2.06	0.56
85:B5:43:VAL:O	85:B5:152:ARG:HA	2.05	0.56
17:Aj:20:ILE:HG21	17:Aj:114:VAL:CG2	2.35	0.56
66:Bn:77:ARG:NE	66:Bn:103:LEU:HB3	2.21	0.56
68:Bp:68:LEU:O	68:Bp:71:ARG:HG2	2.06	0.56
68:Bp:115:ILE:CG2	68:Bp:119:MET:HB2	2.36	0.56
77:Bw:196:LEU:CD1	77:Bw:209:MET:HA	2.32	0.56
77:Bw:228:ASN:HD22	77:Bw:228:ASN:N	2.03	0.56
81:Bz:47:MET:HE3	81:Bz:71:TYR:CE2	2.41	0.56
86:B6:7:THR:HG22	86:B6:8:LYS:H	1.71	0.56
17:Aj:50:VAL:HG13	17:Aj:90:ASP:O	2.05	0.56
17:Aj:61:LEU:HD22	17:Aj:61:LEU:N	2.21	0.56
62:Bj:83:VAL:O	62:Bj:86:MET:HB2	2.06	0.56
77:Bw:245:LYS:HB2	77:Bw:245:LYS:NZ	2.20	0.56
12:Ad:92:PHE:CE2	12:Ad:96:LEU:HD11	2.41	0.56
17:Aj:66:ARG:HG3	17:Aj:77:TRP:HE1	1.67	0.56
66:Bn:193:VAL:HG23	66:Bn:235:MET:C	2.27	0.56
68:Bp:24:LEU:O	68:Bp:26:PRO:HD3	2.06	0.56
70:Bq:26:LEU:H	70:Bq:26:LEU:CD2	2.19	0.56
70:Bq:67:THR:H	70:Bq:72:GLY:H	1.53	0.56
77:Bw:149:LYS:HD2	77:Bw:149:LYS:H	1.71	0.56
77:Bw:191:LEU:N	77:Bw:191:LEU:HD23	2.21	0.56
79:By:55:MET:HB3	79:By:56:PRO:HA	1.87	0.56
81:Bz:42:CYS:C	86:B6:53:PRO:HB3	2.26	0.56
83:B3:43:HIS:CD2	83:B3:46:ARG:H	2.17	0.56
85:B5:201:LYS:HB3	85:B5:207:ALA:HA	1.86	0.56
9:Aa:5:MET:SD	9:Aa:258:ILE:HD11	2.46	0.56
66:Bn:195:ARG:CB	66:Bn:203:VAL:HG11	2.35	0.56
77:Bw:118:ARG:HG2	77:Bw:119:GLY:N	2.21	0.56
77:Bw:144:PHE:CE2	77:Bw:233:PHE:HZ	2.22	0.56
77:Bw:161:TYR:O	77:Bw:162:ILE:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Bw:162:ILE:HD12	77:Bw:162:ILE:C	2.30	0.56
77:Bw:230:LEU:CD1	77:Bw:232:PRO:HD3	2.34	0.56
80:B9:88:LEU:HD13	80:B9:88:LEU:C	2.31	0.56
81:Bz:78:THR:HG23	81:Bz:79:VAL:N	2.20	0.56
83:B3:49:LEU:N	83:B3:49:LEU:HD12	2.21	0.56
86:B6:31:TYR:HA	86:B6:93:THR:CG2	2.29	0.56
17:Aj:29:VAL:HG23	17:Aj:30:LYS:N	2.21	0.56
62:Bj:46:PHE:HD1	62:Bj:135:ALA:HB2	1.69	0.56
66:Bn:89:VAL:HG22	66:Bn:90:GLY:H	1.69	0.56
66:Bn:182:TYR:O	66:Bn:198:ILE:HB	2.05	0.56
77:Bw:133:LEU:HD13	77:Bw:134:LEU:HG	1.87	0.56
77:Bw:144:PHE:CE2	77:Bw:233:PHE:CZ	2.94	0.56
77:Bw:265:LEU:HD12	77:Bw:268:ARG:HH21	1.69	0.56
83:B3:35:ILE:HG23	83:B3:37:TYR:H	1.70	0.56
85:B5:34:LEU:HD13	85:B5:34:LEU:C	2.31	0.56
85:B5:111:MET:HE3	85:B5:131:PRO:HG3	1.88	0.56
86:B6:6:LYS:HG2	86:B6:112:THR:HG21	1.86	0.56
86:B6:79:ILE:CD1	86:B6:79:ILE:H	2.17	0.56
26:B0:4547:G:P	62:Bj:64:ASN:OD1	2.64	0.55
64:Bl:145:VAL:HG13	64:Bl:145:VAL:O	2.05	0.55
66:Bn:49:ARG:HG3	66:Bn:51:ILE:HG23	1.88	0.55
66:Bn:184:SER:HB2	66:Bn:198:ILE:H	1.72	0.55
77:Bw:134:LEU:O	77:Bw:135:ARG:HB2	2.06	0.55
79:By:15:LYS:HD3	79:By:16:ARG:H	1.69	0.55
85:B5:45:GLU:CD	85:B5:188:LEU:HD11	2.30	0.55
86:B6:14:ILE:HG13	86:B6:15:ASN:N	2.20	0.55
9:Aa:56:GLN:HE21	9:Aa:66:VAL:CG2	2.19	0.55
17:Aj:46:LYS:HE3	17:Aj:100:GLN:NE2	2.22	0.55
66:Bn:58:ASP:HA	66:Bn:91:LEU:CD1	2.35	0.55
79:By:45:VAL:HG13	79:By:52:GLN:HE22	1.71	0.55
85:B5:111:MET:O	85:B5:114:ILE:HG22	2.06	0.55
86:B6:46:VAL:HG12	86:B6:72:HIS:HA	1.88	0.55
9:Aa:217:MET:HE2	9:Aa:226:HIS:CD2	2.40	0.55
12:Ad:149:GLU:HG3	12:Ad:152:ARG:NH2	2.17	0.55
64:Bl:97:VAL:O	64:Bl:100:ILE:HG22	2.06	0.55
68:Bp:10:LEU:CB	68:Bp:41:ILE:HD12	2.37	0.55
77:Bw:174:GLU:C	77:Bw:177:TYR:HB3	2.31	0.55
79:By:43:ASN:HB3	79:By:46:ARG:HB2	1.87	0.55
84:B4:23:VAL:HG23	84:B4:70:LEU:CD2	2.34	0.55
85:B5:34:LEU:HD13	85:B5:40:SER:HB2	1.87	0.55
85:B5:121:VAL:HG13	85:B5:125:ARG:NH1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B6:29:LEU:CD2	86:B6:87:LYS:HE3	2.37	0.55
86:B6:67:ALA:O	86:B6:68:LYS:HB3	2.06	0.55
17:Aj:50:VAL:CG1	17:Aj:89:ILE:HG12	2.26	0.55
62:Bj:8:LEU:CD1	62:Bj:18:LEU:HD11	2.32	0.55
66:Bn:184:SER:CB	66:Bn:198:ILE:C	2.80	0.55
68:Bp:14:VAL:HG13	68:Bp:15:LEU:N	2.21	0.55
70:Bq:16:ARG:HH21	70:Bq:44:MET:HB3	1.72	0.55
70:Bq:20:LYS:HD2	70:Bq:20:LYS:N	2.22	0.55
77:Bw:124:SER:O	77:Bw:127:VAL:HB	2.05	0.55
77:Bw:183:LYS:HG3	77:Bw:184:ILE:H	1.71	0.55
81:Bz:11:VAL:HG22	81:Bz:27:LYS:CG	2.35	0.55
81:Bz:42:CYS:HG	86:B6:53:PRO:HB2	1.69	0.55
9:Aa:100:ARG:HE	9:Aa:134:THR:HG23	1.71	0.55
21:An:23:VAL:HG23	21:An:36:LEU:HD11	1.88	0.55
66:Bn:184:SER:N	66:Bn:198:ILE:HG22	2.21	0.55
68:Bp:30:ASN:HD22	68:Bp:30:ASN:N	2.04	0.55
70:Bq:73:ILE:HG23	70:Bq:73:ILE:O	2.05	0.55
77:Bw:218:THR:HG23	77:Bw:218:THR:O	2.06	0.55
79:By:52:GLN:O	79:By:53:ILE:HD13	2.05	0.55
80:B9:81:ASN:ND2	80:B9:83:LYS:HB2	2.20	0.55
81:Bz:26:VAL:O	81:Bz:29:ILE:HG13	2.06	0.55
86:B6:29:LEU:HA	86:B6:94:LEU:CD2	2.36	0.55
17:Aj:106:ILE:HG22	17:Aj:107:GLU:N	2.20	0.55
26:B0:52:G:P	82:B2:49:TRP:CG	3.00	0.55
64:Bl:117:LEU:CD1	64:Bl:136:LYS:HA	2.36	0.55
66:Bn:194:HIS:C	66:Bn:195:ARG:CG	2.79	0.55
80:B9:89:LEU:N	80:B9:89:LEU:HD22	2.21	0.55
85:B5:31:LEU:HB2	85:B5:157:ARG:HB3	1.87	0.55
12:Ad:87:VAL:O	12:Ad:91:VAL:HG23	2.06	0.55
21:An:26:ASN:ND2	21:An:38:MET:HG3	2.21	0.55
64:Bl:89:ASN:HB3	64:Bl:94:LYS:HE2	1.89	0.55
64:Bl:121:PRO:HA	64:Bl:140:VAL:HG13	1.89	0.55
66:Bn:77:ARG:CD	66:Bn:81:GLU:HB3	2.36	0.55
66:Bn:85:TYR:CE1	66:Bn:246:ILE:CG2	2.89	0.55
77:Bw:191:LEU:HG	77:Bw:192:THR:N	2.21	0.55
77:Bw:242:MET:HG2	77:Bw:268:ARG:NH2	2.21	0.55
79:By:17:THR:O	79:By:17:THR:HG23	2.07	0.55
80:B9:80:HIS:H	80:B9:84:GLU:HG3	1.72	0.55
85:B5:16:ALA:HB1	85:B5:202:THR:HG21	1.88	0.55
85:B5:103:PHE:CB	85:B5:145:MET:HE3	2.37	0.55
85:B5:125:ARG:HB3	85:B5:127:LYS:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:173:ILE:O	85:B5:177:ILE:HG13	2.06	0.55
17:Aj:84:ILE:O	17:Aj:84:ILE:HG23	2.06	0.55
70:Bq:10:THR:HG21	70:Bq:54:LYS:HG3	1.89	0.55
70:Bq:49:LYS:HB2	70:Bq:91:ARG:HH12	1.72	0.55
77:Bw:171:SER:O	77:Bw:175:LEU:HD22	2.07	0.55
79:By:55:MET:HE3	79:By:56:PRO:CB	2.36	0.55
86:B6:21:VAL:CG2	86:B6:96:ILE:HD11	2.36	0.55
9:Aa:79:LEU:HD21	9:Aa:89:LEU:HD13	1.87	0.55
17:Aj:54:VAL:O	17:Aj:87:ARG:HA	2.07	0.55
49:BW:14:G:P	64:Bl:135:GLU:OE1	2.65	0.55
64:Bl:98:ALA:HB3	64:Bl:99:PRO:CD	2.37	0.55
81:Bz:50:ARG:HB3	81:Bz:54:ILE:CG2	2.36	0.55
85:B5:45:GLU:HG2	85:B5:188:LEU:CD1	2.36	0.55
86:B6:21:VAL:HG21	86:B6:96:ILE:HD11	1.86	0.55
86:B6:98:ASP:CB	86:B6:99:PRO:HD3	2.28	0.55
62:Bj:18:LEU:HD23	62:Bj:18:LEU:O	2.07	0.55
79:By:12:ILE:O	79:By:12:ILE:HG23	2.06	0.55
84:B4:69:ARG:HG3	84:B4:80:LYS:HD3	1.86	0.55
66:Bn:95:ALA:HB3	66:Bn:194:HIS:HB3	1.89	0.54
68:Bp:84:THR:HG23	68:Bp:87:ALA:H	1.71	0.54
77:Bw:134:LEU:CB	77:Bw:136:LEU:HD13	2.36	0.54
85:B5:74:VAL:HG11	85:B5:142:ILE:HG22	1.87	0.54
9:Aa:282:GLU:HG3	9:Aa:308:ARG:HH12	1.72	0.54
17:Aj:22:ILE:HG12	17:Aj:91:LEU:CD2	2.36	0.54
17:Aj:63:ILE:CG1	17:Aj:80:PHE:HB2	2.37	0.54
21:An:19:ARG:HB2	21:An:37:ASN:ND2	2.22	0.54
62:Bj:46:PHE:HE1	62:Bj:135:ALA:HB1	1.70	0.54
77:Bw:152:ILE:HG13	77:Bw:153:ASN:N	2.21	0.54
81:Bz:57:CYS:SG	81:Bz:59:SER:HB3	2.47	0.54
82:B2:29:LEU:HD22	82:B2:29:LEU:H	1.73	0.54
84:B4:6:LYS:HG3	84:B4:93:LEU:HB3	1.88	0.54
84:B4:57:ARG:H	84:B4:57:ARG:HD2	1.72	0.54
85:B5:45:GLU:HB3	85:B5:183:ARG:HG2	1.89	0.54
12:Ad:127:VAL:HG23	12:Ad:132:VAL:HG22	1.88	0.54
17:Aj:44:LYS:NZ	17:Aj:49:LYS:HD2	2.23	0.54
64:Bl:72:THR:HG22	64:Bl:110:LYS:CG	2.36	0.54
66:Bn:198:ILE:HG13	66:Bn:239:TYR:CE2	2.43	0.54
68:Bp:23:TRP:C	68:Bp:24:LEU:HD12	2.32	0.54
70:Bq:26:LEU:N	70:Bq:26:LEU:HD23	2.22	0.54
70:Bq:66:VAL:HG22	70:Bq:70:ALA:O	2.06	0.54
77:Bw:131:LEU:HD22	77:Bw:136:LEU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Bw:265:LEU:CD1	77:Bw:268:ARG:HH21	2.20	0.54
1:AA:1413:C:P	21:An:27:ARG:HD3	2.47	0.54
66:Bn:200:GLY:HA2	66:Bn:236:GLU:CB	2.38	0.54
70:Bq:41:ILE:CD1	70:Bq:77:LYS:HE2	2.37	0.54
70:Bq:46:THR:HG23	70:Bq:47:VAL:HG23	1.89	0.54
85:B5:34:LEU:H	85:B5:157:ARG:HH11	1.55	0.54
86:B6:19:GLN:O	86:B6:22:MET:HG3	2.08	0.54
9:Aa:17:TRP:HA	9:Aa:305:ASN:CG	2.32	0.54
9:Aa:129:ILE:CG1	9:Aa:143:GLN:HB2	2.38	0.54
17:Aj:101:ILE:HD13	17:Aj:101:ILE:C	2.32	0.54
21:An:31:ILE:HD12	21:An:31:ILE:N	2.21	0.54
26:B0:2866:G:P	68:Bp:75:HIS:CD2	2.96	0.54
70:Bq:26:LEU:H	70:Bq:26:LEU:HD23	1.73	0.54
70:Bq:37:ASP:OD1	70:Bq:63:VAL:HB	2.07	0.54
82:B2:28:HIS:HB3	82:B2:31:LYS:HG2	1.85	0.54
83:B3:27:ILE:HG13	83:B3:31:THR:HG23	1.89	0.54
85:B5:114:ILE:HG23	85:B5:115:GLY:N	2.21	0.54
86:B6:26:LYS:CB	86:B6:97:ILE:HG12	2.33	0.54
66:Bn:198:ILE:HD11	66:Bn:239:TYR:HE2	1.72	0.54
77:Bw:123:VAL:HG21	77:Bw:161:TYR:CE1	2.43	0.54
77:Bw:173:ASN:HB2	77:Bw:209:MET:SD	2.48	0.54
80:B9:79:VAL:CG2	80:B9:84:GLU:HB2	2.24	0.54
85:B5:57:THR:HG22	85:B5:146:LYS:CA	2.37	0.54
86:B6:81:LEU:HD23	86:B6:81:LEU:C	2.33	0.54
86:B6:93:THR:O	86:B6:94:LEU:HD23	2.07	0.54
17:Aj:20:ILE:HG21	17:Aj:114:VAL:HG23	1.89	0.54
17:Aj:63:ILE:CD1	17:Aj:80:PHE:HB2	2.38	0.54
17:Aj:92:HIS:O	17:Aj:93:SER:HB3	2.07	0.54
21:An:10:HIS:CB	21:An:11:PRO:HD3	2.34	0.54
22:Ao:66:LEU:HD11	22:Ao:84:LEU:HD12	1.89	0.54
62:Bj:15:LEU:HG	62:Bj:40:ILE:HD13	1.90	0.54
70:Bq:82:LYS:HG3	70:Bq:86:LYS:CB	2.35	0.54
79:By:55:MET:HB3	79:By:56:PRO:CA	2.38	0.54
84:B4:75:PRO:O	84:B4:76:ASN:HB2	2.06	0.54
85:B5:58:THR:HG23	85:B5:58:THR:O	2.08	0.54
86:B6:18:LEU:HD13	86:B6:18:LEU:C	2.32	0.54
66:Bn:200:GLY:HA2	66:Bn:236:GLU:H	1.73	0.54
77:Bw:125:PRO:C	77:Bw:127:VAL:H	2.16	0.54
77:Bw:196:LEU:H	77:Bw:196:LEU:CD2	2.16	0.54
80:B9:78:LEU:HD23	80:B9:78:LEU:C	2.32	0.54
80:B9:104:SER:O	80:B9:108:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Bz:64:VAL:HG12	81:Bz:65:ALA:N	2.21	0.54
84:B4:53:LYS:HB2	84:B4:54:PRO:CD	2.33	0.54
85:B5:45:GLU:CG	85:B5:188:LEU:HD11	2.36	0.54
17:Aj:66:ARG:HA	17:Aj:77:TRP:CD1	2.43	0.54
64:Bl:24:LYS:HD2	64:Bl:24:LYS:N	2.22	0.54
66:Bn:203:VAL:HG22	66:Bn:236:GLU:OE2	2.08	0.54
66:Bn:243:HIS:HA	66:Bn:246:ILE:HG12	1.90	0.54
70:Bq:92:ILE:CA	70:Bq:95:ILE:HG22	2.38	0.54
81:Bz:20:ALA:HB1	81:Bz:24:LYS:HZ3	1.73	0.54
85:B5:185:HIS:HD2	85:B5:192:PRO:HD3	1.72	0.54
85:B5:195:ILE:HG23	85:B5:195:ILE:O	2.08	0.54
9:Aa:64:HIS:CE1	9:Aa:65:PHE:CD1	2.95	0.54
62:Bj:26:VAL:HG21	62:Bj:101:LEU:CD2	2.38	0.54
64:Bl:137:ILE:CD1	64:Bl:144:CYS:HB2	2.37	0.54
77:Bw:156:ARG:HA	77:Bw:156:ARG:HE	1.71	0.54
77:Bw:226:ALA:O	77:Bw:227:ASN:HB2	2.08	0.54
80:B9:99:ILE:HG22	80:B9:103:VAL:HG21	1.88	0.54
82:B2:29:LEU:HD22	82:B2:29:LEU:N	2.23	0.54
22:Ao:70:GLN:CD	22:Ao:77:TYR:CE2	2.85	0.53
62:Bj:14:LEU:N	62:Bj:14:LEU:HD12	2.24	0.53
64:Bl:117:LEU:HD13	64:Bl:136:LYS:C	2.33	0.53
66:Bn:51:ILE:CG1	66:Bn:62:GLN:HB3	2.38	0.53
69:B7:198:ARG:HB2	69:B7:201:ARG:HH21	1.73	0.53
70:Bq:83:ILE:CG1	70:Bq:84:LEU:H	2.19	0.53
77:Bw:144:PHE:HB2	77:Bw:224:LYS:HD3	1.90	0.53
80:B9:98:GLU:HA	80:B9:123:THR:HG22	1.91	0.53
85:B5:5:ILE:HD11	85:B5:177:ILE:HD13	1.88	0.53
85:B5:64:GLU:HG2	85:B5:65:GLY:N	2.23	0.53
26:B0:1817:U:P	77:Bw:135:ARG:CZ	2.95	0.53
26:B0:4169:G:P	70:Bq:9:GLY:H	2.31	0.53
66:Bn:42:LYS:H	70:Bq:32:ILE:HG12	1.72	0.53
66:Bn:49:ARG:HB3	66:Bn:144:TYR:CE1	2.43	0.53
68:Bp:10:LEU:HB2	68:Bp:41:ILE:HD12	1.91	0.53
77:Bw:165:GLY:HA3	77:Bw:262:ILE:HD11	1.89	0.53
81:Bz:46:LYS:HD3	81:Bz:59:SER:H	1.72	0.53
84:B4:58:LYS:HE2	84:B4:59:LYS:O	2.08	0.53
12:Ad:63:LEU:HD12	12:Ad:74:PHE:CE1	2.43	0.53
26:B0:4676:C:P	54:Bb:275:HIS:HE1	2.23	0.53
62:Bj:26:VAL:CG2	62:Bj:101:LEU:HD21	2.38	0.53
66:Bn:226:ILE:HD13	66:Bn:232:PRO:HG3	1.88	0.53
68:Bp:104:ARG:HA	68:Bp:107:ARG:NE	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Bq:71:VAL:HG22	70:Bq:90:VAL:O	2.08	0.53
77:Bw:123:VAL:HG21	77:Bw:127:VAL:HG11	1.89	0.53
77:Bw:197:ILE:HG13	77:Bw:197:ILE:O	2.08	0.53
79:By:12:ILE:C	79:By:12:ILE:HD13	2.32	0.53
80:B9:75:ARG:HB3	80:B9:95:TYR:CE2	2.43	0.53
83:B3:6:THR:HG23	83:B3:8:ARG:N	2.24	0.53
85:B5:50:PRO:CD	85:B5:179:VAL:HG21	2.38	0.53
12:Ad:127:VAL:HG23	12:Ad:132:VAL:CG2	2.38	0.53
26:B0:363:A:P	82:B2:24:SER:HG	2.25	0.53
62:Bj:18:LEU:HD23	62:Bj:18:LEU:C	2.34	0.53
64:Bl:7:LYS:HA	64:Bl:10:LYS:HG2	1.90	0.53
66:Bn:187:LYS:H	66:Bn:237:GLU:HB3	1.73	0.53
68:Bp:45:ILE:HG22	68:Bp:50:ILE:HB	1.90	0.53
68:Bp:104:ARG:HB2	68:Bp:107:ARG:HH21	1.73	0.53
77:Bw:169:LEU:N	77:Bw:169:LEU:HD23	2.23	0.53
12:Ad:63:LEU:HD13	12:Ad:63:LEU:O	2.09	0.53
64:Bl:79:TRP:HB2	64:Bl:118:PRO:CA	2.38	0.53
69:B7:198:ARG:HA	69:B7:201:ARG:NE	2.18	0.53
70:Bq:41:ILE:HG12	70:Bq:77:LYS:NZ	2.23	0.53
83:B3:35:ILE:HG12	83:B3:37:TYR:HD1	1.73	0.53
17:Aj:24:LEU:CD2	17:Aj:112:VAL:HG22	2.37	0.53
17:Aj:93:SER:HB2	17:Aj:94:PRO:HD2	1.91	0.53
77:Bw:166:TYR:O	77:Bw:259:GLU:HG3	2.09	0.53
81:Bz:11:VAL:CG2	81:Bz:23:ARG:HG3	2.37	0.53
82:B2:33:THR:O	82:B2:33:THR:HG23	2.07	0.53
86:B6:48:LEU:HB2	86:B6:74:TYR:CD2	2.44	0.53
86:B6:81:LEU:HD21	86:B6:94:LEU:HD11	1.90	0.53
12:Ad:149:GLU:CD	12:Ad:149:GLU:H	2.16	0.53
66:Bn:77:ARG:CZ	66:Bn:82:LEU:HA	2.39	0.53
66:Bn:79:ALA:HB1	66:Bn:91:LEU:HD22	1.91	0.53
66:Bn:102:LEU:HD22	66:Bn:246:ILE:CD1	2.33	0.53
68:Bp:73:GLY:HA2	68:Bp:76:MET:HE2	1.90	0.53
77:Bw:127:VAL:O	77:Bw:128:ARG:HB3	2.09	0.53
79:By:6:PRO:O	79:By:7:LEU:HB2	2.08	0.53
80:B9:99:ILE:HG22	80:B9:103:VAL:CG2	2.39	0.53
82:B2:10:LYS:HE3	82:B2:12:ARG:H	1.71	0.53
86:B6:18:LEU:HD21	86:B6:94:LEU:HD13	1.90	0.53
26:B0:4586:A:P	54:Bb:223:LYS:HZ3	2.32	0.53
62:Bj:33:VAL:O	62:Bj:33:VAL:HG13	2.08	0.53
62:Bj:37:CYS:SG	62:Bj:137:LEU:HD22	2.48	0.53
66:Bn:199:MET:O	66:Bn:199:MET:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:242:ALA:O	66:Bn:246:ILE:HG23	2.08	0.53
70:Bq:11:ARG:HB3	70:Bq:11:ARG:HH11	1.74	0.53
77:Bw:216:ILE:HG22	77:Bw:216:ILE:O	2.08	0.53
85:B5:60:VAL:HG22	85:B5:104:PHE:HA	1.88	0.53
86:B6:37:MET:HE3	86:B6:42:LYS:HB3	1.89	0.53
9:Aa:79:LEU:HD21	9:Aa:89:LEU:CD1	2.39	0.53
62:Bj:118:VAL:HG22	62:Bj:120:PRO:CD	2.38	0.53
66:Bn:84:LYS:HB2	66:Bn:103:LEU:HD11	1.90	0.53
66:Bn:194:HIS:C	66:Bn:195:ARG:HG2	2.34	0.53
77:Bw:136:LEU:HD11	77:Bw:143:THR:CG2	2.39	0.53
79:By:55:MET:CB	79:By:56:PRO:HA	2.39	0.53
86:B6:7:THR:N	86:B6:10:SER:HB2	2.24	0.53
86:B6:51:ASN:CB	86:B6:78:ASN:HD21	2.14	0.53
86:B6:59:GLU:HB3	86:B6:63:TYR:CE1	2.43	0.53
8:AH:10:G:P	21:An:13:LYS:NZ	2.82	0.53
21:An:30:LEU:HD12	21:An:31:ILE:N	2.24	0.53
26:B0:1817:U:P	77:Bw:135:ARG:HH11	2.30	0.53
26:B0:4013:G:P	85:B5:124:PRO:CG	2.97	0.53
62:Bj:15:LEU:HD11	62:Bj:40:ILE:HG23	1.91	0.53
62:Bj:35:VAL:HB	62:Bj:115:LYS:CG	2.28	0.53
62:Bj:55:ALA:H	62:Bj:58:ARG:CG	2.18	0.53
70:Bq:71:VAL:HG23	70:Bq:71:VAL:O	2.08	0.53
77:Bw:155:LEU:CA	77:Bw:158:VAL:HG12	2.39	0.53
26:B0:2611:C:P	68:Bp:60:ARG:CB	2.96	0.52
26:B0:4013:G:P	85:B5:124:PRO:CB	2.97	0.52
64:Bl:37:GLY:HA3	64:Bl:47:LYS:CD	2.37	0.52
66:Bn:191:ALA:CB	66:Bn:238:MET:SD	2.95	0.52
86:B6:6:LYS:CD	86:B6:14:ILE:HD13	2.39	0.52
26:B0:4586:A:P	54:Bb:223:LYS:NZ	2.82	0.52
66:Bn:77:ARG:HA	66:Bn:81:GLU:CD	2.35	0.52
68:Bp:62:ARG:HB2	68:Bp:62:ARG:CZ	2.38	0.52
70:Bq:73:ILE:CG1	70:Bq:87:ARG:HG3	2.38	0.52
70:Bq:78:GLN:HA	70:Bq:82:LYS:CE	2.38	0.52
77:Bw:154:MET:O	77:Bw:155:LEU:HB3	2.09	0.52
77:Bw:194:ASN:CA	77:Bw:197:ILE:HG12	2.39	0.52
79:By:29:VAL:HG13	79:By:30:LYS:N	2.24	0.52
85:B5:34:LEU:HB3	85:B5:157:ARG:CG	2.40	0.52
86:B6:28:VAL:HG21	86:B6:37:MET:SD	2.49	0.52
17:Aj:89:ILE:O	17:Aj:89:ILE:HG23	2.08	0.52
64:Bl:103:VAL:HG22	64:Bl:103:VAL:O	2.09	0.52
66:Bn:239:TYR:C	66:Bn:239:TYR:CD2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Bz:38:THR:HG23	81:Bz:38:THR:O	2.08	0.52
82:B2:18:LEU:CG	82:B2:19:CYS:H	2.22	0.52
84:B4:93:LEU:HD22	84:B4:93:LEU:N	2.24	0.52
85:B5:32:ARG:HG2	85:B5:33:ASP:N	2.24	0.52
9:Aa:188:HIS:NE2	9:Aa:219:TRP:CD1	2.78	0.52
66:Bn:40:LYS:HG3	70:Bq:67:THR:O	1.99	0.52
77:Bw:125:PRO:O	77:Bw:126:LYS:HB2	2.10	0.52
9:Aa:284:PRO:CG	9:Aa:304:ASP:HB2	2.39	0.52
26:B0:4022:C:P	85:B5:196:ASP:HB2	2.49	0.52
62:Bj:25:GLN:NE2	62:Bj:32:VAL:HG22	2.24	0.52
62:Bj:50:LYS:HE3	62:Bj:51:LEU:HD23	1.90	0.52
62:Bj:140:LEU:HD23	62:Bj:140:LEU:C	2.34	0.52
64:Bl:88:VAL:HG11	64:Bl:95:THR:HG22	1.92	0.52
66:Bn:198:ILE:CG1	66:Bn:239:TYR:CE2	2.92	0.52
70:Bq:17:PRO:HB2	70:Bq:20:LYS:CD	2.16	0.52
70:Bq:39:VAL:CB	70:Bq:95:ILE:HD11	2.39	0.52
79:By:37:LYS:CG	79:By:38:PRO:HD2	2.38	0.52
80:B9:70:LEU:HD12	80:B9:70:LEU:N	2.24	0.52
85:B5:177:ILE:O	85:B5:180:ILE:HG12	2.10	0.52
9:Aa:201:SER:HB2	9:Aa:206:LEU:CD1	2.40	0.52
62:Bj:13:HIS:CD2	62:Bj:122:ALA:HA	2.45	0.52
77:Bw:155:LEU:HA	77:Bw:158:VAL:HG11	1.89	0.52
79:By:62:SER:OG	79:By:67:LYS:HA	2.10	0.52
85:B5:74:VAL:O	85:B5:74:VAL:HG12	2.10	0.52
22:Ao:66:LEU:HB3	22:Ao:77:TYR:CE1	2.45	0.52
62:Bj:21:ILE:HG23	62:Bj:22:VAL:N	2.24	0.52
64:Bl:109:TYR:CE2	64:Bl:111:VAL:HG22	2.45	0.52
77:Bw:134:LEU:HB3	77:Bw:136:LEU:HD13	1.91	0.52
82:B2:11:ARG:HG3	82:B2:12:ARG:HG3	1.92	0.52
83:B3:23:ILE:H	83:B3:23:ILE:CD1	2.22	0.52
9:Aa:14:HIS:HB2	9:Aa:18:VAL:N	2.25	0.52
17:Aj:25:THR:HG22	17:Aj:86:LYS:CD	2.36	0.52
26:B0:429:G:P	79:By:19:LYS:CE	2.97	0.52
79:By:11:LYS:HE2	79:By:66:THR:HG21	1.92	0.52
80:B9:79:VAL:HG13	80:B9:79:VAL:O	2.08	0.52
80:B9:79:VAL:CG1	80:B9:99:ILE:HA	2.40	0.52
80:B9:122:VAL:HG23	80:B9:122:VAL:O	2.10	0.52
84:B4:33:LEU:O	84:B4:38:LYS:HD2	2.09	0.52
21:An:24:CYS:O	21:An:25:SER:HB3	2.10	0.52
26:B0:4013:G:P	85:B5:124:PRO:HG3	2.50	0.52
62:Bj:15:LEU:HD21	62:Bj:137:LEU:CG	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:By:28:TYR:HE2	79:By:30:LYS:CD	2.17	0.52
86:B6:6:LYS:HB3	86:B6:10:SER:HB3	1.90	0.52
9:Aa:14:HIS:CD2	9:Aa:34:ALA:C	2.88	0.52
17:Aj:46:LYS:HG2	17:Aj:100:GLN:HE21	1.74	0.52
17:Aj:64:THR:O	17:Aj:64:THR:HG23	2.10	0.52
62:Bj:40:ILE:CG2	62:Bj:137:LEU:HD22	2.40	0.52
68:Bp:30:ASN:HD22	68:Bp:30:ASN:H	1.56	0.52
77:Bw:133:LEU:HD22	77:Bw:133:LEU:O	2.10	0.52
81:Bz:52:VAL:HG23	81:Bz:52:VAL:O	2.08	0.52
85:B5:45:GLU:CB	85:B5:183:ARG:HG2	2.40	0.52
85:B5:188:LEU:O	85:B5:189:GLU:HG2	2.09	0.52
9:Aa:139:LYS:HZ2	9:Aa:142:VAL:HG22	1.74	0.51
12:Ad:99:ARG:CZ	12:Ad:136:SER:HA	2.40	0.51
21:An:26:ASN:O	21:An:38:MET:HA	2.11	0.51
62:Bj:21:ILE:O	62:Bj:24:LYS:HG2	2.09	0.51
62:Bj:44:GLY:O	62:Bj:133:LYS:HB2	2.09	0.51
66:Bn:207:MET:CG	66:Bn:233:ASP:HA	2.38	0.51
68:Bp:94:THR:HG23	68:Bp:95:TRP:N	2.25	0.51
77:Bw:114:VAL:HG23	77:Bw:136:LEU:HD21	1.91	0.51
77:Bw:127:VAL:CG2	77:Bw:157:ILE:HD11	2.27	0.51
77:Bw:136:LEU:CD1	77:Bw:143:THR:HG21	2.40	0.51
77:Bw:190:ALA:HA	77:Bw:195:SER:CB	2.40	0.51
82:B2:18:LEU:HD12	82:B2:27:TYR:CB	2.33	0.51
85:B5:111:MET:HE1	85:B5:131:PRO:CG	2.38	0.51
86:B6:24:SER:HB2	86:B6:26:LYS:HD2	1.91	0.51
9:Aa:256:ILE:HD11	9:Aa:300:ALA:CB	2.39	0.51
17:Aj:81:GLN:O	17:Aj:81:GLN:HG3	2.10	0.51
26:B0:3840:A:P	54:Bb:260:ARG:HD2	2.50	0.51
62:Bj:35:VAL:HG11	62:Bj:109:PRO:HB3	1.92	0.51
64:Bl:103:VAL:O	64:Bl:103:VAL:HG13	2.10	0.51
66:Bn:81:GLU:CD	66:Bn:103:LEU:HD22	2.36	0.51
66:Bn:108:LEU:C	66:Bn:108:LEU:CD2	2.83	0.51
70:Bq:39:VAL:HB	70:Bq:95:ILE:HD11	1.92	0.51
77:Bw:116:ARG:HD2	77:Bw:161:TYR:CD2	2.46	0.51
77:Bw:158:VAL:HG22	77:Bw:162:ILE:CG2	2.39	0.51
79:By:9:LYS:HA	79:By:9:LYS:HE3	1.91	0.51
82:B2:17:THR:O	82:B2:27:TYR:HB3	2.10	0.51
84:B4:72:CYS:HB3	84:B4:77:CYS:O	2.09	0.51
85:B5:60:VAL:HG23	85:B5:60:VAL:O	2.09	0.51
17:Aj:47:ASN:HB2	17:Aj:97:ILE:CG2	2.40	0.51
26:B0:2650:G:P	86:B6:91:VAL:CA	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:222:PHE:HB2	66:Bn:231:THR:HG22	1.93	0.51
85:B5:34:LEU:HB3	85:B5:157:ARG:HG2	1.92	0.51
85:B5:137:ASP:OD1	85:B5:139:VAL:HG23	2.11	0.51
85:B5:198:VAL:HG23	85:B5:210:VAL:HG13	1.92	0.51
9:Aa:14:HIS:CB	9:Aa:35:SER:CB	2.89	0.51
9:Aa:162:ASN:HB3	9:Aa:163:PRO:CD	2.40	0.51
21:An:23:VAL:HG23	21:An:36:LEU:CD1	2.40	0.51
62:Bj:26:VAL:CG2	62:Bj:97:ALA:HB1	2.39	0.51
62:Bj:36:ARG:CG	62:Bj:107:ILE:HA	2.40	0.51
64:Bl:43:ILE:HG23	64:Bl:43:ILE:O	2.09	0.51
66:Bn:110:ASN:HB3	66:Bn:138:PRO:CB	2.41	0.51
66:Bn:194:HIS:O	66:Bn:195:ARG:HD2	2.10	0.51
68:Bp:11:ALA:HA	68:Bp:14:VAL:HG12	1.93	0.51
70:Bq:38:ILE:CD1	70:Bq:60:THR:HG23	2.39	0.51
77:Bw:244:LYS:HD3	77:Bw:246:THR:H	1.73	0.51
80:B9:84:GLU:OE1	80:B9:84:GLU:HA	2.10	0.51
9:Aa:102:VAL:CG1	9:Aa:132:TRP:CZ3	2.94	0.51
9:Aa:239:LEU:HD23	9:Aa:239:LEU:C	2.35	0.51
9:Aa:305:ASN:O	9:Aa:306:LEU:HD12	2.11	0.51
26:B0:2776:G:P	82:B2:3:LYS:N	2.83	0.51
62:Bj:18:LEU:HD23	62:Bj:22:VAL:CG2	2.39	0.51
70:Bq:68:GLN:HG2	70:Bq:69:HIS:H	1.76	0.51
81:Bz:22:LEU:O	81:Bz:26:VAL:HG23	2.11	0.51
81:Bz:64:VAL:HG11	81:Bz:71:TYR:CZ	2.46	0.51
86:B6:68:LYS:HG2	86:B6:68:LYS:O	2.09	0.51
1:AA:1800:U:P	17:Aj:77:TRP:HZ2	2.26	0.51
9:Aa:248:LEU:HD21	9:Aa:298:LEU:HD21	1.92	0.51
62:Bj:31:LYS:HG3	62:Bj:100:ARG:O	2.10	0.51
62:Bj:134:PHE:HE1	62:Bj:136:TYR:CZ	2.28	0.51
70:Bq:29:TYR:HB2	70:Bq:93:GLU:CD	2.36	0.51
70:Bq:67:THR:HG22	70:Bq:68:GLN:N	2.26	0.51
77:Bw:123:VAL:HG11	77:Bw:128:ARG:HB2	1.92	0.51
77:Bw:175:LEU:HD21	77:Bw:266:ILE:HD13	1.93	0.51
81:Bz:55:TRP:NE1	81:Bz:71:TYR:HA	2.26	0.51
86:B6:18:LEU:CD1	86:B6:85:CYS:HA	2.40	0.51
26:B0:1860:U:P	79:By:47:ARG:HH11	2.33	0.51
84:B4:2:VAL:HG23	84:B4:3:ASN:N	2.26	0.51
85:B5:50:PRO:HD3	85:B5:179:VAL:HG21	1.91	0.51
85:B5:70:ARG:CG	85:B5:137:ASP:HA	2.41	0.51
85:B5:120:THR:HG23	85:B5:121:VAL:N	2.26	0.51
66:Bn:48:TYR:CB	66:Bn:63:ILE:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:124:VAL:HG11	66:Bn:128:GLU:HB2	1.93	0.51
79:By:5:ARG:HB2	79:By:6:PRO:CD	2.38	0.51
83:B3:35:ILE:HD13	83:B3:37:TYR:CD1	2.46	0.51
84:B4:24:THR:HG22	84:B4:25:GLN:O	2.11	0.51
86:B6:45:LEU:HD13	86:B6:109:PRO:HD3	1.93	0.51
9:Aa:10:THR:CG2	9:Aa:306:LEU:HD23	2.40	0.51
17:Aj:68:THR:HG22	17:Aj:69:PRO:N	2.24	0.51
64:Bl:109:TYR:CE2	64:Bl:111:VAL:CG2	2.94	0.51
66:Bn:50:MET:SD	66:Bn:172:ILE:HD13	2.50	0.51
66:Bn:184:SER:HB2	66:Bn:198:ILE:N	2.26	0.51
68:Bp:28:GLU:OE1	68:Bp:28:GLU:HA	2.09	0.51
68:Bp:51:ILE:HG12	68:Bp:52:ARG:N	2.26	0.51
70:Bq:39:VAL:HB	70:Bq:95:ILE:CD1	2.41	0.51
79:By:21:ILE:HG22	79:By:22:ARG:N	2.26	0.51
26:B0:1511:G:P	82:B2:16:HIS:NE2	2.81	0.51
62:Bj:7:VAL:HG23	62:Bj:7:VAL:O	2.09	0.51
62:Bj:8:LEU:HD12	62:Bj:18:LEU:CD1	2.34	0.51
66:Bn:84:LYS:NZ	66:Bn:107:ARG:HH12	2.08	0.51
68:Bp:66:ASN:O	68:Bp:70:ARG:HG2	2.11	0.51
70:Bq:38:ILE:HG23	70:Bq:38:ILE:O	2.11	0.51
81:Bz:29:ILE:HD12	81:Bz:29:ILE:C	2.36	0.51
84:B4:69:ARG:HD2	84:B4:80:LYS:CD	2.36	0.51
85:B5:47:VAL:HG13	85:B5:179:VAL:HG12	1.92	0.51
85:B5:64:GLU:HG2	85:B5:65:GLY:H	1.76	0.51
85:B5:150:GLN:HE21	85:B5:152:ARG:CD	2.22	0.51
26:B0:4259:U:P	70:Bq:87:ARG:NH1	2.84	0.50
64:Bl:82:VAL:HA	64:Bl:85:GLN:HG2	1.93	0.50
66:Bn:48:TYR:CE2	66:Bn:140:ALA:HB1	2.46	0.50
66:Bn:207:MET:O	66:Bn:210:LEU:HB2	2.11	0.50
77:Bw:158:VAL:CG2	77:Bw:162:ILE:HG21	2.41	0.50
85:B5:62:PHE:CE2	85:B5:110:LEU:CD2	2.94	0.50
9:Aa:248:LEU:HD11	9:Aa:256:ILE:HG22	1.93	0.50
64:Bl:117:LEU:HD11	64:Bl:136:LYS:CD	2.41	0.50
70:Bq:8:ARG:HB3	70:Bq:8:ARG:CZ	2.40	0.50
70:Bq:92:ILE:HD13	70:Bq:95:ILE:CG2	2.42	0.50
83:B3:21:ARG:HD2	83:B3:21:ARG:C	2.36	0.50
86:B6:66:LEU:HD13	86:B6:66:LEU:O	2.10	0.50
9:Aa:148:SER:HB2	9:Aa:170:TRP:HB2	1.94	0.50
9:Aa:248:LEU:CD1	9:Aa:256:ILE:HG22	2.41	0.50
17:Aj:72:GLU:CD	21:An:54:LYS:CG	2.82	0.50
26:B0:2867:C:P	68:Bp:74:ARG:HH22	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bj:26:VAL:HG11	62:Bj:87:LEU:CD1	2.38	0.50
62:Bj:53:TYR:O	62:Bj:58:ARG:HA	2.11	0.50
64:Bl:96:GLY:O	64:Bl:99:PRO:HG2	2.12	0.50
66:Bn:187:LYS:CB	66:Bn:237:GLU:HG3	2.40	0.50
77:Bw:219:VAL:CB	77:Bw:222:ARG:HB3	2.30	0.50
79:By:28:TYR:CZ	79:By:31:ILE:CG1	2.95	0.50
81:Bz:39:CYS:SG	81:Bz:42:CYS:HB3	2.50	0.50
84:B4:56:PHE:CZ	84:B4:57:ARG:HD3	2.46	0.50
1:AA:1654:C:P	21:An:29:GLY:O	2.70	0.50
9:Aa:102:VAL:HG11	9:Aa:132:TRP:CD2	2.47	0.50
68:Bp:106:LEU:CB	68:Bp:120:TYR:HE1	2.24	0.50
77:Bw:127:VAL:C	77:Bw:129:LYS:H	2.19	0.50
77:Bw:247:THR:HG23	77:Bw:255:ALA:CB	2.41	0.50
81:Bz:49:ARG:HH12	81:Bz:52:VAL:HG12	1.76	0.50
83:B3:9:ILE:HG23	83:B3:10:LYS:N	2.27	0.50
85:B5:62:PHE:CE1	85:B5:110:LEU:CB	2.92	0.50
9:Aa:13:GLY:HA3	9:Aa:41:ILE:HD12	1.94	0.50
9:Aa:70:VAL:HG22	9:Aa:79:LEU:HB2	1.93	0.50
9:Aa:100:ARG:NH2	9:Aa:102:VAL:HG21	2.27	0.50
66:Bn:191:ALA:CA	66:Bn:238:MET:SD	3.00	0.50
68:Bp:69:ALA:HB1	68:Bp:74:ARG:HB2	1.92	0.50
77:Bw:116:ARG:CD	77:Bw:161:TYR:CD2	2.95	0.50
77:Bw:118:ARG:CG	77:Bw:119:GLY:H	2.17	0.50
77:Bw:157:ILE:HD13	77:Bw:157:ILE:C	2.36	0.50
9:Aa:17:TRP:CA	9:Aa:305:ASN:CG	2.85	0.50
9:Aa:102:VAL:HG11	9:Aa:132:TRP:CE3	2.46	0.50
9:Aa:230:LEU:HD13	9:Aa:259:TRP:CB	2.41	0.50
77:Bw:247:THR:HG1	77:Bw:253:GLY:C	2.20	0.50
79:By:28:TYR:CD2	79:By:31:ILE:HG12	2.45	0.50
83:B3:6:THR:N	83:B3:9:ILE:HG22	2.27	0.50
85:B5:62:PHE:CE1	85:B5:110:LEU:CG	2.95	0.50
9:Aa:62:HIS:HB3	9:Aa:84:ASP:OD2	2.12	0.50
9:Aa:173:LEU:CD2	9:Aa:189:ILE:HG22	2.41	0.50
12:Ad:100:LEU:CD2	12:Ad:120:VAL:HG21	2.32	0.50
21:An:20:SER:HB3	21:An:25:SER:CA	2.42	0.50
62:Bj:119:VAL:HG13	62:Bj:120:PRO:CD	2.41	0.50
66:Bn:207:MET:CB	66:Bn:233:ASP:HA	2.42	0.50
68:Bp:23:TRP:HB3	68:Bp:51:ILE:HG22	1.94	0.50
68:Bp:69:ALA:HB1	68:Bp:75:HIS:ND1	2.27	0.50
70:Bq:6:LYS:HD2	70:Bq:6:LYS:N	2.27	0.50
83:B3:35:ILE:CD1	83:B3:37:TYR:CD1	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B6:6:LYS:HZ2	86:B6:14:ILE:HG21	1.75	0.50
62:Bj:26:VAL:HG22	62:Bj:97:ALA:HB1	1.94	0.50
62:Bj:78:ILE:HD13	62:Bj:78:ILE:C	2.37	0.50
66:Bn:187:LYS:HB2	66:Bn:237:GLU:HG3	1.94	0.50
66:Bn:194:HIS:C	66:Bn:195:ARG:HD2	2.37	0.50
66:Bn:200:GLY:HA2	66:Bn:236:GLU:CD	2.37	0.50
68:Bp:28:GLU:CG	68:Bp:49:LEU:HG	2.34	0.50
77:Bw:117:ILE:C	77:Bw:245:LYS:HE3	2.37	0.50
77:Bw:123:VAL:HG21	77:Bw:127:VAL:HG12	1.93	0.50
79:By:9:LYS:CB	79:By:10:PRO:HD3	2.32	0.50
82:B2:16:HIS:HB3	82:B2:25:LYS:O	2.11	0.50
84:B4:4:VAL:HG12	84:B4:5:PRO:N	2.25	0.50
85:B5:151:LEU:CD1	85:B5:159:PHE:CD2	2.95	0.50
86:B6:18:LEU:HD11	86:B6:85:CYS:HA	1.94	0.50
86:B6:29:LEU:HA	86:B6:94:LEU:HD23	1.93	0.50
86:B6:30:GLY:C	86:B6:93:THR:HG23	2.37	0.50
9:Aa:17:TRP:CA	9:Aa:305:ASN:HB3	2.37	0.50
9:Aa:156:PHE:CE1	9:Aa:166:VAL:HG13	2.46	0.50
9:Aa:188:HIS:NE2	9:Aa:226:HIS:CD2	2.80	0.50
17:Aj:20:ILE:CG2	17:Aj:114:VAL:HG23	2.42	0.50
22:Ao:70:GLN:CG	22:Ao:77:TYR:CG	2.95	0.50
66:Bn:108:LEU:CD2	66:Bn:170:LEU:HD11	2.36	0.50
66:Bn:182:TYR:HE2	66:Bn:198:ILE:HG21	1.72	0.50
66:Bn:191:ALA:O	66:Bn:238:MET:SD	2.69	0.50
77:Bw:136:LEU:HD11	77:Bw:143:THR:HG21	1.94	0.50
77:Bw:162:ILE:HD11	77:Bw:164:TRP:CD1	2.47	0.50
77:Bw:222:ARG:HD3	77:Bw:222:ARG:N	2.27	0.50
85:B5:5:ILE:HD13	85:B5:177:ILE:CG2	2.35	0.50
9:Aa:25:PRO:HG2	9:Aa:30:MET:HB2	1.94	0.49
9:Aa:188:HIS:CE1	9:Aa:219:TRP:CD1	3.00	0.49
9:Aa:230:LEU:HD13	9:Aa:259:TRP:CG	2.47	0.49
17:Aj:66:ARG:HA	17:Aj:77:TRP:HD1	1.77	0.49
21:An:20:SER:HB3	21:An:25:SER:C	2.36	0.49
26:B0:4526:U:P	54:Bb:263:PHE:HE1	2.35	0.49
62:Bj:78:ILE:CG2	62:Bj:137:LEU:HD23	2.41	0.49
66:Bn:108:LEU:CD2	66:Bn:140:ALA:HB3	2.39	0.49
66:Bn:198:ILE:O	66:Bn:236:GLU:HB2	2.12	0.49
77:Bw:158:VAL:HG21	77:Bw:162:ILE:HG21	1.94	0.49
77:Bw:176:ILE:HD13	77:Bw:233:PHE:CE2	2.47	0.49
79:By:12:ILE:HG12	79:By:17:THR:HG21	1.92	0.49
79:By:66:THR:C	80:B9:69:MET:SD	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Bz:46:LYS:HD3	81:Bz:59:SER:CA	2.42	0.49
9:Aa:307:VAL:HG12	9:Aa:308:ARG:N	2.26	0.49
64:Bl:45:PHE:HB3	64:Bl:47:LYS:HG2	1.93	0.49
66:Bn:85:TYR:OH	66:Bn:106:ARG:HD3	2.12	0.49
82:B2:18:LEU:HD21	82:B2:22:CYS:CB	2.42	0.49
82:B2:18:LEU:CB	82:B2:25:LYS:HA	2.23	0.49
86:B6:80:GLU:O	86:B6:83:THR:HG22	2.11	0.49
9:Aa:89:LEU:HD22	9:Aa:100:ARG:HE	1.77	0.49
12:Ad:140:ARG:HG2	12:Ad:143:ASP:OD2	2.12	0.49
21:An:21:CYS:HB3	21:An:37:ASN:N	2.27	0.49
21:An:26:ASN:C	21:An:38:MET:HA	2.36	0.49
26:B0:2278:C:P	80:B9:104:SER:N	2.83	0.49
64:Bl:93:ASN:OD1	64:Bl:95:THR:HG23	2.12	0.49
64:Bl:116:LYS:C	64:Bl:117:LEU:HD23	2.37	0.49
66:Bn:193:VAL:CG2	66:Bn:235:MET:HB3	2.42	0.49
70:Bq:35:LYS:HD2	70:Bq:65:ASN:CA	2.40	0.49
70:Bq:79:VAL:HG22	70:Bq:80:LYS:H	1.76	0.49
85:B5:69:LEU:H	85:B5:69:LEU:CD2	2.24	0.49
86:B6:6:LYS:HD3	86:B6:14:ILE:CG2	2.43	0.49
9:Aa:162:ASN:CB	9:Aa:163:PRO:CD	2.91	0.49
9:Aa:173:LEU:HD22	9:Aa:189:ILE:HG22	1.94	0.49
17:Aj:39:LEU:HD11	17:Aj:91:LEU:HD21	1.95	0.49
26:B0:2381:A:P	82:B2:14:LYS:CE	3.00	0.49
62:Bj:54:LEU:HA	62:Bj:58:ARG:HG3	1.90	0.49
68:Bp:70:ARG:HD2	68:Bp:75:HIS:HB2	1.94	0.49
70:Bq:78:GLN:HB2	70:Bq:82:LYS:HE3	1.93	0.49
77:Bw:127:VAL:CG1	77:Bw:161:TYR:CE1	2.94	0.49
77:Bw:196:LEU:HD11	77:Bw:209:MET:N	2.27	0.49
81:Bz:81:SER:O	81:Bz:82:ALA:HB2	2.12	0.49
82:B2:18:LEU:HB3	82:B2:24:SER:O	2.12	0.49
17:Aj:29:VAL:HG12	17:Aj:85:HIS:CE1	2.47	0.49
17:Aj:70:CYS:O	17:Aj:72:GLU:HG3	2.12	0.49
64:Bl:72:THR:HG22	64:Bl:110:LYS:HG2	1.93	0.49
66:Bn:84:LYS:HZ3	66:Bn:107:ARG:HH22	1.60	0.49
68:Bp:95:TRP:HE1	68:Bp:99:MET:CE	2.25	0.49
84:B4:39:ARG:HD3	84:B4:39:ARG:N	2.27	0.49
84:B4:89:LYS:HG3	84:B4:90:HIS:CD2	2.48	0.49
85:B5:151:LEU:CD1	85:B5:159:PHE:CE2	2.95	0.49
86:B6:37:MET:CE	86:B6:42:LYS:HB3	2.43	0.49
12:Ad:151:SER:O	12:Ad:154:LEU:HG	2.12	0.49
17:Aj:40:ILE:HD12	17:Aj:50:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:224:GLN:CG	66:Bn:231:THR:HB	2.40	0.49
70:Bq:82:LYS:HD2	70:Bq:83:ILE:O	2.12	0.49
81:Bz:64:VAL:HG12	81:Bz:65:ALA:O	2.13	0.49
82:B2:24:SER:O	82:B2:25:LYS:HD2	2.11	0.49
8:AH:17:C:P	21:An:18:SER:OG	2.71	0.49
9:Aa:81:GLY:HA3	9:Aa:109:LEU:HD23	1.93	0.49
9:Aa:282:GLU:HG3	9:Aa:308:ARG:NH2	2.27	0.49
17:Aj:32:LEU:HD21	17:Aj:87:ARG:CG	2.40	0.49
26:B0:4306:U:P	84:B4:80:LYS:HZ2	2.33	0.49
62:Bj:14:LEU:HD12	62:Bj:14:LEU:H	1.78	0.49
62:Bj:36:ARG:HH11	62:Bj:107:ILE:CG2	2.26	0.49
66:Bn:193:VAL:HG21	66:Bn:235:MET:N	2.27	0.49
77:Bw:169:LEU:O	77:Bw:170:LYS:HB2	2.11	0.49
85:B5:141:VAL:HG23	85:B5:142:ILE:N	2.27	0.49
86:B6:20:LEU:HD23	86:B6:20:LEU:C	2.37	0.49
22:Ao:26:VAL:HG12	22:Ao:30:LEU:HD23	1.94	0.49
62:Bj:97:ALA:HA	62:Bj:100:ARG:HD2	1.93	0.49
66:Bn:38:GLN:OE1	70:Bq:29:TYR:CD2	2.46	0.49
81:Bz:76:ALA:O	81:Bz:79:VAL:HG22	2.13	0.49
82:B2:39:TYR:OH	82:B2:43:ARG:HA	2.12	0.49
85:B5:62:PHE:HE1	85:B5:81:GLU:HG2	1.71	0.49
17:Aj:72:GLU:OE2	21:An:54:LYS:HG2	2.13	0.49
21:An:36:LEU:HB3	21:An:39:CYS:O	2.13	0.49
62:Bj:88:PRO:O	62:Bj:91:THR:HG22	2.13	0.49
77:Bw:190:ALA:O	77:Bw:191:LEU:HB3	2.13	0.49
77:Bw:223:PHE:C	77:Bw:224:LYS:HG3	2.37	0.49
82:B2:19:CYS:HB2	82:B2:34:CYS:SG	2.53	0.49
84:B4:23:VAL:HG21	84:B4:68:LEU:HD13	1.93	0.49
84:B4:74:GLU:N	84:B4:75:PRO:HD2	2.28	0.49
86:B6:83:THR:HG23	86:B6:84:ALA:N	2.26	0.49
9:Aa:113:PHE:C	9:Aa:120:ILE:HD12	2.36	0.49
21:An:34:TYR:CD1	21:An:43:PHE:CD1	3.01	0.49
26:B0:2383:G:P	83:B3:49:LEU:HD13	2.53	0.49
26:B0:4238:C:P	70:Bq:21:HIS:CD2	3.06	0.49
64:Bl:111:VAL:HG21	64:Bl:129:PHE:CE2	2.48	0.49
66:Bn:84:LYS:HZ2	66:Bn:107:ARG:NH1	2.10	0.49
79:By:13:VAL:HG23	79:By:14:LYS:H	1.78	0.49
79:By:23:HIS:C	79:By:24:GLN:HG3	2.38	0.49
82:B2:18:LEU:HD12	82:B2:19:CYS:N	2.14	0.49
85:B5:36:LEU:HD23	85:B5:36:LEU:C	2.38	0.49
85:B5:105:ILE:HA	85:B5:130:GLU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B6:53:PRO:O	86:B6:54:ALA:HB3	2.12	0.49
86:B6:59:GLU:HB3	86:B6:63:TYR:HE1	1.78	0.49
9:Aa:88:ARG:HD3	9:Aa:88:ARG:N	2.28	0.48
9:Aa:188:HIS:NE2	9:Aa:226:HIS:CE1	2.81	0.48
22:Ao:77:TYR:CD2	22:Ao:77:TYR:C	2.91	0.48
62:Bj:72:PHE:HB2	62:Bj:77:ARG:CG	2.31	0.48
64:Bl:81:LEU:CD1	64:Bl:100:ILE:HD11	2.43	0.48
64:Bl:101:ILE:HG12	64:Bl:104:VAL:HG22	1.90	0.48
66:Bn:84:LYS:HB2	66:Bn:103:LEU:CD1	2.43	0.48
68:Bp:45:ILE:HG13	68:Bp:46:LYS:HD2	1.95	0.48
77:Bw:248:HIS:CA	77:Bw:255:ALA:HB3	2.43	0.48
79:By:64:LYS:HA	79:By:67:LYS:CE	2.43	0.48
9:Aa:257:LYS:HB2	9:Aa:259:TRP:CH2	2.49	0.48
26:B0:2866:G:P	68:Bp:75:HIS:CE1	2.98	0.48
64:Bl:117:LEU:CD2	64:Bl:136:LYS:HD2	2.26	0.48
66:Bn:162:LEU:C	66:Bn:162:LEU:HD13	2.39	0.48
66:Bn:198:ILE:HG23	66:Bn:199:MET:H	1.78	0.48
79:By:53:ILE:HG22	79:By:54:LEU:N	2.28	0.48
80:B9:83:LYS:H	80:B9:83:LYS:CD	2.24	0.48
84:B4:68:LEU:CD1	84:B4:91:PHE:CZ	2.95	0.48
85:B5:161:THR:HG21	85:B5:180:ILE:CD1	2.42	0.48
22:Ao:70:GLN:HG3	22:Ao:77:TYR:CD2	2.47	0.48
62:Bj:9:ASP:N	62:Bj:115:LYS:HB3	2.28	0.48
62:Bj:26:VAL:HG22	62:Bj:26:VAL:O	2.13	0.48
64:Bl:37:GLY:O	64:Bl:42:ARG:HB2	2.13	0.48
64:Bl:76:ASP:CA	64:Bl:79:TRP:HD1	2.20	0.48
66:Bn:89:VAL:CG2	66:Bn:193:VAL:HA	2.43	0.48
77:Bw:245:LYS:O	77:Bw:247:THR:HB	2.13	0.48
82:B2:12:ARG:NE	83:B3:4:HIS:CD2	2.81	0.48
84:B4:22:LYS:HE3	84:B4:71:GLU:CD	2.38	0.48
84:B4:62:THR:HG23	84:B4:63:THR:N	2.28	0.48
9:Aa:239:LEU:HD22	9:Aa:291:TRP:HB2	1.95	0.48
9:Aa:284:PRO:HG3	9:Aa:304:ASP:HB2	1.96	0.48
62:Bj:140:LEU:HD23	62:Bj:140:LEU:O	2.14	0.48
66:Bn:51:ILE:HG13	66:Bn:62:GLN:HB3	1.96	0.48
66:Bn:233:ASP:C	66:Bn:234:MET:HG3	2.37	0.48
70:Bq:3:THR:HG22	70:Bq:4:LYS:H	1.77	0.48
85:B5:58:THR:HG23	85:B5:101:THR:CA	2.41	0.48
85:B5:151:LEU:CD1	85:B5:159:PHE:CZ	2.95	0.48
26:B0:2813:A:P	54:Bb:248:ARG:CD	3.02	0.48
70:Bq:71:VAL:C	70:Bq:74:ILE:HG12	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Bw:196:LEU:HD11	77:Bw:208:CYS:O	2.13	0.48
86:B6:61:GLU:HG3	86:B6:62:TYR:N	2.28	0.48
9:Aa:102:VAL:CG1	9:Aa:132:TRP:CE3	2.96	0.48
26:B0:2251:G:P	77:Bw:186:LYS:N	2.86	0.48
26:B0:4608:A:P	68:Bp:62:ARG:HH22	2.36	0.48
62:Bj:58:ARG:N	62:Bj:58:ARG:HD3	2.29	0.48
66:Bn:58:ASP:HA	66:Bn:91:LEU:HD12	1.95	0.48
70:Bq:59:LYS:N	70:Bq:59:LYS:HD2	2.28	0.48
77:Bw:116:ARG:NH2	77:Bw:131:LEU:HD23	2.29	0.48
77:Bw:201:LEU:HD12	77:Bw:201:LEU:N	2.28	0.48
77:Bw:259:GLU:O	77:Bw:262:ILE:HG12	2.13	0.48
79:By:45:VAL:HG12	79:By:52:GLN:O	2.14	0.48
79:By:64:LYS:HD2	79:By:64:LYS:O	2.13	0.48
83:B3:5:LYS:HB2	83:B3:9:ILE:HG23	1.93	0.48
83:B3:15:LYS:HD2	83:B3:15:LYS:O	2.14	0.48
85:B5:31:LEU:HD23	85:B5:195:ILE:HA	1.95	0.48
85:B5:43:VAL:HG22	85:B5:188:LEU:HD13	1.96	0.48
85:B5:151:LEU:CD1	85:B5:159:PHE:CG	2.96	0.48
86:B6:6:LYS:NZ	86:B6:71:VAL:HG11	2.29	0.48
86:B6:71:VAL:O	86:B6:71:VAL:HG12	2.12	0.48
22:Ao:66:LEU:CA	22:Ao:77:TYR:CE1	2.97	0.48
26:B0:52:G:P	82:B2:49:TRP:H	2.36	0.48
26:B0:4303:U:P	84:B4:37:GLY:HA3	2.53	0.48
66:Bn:85:TYR:OH	66:Bn:103:LEU:HG	2.12	0.48
66:Bn:235:MET:CG	66:Bn:237:GLU:HB2	2.43	0.48
68:Bp:64:ARG:HA	68:Bp:67:THR:HG22	1.95	0.48
70:Bq:8:ARG:HB3	70:Bq:8:ARG:HH11	1.76	0.48
70:Bq:62:ARG:HB3	70:Bq:64:TYR:CE1	2.49	0.48
70:Bq:92:ILE:C	70:Bq:95:ILE:HG22	2.38	0.48
82:B2:28:HIS:CA	82:B2:31:LYS:HE2	2.43	0.48
9:Aa:164:ILE:CD1	9:Aa:178:ASN:HA	2.43	0.48
9:Aa:284:PRO:HG2	9:Aa:304:ASP:H	1.79	0.48
17:Aj:114:VAL:O	17:Aj:114:VAL:HG13	2.12	0.48
62:Bj:23:ALA:O	62:Bj:27:LEU:HG	2.14	0.48
70:Bq:66:VAL:HG23	70:Bq:71:VAL:HG12	1.96	0.48
77:Bw:248:HIS:O	77:Bw:255:ALA:HB3	2.13	0.48
81:Bz:11:VAL:CG2	81:Bz:27:LYS:HG2	2.44	0.48
83:B3:27:ILE:HG23	83:B3:28:ARG:N	2.29	0.48
85:B5:62:PHE:CZ	85:B5:110:LEU:CD2	2.97	0.48
86:B6:46:VAL:HG12	86:B6:72:HIS:HB3	1.95	0.48
12:Ad:58:ARG:NH2	12:Ad:61:GLN:HG3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:An:20:SER:HB3	21:An:25:SER:HB2	1.94	0.48
62:Bj:74:ALA:H	62:Bj:77:ARG:HE	1.62	0.48
62:Bj:128:LEU:HD22	62:Bj:128:LEU:N	2.29	0.48
66:Bn:184:SER:OG	66:Bn:200:GLY:N	2.35	0.48
68:Bp:29:THR:HA	68:Bp:32:ILE:HG22	1.96	0.48
79:By:50:LYS:NZ	79:By:51:GLY:H	2.12	0.48
79:By:66:THR:HG23	80:B9:69:MET:HG3	1.43	0.48
84:B4:67:VAL:HG22	84:B4:85:ILE:CD1	2.43	0.48
85:B5:78:VAL:O	85:B5:79:LEU:HD12	2.14	0.48
26:B0:4190:C:P	84:B4:89:LYS:H	2.37	0.48
64:Bl:117:LEU:HD13	64:Bl:136:LYS:O	2.14	0.48
79:By:28:TYR:CZ	79:By:31:ILE:HG12	2.48	0.48
80:B9:79:VAL:HG13	80:B9:99:ILE:HA	1.96	0.48
80:B9:81:ASN:ND2	80:B9:83:LYS:HD3	2.29	0.48
81:Bz:42:CYS:HA	86:B6:53:PRO:CA	2.40	0.48
85:B5:62:PHE:CD1	85:B5:62:PHE:C	2.92	0.48
85:B5:87:LEU:CB	85:B5:117:TYR:CE2	2.97	0.48
85:B5:190:LYS:H	85:B5:190:LYS:CD	2.23	0.48
9:Aa:217:MET:CE	9:Aa:226:HIS:CD2	2.96	0.47
22:Ao:66:LEU:HD11	22:Ao:84:LEU:CD1	2.44	0.47
22:Ao:70:GLN:HG3	22:Ao:77:TYR:CG	2.48	0.47
26:B0:1495:G:P	64:Bl:32:ARG:HH11	2.37	0.47
70:Bq:24:VAL:CG2	70:Bq:25:PRO:HD2	2.44	0.47
70:Bq:82:LYS:HD3	70:Bq:85:ALA:HA	1.94	0.47
77:Bw:139:ILE:HG22	77:Bw:140:PHE:CD1	2.49	0.47
77:Bw:162:ILE:CD1	77:Bw:164:TRP:CD1	2.95	0.47
77:Bw:191:LEU:HG	77:Bw:192:THR:H	1.78	0.47
79:By:16:ARG:NE	79:By:16:ARG:HA	2.27	0.47
80:B9:87:VAL:HG11	80:B9:89:LEU:HD23	1.95	0.47
85:B5:43:VAL:CG1	85:B5:188:LEU:HD12	2.43	0.47
9:Aa:34:ALA:CB	9:Aa:69:VAL:HB	2.44	0.47
9:Aa:100:ARG:HH21	9:Aa:102:VAL:HG21	1.79	0.47
9:Aa:164:ILE:HG21	9:Aa:179:LEU:H	1.79	0.47
12:Ad:107:LEU:CD1	12:Ad:109:PHE:CE2	2.96	0.47
22:Ao:66:LEU:C	22:Ao:77:TYR:CE1	2.92	0.47
62:Bj:33:VAL:HG21	62:Bj:111:TYR:CE1	2.49	0.47
62:Bj:78:ILE:HG23	62:Bj:79:PHE:N	2.28	0.47
66:Bn:53:ARG:HG2	66:Bn:60:ILE:CG2	2.45	0.47
66:Bn:53:ARG:HG2	66:Bn:60:ILE:HG22	1.96	0.47
77:Bw:145:VAL:HG12	77:Bw:146:LYS:N	2.29	0.47
77:Bw:219:VAL:HG23	77:Bw:220:GLY:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Bw:222:ARG:HD3	77:Bw:222:ARG:H	1.79	0.47
79:By:45:VAL:O	79:By:53:ILE:HD12	2.15	0.47
81:Bz:29:ILE:CD1	81:Bz:30:GLU:HG2	2.44	0.47
83:B3:6:THR:HG23	83:B3:9:ILE:H	1.79	0.47
85:B5:62:PHE:CZ	85:B5:110:LEU:CG	2.96	0.47
86:B6:18:LEU:HG	86:B6:94:LEU:HD12	1.95	0.47
86:B6:46:VAL:CG1	86:B6:72:HIS:HB3	2.44	0.47
9:Aa:254:PRO:HG3	9:Aa:285:GLN:N	2.30	0.47
62:Bj:75:PRO:HA	62:Bj:78:ILE:HG22	1.96	0.47
64:Bl:77:LYS:HB2	64:Bl:78:PRO:HD2	1.95	0.47
66:Bn:81:GLU:HG2	66:Bn:103:LEU:HD13	1.96	0.47
80:B9:81:ASN:HD22	80:B9:83:LYS:N	2.09	0.47
82:B2:43:ARG:HG2	82:B2:44:LYS:H	1.79	0.47
83:B3:5:LYS:CB	83:B3:9:ILE:HG21	2.44	0.47
8:AH:10:G:P	21:An:13:LYS:HZ2	2.36	0.47
12:Ad:106:ARG:HH21	12:Ad:113:ARG:HH21	1.62	0.47
26:B0:2713:G:P	81:Bz:34:HIS:ND1	2.88	0.47
62:Bj:23:ALA:HB1	62:Bj:87:LEU:CD2	2.42	0.47
62:Bj:61:MET:HA	62:Bj:61:MET:CE	2.32	0.47
64:Bl:109:TYR:CZ	64:Bl:111:VAL:HG22	2.49	0.47
79:By:28:TYR:CE2	79:By:30:LYS:HG3	2.46	0.47
82:B2:29:LEU:H	82:B2:29:LEU:CD2	2.27	0.47
82:B2:32:SER:O	82:B2:40:PRO:HD2	2.15	0.47
83:B3:18:LYS:O	83:B3:21:ARG:HG3	2.14	0.47
85:B5:74:VAL:HG21	85:B5:142:ILE:HB	1.95	0.47
86:B6:17:ARG:NH1	86:B6:108:MET:HB2	2.23	0.47
62:Bj:15:LEU:CG	62:Bj:40:ILE:HG12	2.43	0.47
62:Bj:25:GLN:O	62:Bj:28:LEU:HB2	2.15	0.47
66:Bn:78:TYR:CD2	66:Bn:80:HIS:HB2	2.50	0.47
70:Bq:65:ASN:C	70:Bq:74:ILE:HG21	2.39	0.47
77:Bw:210:GLU:O	77:Bw:213:ILE:HG12	2.14	0.47
82:B2:15:THR:HG23	82:B2:28:HIS:NE2	2.30	0.47
83:B3:35:ILE:CG2	83:B3:37:TYR:HB2	2.44	0.47
85:B5:43:VAL:HA	85:B5:188:LEU:HD13	1.97	0.47
9:Aa:21:ILE:CG2	9:Aa:307:VAL:HG21	2.44	0.47
9:Aa:162:ASN:HB3	9:Aa:163:PRO:HD2	1.96	0.47
12:Ad:152:ARG:HB3	12:Ad:152:ARG:NH1	2.30	0.47
17:Aj:35:VAL:HG21	17:Aj:107:GLU:HB3	1.97	0.47
62:Bj:115:LYS:HD3	62:Bj:115:LYS:N	2.30	0.47
66:Bn:41:ASN:HB2	70:Bq:66:VAL:HG21	1.96	0.47
68:Bp:129:GLY:O	68:Bp:130:ASN:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:B7:192:ARG:HG3	69:B7:193:MET:N	2.30	0.47
70:Bq:41:ILE:HG12	70:Bq:77:LYS:CE	2.45	0.47
77:Bw:216:ILE:HD11	77:Bw:223:PHE:HD2	1.80	0.47
77:Bw:239:ARG:N	77:Bw:268:ARG:HB2	2.20	0.47
84:B4:23:VAL:HG22	84:B4:68:LEU:HB3	1.97	0.47
9:Aa:107:ASP:HB3	9:Aa:125:ARG:HB3	1.97	0.47
9:Aa:262:GLU:CA	9:Aa:270:LEU:HD23	2.42	0.47
26:B0:1634:C:P	64:Bl:24:LYS:HZ2	2.38	0.47
62:Bj:50:LYS:HD2	62:Bj:50:LYS:C	2.39	0.47
64:Bl:7:LYS:HG3	64:Bl:8:THR:N	2.29	0.47
64:Bl:71:PRO:HD2	64:Bl:108:TYR:O	2.15	0.47
66:Bn:77:ARG:NH2	66:Bn:82:LEU:HA	2.29	0.47
66:Bn:89:VAL:CG2	66:Bn:193:VAL:HG12	2.44	0.47
66:Bn:187:LYS:HE3	66:Bn:188:GLU:H	1.78	0.47
66:Bn:243:HIS:O	66:Bn:246:ILE:HG12	2.15	0.47
66:Bn:246:ILE:HG21	66:Bn:246:ILE:HD13	1.64	0.47
68:Bp:98:ARG:HG3	68:Bp:99:MET:N	2.30	0.47
70:Bq:11:ARG:HB3	70:Bq:11:ARG:NH1	2.29	0.47
70:Bq:38:ILE:CD1	70:Bq:60:THR:CG2	2.93	0.47
70:Bq:73:ILE:HG13	70:Bq:87:ARG:CG	2.45	0.47
77:Bw:169:LEU:H	77:Bw:169:LEU:CD2	2.28	0.47
77:Bw:245:LYS:HB2	77:Bw:245:LYS:HZ3	1.80	0.47
79:By:35:TRP:CD1	79:By:36:ARG:N	2.83	0.47
80:B9:87:VAL:HG12	80:B9:89:LEU:HD23	1.94	0.47
85:B5:57:THR:HG21	85:B5:145:MET:O	2.15	0.47
85:B5:74:VAL:HG12	85:B5:146:LYS:HD3	1.96	0.47
85:B5:104:PHE:CZ	85:B5:122:LEU:CD2	2.94	0.47
86:B6:44:LYS:HD3	86:B6:98:ASP:CA	2.38	0.47
21:An:19:ARG:HB2	21:An:37:ASN:HD21	1.79	0.47
66:Bn:40:LYS:HE3	70:Bq:67:THR:H	1.72	0.47
66:Bn:61:CYS:SG	66:Bn:104:LEU:HD22	2.54	0.47
66:Bn:89:VAL:CG2	66:Bn:90:GLY:N	2.77	0.47
70:Bq:82:LYS:HD2	70:Bq:83:ILE:C	2.39	0.47
77:Bw:133:LEU:CD1	77:Bw:134:LEU:HG	2.45	0.47
77:Bw:216:ILE:HD13	77:Bw:222:ARG:HB2	1.95	0.47
79:By:64:LYS:CB	79:By:67:LYS:HE3	2.44	0.47
86:B6:17:ARG:HD2	86:B6:21:VAL:HG21	1.97	0.47
86:B6:17:ARG:HH22	86:B6:45:LEU:HD11	1.77	0.47
9:Aa:14:HIS:HB2	9:Aa:18:VAL:HG22	1.97	0.47
9:Aa:149:GLU:HB3	9:Aa:170:TRP:CD2	2.50	0.47
26:B0:2611:C:P	68:Bp:60:ARG:N	2.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B0:2867:C:P	68:Bp:74:ARG:HH12	2.33	0.47
62:Bj:15:LEU:HD12	62:Bj:41:ASN:O	2.15	0.47
64:Bl:79:TRP:HB2	64:Bl:118:PRO:HA	1.97	0.47
66:Bn:198:ILE:CG2	66:Bn:199:MET:N	2.77	0.47
68:Bp:89:MET:HB3	68:Bp:90:PRO:CD	2.38	0.47
68:Bp:103:ARG:HG2	68:Bp:124:TYR:HE1	1.79	0.47
70:Bq:33:TYR:HE1	70:Bq:92:ILE:CD1	2.27	0.47
82:B2:18:LEU:CG	82:B2:19:CYS:N	2.78	0.47
84:B4:32:SER:O	84:B4:33:LEU:HB2	2.13	0.47
85:B5:60:VAL:N	85:B5:101:THR:HG21	2.29	0.47
12:Ad:125:ILE:HG22	12:Ad:126:THR:N	2.29	0.47
62:Bj:123:LEU:HG	62:Bj:130:PRO:HG2	1.97	0.47
66:Bn:184:SER:HB3	66:Bn:198:ILE:HG22	1.97	0.47
66:Bn:195:ARG:NH2	66:Bn:234:MET:HG2	2.30	0.47
68:Bp:14:VAL:HG21	68:Bp:42:ARG:HG2	1.96	0.47
68:Bp:71:ARG:NH1	68:Bp:71:ARG:HB2	2.29	0.47
70:Bq:29:TYR:O	70:Bq:92:ILE:HG21	2.14	0.47
70:Bq:79:VAL:CG1	70:Bq:82:LYS:H	2.10	0.47
77:Bw:186:LYS:HD3	77:Bw:186:LYS:N	2.23	0.47
85:B5:34:LEU:HD22	85:B5:40:SER:HB3	1.95	0.47
85:B5:62:PHE:CD1	85:B5:110:LEU:CG	2.93	0.47
9:Aa:18:VAL:CG2	9:Aa:305:ASN:O	2.62	0.46
17:Aj:44:LYS:HZ2	17:Aj:49:LYS:HD2	1.80	0.46
21:An:21:CYS:SG	21:An:38:MET:CB	3.03	0.46
26:B0:2029:C:P	62:Bj:53:TYR:OH	2.73	0.46
64:Bl:109:TYR:HD2	64:Bl:126:ALA:HB1	1.79	0.46
77:Bw:157:ILE:HG23	77:Bw:158:VAL:N	2.29	0.46
12:Ad:124:HIS:CE1	12:Ad:154:LEU:HD11	2.50	0.46
17:Aj:40:ILE:HD11	17:Aj:49:LYS:O	2.16	0.46
17:Aj:95:SER:O	17:Aj:98:VAL:HB	2.14	0.46
51:BY:7:G:P	66:Bn:27:THR:CB	3.02	0.46
64:Bl:122:VAL:O	64:Bl:122:VAL:HG23	2.14	0.46
70:Bq:31:ARG:HB2	70:Bq:92:ILE:HD11	1.96	0.46
77:Bw:214:HIS:CA	77:Bw:217:TYR:CD2	2.94	0.46
80:B9:78:LEU:HD22	80:B9:80:HIS:NE2	2.31	0.46
82:B2:16:HIS:CE1	82:B2:28:HIS:HB2	2.50	0.46
85:B5:29:VAL:HG22	85:B5:198:VAL:CG1	2.44	0.46
9:Aa:7:LEU:CD1	9:Aa:308:ARG:HB3	2.45	0.46
9:Aa:100:ARG:HH21	9:Aa:102:VAL:HG23	1.80	0.46
9:Aa:104:HIS:CE1	9:Aa:139:LYS:NZ	2.83	0.46
64:Bl:97:VAL:HG12	64:Bl:97:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:48:TYR:CD2	66:Bn:140:ALA:HB1	2.50	0.46
66:Bn:67:ARG:HB3	66:Bn:70:GLY:O	2.16	0.46
79:By:43:ASN:H	79:By:43:ASN:HD22	1.63	0.46
81:Bz:37:TYR:CZ	81:Bz:70:THR:HG23	2.50	0.46
82:B2:31:LYS:CE	82:B2:33:THR:N	2.78	0.46
85:B5:45:GLU:CG	85:B5:183:ARG:HG3	2.45	0.46
48:BV:12:C:P	64:Bl:136:LYS:HZ2	2.36	0.46
66:Bn:37:ILE:HG22	66:Bn:45:THR:N	2.28	0.46
66:Bn:76:ALA:O	66:Bn:81:GLU:OE1	2.34	0.46
66:Bn:78:TYR:HD2	66:Bn:80:HIS:H	1.61	0.46
66:Bn:191:ALA:O	66:Bn:238:MET:HB3	2.15	0.46
82:B2:18:LEU:HG	82:B2:22:CYS:HB2	1.98	0.46
83:B3:21:ARG:HA	83:B3:22:PRO:HD3	1.65	0.46
84:B4:4:VAL:HG13	84:B4:5:PRO:HD2	1.97	0.46
84:B4:78:ARG:HG2	84:B4:78:ARG:O	2.16	0.46
85:B5:16:ALA:CB	85:B5:202:THR:HG21	2.45	0.46
85:B5:98:ALA:CB	85:B5:121:VAL:CG1	2.93	0.46
9:Aa:14:HIS:CE1	9:Aa:33:SER:HB3	2.50	0.46
9:Aa:14:HIS:HB2	9:Aa:18:VAL:CG2	2.46	0.46
12:Ad:104:VAL:HG13	12:Ad:109:PHE:HB2	1.97	0.46
21:An:38:MET:O	21:An:39:CYS:HB3	2.15	0.46
66:Bn:33:LYS:O	66:Bn:37:ILE:HA	2.15	0.46
66:Bn:38:GLN:O	70:Bq:29:TYR:OH	2.34	0.46
66:Bn:200:GLY:HA2	66:Bn:236:GLU:N	2.31	0.46
70:Bq:16:ARG:NH2	70:Bq:44:MET:HB3	2.30	0.46
70:Bq:65:ASN:O	70:Bq:74:ILE:HB	2.15	0.46
85:B5:151:LEU:HD12	85:B5:159:PHE:CE2	2.50	0.46
85:B5:198:VAL:CG2	85:B5:210:VAL:CG2	2.93	0.46
9:Aa:7:LEU:CD2	9:Aa:308:ARG:HD2	2.46	0.46
21:An:31:ILE:HD11	21:An:40:ARG:HG2	1.97	0.46
25:B1:54:A:P	83:B3:21:ARG:HD3	2.52	0.46
62:Bj:13:HIS:CE1	62:Bj:117:MET:HB3	2.50	0.46
62:Bj:60:ARG:HB3	62:Bj:71:ASP:OD2	2.16	0.46
66:Bn:79:ALA:HB3	66:Bn:91:LEU:CD1	2.44	0.46
66:Bn:181:GLY:O	66:Bn:197:HIS:CD2	2.69	0.46
70:Bq:31:ARG:O	70:Bq:92:ILE:HG13	2.15	0.46
70:Bq:79:VAL:H	70:Bq:82:LYS:HB3	1.81	0.46
8:AH:9:G:P	21:An:13:LYS:CB	3.03	0.46
12:Ad:87:VAL:O	12:Ad:87:VAL:HG13	2.14	0.46
62:Bj:46:PHE:CD1	62:Bj:135:ALA:CB	2.98	0.46
66:Bn:184:SER:HB3	66:Bn:198:ILE:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Bw:134:LEU:CB	77:Bw:136:LEU:CD1	2.94	0.46
79:By:9:LYS:HB3	79:By:10:PRO:CD	2.36	0.46
81:Bz:11:VAL:CG2	81:Bz:23:ARG:CG	2.94	0.46
9:Aa:301:GLY:HA2	9:Aa:307:VAL:HG22	1.98	0.46
26:B0:1639:U:P	64:Bl:15:VAL:CA	3.04	0.46
26:B0:3895:C:P	84:B4:50:GLY:N	2.89	0.46
26:B0:4608:A:P	68:Bp:62:ARG:CZ	3.04	0.46
62:Bj:35:VAL:CG1	62:Bj:115:LYS:HD2	2.38	0.46
62:Bj:127:ARG:NH1	62:Bj:136:TYR:HE2	2.14	0.46
70:Bq:42:LYS:HB3	70:Bq:42:LYS:NZ	2.31	0.46
77:Bw:263:ASN:O	77:Bw:264:ARG:HB2	2.15	0.46
77:Bw:266:ILE:HD12	77:Bw:267:ARG:CA	2.46	0.46
79:By:55:MET:CE	79:By:56:PRO:HA	2.42	0.46
80:B9:70:LEU:H	80:B9:70:LEU:CD1	2.29	0.46
82:B2:18:LEU:CD2	82:B2:22:CYS:CB	2.94	0.46
83:B3:30:LYS:HG3	83:B3:31:THR:N	2.31	0.46
9:Aa:57:ARG:C	9:Aa:63:SER:CB	2.89	0.46
17:Aj:19:ARG:HG3	17:Aj:92:HIS:NE2	2.30	0.46
26:B0:1817:U:P	77:Bw:135:ARG:HH12	2.27	0.46
51:BY:49:A:P	66:Bn:219:LYS:CG	2.78	0.46
62:Bj:11:ARG:HD2	62:Bj:107:ILE:CD1	2.46	0.46
64:Bl:101:ILE:HD13	64:Bl:109:TYR:CB	2.43	0.46
66:Bn:52:VAL:CG2	66:Bn:158:VAL:HG23	2.32	0.46
66:Bn:77:ARG:HD3	66:Bn:81:GLU:CD	2.41	0.46
66:Bn:98:TYR:CD2	66:Bn:102:LEU:HD11	2.51	0.46
66:Bn:195:ARG:CZ	66:Bn:234:MET:HB3	2.46	0.46
68:Bp:74:ARG:HH11	68:Bp:74:ARG:HG3	1.80	0.46
79:By:7:LEU:C	79:By:10:PRO:HD2	2.41	0.46
85:B5:139:VAL:O	85:B5:143:GLU:HG3	2.15	0.46
86:B6:11:LEU:HD13	86:B6:75:SER:HB3	1.97	0.46
86:B6:31:TYR:CD1	86:B6:57:LYS:HA	2.50	0.46
9:Aa:282:GLU:HG2	9:Aa:302:TYR:CD2	2.51	0.46
26:B0:4323:A:P	84:B4:36:GLN:CB	3.04	0.46
69:B7:193:MET:HE3	69:B7:197:ARG:HH21	1.81	0.46
70:Bq:54:LYS:N	70:Bq:54:LYS:HE3	2.30	0.46
82:B2:26:ALA:O	82:B2:34:CYS:HA	2.16	0.46
82:B2:27:TYR:CD1	82:B2:29:LEU:CD2	2.95	0.46
85:B5:104:PHE:CE2	85:B5:122:LEU:HD21	2.51	0.46
86:B6:45:LEU:CD2	86:B6:96:ILE:CG2	2.94	0.46
9:Aa:146:SER:HA	9:Aa:150:TRP:CD1	2.50	0.45
9:Aa:217:MET:HG2	9:Aa:229:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ao:21:THR:HG22	22:Ao:23:SER:H	1.81	0.45
64:Bl:16:SER:CB	64:Bl:19:HIS:HB2	2.45	0.45
64:Bl:126:ALA:C	64:Bl:147:VAL:HG22	2.41	0.45
66:Bn:77:ARG:NE	66:Bn:103:LEU:CB	2.75	0.45
66:Bn:98:TYR:CZ	66:Bn:102:LEU:HD11	2.51	0.45
70:Bq:73:ILE:CG1	70:Bq:87:ARG:CG	2.94	0.45
77:Bw:136:LEU:CD1	77:Bw:143:THR:CG2	2.94	0.45
79:By:35:TRP:CG	79:By:36:ARG:N	2.83	0.45
81:Bz:26:VAL:O	81:Bz:30:GLU:HG3	2.15	0.45
83:B3:6:THR:CG2	83:B3:9:ILE:H	2.28	0.45
84:B4:10:THR:HG22	84:B4:21:HIS:ND1	2.31	0.45
85:B5:49:LEU:HD22	85:B5:176:ASN:HB3	1.98	0.45
85:B5:105:ILE:CG2	85:B5:132:LEU:CG	2.94	0.45
85:B5:105:ILE:CG2	85:B5:132:LEU:CD2	2.94	0.45
85:B5:118:LEU:HD22	85:B5:118:LEU:N	2.31	0.45
85:B5:151:LEU:HD12	85:B5:159:PHE:CD2	2.51	0.45
86:B6:3:ALA:HB3	86:B6:74:TYR:CD1	2.51	0.45
62:Bj:15:LEU:HG	62:Bj:40:ILE:CG1	2.47	0.45
62:Bj:53:TYR:O	62:Bj:58:ARG:HB3	2.17	0.45
62:Bj:123:LEU:HG	62:Bj:130:PRO:CG	2.47	0.45
66:Bn:77:ARG:CD	66:Bn:81:GLU:CB	2.94	0.45
66:Bn:108:LEU:HD23	66:Bn:108:LEU:O	2.16	0.45
70:Bq:67:THR:HG22	70:Bq:68:GLN:H	1.81	0.45
70:Bq:73:ILE:CD1	70:Bq:87:ARG:HG3	2.46	0.45
77:Bw:116:ARG:HD3	77:Bw:161:TYR:O	2.15	0.45
79:By:5:ARG:CB	79:By:6:PRO:HD3	2.36	0.45
79:By:43:ASN:CB	79:By:46:ARG:HB3	2.47	0.45
85:B5:163:VAL:HG12	85:B5:163:VAL:O	2.16	0.45
86:B6:15:ASN:OD1	86:B6:84:ALA:HB2	2.16	0.45
86:B6:45:LEU:HD23	86:B6:45:LEU:C	2.41	0.45
86:B6:47:ILE:O	86:B6:48:LEU:HD23	2.16	0.45
9:Aa:254:PRO:CG	9:Aa:284:PRO:C	2.89	0.45
12:Ad:147:VAL:HG12	12:Ad:148:ALA:N	2.30	0.45
21:An:26:ASN:CA	21:An:38:MET:HA	2.46	0.45
21:An:31:ILE:HG22	21:An:33:LYS:H	1.80	0.45
64:Bl:120:GLN:CG	64:Bl:121:PRO:HD2	2.43	0.45
66:Bn:105:ALA:CB	66:Bn:165:ALA:HA	2.46	0.45
68:Bp:23:TRP:HB3	68:Bp:51:ILE:CG2	2.46	0.45
70:Bq:24:VAL:HG23	70:Bq:25:PRO:HD2	1.97	0.45
77:Bw:166:TYR:CE2	77:Bw:259:GLU:CD	2.95	0.45
77:Bw:265:LEU:HD12	77:Bw:268:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:B3:20:ASN:HD21	83:B3:42:ARG:HB3	1.81	0.45
84:B4:38:LYS:HG2	84:B4:39:ARG:CD	2.46	0.45
86:B6:29:LEU:CB	86:B6:94:LEU:CD2	2.94	0.45
86:B6:81:LEU:HD22	86:B6:91:VAL:CB	2.24	0.45
26:B0:4191:C:P	84:B4:2:VAL:HG13	2.55	0.45
62:Bj:118:VAL:HG13	62:Bj:121:ALA:CB	2.46	0.45
64:Bl:96:GLY:HA2	64:Bl:125:LYS:HB2	1.98	0.45
66:Bn:199:MET:O	66:Bn:237:GLU:N	2.50	0.45
70:Bq:35:LYS:HA	70:Bq:63:VAL:O	2.17	0.45
77:Bw:116:ARG:HH12	77:Bw:131:LEU:HB2	1.79	0.45
77:Bw:158:VAL:CG2	77:Bw:162:ILE:CG2	2.94	0.45
77:Bw:170:LYS:HA	77:Bw:173:ASN:ND2	2.26	0.45
77:Bw:176:ILE:CD1	77:Bw:233:PHE:HE2	2.29	0.45
79:By:43:ASN:CB	79:By:46:ARG:CB	2.94	0.45
1:AA:1654:C:P	21:An:29:GLY:CA	3.05	0.45
9:Aa:54:ILE:HG23	9:Aa:96:THR:CG2	2.47	0.45
17:Aj:47:ASN:CB	17:Aj:97:ILE:CG2	2.94	0.45
62:Bj:7:VAL:HG12	62:Bj:33:VAL:HG12	1.90	0.45
66:Bn:77:ARG:HH21	66:Bn:103:LEU:HB2	1.81	0.45
66:Bn:203:VAL:HB	66:Bn:234:MET:SD	2.57	0.45
68:Bp:95:TRP:NE1	68:Bp:99:MET:CE	2.79	0.45
77:Bw:169:LEU:HD23	77:Bw:169:LEU:H	1.80	0.45
77:Bw:172:VAL:HG21	77:Bw:213:ILE:HB	1.97	0.45
77:Bw:201:LEU:HB2	77:Bw:228:ASN:HB3	1.97	0.45
85:B5:45:GLU:HB3	85:B5:183:ARG:CG	2.47	0.45
85:B5:60:VAL:CG2	85:B5:104:PHE:CD2	2.94	0.45
85:B5:98:ALA:HB3	85:B5:121:VAL:HG12	1.97	0.45
62:Bj:15:LEU:HD11	62:Bj:137:LEU:HD13	1.97	0.45
62:Bj:58:ARG:HD3	62:Bj:58:ARG:H	1.80	0.45
70:Bq:66:VAL:N	70:Bq:74:ILE:HG21	2.32	0.45
77:Bw:116:ARG:CZ	77:Bw:162:ILE:CG2	2.94	0.45
77:Bw:217:TYR:CD1	77:Bw:217:TYR:C	2.94	0.45
79:By:28:TYR:CZ	79:By:31:ILE:CD1	3.00	0.45
79:By:40:GLY:HA3	79:By:43:ASN:HD21	1.79	0.45
81:Bz:11:VAL:CG2	81:Bz:27:LYS:CG	2.95	0.45
81:Bz:22:LEU:N	81:Bz:22:LEU:HD12	2.31	0.45
82:B2:27:TYR:CD1	82:B2:27:TYR:C	2.95	0.45
9:Aa:18:VAL:N	9:Aa:305:ASN:CB	2.79	0.45
9:Aa:129:ILE:HG12	9:Aa:143:GLN:HB2	1.97	0.45
9:Aa:230:LEU:HD12	9:Aa:247:TRP:CE3	2.51	0.45
9:Aa:239:LEU:HD23	9:Aa:240:CYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:An:21:CYS:CB	21:An:37:ASN:N	2.80	0.45
54:Bb:219:ILE:HG23	54:Bb:275:HIS:CE1	2.51	0.45
62:Bj:119:VAL:HG13	62:Bj:120:PRO:N	2.31	0.45
64:Bl:11:LEU:HG	64:Bl:17:HIS:CD2	2.52	0.45
64:Bl:117:LEU:HD13	64:Bl:136:LYS:CB	2.46	0.45
68:Bp:42:ARG:HA	68:Bp:45:ILE:HG12	1.98	0.45
79:By:7:LEU:HD21	79:By:64:LYS:O	2.16	0.45
79:By:64:LYS:CA	79:By:67:LYS:HE3	2.45	0.45
81:Bz:42:CYS:SG	81:Bz:44:LYS:HG3	2.57	0.45
83:B3:35:ILE:CG1	83:B3:37:TYR:HD1	2.30	0.45
85:B5:196:ASP:C	85:B5:197:THR:HG23	2.42	0.45
9:Aa:139:LYS:HZ2	9:Aa:142:VAL:CG2	2.30	0.45
9:Aa:208:ALA:HB1	9:Aa:247:TRP:CH2	2.51	0.45
9:Aa:230:LEU:HD23	9:Aa:272:GLN:HB3	1.99	0.45
62:Bj:47:TYR:O	62:Bj:51:LEU:HG	2.17	0.45
62:Bj:53:TYR:HB3	62:Bj:54:LEU:H	1.21	0.45
64:Bl:109:TYR:HE2	64:Bl:111:VAL:CG2	2.29	0.45
66:Bn:83:PRO:HA	66:Bn:87:VAL:HG22	1.98	0.45
70:Bq:33:TYR:CE1	70:Bq:92:ILE:CG1	2.94	0.45
70:Bq:78:GLN:CB	70:Bq:82:LYS:CE	2.95	0.45
82:B2:20:ARG:HD3	82:B2:20:ARG:H	1.81	0.45
84:B4:11:PHE:CZ	84:B4:16:GLY:HA2	2.52	0.45
84:B4:56:PHE:CZ	84:B4:57:ARG:CD	2.99	0.45
9:Aa:64:HIS:CD2	9:Aa:65:PHE:N	2.84	0.45
9:Aa:170:TRP:CG	9:Aa:194:TYR:CD2	3.04	0.45
12:Ad:79:GLU:HA	12:Ad:79:GLU:OE1	2.17	0.45
62:Bj:134:PHE:CD1	62:Bj:134:PHE:C	2.95	0.45
77:Bw:134:LEU:HB2	77:Bw:136:LEU:HD13	1.99	0.45
77:Bw:224:LYS:HB3	77:Bw:231:TRP:CB	2.38	0.45
80:B9:81:ASN:ND2	80:B9:83:LYS:H	2.09	0.45
80:B9:101:HIS:HA	80:B9:108:ARG:NH2	2.31	0.45
82:B2:4:GLY:CA	82:B2:8:PHE:CZ	2.96	0.45
85:B5:47:VAL:CG1	85:B5:179:VAL:CG1	2.95	0.45
85:B5:58:THR:C	85:B5:101:THR:HG23	2.42	0.45
85:B5:98:ALA:HB3	85:B5:121:VAL:CG1	2.47	0.45
21:An:53:ILE:HG12	21:An:54:LYS:N	2.32	0.45
26:B0:1494:A:P	64:Bl:32:ARG:C	3.00	0.45
26:B0:4192:U:P	84:B4:2:VAL:CB	3.03	0.45
62:Bj:26:VAL:CG2	62:Bj:101:LEU:CD2	2.95	0.45
62:Bj:46:PHE:CE1	62:Bj:135:ALA:CB	3.00	0.45
62:Bj:50:LYS:HD2	62:Bj:51:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Bl:7:LYS:O	64:Bl:10:LYS:HB2	2.17	0.45
66:Bn:78:TYR:HB3	66:Bn:80:HIS:HB3	1.99	0.45
66:Bn:85:TYR:CZ	66:Bn:246:ILE:HG22	2.52	0.45
77:Bw:248:HIS:N	77:Bw:255:ALA:HB2	2.32	0.45
77:Bw:250:VAL:O	77:Bw:251:GLU:HB3	2.17	0.45
79:By:52:GLN:C	79:By:53:ILE:HG12	2.41	0.45
79:By:64:LYS:HB2	79:By:67:LYS:HE3	1.99	0.45
81:Bz:42:CYS:SG	86:B6:53:PRO:HB3	2.34	0.45
82:B2:18:LEU:HD23	82:B2:24:SER:CB	2.47	0.45
85:B5:43:VAL:HG11	85:B5:151:LEU:HD23	1.97	0.45
85:B5:47:VAL:HG11	85:B5:179:VAL:HG12	1.99	0.45
85:B5:184:LEU:HD23	85:B5:184:LEU:C	2.42	0.45
9:Aa:168:CYS:SG	9:Aa:198:VAL:HB	2.57	0.44
12:Ad:61:GLN:O	12:Ad:65:ARG:HG3	2.18	0.44
26:B0:1490:U:P	64:Bl:8:THR:OG1	2.75	0.44
62:Bj:15:LEU:HG	62:Bj:40:ILE:CD1	2.47	0.44
62:Bj:18:LEU:CD2	62:Bj:22:VAL:CG2	2.94	0.44
64:Bl:98:ALA:HB3	64:Bl:99:PRO:HD3	1.99	0.44
68:Bp:26:PRO:O	68:Bp:29:THR:HG23	2.16	0.44
79:By:22:ARG:HD2	79:By:31:ILE:HG21	2.00	0.44
81:Bz:37:TYR:O	81:Bz:45:THR:HA	2.17	0.44
85:B5:61:VAL:HG13	85:B5:132:LEU:HD11	1.99	0.44
86:B6:27:TYR:CD1	86:B6:27:TYR:C	2.94	0.44
9:Aa:79:LEU:HD23	9:Aa:88:ARG:O	2.17	0.44
17:Aj:66:ARG:HA	17:Aj:77:TRP:HA	1.99	0.44
64:Bl:89:ASN:HB2	64:Bl:94:LYS:HB3	1.99	0.44
66:Bn:39:ASP:C	70:Bq:69:HIS:HB3	2.42	0.44
66:Bn:102:LEU:H	66:Bn:102:LEU:HD12	1.83	0.44
66:Bn:203:VAL:CG2	66:Bn:236:GLU:OE2	2.65	0.44
70:Bq:82:LYS:CG	70:Bq:86:LYS:HB2	2.39	0.44
77:Bw:214:HIS:HA	77:Bw:217:TYR:CE2	2.52	0.44
80:B9:92:ASN:ND2	80:B9:120:ILE:HG12	2.29	0.44
82:B2:18:LEU:HD13	82:B2:26:ALA:N	2.32	0.44
84:B4:24:THR:HG22	84:B4:25:GLN:N	2.32	0.44
85:B5:190:LYS:HD3	85:B5:190:LYS:N	2.26	0.44
86:B6:17:ARG:HD3	86:B6:105:ILE:HD13	1.97	0.44
86:B6:34:THR:HG23	86:B6:35:LEU:N	2.31	0.44
9:Aa:14:HIS:CA	9:Aa:35:SER:CB	2.92	0.44
9:Aa:156:PHE:CD2	9:Aa:163:PRO:HB2	2.52	0.44
62:Bj:57:LEU:HD23	62:Bj:57:LEU:C	2.42	0.44
64:Bl:101:ILE:HD13	64:Bl:109:TYR:HD1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Bl:109:TYR:CE2	64:Bl:126:ALA:CB	3.01	0.44
66:Bn:103:LEU:HD23	66:Bn:103:LEU:O	2.18	0.44
68:Bp:70:ARG:CD	68:Bp:75:HIS:HB2	2.47	0.44
77:Bw:116:ARG:HH12	77:Bw:158:VAL:HG23	1.82	0.44
79:By:28:TYR:CE2	79:By:31:ILE:CG1	2.95	0.44
83:B3:11:ARG:HG3	83:B3:12:PHE:N	2.32	0.44
84:B4:22:LYS:HE3	84:B4:71:GLU:OE1	2.16	0.44
85:B5:30:ASN:HD22	85:B5:31:LEU:N	2.14	0.44
85:B5:51:ALA:HB3	85:B5:168:MET:HE1	1.98	0.44
85:B5:156:ARG:HD3	85:B5:158:THR:CG2	2.48	0.44
17:Aj:20:ILE:CG2	17:Aj:114:VAL:CG2	2.96	0.44
25:B1:54:A:P	83:B3:21:ARG:HB2	2.57	0.44
26:B0:4192:U:P	84:B4:2:VAL:HG11	2.57	0.44
62:Bj:118:VAL:CG1	62:Bj:121:ALA:HB2	2.48	0.44
64:Bl:124:VAL:HG12	64:Bl:129:PHE:HZ	1.83	0.44
66:Bn:237:GLU:HB2	66:Bn:238:MET:HE3	2.00	0.44
77:Bw:123:VAL:CG2	77:Bw:127:VAL:HG11	2.47	0.44
77:Bw:194:ASN:HA	77:Bw:197:ILE:CG1	2.45	0.44
77:Bw:248:HIS:CA	77:Bw:255:ALA:CB	2.96	0.44
80:B9:118:LEU:O	80:B9:119:ALA:HB3	2.18	0.44
85:B5:45:GLU:CB	85:B5:183:ARG:CG	2.95	0.44
86:B6:21:VAL:HG13	86:B6:26:LYS:HB2	1.98	0.44
9:Aa:109:LEU:HD11	9:Aa:122:SER:HB2	2.00	0.44
9:Aa:304:ASP:O	9:Aa:305:ASN:HB2	2.17	0.44
12:Ad:99:ARG:NH2	12:Ad:117:ARG:HH12	2.16	0.44
26:B0:4546:G:P	62:Bj:61:MET:CE	3.06	0.44
62:Bj:78:ILE:CG2	62:Bj:79:PHE:N	2.81	0.44
66:Bn:105:ALA:HB1	66:Bn:170:LEU:CD2	2.46	0.44
77:Bw:111:LEU:C	77:Bw:111:LEU:HD12	2.42	0.44
79:By:50:LYS:HE2	79:By:50:LYS:CA	2.43	0.44
82:B2:28:HIS:N	82:B2:31:LYS:HE2	2.32	0.44
84:B4:21:HIS:HA	84:B4:71:GLU:O	2.17	0.44
85:B5:47:VAL:HG13	85:B5:179:VAL:CG1	2.47	0.44
85:B5:48:VAL:HG21	85:B5:144:ARG:NE	2.26	0.44
85:B5:67:THR:HG22	85:B5:67:THR:O	2.16	0.44
17:Aj:22:ILE:CG1	17:Aj:91:LEU:CD2	2.95	0.44
17:Aj:72:GLU:CG	21:An:54:LYS:HG3	2.18	0.44
21:An:12:ARG:HG2	21:An:14:PHE:O	2.18	0.44
21:An:19:ARG:NH2	21:An:32:ARG:HH12	2.15	0.44
62:Bj:15:LEU:HD13	62:Bj:42:ILE:CG1	2.43	0.44
62:Bj:35:VAL:HG12	62:Bj:36:ARG:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bj:72:PHE:CD2	62:Bj:81:ARG:CG	2.94	0.44
66:Bn:38:GLN:OE1	70:Bq:30:MET:N	2.46	0.44
66:Bn:226:ILE:CD1	66:Bn:232:PRO:HG3	2.47	0.44
77:Bw:158:VAL:HG13	77:Bw:159:GLU:N	2.31	0.44
79:By:35:TRP:CD1	79:By:36:ARG:H	2.35	0.44
79:By:35:TRP:CG	79:By:36:ARG:H	2.36	0.44
85:B5:143:GLU:HG2	85:B5:146:LYS:CE	2.45	0.44
85:B5:149:VAL:HG22	85:B5:150:GLN:N	2.33	0.44
85:B5:151:LEU:HA	85:B5:159:PHE:HE1	1.77	0.44
9:Aa:14:HIS:CE1	9:Aa:33:SER:C	2.96	0.44
9:Aa:65:PHE:O	9:Aa:82:SER:HB2	2.18	0.44
21:An:23:VAL:HG21	21:An:42:CYS:SG	2.58	0.44
62:Bj:64:ASN:HD22	62:Bj:64:ASN:C	2.26	0.44
62:Bj:118:VAL:CG1	62:Bj:121:ALA:CB	2.95	0.44
62:Bj:124:LYS:HB2	62:Bj:130:PRO:CG	2.48	0.44
66:Bn:89:VAL:HG11	66:Bn:194:HIS:ND1	2.33	0.44
66:Bn:105:ALA:CB	66:Bn:170:LEU:HD23	2.47	0.44
66:Bn:183:ASP:O	66:Bn:197:HIS:CD2	2.71	0.44
66:Bn:231:THR:HG23	66:Bn:231:THR:O	2.17	0.44
70:Bq:64:TYR:N	70:Bq:64:TYR:CD1	2.86	0.44
77:Bw:135:ARG:HA	77:Bw:135:ARG:NE	2.33	0.44
9:Aa:65:PHE:C	9:Aa:66:VAL:CG2	2.91	0.44
17:Aj:32:LEU:HG	17:Aj:87:ARG:HG3	1.99	0.44
17:Aj:68:THR:HG23	17:Aj:69:PRO:HD2	1.99	0.44
26:B0:3895:C:P	84:B4:50:GLY:H	2.41	0.44
62:Bj:35:VAL:CG1	62:Bj:36:ARG:N	2.80	0.44
62:Bj:64:ASN:HA	62:Bj:69:PRO:CB	2.32	0.44
62:Bj:68:GLY:HA2	62:Bj:69:PRO:HD2	1.62	0.44
62:Bj:134:PHE:HE1	62:Bj:136:TYR:OH	2.00	0.44
68:Bp:56:THR:HG23	68:Bp:56:THR:O	2.17	0.44
70:Bq:71:VAL:CB	70:Bq:74:ILE:HD11	2.42	0.44
77:Bw:130:VAL:HG13	77:Bw:131:LEU:H	1.79	0.44
79:By:65:LYS:HG3	79:By:65:LYS:O	2.17	0.44
85:B5:174:ALA:HA	85:B5:177:ILE:HD12	1.99	0.44
86:B6:31:TYR:CA	86:B6:93:THR:CG2	2.94	0.44
1:AA:1654:C:P	21:An:40:ARG:HG3	2.58	0.44
9:Aa:262:GLU:HG2	9:Aa:270:LEU:HD23	2.00	0.44
12:Ad:71:GLU:OE1	12:Ad:71:GLU:HA	2.18	0.44
12:Ad:106:ARG:HH21	12:Ad:113:ARG:NH2	2.16	0.44
12:Ad:122:HIS:CB	12:Ad:124:HIS:CD2	2.99	0.44
17:Aj:71:GLY:HA2	17:Aj:74:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Aj:93:SER:HB2	17:Aj:94:PRO:CD	2.48	0.44
17:Aj:94:PRO:O	17:Aj:97:ILE:HG23	2.18	0.44
21:An:17:GLY:C	21:An:19:ARG:HD2	2.43	0.44
66:Bn:221:GLN:HB2	66:Bn:230:VAL:HG22	1.99	0.44
68:Bp:99:MET:HE3	68:Bp:103:ARG:HH21	1.81	0.44
77:Bw:136:LEU:HG	77:Bw:143:THR:HG23	1.98	0.44
77:Bw:166:TYR:HA	77:Bw:167:PRO:HD2	1.82	0.44
77:Bw:173:ASN:CB	77:Bw:213:ILE:HG21	2.47	0.44
81:Bz:41:PHE:HE2	86:B6:54:ALA:HA	1.83	0.44
82:B2:28:HIS:N	82:B2:31:LYS:CE	2.81	0.44
84:B4:19:GLN:HB2	84:B4:72:CYS:SG	2.58	0.44
84:B4:55:ILE:HG22	84:B4:56:PHE:N	2.32	0.44
86:B6:7:THR:CG2	86:B6:8:LYS:N	2.81	0.44
9:Aa:65:PHE:O	9:Aa:82:SER:HB3	2.17	0.43
12:Ad:69:ILE:HD13	12:Ad:99:ARG:CZ	2.48	0.43
17:Aj:50:VAL:CG2	17:Aj:91:LEU:CD1	2.94	0.43
22:Ao:70:GLN:HG2	22:Ao:77:TYR:CG	2.52	0.43
64:Bl:37:GLY:HA3	64:Bl:47:LYS:CE	2.47	0.43
68:Bp:94:THR:CG2	68:Bp:95:TRP:N	2.81	0.43
77:Bw:123:VAL:CG2	77:Bw:127:VAL:CG1	2.95	0.43
82:B2:18:LEU:HD23	82:B2:24:SER:HB3	2.00	0.43
82:B2:49:TRP:O	82:B2:50:SER:HB2	2.16	0.43
83:B3:6:THR:H	83:B3:9:ILE:CG2	2.31	0.43
83:B3:35:ILE:HG21	83:B3:37:TYR:HB2	2.00	0.43
84:B4:26:TYR:CD1	84:B4:26:TYR:C	2.96	0.43
9:Aa:24:THR:OG1	9:Aa:28:PRO:HA	2.17	0.43
9:Aa:70:VAL:CG2	9:Aa:79:LEU:HB2	2.49	0.43
9:Aa:284:PRO:HD3	9:Aa:304:ASP:HB2	1.98	0.43
62:Bj:127:ARG:NH1	62:Bj:136:TYR:CE2	2.86	0.43
64:Bl:101:ILE:O	64:Bl:104:VAL:HG23	2.19	0.43
66:Bn:198:ILE:CG2	66:Bn:199:MET:H	2.31	0.43
77:Bw:260:ASP:C	77:Bw:262:ILE:H	2.25	0.43
79:By:22:ARG:CZ	79:By:36:ARG:HD3	2.48	0.43
80:B9:70:LEU:HD11	80:B9:76:LYS:N	2.33	0.43
84:B4:38:LYS:HG3	84:B4:39:ARG:HD3	2.00	0.43
86:B6:52:CYS:HB2	86:B6:57:LYS:HD3	1.99	0.43
9:Aa:164:ILE:HG21	9:Aa:179:LEU:CB	2.48	0.43
12:Ad:100:LEU:CD2	12:Ad:120:VAL:CG2	2.95	0.43
62:Bj:26:VAL:HG22	62:Bj:97:ALA:CB	2.47	0.43
62:Bj:54:LEU:HD12	62:Bj:58:ARG:CD	2.47	0.43
62:Bj:109:PRO:HD3	62:Bj:115:LYS:HZ3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:40:LYS:HZ2	70:Bq:72:GLY:N	2.16	0.43
66:Bn:184:SER:HG	66:Bn:200:GLY:H	1.62	0.43
70:Bq:51:MET:HA	70:Bq:52:PRO:HD3	1.78	0.43
77:Bw:242:MET:HE3	77:Bw:268:ARG:HH22	1.79	0.43
81:Bz:70:THR:CG2	81:Bz:71:TYR:N	2.81	0.43
82:B2:16:HIS:HA	82:B2:27:TYR:O	2.18	0.43
86:B6:15:ASN:CG	86:B6:84:ALA:HB2	2.44	0.43
62:Bj:26:VAL:HG13	62:Bj:27:LEU:N	2.32	0.43
62:Bj:36:ARG:NE	62:Bj:39:GLY:HA3	2.33	0.43
66:Bn:39:ASP:CA	70:Bq:29:TYR:OH	2.67	0.43
77:Bw:181:TYR:HE1	77:Bw:234:LYS:HB2	1.82	0.43
82:B2:18:LEU:CD2	82:B2:24:SER:CB	2.93	0.43
84:B4:58:LYS:O	84:B4:58:LYS:HG3	2.17	0.43
85:B5:143:GLU:CG	85:B5:146:LYS:HE2	2.46	0.43
62:Bj:72:PHE:CB	62:Bj:77:ARG:CG	2.93	0.43
66:Bn:102:LEU:HB3	66:Bn:246:ILE:HD12	2.00	0.43
77:Bw:120:ILE:O	77:Bw:121:ASN:HB3	2.18	0.43
81:Bz:42:CYS:CA	86:B6:53:PRO:CB	2.44	0.43
8:AH:9:G:P	21:An:13:LYS:CG	3.00	0.43
9:Aa:14:HIS:CE1	9:Aa:33:SER:CA	3.01	0.43
26:B0:23:C:P	82:B2:44:LYS:CE	2.92	0.43
26:B0:4478:A:P	54:Bb:257:HIS:CA	3.06	0.43
66:Bn:63:ILE:HD12	66:Bn:63:ILE:HA	1.85	0.43
68:Bp:62:ARG:CZ	68:Bp:62:ARG:CB	2.96	0.43
70:Bq:71:VAL:CG2	70:Bq:74:ILE:HD11	2.48	0.43
70:Bq:73:ILE:HD11	70:Bq:87:ARG:CG	2.48	0.43
77:Bw:191:LEU:CG	77:Bw:192:THR:N	2.82	0.43
77:Bw:247:THR:CB	77:Bw:255:ALA:HB2	2.49	0.43
79:By:11:LYS:HE2	80:B9:69:MET:HE2	0.44	0.43
82:B2:12:ARG:HE	83:B3:4:HIS:CD2	2.36	0.43
82:B2:19:CYS:CB	82:B2:34:CYS:SG	3.06	0.43
85:B5:26:ASP:OD1	85:B5:201:LYS:HG3	2.18	0.43
9:Aa:104:HIS:CE1	9:Aa:139:LYS:HZ3	2.37	0.43
9:Aa:148:SER:HB2	9:Aa:170:TRP:CB	2.47	0.43
66:Bn:39:ASP:C	70:Bq:29:TYR:HH	2.23	0.43
66:Bn:77:ARG:NH1	66:Bn:82:LEU:HB2	2.34	0.43
68:Bp:42:ARG:O	68:Bp:46:LYS:HD3	2.19	0.43
79:By:23:HIS:HB3	79:By:45:VAL:HG11	1.99	0.43
80:B9:87:VAL:HB	80:B9:90:MET:H	1.83	0.43
82:B2:27:TYR:CE1	82:B2:29:LEU:CD1	2.95	0.43
82:B2:30:GLN:HB3	82:B2:31:LYS:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Aa:62:HIS:CB	9:Aa:84:ASP:OD2	2.67	0.43
54:Bb:216:ILE:O	54:Bb:280:ASN:HA	2.19	0.43
64:Bl:129:PHE:CE1	64:Bl:144:CYS:SG	3.12	0.43
66:Bn:51:ILE:HB	66:Bn:53:ARG:NH1	2.34	0.43
70:Bq:3:THR:HB	70:Bq:8:ARG:NE	2.34	0.43
77:Bw:217:TYR:O	77:Bw:218:THR:HG22	2.18	0.43
79:By:32:LYS:HD2	79:By:32:LYS:N	2.34	0.43
85:B5:114:ILE:CG2	85:B5:115:GLY:N	2.82	0.43
86:B6:22:MET:HA	86:B6:27:TYR:CE2	2.51	0.43
1:AA:1217:G:P	22:Ao:47:LYS:HG3	2.59	0.43
12:Ad:126:THR:HG22	12:Ad:146:ALA:C	2.44	0.43
17:Aj:32:LEU:CD2	17:Aj:87:ARG:CG	2.95	0.43
64:Bl:76:ASP:CA	64:Bl:79:TRP:CD1	2.93	0.43
66:Bn:182:TYR:CE2	66:Bn:198:ILE:CG2	2.97	0.43
77:Bw:135:ARG:HG3	77:Bw:231:TRP:CE2	2.48	0.43
79:By:36:ARG:HG3	79:By:36:ARG:O	2.18	0.43
80:B9:89:LEU:H	80:B9:89:LEU:CD2	2.32	0.43
81:Bz:11:VAL:HG21	81:Bz:23:ARG:HG3	1.99	0.43
81:Bz:72:ASN:OD1	81:Bz:77:VAL:HG23	2.18	0.43
82:B2:15:THR:CG2	82:B2:16:HIS:H	2.21	0.43
86:B6:3:ALA:N	86:B6:74:TYR:CD1	2.86	0.43
9:Aa:13:GLY:CA	9:Aa:41:ILE:HD12	2.49	0.43
9:Aa:14:HIS:HB3	9:Aa:35:SER:CB	2.47	0.43
12:Ad:125:ILE:CG2	12:Ad:126:THR:N	2.82	0.43
17:Aj:29:VAL:CG2	17:Aj:30:LYS:N	2.82	0.43
26:B0:4526:U:P	54:Bb:263:PHE:CE1	3.12	0.43
62:Bj:50:LYS:CE	62:Bj:51:LEU:CD2	2.95	0.43
77:Bw:157:ILE:CG2	77:Bw:158:VAL:N	2.82	0.43
79:By:8:VAL:CG1	79:By:9:LYS:N	2.82	0.43
79:By:18:LYS:HA	79:By:18:LYS:HZ2	1.81	0.43
79:By:22:ARG:HH11	79:By:31:ILE:HG23	1.82	0.43
85:B5:60:VAL:HG13	85:B5:101:THR:OG1	2.19	0.43
85:B5:193:LEU:HD12	85:B5:193:LEU:N	2.33	0.43
9:Aa:254:PRO:HG2	9:Aa:284:PRO:CA	2.49	0.42
26:B0:2279:C:P	80:B9:104:SER:CB	3.07	0.42
26:B0:2383:G:P	83:B3:48:LYS:NZ	2.92	0.42
62:Bj:13:HIS:CE1	62:Bj:117:MET:HG2	2.54	0.42
66:Bn:82:LEU:CG	66:Bn:87:VAL:HG21	2.46	0.42
66:Bn:182:TYR:CD2	66:Bn:182:TYR:C	2.97	0.42
70:Bq:79:VAL:CG1	70:Bq:82:LYS:CB	2.94	0.42
79:By:28:TYR:CE2	79:By:30:LYS:CD	2.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:By:37:LYS:HD2	79:By:38:PRO:CD	2.27	0.42
79:By:45:VAL:CG2	79:By:46:ARG:N	2.82	0.42
80:B9:85:LEU:O	80:B9:90:MET:HG2	2.19	0.42
83:B3:35:ILE:CD1	83:B3:37:TYR:HD1	2.31	0.42
9:Aa:132:TRP:CZ3	9:Aa:139:LYS:HB2	2.54	0.42
17:Aj:50:VAL:CG1	17:Aj:51:LYS:N	2.82	0.42
66:Bn:102:LEU:CD2	66:Bn:246:ILE:HD11	2.36	0.42
66:Bn:203:VAL:CG2	66:Bn:204:ALA:N	2.82	0.42
70:Bq:26:LEU:CD2	70:Bq:26:LEU:N	2.82	0.42
70:Bq:29:TYR:HA	70:Bq:93:GLU:HG2	2.00	0.42
70:Bq:29:TYR:C	70:Bq:92:ILE:HG21	2.44	0.42
84:B4:4:VAL:O	84:B4:93:LEU:HD13	2.19	0.42
84:B4:38:LYS:CG	84:B4:39:ARG:N	2.81	0.42
85:B5:138:VAL:HB	85:B5:141:VAL:HG22	2.01	0.42
9:Aa:11:LEU:CD1	9:Aa:31:ILE:HD13	2.49	0.42
12:Ad:67:TYR:N	12:Ad:67:TYR:CD1	2.85	0.42
17:Aj:29:VAL:CG1	17:Aj:85:HIS:CE1	3.03	0.42
26:B0:4418:C:P	54:Bb:237:LYS:H	2.42	0.42
64:Bl:134:GLU:O	64:Bl:137:ILE:HG12	2.19	0.42
66:Bn:47:LYS:HG3	66:Bn:142:THR:CG2	2.48	0.42
66:Bn:47:LYS:HG3	66:Bn:142:THR:HG23	2.01	0.42
68:Bp:89:MET:CE	68:Bp:90:PRO:HB3	2.50	0.42
70:Bq:31:ARG:HB2	70:Bq:92:ILE:HG13	1.99	0.42
70:Bq:73:ILE:HD11	70:Bq:87:ARG:HG3	2.00	0.42
77:Bw:116:ARG:CZ	77:Bw:131:LEU:HD23	2.50	0.42
77:Bw:242:MET:SD	77:Bw:254:ASP:CB	3.07	0.42
79:By:21:ILE:CG2	79:By:22:ARG:N	2.82	0.42
79:By:42:ASP:CG	79:By:43:ASN:H	2.28	0.42
82:B2:20:ARG:HG2	82:B2:21:ARG:H	1.84	0.42
83:B3:9:ILE:CG2	83:B3:10:LYS:N	2.82	0.42
85:B5:62:PHE:CZ	85:B5:81:GLU:CG	2.94	0.42
85:B5:110:LEU:HD13	85:B5:110:LEU:C	2.43	0.42
86:B6:17:ARG:HG3	86:B6:17:ARG:HH11	1.84	0.42
86:B6:28:VAL:CG2	86:B6:37:MET:SD	3.07	0.42
9:Aa:58:ALA:HA	9:Aa:101:PHE:CZ	2.55	0.42
12:Ad:62:LYS:HB2	12:Ad:62:LYS:NZ	2.34	0.42
12:Ad:87:VAL:HG13	12:Ad:90:SER:H	1.85	0.42
17:Aj:91:LEU:N	17:Aj:91:LEU:CD2	2.83	0.42
22:Ao:35:ILE:HD11	22:Ao:62:ARG:CZ	2.49	0.42
64:Bl:16:SER:HB3	64:Bl:19:HIS:HB2	2.00	0.42
64:Bl:124:VAL:HG12	64:Bl:129:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:82:LEU:HB3	66:Bn:83:PRO:HD3	2.01	0.42
66:Bn:89:VAL:CG2	66:Bn:90:GLY:H	2.33	0.42
79:By:28:TYR:CE2	79:By:30:LYS:CG	3.01	0.42
84:B4:8:ARG:HG2	84:B4:9:ARG:N	2.35	0.42
84:B4:82:MET:HE2	84:B4:83:LEU:O	2.19	0.42
85:B5:142:ILE:O	85:B5:146:LYS:HG3	2.20	0.42
85:B5:143:GLU:CB	85:B5:146:LYS:HE2	2.49	0.42
85:B5:185:HIS:HD2	85:B5:192:PRO:CD	2.32	0.42
86:B6:81:LEU:CD2	86:B6:94:LEU:HD11	2.49	0.42
62:Bj:6:LEU:HB2	62:Bj:25:GLN:HE22	1.84	0.42
66:Bn:77:ARG:HH22	66:Bn:82:LEU:HD12	1.85	0.42
68:Bp:88:ARG:HH11	68:Bp:88:ARG:HD3	1.72	0.42
70:Bq:90:VAL:HG22	70:Bq:91:ARG:O	2.19	0.42
77:Bw:126:LYS:H	77:Bw:129:LYS:HG2	1.84	0.42
81:Bz:64:VAL:CG1	81:Bz:65:ALA:N	2.81	0.42
86:B6:96:ILE:HG23	86:B6:96:ILE:O	2.20	0.42
21:An:21:CYS:O	21:An:25:SER:HA	2.20	0.42
21:An:23:VAL:CG2	21:An:36:LEU:CD1	2.97	0.42
62:Bj:13:HIS:HD2	62:Bj:122:ALA:HA	1.85	0.42
64:Bl:146:LEU:HD12	64:Bl:146:LEU:N	2.35	0.42
66:Bn:48:TYR:HE1	66:Bn:135:ASP:HB2	1.85	0.42
70:Bq:74:ILE:CD1	70:Bq:75:VAL:CG2	2.97	0.42
77:Bw:116:ARG:CZ	77:Bw:162:ILE:HG22	2.49	0.42
77:Bw:191:LEU:N	77:Bw:191:LEU:CD2	2.82	0.42
79:By:43:ASN:HB3	79:By:46:ARG:HB3	1.98	0.42
81:Bz:78:THR:CG2	81:Bz:79:VAL:N	2.82	0.42
82:B2:10:LYS:HE3	82:B2:11:ARG:N	2.34	0.42
9:Aa:7:LEU:CD1	9:Aa:308:ARG:HD2	2.49	0.42
9:Aa:18:VAL:CA	9:Aa:305:ASN:HA	2.50	0.42
9:Aa:25:PRO:HG3	9:Aa:71:ILE:HG21	2.01	0.42
9:Aa:206:LEU:C	9:Aa:206:LEU:HD12	2.44	0.42
9:Aa:259:TRP:CD1	9:Aa:274:VAL:HG22	2.55	0.42
26:B0:22:G:P	82:B2:44:LYS:HZ2	2.41	0.42
62:Bj:115:LYS:N	62:Bj:115:LYS:CD	2.83	0.42
62:Bj:127:ARG:O	62:Bj:130:PRO:HD2	2.20	0.42
64:Bl:109:TYR:CE2	64:Bl:126:ALA:HB1	2.54	0.42
77:Bw:217:TYR:CE1	77:Bw:218:THR:HG22	2.54	0.42
77:Bw:219:VAL:CG2	77:Bw:220:GLY:N	2.81	0.42
82:B2:8:PHE:HB3	82:B2:9:GLY:H	1.50	0.42
82:B2:10:LYS:HD2	82:B2:10:LYS:C	2.44	0.42
82:B2:42:LYS:HB3	82:B2:43:ARG:H	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:B3:6:THR:HG23	83:B3:8:ARG:H	1.83	0.42
84:B4:11:PHE:CE1	84:B4:16:GLY:C	2.98	0.42
84:B4:74:GLU:C	84:B4:76:ASN:H	2.28	0.42
85:B5:34:LEU:HD11	85:B5:41:ASN:N	2.35	0.42
86:B6:15:ASN:ND2	86:B6:84:ALA:HB2	2.35	0.42
86:B6:44:LYS:HZ2	86:B6:44:LYS:HB3	1.84	0.42
9:Aa:282:GLU:CD	9:Aa:302:TYR:HB3	2.45	0.42
12:Ad:78:PHE:HA	12:Ad:92:PHE:CE1	2.54	0.42
17:Aj:68:THR:CG2	17:Aj:69:PRO:N	2.82	0.42
26:B0:1704:U:P	77:Bw:126:LYS:NZ	2.93	0.42
26:B0:1712:G:P	70:Bq:42:LYS:HE3	2.59	0.42
26:B0:4608:A:P	68:Bp:62:ARG:NH2	2.93	0.42
62:Bj:54:LEU:HD22	62:Bj:73:ARG:HB3	2.02	0.42
62:Bj:58:ARG:CB	62:Bj:61:MET:CB	2.94	0.42
62:Bj:140:LEU:CD2	62:Bj:140:LEU:C	2.93	0.42
66:Bn:77:ARG:HG2	66:Bn:100:THR:HA	2.01	0.42
66:Bn:195:ARG:CB	66:Bn:203:VAL:CG1	2.98	0.42
66:Bn:224:GLN:HG3	66:Bn:231:THR:CB	2.41	0.42
77:Bw:131:LEU:HD21	77:Bw:136:LEU:CB	2.33	0.42
77:Bw:172:VAL:CG2	77:Bw:173:ASN:N	2.82	0.42
80:B9:78:LEU:C	80:B9:78:LEU:CD2	2.92	0.42
80:B9:99:ILE:HG21	80:B9:103:VAL:HG21	2.00	0.42
85:B5:79:LEU:HD12	85:B5:79:LEU:N	2.34	0.42
85:B5:184:LEU:C	85:B5:184:LEU:CD2	2.93	0.42
9:Aa:21:ILE:HG23	9:Aa:307:VAL:CG2	2.49	0.42
9:Aa:32:LEU:HD13	9:Aa:71:ILE:HG12	2.01	0.42
9:Aa:284:PRO:HG2	9:Aa:304:ASP:N	2.35	0.42
17:Aj:35:VAL:CG2	17:Aj:107:GLU:HB3	2.50	0.42
17:Aj:101:ILE:CG2	17:Aj:102:THR:N	2.82	0.42
26:B0:2292:G:P	80:B9:71:PRO:CB	3.08	0.42
64:Bl:109:TYR:CD2	64:Bl:109:TYR:C	2.95	0.42
68:Bp:38:ARG:CZ	68:Bp:38:ARG:HB3	2.50	0.42
77:Bw:173:ASN:H	77:Bw:173:ASN:ND2	2.15	0.42
77:Bw:183:LYS:CG	77:Bw:184:ILE:H	2.32	0.42
77:Bw:219:VAL:CG2	77:Bw:222:ARG:HD2	2.50	0.42
84:B4:53:LYS:CB	84:B4:54:PRO:HD3	2.36	0.42
86:B6:31:TYR:N	86:B6:93:THR:CG2	2.83	0.42
9:Aa:248:LEU:HD13	9:Aa:258:ILE:HG12	2.02	0.42
12:Ad:120:VAL:O	12:Ad:133:ASP:HA	2.19	0.42
62:Bj:57:LEU:C	62:Bj:57:LEU:CD2	2.93	0.42
64:Bl:36:GLY:C	64:Bl:41:HIS:HB3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:101:GLY:O	66:Bn:104:LEU:HD23	2.20	0.42
66:Bn:106:ARG:CZ	66:Bn:246:ILE:O	2.68	0.42
66:Bn:236:GLU:O	66:Bn:239:TYR:HB3	2.20	0.42
68:Bp:10:LEU:HB3	68:Bp:41:ILE:HD12	2.01	0.42
68:Bp:30:ASN:ND2	68:Bp:31:GLU:H	2.18	0.42
70:Bq:3:THR:CG2	70:Bq:4:LYS:N	2.82	0.42
70:Bq:20:LYS:HD2	70:Bq:20:LYS:H	1.85	0.42
79:By:19:LYS:HD2	79:By:19:LYS:O	2.19	0.42
81:Bz:29:ILE:HD12	81:Bz:30:GLU:CA	2.48	0.42
82:B2:46:LYS:N	82:B2:46:LYS:CD	2.83	0.42
85:B5:138:VAL:HB	85:B5:141:VAL:CG2	2.50	0.42
1:AA:1653:C:P	21:An:42:CYS:CB	2.96	0.41
21:An:36:LEU:HD22	21:An:36:LEU:N	2.35	0.41
26:B0:1634:C:P	64:Bl:24:LYS:HZ3	2.42	0.41
62:Bj:15:LEU:HG	62:Bj:40:ILE:HG12	2.02	0.41
62:Bj:26:VAL:HG22	62:Bj:97:ALA:HA	2.02	0.41
62:Bj:72:PHE:HA	62:Bj:77:ARG:HD2	2.02	0.41
62:Bj:126:VAL:O	62:Bj:130:PRO:HD2	2.20	0.41
66:Bn:103:LEU:HD23	66:Bn:103:LEU:C	2.45	0.41
68:Bp:52:ARG:HG2	68:Bp:53:LYS:O	2.20	0.41
70:Bq:82:LYS:HZ3	70:Bq:85:ALA:HA	1.84	0.41
82:B2:18:LEU:CD2	82:B2:24:SER:C	2.93	0.41
9:Aa:82:SER:C	9:Aa:108:VAL:HG13	2.45	0.41
9:Aa:262:GLU:CG	9:Aa:270:LEU:HD23	2.50	0.41
9:Aa:302:TYR:CE1	9:Aa:304:ASP:HB3	2.54	0.41
12:Ad:102:ASN:O	12:Ad:105:TYR:HB3	2.21	0.41
62:Bj:21:ILE:CG2	62:Bj:22:VAL:N	2.82	0.41
62:Bj:42:ILE:HG22	62:Bj:43:SER:O	2.20	0.41
62:Bj:82:THR:CG2	62:Bj:83:VAL:N	2.82	0.41
64:Bl:82:VAL:HG23	64:Bl:83:SER:H	1.84	0.41
77:Bw:116:ARG:HD3	77:Bw:161:TYR:CD2	2.54	0.41
77:Bw:148:ASN:H	77:Bw:151:SER:HB3	1.84	0.41
77:Bw:203:LYS:HE3	77:Bw:204:PHE:CZ	2.55	0.41
82:B2:18:LEU:CB	82:B2:24:SER:C	2.93	0.41
83:B3:15:LYS:O	83:B3:18:LYS:HB2	2.20	0.41
85:B5:78:VAL:HG12	85:B5:79:LEU:N	2.35	0.41
86:B6:24:SER:CB	86:B6:26:LYS:HD2	2.49	0.41
9:Aa:191:HIS:CD2	9:Aa:195:LEU:HD21	2.54	0.41
22:Ao:35:ILE:CG2	22:Ao:58:MET:HB3	2.50	0.41
39:BM:2688:C:P	68:Bp:39:GLN:CD	3.03	0.41
64:Bl:16:SER:HB3	64:Bl:19:HIS:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Bl:43:ILE:O	64:Bl:45:PHE:CD1	2.74	0.41
64:Bl:73:VAL:HG12	64:Bl:74:ASN:N	2.34	0.41
66:Bn:222:PHE:HB2	66:Bn:231:THR:CG2	2.50	0.41
68:Bp:45:ILE:HG13	68:Bp:46:LYS:N	2.34	0.41
70:Bq:51:MET:SD	70:Bq:54:LYS:CE	3.07	0.41
77:Bw:162:ILE:CD1	77:Bw:162:ILE:C	2.93	0.41
77:Bw:169:LEU:N	77:Bw:169:LEU:CD2	2.83	0.41
79:By:38:PRO:HB3	79:By:45:VAL:HG21	2.02	0.41
80:B9:87:VAL:CG1	80:B9:89:LEU:CD2	2.95	0.41
80:B9:87:VAL:CG1	80:B9:88:LEU:N	2.83	0.41
80:B9:123:THR:CG2	80:B9:124:ASN:N	2.83	0.41
82:B2:10:LYS:CE	82:B2:12:ARG:H	2.33	0.41
85:B5:141:VAL:CG2	85:B5:142:ILE:N	2.83	0.41
86:B6:79:ILE:HG12	86:B6:80:GLU:N	2.35	0.41
9:Aa:14:HIS:CE1	9:Aa:34:ALA:N	2.89	0.41
9:Aa:20:GLN:CB	9:Aa:68:ASP:HA	2.50	0.41
9:Aa:109:LEU:CD1	9:Aa:122:SER:HB2	2.50	0.41
9:Aa:208:ALA:HB1	9:Aa:247:TRP:CE2	2.56	0.41
26:B0:2642:U:P	68:Bp:124:TYR:HH	2.42	0.41
62:Bj:18:LEU:C	62:Bj:18:LEU:CD2	2.94	0.41
62:Bj:109:PRO:HG2	62:Bj:111:TYR:O	2.21	0.41
64:Bl:41:HIS:O	64:Bl:45:PHE:CE1	2.73	0.41
66:Bn:55:THR:HB	66:Bn:58:ASP:OD1	2.20	0.41
66:Bn:61:CYS:C	66:Bn:104:LEU:HD13	2.45	0.41
77:Bw:130:VAL:CG1	77:Bw:131:LEU:N	2.82	0.41
77:Bw:168:ASN:OD1	77:Bw:169:LEU:HD23	2.19	0.41
81:Bz:11:VAL:CG1	81:Bz:23:ARG:HG3	2.50	0.41
82:B2:10:LYS:NZ	82:B2:11:ARG:HB3	2.35	0.41
83:B3:27:ILE:CG2	83:B3:28:ARG:N	2.83	0.41
85:B5:62:PHE:CE2	85:B5:110:LEU:CG	3.03	0.41
85:B5:87:LEU:O	85:B5:117:TYR:CE1	2.73	0.41
86:B6:31:TYR:CE2	86:B6:35:LEU:HD11	2.55	0.41
9:Aa:162:ASN:HB2	9:Aa:163:PRO:HD2	2.03	0.41
62:Bj:92:LYS:HD2	62:Bj:92:LYS:HA	1.87	0.41
66:Bn:207:MET:HG2	66:Bn:233:ASP:CA	2.49	0.41
68:Bp:98:ARG:O	68:Bp:102:LEU:HD13	2.20	0.41
69:B7:192:ARG:O	69:B7:196:LEU:HD13	2.20	0.41
70:Bq:6:LYS:HG2	70:Bq:7:ARG:N	2.35	0.41
79:By:16:ARG:HA	79:By:16:ARG:HE	1.84	0.41
79:By:60:TYR:CD2	79:By:60:TYR:O	2.73	0.41
81:Bz:36:LYS:HD3	81:Bz:45:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:B4:35:ALA:H	84:B4:38:LYS:HB3	1.85	0.41
85:B5:34:LEU:CD2	85:B5:40:SER:CB	2.93	0.41
85:B5:34:LEU:CD1	85:B5:40:SER:CB	2.95	0.41
85:B5:120:THR:CG2	85:B5:121:VAL:N	2.83	0.41
9:Aa:14:HIS:NE2	9:Aa:18:VAL:HG13	2.33	0.41
9:Aa:188:HIS:CE1	9:Aa:226:HIS:CD2	3.09	0.41
9:Aa:239:LEU:HD21	9:Aa:291:TRP:HB3	2.02	0.41
9:Aa:256:ILE:HB	9:Aa:279:SER:HB3	2.02	0.41
17:Aj:55:ARG:HA	17:Aj:87:ARG:HH11	1.85	0.41
26:B0:2713:G:P	81:Bz:34:HIS:HE1	2.43	0.41
64:Bl:7:LYS:HA	64:Bl:10:LYS:CG	2.51	0.41
66:Bn:42:LYS:HA	70:Bq:32:ILE:HD11	1.55	0.41
66:Bn:50:MET:HE2	66:Bn:52:VAL:CG1	2.51	0.41
66:Bn:224:GLN:HG3	66:Bn:231:THR:CA	2.50	0.41
68:Bp:36:ASN:H	68:Bp:40:GLN:CD	2.28	0.41
68:Bp:51:ILE:CG1	68:Bp:52:ARG:N	2.83	0.41
79:By:54:LEU:N	79:By:54:LEU:CD2	2.83	0.41
81:Bz:20:ALA:O	81:Bz:24:LYS:HG3	2.20	0.41
85:B5:3:GLN:O	85:B5:6:GLU:HG3	2.21	0.41
85:B5:151:LEU:HD13	85:B5:159:PHE:CE2	2.55	0.41
9:Aa:248:LEU:HD11	9:Aa:256:ILE:CG2	2.50	0.41
17:Aj:40:ILE:CG2	17:Aj:41:ARG:N	2.82	0.41
17:Aj:47:ASN:HB3	17:Aj:93:SER:HB2	1.90	0.41
62:Bj:72:PHE:CD1	62:Bj:72:PHE:O	2.74	0.41
64:Bl:97:VAL:HG11	64:Bl:109:TYR:HH	1.85	0.41
70:Bq:38:ILE:CD1	70:Bq:38:ILE:C	2.94	0.41
77:Bw:123:VAL:CG2	77:Bw:124:SER:N	2.83	0.41
77:Bw:247:THR:HB	77:Bw:254:ASP:OD1	2.21	0.41
79:By:7:LEU:HD21	79:By:63:ASN:HB3	2.02	0.41
79:By:11:LYS:HE2	80:B9:69:MET:SD	2.44	0.41
85:B5:36:LEU:C	85:B5:36:LEU:CD2	2.93	0.41
85:B5:184:LEU:HD23	85:B5:184:LEU:O	2.21	0.41
9:Aa:18:VAL:HB	9:Aa:305:ASN:HA	2.03	0.41
12:Ad:105:TYR:CD1	12:Ad:112:SER:C	2.99	0.41
12:Ad:118:GLN:CG	12:Ad:122:HIS:CD2	2.98	0.41
21:An:36:LEU:CD1	21:An:42:CYS:SG	3.07	0.41
66:Bn:62:GLN:HG3	66:Bn:76:ALA:HB2	2.02	0.41
66:Bn:102:LEU:HD12	66:Bn:164:GLY:HA3	2.03	0.41
68:Bp:14:VAL:CG1	68:Bp:15:LEU:N	2.83	0.41
68:Bp:123:LEU:O	68:Bp:127:VAL:HG23	2.20	0.41
70:Bq:10:THR:O	70:Bq:14:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Bq:38:ILE:HD11	70:Bq:60:THR:HG21	2.00	0.41
70:Bq:73:ILE:HG13	70:Bq:87:ARG:HB2	2.03	0.41
77:Bw:135:ARG:HG3	77:Bw:231:TRP:CH2	2.54	0.41
77:Bw:158:VAL:CG1	77:Bw:159:GLU:N	2.82	0.41
77:Bw:161:TYR:O	77:Bw:161:TYR:CD2	2.74	0.41
77:Bw:217:TYR:CD1	77:Bw:218:THR:HG22	2.55	0.41
84:B4:32:SER:O	84:B4:34:TYR:CD1	2.74	0.41
85:B5:159:PHE:HZ	85:B5:161:THR:HB	1.71	0.41
86:B6:48:LEU:CD2	86:B6:60:ILE:CD1	2.98	0.41
86:B6:64:ALA:HB1	86:B6:72:HIS:ND1	2.36	0.41
86:B6:67:ALA:HB1	86:B6:69:THR:OG1	2.20	0.41
86:B6:81:LEU:C	86:B6:81:LEU:CD2	2.93	0.41
12:Ad:100:LEU:CD2	12:Ad:132:VAL:HG23	2.50	0.41
12:Ad:100:LEU:HD21	12:Ad:132:VAL:HG23	2.02	0.41
12:Ad:148:ALA:HB3	12:Ad:151:SER:HB2	2.02	0.41
62:Bj:8:LEU:C	62:Bj:8:LEU:CD1	2.94	0.41
64:Bl:6:ARG:HA	64:Bl:9:ARG:HD2	2.03	0.41
64:Bl:38:MET:C	64:Bl:42:ARG:HB2	2.46	0.41
64:Bl:109:TYR:CE1	64:Bl:110:LYS:O	2.74	0.41
66:Bn:48:TYR:CE1	66:Bn:135:ASP:HB2	2.55	0.41
66:Bn:102:LEU:CD1	66:Bn:164:GLY:HA2	2.51	0.41
66:Bn:184:SER:H	66:Bn:198:ILE:HG22	1.84	0.41
66:Bn:235:MET:HG2	66:Bn:238:MET:HG2	2.03	0.41
69:B7:193:MET:CE	69:B7:197:ARG:HH21	2.34	0.41
70:Bq:41:ILE:N	70:Bq:41:ILE:CD1	2.83	0.41
70:Bq:64:TYR:CE1	70:Bq:76:ASN:CB	2.94	0.41
70:Bq:65:ASN:C	70:Bq:74:ILE:CG2	2.94	0.41
70:Bq:92:ILE:HG23	70:Bq:93:GLU:N	2.34	0.41
70:Bq:92:ILE:CG2	70:Bq:93:GLU:N	2.84	0.41
77:Bw:114:VAL:HG23	77:Bw:114:VAL:O	2.20	0.41
77:Bw:116:ARG:CZ	77:Bw:131:LEU:HG	2.51	0.41
77:Bw:173:ASN:HA	77:Bw:213:ILE:CG2	2.43	0.41
77:Bw:193:ASP:CA	77:Bw:196:LEU:CD2	2.94	0.41
77:Bw:209:MET:SD	77:Bw:210:GLU:N	2.94	0.41
79:By:11:LYS:HD2	79:By:66:THR:HG21	2.02	0.41
79:By:21:ILE:CD1	79:By:21:ILE:N	2.83	0.41
84:B4:62:THR:CG2	84:B4:63:THR:N	2.83	0.41
84:B4:69:ARG:HB3	84:B4:80:LYS:HE2	2.03	0.41
86:B6:20:LEU:C	86:B6:20:LEU:CD2	2.94	0.41
86:B6:29:LEU:C	86:B6:29:LEU:CD1	2.94	0.41
86:B6:78:ASN:ND2	86:B6:78:ASN:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Aa:34:ALA:HB1	9:Aa:66:VAL:HG11	2.02	0.41
9:Aa:161:SER:HA	9:Aa:164:ILE:HD11	2.03	0.41
9:Aa:271:LYS:HD3	9:Aa:271:LYS:O	2.20	0.41
9:Aa:284:PRO:CG	9:Aa:304:ASP:N	2.84	0.41
62:Bj:115:LYS:CD	62:Bj:115:LYS:H	2.33	0.41
66:Bn:77:ARG:NH1	66:Bn:100:THR:HA	2.36	0.41
66:Bn:186:SER:OG	66:Bn:240:LYS:HG2	2.21	0.41
66:Bn:213:GLU:HA	66:Bn:217:ALA:HB1	2.03	0.41
70:Bq:46:THR:HG23	70:Bq:47:VAL:N	2.35	0.41
77:Bw:140:PHE:CD2	77:Bw:140:PHE:O	2.74	0.41
77:Bw:159:GLU:OE2	77:Bw:164:TRP:CD1	2.74	0.41
79:By:44:ARG:HA	79:By:44:ARG:NE	2.35	0.41
80:B9:85:LEU:HD11	80:B9:111:ILE:HG23	2.03	0.41
80:B9:88:LEU:C	80:B9:88:LEU:CD1	2.94	0.41
80:B9:89:LEU:N	80:B9:89:LEU:CD2	2.83	0.41
83:B3:21:ARG:CD	83:B3:21:ARG:C	2.94	0.41
84:B4:38:LYS:CG	84:B4:39:ARG:CD	2.98	0.41
85:B5:105:ILE:HG22	85:B5:132:LEU:CG	2.38	0.41
85:B5:168:MET:HB2	85:B5:173:ILE:HD11	2.03	0.41
85:B5:185:HIS:HA	85:B5:189:GLU:O	2.21	0.41
12:Ad:63:LEU:HD12	12:Ad:74:PHE:CZ	2.56	0.40
17:Aj:66:ARG:HG2	17:Aj:71:GLY:HA3	2.03	0.40
21:An:31:ILE:HG22	21:An:33:LYS:N	2.36	0.40
26:B0:1704:U:P	77:Bw:126:LYS:HZ3	2.44	0.40
26:B0:4306:U:P	84:B4:80:LYS:HZ1	2.43	0.40
62:Bj:8:LEU:CD1	62:Bj:18:LEU:CD1	2.95	0.40
64:Bl:86:THR:C	64:Bl:88:VAL:H	2.28	0.40
64:Bl:120:GLN:O	64:Bl:140:VAL:HG21	2.21	0.40
66:Bn:38:GLN:CB	70:Bq:29:TYR:CD2	3.03	0.40
68:Bp:93:VAL:CG2	68:Bp:94:THR:N	2.83	0.40
77:Bw:116:ARG:HD2	77:Bw:161:TYR:HE2	1.84	0.40
77:Bw:118:ARG:HA	77:Bw:245:LYS:HE2	2.03	0.40
77:Bw:173:ASN:HB3	77:Bw:213:ILE:HG21	2.04	0.40
77:Bw:210:GLU:C	77:Bw:213:ILE:HG12	2.47	0.40
79:By:11:LYS:CD	79:By:66:THR:HG21	2.51	0.40
80:B9:89:LEU:H	80:B9:89:LEU:HD22	1.85	0.40
85:B5:87:LEU:C	85:B5:117:TYR:CE1	2.99	0.40
86:B6:66:LEU:C	86:B6:66:LEU:CD1	2.94	0.40
1:AA:660:A:P	12:Ad:72:ARG:HH12	2.36	0.40
9:Aa:164:ILE:HD12	9:Aa:178:ASN:CA	2.49	0.40
9:Aa:217:MET:HB2	9:Aa:226:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Aa:248:LEU:HD21	9:Aa:298:LEU:CD2	2.51	0.40
9:Aa:282:GLU:HG3	9:Aa:308:ARG:NH1	2.34	0.40
17:Aj:53:PRO:CA	17:Aj:89:ILE:HB	2.50	0.40
22:Ao:21:THR:OG1	22:Ao:26:VAL:HG11	2.21	0.40
66:Bn:235:MET:HG3	66:Bn:237:GLU:CG	2.51	0.40
68:Bp:32:ILE:HA	68:Bp:44:LEU:CD1	2.51	0.40
68:Bp:32:ILE:HA	68:Bp:44:LEU:HD11	2.02	0.40
70:Bq:29:TYR:HD1	70:Bq:93:GLU:HG3	1.84	0.40
79:By:5:ARG:HB2	79:By:5:ARG:CZ	2.50	0.40
82:B2:19:CYS:SG	82:B2:20:ARG:N	2.94	0.40
83:B3:6:THR:N	83:B3:9:ILE:CG2	2.83	0.40
9:Aa:130:LYS:HD3	9:Aa:139:LYS:CD	2.51	0.40
17:Aj:34:LYS:HE2	17:Aj:106:ILE:HD13	2.02	0.40
62:Bj:13:HIS:CE1	62:Bj:117:MET:CB	3.04	0.40
66:Bn:204:ALA:O	66:Bn:207:MET:HG3	2.21	0.40
68:Bp:62:ARG:HB2	68:Bp:62:ARG:HH11	1.83	0.40
68:Bp:119:MET:HA	68:Bp:119:MET:CE	2.34	0.40
70:Bq:62:ARG:O	70:Bq:64:TYR:CD1	2.74	0.40
70:Bq:73:ILE:CG1	70:Bq:87:ARG:HD2	2.52	0.40
77:Bw:175:LEU:HD22	77:Bw:175:LEU:H	1.87	0.40
77:Bw:191:LEU:CG	77:Bw:192:THR:H	2.34	0.40
77:Bw:214:HIS:O	77:Bw:217:TYR:CD2	2.74	0.40
79:By:5:ARG:O	79:By:8:VAL:HG12	2.21	0.40
79:By:18:LYS:CG	79:By:19:LYS:HE2	2.47	0.40
81:Bz:29:ILE:HD12	81:Bz:30:GLU:HG2	2.02	0.40
82:B2:3:LYS:C	82:B2:8:PHE:CZ	2.93	0.40
85:B5:70:ARG:O	85:B5:139:VAL:HG22	2.21	0.40
86:B6:29:LEU:CD2	86:B6:87:LYS:CE	2.98	0.40
86:B6:30:GLY:C	86:B6:93:THR:CG2	2.94	0.40
9:Aa:14:HIS:HA	9:Aa:35:SER:OG	2.22	0.40
9:Aa:17:TRP:CB	9:Aa:305:ASN:CG	2.95	0.40
9:Aa:21:ILE:HD13	9:Aa:307:VAL:CG1	2.47	0.40
9:Aa:32:LEU:HD22	9:Aa:78:ALA:HB2	2.03	0.40
9:Aa:259:TRP:NE1	9:Aa:274:VAL:HG22	2.36	0.40
17:Aj:26:SER:OG	17:Aj:110:VAL:HA	2.21	0.40
17:Aj:49:LYS:O	17:Aj:50:VAL:HB	2.21	0.40
17:Aj:84:ILE:C	17:Aj:84:ILE:CD1	2.95	0.40
21:An:21:CYS:CA	21:An:37:ASN:H	2.30	0.40
62:Bj:118:VAL:HG13	62:Bj:118:VAL:O	2.20	0.40
64:Bl:110:LYS:HE2	64:Bl:112:LEU:CD2	2.51	0.40
66:Bn:38:GLN:HB3	70:Bq:29:TYR:CE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Bn:67:ARG:HD3	66:Bn:72:MET:CG	2.52	0.40
66:Bn:154:THR:HG23	66:Bn:155:GLY:N	2.36	0.40
66:Bn:187:LYS:HG3	66:Bn:188:GLU:N	2.37	0.40
70:Bq:42:LYS:HD2	70:Bq:42:LYS:HA	1.98	0.40
70:Bq:49:LYS:HB2	70:Bq:91:ARG:NH1	2.35	0.40
77:Bw:216:ILE:C	77:Bw:219:VAL:CG1	2.94	0.40
79:By:64:LYS:C	79:By:64:LYS:CD	2.94	0.40
82:B2:43:ARG:CG	82:B2:44:LYS:N	2.83	0.40
84:B4:69:ARG:HB3	84:B4:80:LYS:CG	2.51	0.40
85:B5:58:THR:HG23	85:B5:102:ASP:N	2.33	0.40
86:B6:44:LYS:HA	86:B6:44:LYS:HD2	1.95	0.40
9:Aa:156:PHE:CE2	9:Aa:163:PRO:HB2	2.57	0.40
9:Aa:216:ALA:HB1	9:Aa:247:TRP:CZ3	2.56	0.40
17:Aj:26:SER:HG	17:Aj:110:VAL:HA	1.87	0.40
17:Aj:39:LEU:C	17:Aj:39:LEU:CD1	2.95	0.40
17:Aj:46:LYS:HD3	17:Aj:46:LYS:HA	1.91	0.40
17:Aj:60:THR:C	17:Aj:61:LEU:HD22	2.46	0.40
62:Bj:26:VAL:CG2	62:Bj:97:ALA:CA	2.99	0.40
62:Bj:50:LYS:C	62:Bj:50:LYS:CD	2.95	0.40
62:Bj:78:ILE:C	62:Bj:78:ILE:CD1	2.95	0.40
62:Bj:115:LYS:H	62:Bj:115:LYS:HE2	1.86	0.40
66:Bn:230:VAL:O	66:Bn:231:THR:C	2.63	0.40
68:Bp:104:ARG:CB	68:Bp:107:ARG:HH21	2.35	0.40
77:Bw:115:ILE:HG22	77:Bw:116:ARG:N	2.36	0.40
77:Bw:234:LYS:HD2	77:Bw:234:LYS:HA	1.98	0.40
82:B2:18:LEU:HG	82:B2:19:CYS:N	2.36	0.40
86:B6:29:LEU:HA	86:B6:94:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Aa	300/317 (95%)	256 (85%)	31 (10%)	13 (4%)	2	17
10	Ab	188/295 (64%)	180 (96%)	5 (3%)	3 (2%)	7	38
11	Ac	190/243 (78%)	171 (90%)	12 (6%)	7 (4%)	2	20
12	Ad	101/209 (48%)	100 (99%)	1 (1%)	0	100	100
13	Ae	144/179 (80%)	136 (94%)	6 (4%)	2 (1%)	9	40
14	Ag	153/204 (75%)	147 (96%)	4 (3%)	2 (1%)	9	42
15	Ah	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
16	Ai	134/146 (92%)	120 (90%)	11 (8%)	3 (2%)	5	29
17	Aj	95/119 (80%)	87 (92%)	3 (3%)	5 (5%)	1	15
18	Ak	123/151 (82%)	86 (70%)	31 (25%)	6 (5%)	1	16
19	Al	113/143 (79%)	88 (78%)	17 (15%)	8 (7%)	1	11
20	Am	138/152 (91%)	125 (91%)	9 (6%)	4 (3%)	3	23
21	An	47/56 (84%)	42 (89%)	4 (8%)	1 (2%)	5	30
22	Ao	83/89 (93%)	67 (81%)	15 (18%)	1 (1%)	10	44
23	Aq	70/158 (44%)	65 (93%)	4 (6%)	1 (1%)	9	40
24	As	86/145 (59%)	75 (87%)	7 (8%)	4 (5%)	2	16
53	Ba	240/257 (93%)	219 (91%)	14 (6%)	7 (3%)	3	23
54	Bb	343/403 (85%)	255 (74%)	58 (17%)	30 (9%)	0	9
55	Bc	255/421 (61%)	211 (83%)	33 (13%)	11 (4%)	2	17
56	Bd	163/178 (92%)	140 (86%)	19 (12%)	4 (2%)	4	26
57	Be	173/192 (90%)	155 (90%)	14 (8%)	4 (2%)	5	28
58	Bf	118/266 (44%)	103 (87%)	8 (7%)	7 (6%)	1	13
59	Bg	46/317 (14%)	37 (80%)	8 (17%)	1 (2%)	5	29
60	Bh	164/214 (77%)	154 (94%)	8 (5%)	2 (1%)	10	44
61	Bi	72/165 (44%)	67 (93%)	4 (6%)	1 (1%)	9	40
62	Bj	134/203 (66%)	129 (96%)	4 (3%)	1 (1%)	18	56
63	Bk	122/140 (87%)	114 (93%)	6 (5%)	2 (2%)	7	38
64	Bl	116/148 (78%)	110 (95%)	4 (3%)	2 (2%)	7	36
65	Bm	173/204 (85%)	164 (95%)	8 (5%)	1 (1%)	21	59
66	Bn	232/297 (78%)	186 (80%)	30 (13%)	16 (7%)	1	11
67	Bo	116/188 (62%)	109 (94%)	5 (4%)	2 (2%)	7	36
68	Bp	151/196 (77%)	141 (93%)	6 (4%)	4 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	B7	11/13 (85%)	11 (100%)	0	0	100	100
70	Bq	94/160 (59%)	86 (92%)	7 (7%)	1 (1%)	11	46
71	Br	144/184 (78%)	137 (95%)	6 (4%)	1 (1%)	18	56
72	Bs	76/156 (49%)	74 (97%)	2 (3%)	0	100	100
73	Bt	100/145 (69%)	95 (95%)	3 (3%)	2 (2%)	6	31
74	Bu	51/157 (32%)	49 (96%)	2 (4%)	0	100	100
75	Bv	59/123 (48%)	59 (100%)	0	0	100	100
76	B8	8/10 (80%)	8 (100%)	0	0	100	100
77	Bw	152/270 (56%)	119 (78%)	22 (14%)	11 (7%)	1	11
78	Bx	78/125 (62%)	66 (85%)	7 (9%)	5 (6%)	1	12
79	By	52/135 (38%)	39 (75%)	7 (14%)	6 (12%)	0	5
80	B9	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
81	Bz	70/92 (76%)	65 (93%)	5 (7%)	0	100	100
82	B2	49/97 (50%)	33 (67%)	10 (20%)	6 (12%)	0	4
83	B3	46/51 (90%)	46 (100%)	0	0	100	100
84	B4	90/106 (85%)	87 (97%)	2 (2%)	1 (1%)	11	46
85	B5	208/212 (98%)	199 (96%)	7 (3%)	2 (1%)	12	49
86	B6	111/115 (96%)	104 (94%)	5 (4%)	2 (2%)	6	34
All	All	6163/8734 (71%)	5492 (89%)	479 (8%)	192 (3%)	5	22

All (192) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	Aa	65	PHE
9	Aa	162	ASN
9	Aa	270	LEU
11	Ac	48	ILE
11	Ac	131	ALA
11	Ac	152	PHE
13	Ae	20	VAL
13	Ae	117	VAL
17	Aj	50	VAL
17	Aj	89	ILE
19	Al	87	ASN
19	Al	103	ALA
19	Al	105	PHE

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Mol	Chain	Res	Type
20	Am	17	ASN
21	An	25	SER
23	Aq	82	MET
24	As	54	HIS
24	As	70	MET
53	Ba	37	ARG
53	Ba	223	SER
54	Bb	154	LYS
54	Bb	159	ILE
54	Bb	203	GLN
54	Bb	213	ASP
54	Bb	247	LEU
54	Bb	320	VAL
54	Bb	327	ASN
56	Bd	28	GLU
57	Be	130	PRO
58	Bf	136	LEU
58	Bf	137	ARG
58	Bf	162	ASP
58	Bf	196	ARG
63	Bk	21	PRO
63	Bk	41	SER
64	Bl	15	VAL
66	Bn	17	VAL
66	Bn	37	ILE
66	Bn	56	ASN
66	Bn	67	ARG
66	Bn	110	ASN
66	Bn	210	LEU
66	Bn	233	ASP
67	Bo	89	VAL
67	Bo	96	LYS
68	Bp	89	MET
68	Bp	182	GLU
71	Br	123	PRO
77	Bw	138	GLN
77	Bw	208	CYS
79	By	13	VAL
79	By	53	ILE
82	B2	30	GLN
85	B5	190	LYS
86	B6	57	LYS

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Mol	Chain	Res	Type
86	B6	71	VAL
9	Aa	45	LEU
9	Aa	104	HIS
9	Aa	145	GLU
10	Ab	152	PRO
11	Ac	81	GLU
11	Ac	93	THR
14	Ag	85	LYS
16	Ai	14	GLY
16	Ai	103	ALA
17	Aj	106	ILE
18	Ak	68	GLU
20	Am	76	GLN
24	As	75	VAL
53	Ba	123	ARG
53	Ba	231	ALA
54	Bb	14	GLY
54	Bb	44	ALA
54	Bb	85	ILE
54	Bb	116	ARG
54	Bb	187	GLY
54	Bb	243	THR
54	Bb	296	LYS
54	Bb	308	LEU
54	Bb	310	ASP
54	Bb	347	ARG
55	Bc	86	SER
55	Bc	97	GLY
55	Bc	182	VAL
56	Bd	34	THR
57	Be	141	LYS
65	Bm	90	ASN
66	Bn	79	ALA
66	Bn	197	HIS
66	Bn	198	ILE
66	Bn	213	GLU
68	Bp	181	LYS
73	Bt	112	ASP
77	Bw	118	ARG
77	Bw	132	GLN
77	Bw	191	LEU
77	Bw	224	LYS

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Mol	Chain	Res	Type
77	Bw	231	TRP
78	Bx	37	GLY
78	Bx	42	ALA
79	By	7	LEU
79	By	36	ARG
79	By	57	ASN
82	B2	8	PHE
82	B2	11	ARG
82	B2	22	CYS
9	Aa	284	PRO
10	Ab	189	SER
11	Ac	157	MET
17	Aj	47	ASN
18	Ak	127	GLY
18	Ak	137	SER
19	Al	92	ASN
20	Am	142	ARG
53	Ba	66	PRO
54	Bb	153	LYS
54	Bb	156	CYS
54	Bb	157	GLN
54	Bb	242	LYS
54	Bb	290	TYR
55	Bc	193	GLY
59	Bg	285	THR
60	Bh	103	SER
62	Bj	55	ALA
66	Bn	216	ASP
66	Bn	228	ASN
78	Bx	62	VAL
79	By	43	ASN
9	Aa	23	THR
9	Aa	137	VAL
9	Aa	254	PRO
10	Ab	97	PRO
11	Ac	32	ASP
14	Ag	82	ASN
18	Ak	61	LYS
18	Ak	104	ARG
18	Ak	143	LYS
19	Al	41	PHE
19	Al	65	ALA

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Mol	Chain	Res	Type
19	Al	134	TYR
53	Ba	65	ASP
54	Bb	42	LEU
54	Bb	173	ARG
55	Bc	77	ARG
55	Bc	145	GLU
57	Be	53	LYS
58	Bf	125	LYS
60	Bh	118	PHE
64	Bl	91	ALA
68	Bp	184	ILE
70	Bq	83	ILE
77	Bw	180	GLY
84	B4	42	ASP
9	Aa	46	THR
22	Ao	20	ASP
54	Bb	32	PRO
54	Bb	38	LYS
54	Bb	208	GLN
54	Bb	259	ALA
55	Bc	147	PRO
55	Bc	205	GLY
56	Bd	55	TYR
77	Bw	140	PHE
77	Bw	183	LYS
77	Bw	251	GLU
78	Bx	38	PHE
82	B2	7	SER
82	B2	24	SER
16	Ai	102	GLU
19	Al	102	VAL
20	Am	119	ALA
53	Ba	80	GLU
55	Bc	76	PRO
78	Bx	92	ARG
17	Aj	71	GLY
24	As	69	PRO
54	Bb	158	VAL
54	Bb	171	PRO
58	Bf	126	GLY
55	Bc	80	GLY
73	Bt	67	ILE

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Mol	Chain	Res	Type
9	Aa	263	GLY
56	Bd	124	GLY
61	Bi	89	PRO
66	Bn	138	PRO
9	Aa	18	VAL
55	Bc	78	VAL
57	Be	62	GLY
66	Bn	136	GLY
66	Bn	231	THR
85	B5	154	GLY
58	Bf	129	PRO

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	
9	Aa	265/275 (96%)	262 (99%)	3 (1%)	65	76
10	Ab	160/244 (66%)	153 (96%)	7 (4%)	25	47
11	Ac	157/202 (78%)	148 (94%)	9 (6%)	18	40
12	Ad	89/181 (49%)	87 (98%)	2 (2%)	45	64
13	Ae	117/146 (80%)	111 (95%)	6 (5%)	21	42
14	Ag	138/170 (81%)	133 (96%)	5 (4%)	31	52
15	Ah	110/113 (97%)	106 (96%)	4 (4%)	31	52
16	Ai	114/121 (94%)	110 (96%)	4 (4%)	32	53
17	Aj	90/107 (84%)	83 (92%)	7 (8%)	11	32
18	Ak	98/119 (82%)	91 (93%)	7 (7%)	13	35
19	Al	90/115 (78%)	85 (94%)	5 (6%)	19	40
20	Am	120/132 (91%)	114 (95%)	6 (5%)	22	43
21	An	43/49 (88%)	41 (95%)	2 (5%)	23	45
22	Ao	77/80 (96%)	72 (94%)	5 (6%)	15	37
23	Aq	72/142 (51%)	67 (93%)	5 (7%)	14	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	As	79/130 (61%)	71 (90%)	8 (10%)	7	23
53	Ba	187/199 (94%)	179 (96%)	8 (4%)	26	47
54	Bb	298/348 (86%)	273 (92%)	25 (8%)	10	30
55	Bc	214/351 (61%)	206 (96%)	8 (4%)	30	51
56	Bd	139/149 (93%)	132 (95%)	7 (5%)	22	43
57	Be	156/171 (91%)	148 (95%)	8 (5%)	21	42
58	Bf	100/223 (45%)	86 (86%)	14 (14%)	3	13
59	Bg	29/258 (11%)	29 (100%)	0	100	100
60	Bh	141/181 (78%)	137 (97%)	4 (3%)	38	60
61	Bi	64/137 (47%)	62 (97%)	2 (3%)	35	56
62	Bj	114/174 (66%)	110 (96%)	4 (4%)	32	53
63	Bk	97/107 (91%)	91 (94%)	6 (6%)	16	38
64	Bl	99/122 (81%)	98 (99%)	1 (1%)	68	78
65	Bm	148/172 (86%)	144 (97%)	4 (3%)	39	61
66	Bn	197/251 (78%)	181 (92%)	16 (8%)	11	31
67	Bo	108/165 (66%)	104 (96%)	4 (4%)	30	51
68	Bp	141/175 (81%)	136 (96%)	5 (4%)	32	53
69	B7	13/13 (100%)	13 (100%)	0	100	100
70	Bq	82/139 (59%)	75 (92%)	7 (8%)	10	29
71	Br	131/163 (80%)	123 (94%)	8 (6%)	17	38
72	Bs	69/133 (52%)	67 (97%)	2 (3%)	37	58
73	Bt	103/135 (76%)	100 (97%)	3 (3%)	37	58
74	Bu	46/126 (36%)	45 (98%)	1 (2%)	45	64
75	Bv	53/110 (48%)	50 (94%)	3 (6%)	18	40
76	B8	9/9 (100%)	9 (100%)	0	100	100
77	Bw	137/234 (58%)	121 (88%)	16 (12%)	5	18
78	Bx	71/110 (64%)	66 (93%)	5 (7%)	14	35
79	By	56/121 (46%)	47 (84%)	9 (16%)	2	11
80	B9	51/51 (100%)	49 (96%)	2 (4%)	28	49
81	Bz	57/75 (76%)	55 (96%)	2 (4%)	32	53
82	B2	42/80 (52%)	38 (90%)	4 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
83	B3	45/48 (94%)	44 (98%)	1 (2%)	45 64
84	B4	83/94 (88%)	78 (94%)	5 (6%)	17 39
85	B5	177/178 (99%)	175 (99%)	2 (1%)	65 76
86	B6	95/97 (98%)	90 (95%)	5 (5%)	20 41
All	All	5371/7425 (72%)	5095 (95%)	276 (5%)	23 42

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Aa	35	SER
9	Aa	271	LYS
9	Aa	284	PRO
10	Ab	16	LYS
10	Ab	84	ARG
10	Ab	110	GLN
10	Ab	123	VAL
10	Ab	153	LEU
10	Ab	173	MET
10	Ab	188	ILE
11	Ac	5	ILE
11	Ac	51	LEU
11	Ac	62	LYS
11	Ac	89	GLU
11	Ac	126	ILE
11	Ac	157	MET
11	Ac	179	GLN
11	Ac	182	LEU
11	Ac	187	LYS
12	Ad	62	LYS
12	Ad	121	ARG
13	Ae	23	GLN
13	Ae	25	ARG
13	Ae	28	GLN
13	Ae	59	ILE
13	Ae	78	TRP
13	Ae	84	LYS
14	Ag	63	LYS
14	Ag	128	ILE
14	Ag	166	ILE
14	Ag	190	ILE
14	Ag	193	LYS

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Mol	Chain	Res	Type
15	Ah	57	ARG
15	Ah	61	ILE
15	Ah	94	LEU
15	Ah	126	LEU
16	Ai	60	LYS
16	Ai	97	GLN
16	Ai	108	ILE
16	Ai	113	ILE
17	Aj	47	ASN
17	Aj	75	LYS
17	Aj	83	ARG
17	Aj	84	ILE
17	Aj	91	LEU
17	Aj	101	ILE
17	Aj	104	ILE
18	Ak	25	GLU
18	Ak	76	LEU
18	Ak	103	ASN
18	Ak	104	ARG
18	Ak	121	ARG
18	Ak	125	LYS
18	Ak	147	ARG
19	Al	26	GLN
19	Al	36	LEU
19	Al	52	LEU
19	Al	60	LYS
19	Al	115	ILE
20	Am	78	LYS
20	Am	86	ARG
20	Am	91	LYS
20	Am	94	LYS
20	Am	114	LEU
20	Am	130	ARG
21	An	22	ARG
21	An	54	LYS
22	Ao	6	GLU
22	Ao	21	THR
22	Ao	23	SER
22	Ao	31	LEU
22	Ao	69	LEU
23	Aq	81	LYS
23	Aq	86	ILE

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Mol	Chain	Res	Type
23	Aq	98	LYS
23	Aq	132	ARG
23	Aq	144	LYS
24	As	51	ARG
24	As	52	LYS
24	As	77	LYS
24	As	78	THR
24	As	107	ILE
24	As	108	LYS
24	As	112	ILE
24	As	130	ARG
53	Ba	8	GLN
53	Ba	46	LYS
53	Ba	60	LYS
53	Ba	126	LEU
53	Ba	177	LYS
53	Ba	179	ILE
53	Ba	190	LYS
53	Ba	200	ARG
54	Bb	33	LYS
54	Bb	36	SER
54	Bb	38	LYS
54	Bb	40	VAL
54	Bb	42	LEU
54	Bb	43	THR
54	Bb	75	VAL
54	Bb	98	LEU
54	Bb	119	LYS
54	Bb	123	LYS
54	Bb	134	LYS
54	Bb	135	LYS
54	Bb	136	TRP
54	Bb	137	GLN
54	Bb	142	LYS
54	Bb	179	LEU
54	Bb	185	ASN
54	Bb	197	ARG
54	Bb	212	GLN
54	Bb	225	LYS
54	Bb	280	ASN
54	Bb	296	LYS
54	Bb	300	ASN

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Mol	Chain	Res	Type
54	Bb	340	LYS
54	Bb	350	LEU
55	Bc	28	LYS
55	Bc	151	LEU
55	Bc	198	ARG
55	Bc	208	ILE
55	Bc	209	ILE
55	Bc	228	LEU
55	Bc	229	LEU
55	Bc	238	LYS
56	Bd	15	LEU
56	Bd	20	LEU
56	Bd	63	ARG
56	Bd	85	LYS
56	Bd	107	PHE
56	Bd	109	ILE
56	Bd	118	LYS
57	Be	18	ILE
57	Be	21	LYS
57	Be	28	LYS
57	Be	50	LYS
57	Be	51	LYS
57	Be	113	GLU
57	Be	143	GLU
57	Be	170	LYS
58	Bf	107	LYS
58	Bf	110	LYS
58	Bf	131	LYS
58	Bf	136	LEU
58	Bf	137	ARG
58	Bf	164	ILE
58	Bf	176	LYS
58	Bf	183	ILE
58	Bf	184	ILE
58	Bf	190	LEU
58	Bf	193	LEU
58	Bf	196	ARG
58	Bf	204	PHE
58	Bf	215	LEU
60	Bh	31	ARG
60	Bh	120	LYS
60	Bh	137	ILE

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Mol	Chain	Res	Type
60	Bh	166	ILE
61	Bi	94	LYS
61	Bi	103	ASN
62	Bj	50	LYS
62	Bj	64	ASN
62	Bj	78	ILE
62	Bj	140	LEU
63	Bk	39	ILE
63	Bk	74	LYS
63	Bk	92	ASP
63	Bk	106	VAL
63	Bk	111	GLU
63	Bk	112	MET
64	Bl	123	ILE
65	Bm	13	LYS
65	Bm	19	MET
65	Bm	36	LEU
65	Bm	64	ILE
66	Bn	13	LYS
66	Bn	16	GLN
66	Bn	26	LYS
66	Bn	32	ARG
66	Bn	47	LYS
66	Bn	53	ARG
66	Bn	91	LEU
66	Bn	104	LEU
66	Bn	121	GLN
66	Bn	187	LYS
66	Bn	193	VAL
66	Bn	195	ARG
66	Bn	197	HIS
66	Bn	233	ASP
66	Bn	236	GLU
66	Bn	238	MET
67	Bo	36	ARG
67	Bo	60	LEU
67	Bo	91	ILE
67	Bo	136	VAL
68	Bp	9	ARG
68	Bp	21	LYS
68	Bp	30	ASN
68	Bp	162	ARG

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Mol	Chain	Res	Type
68	Bp	183	GLU
70	Bq	6	LYS
70	Bq	13	MET
70	Bq	38	ILE
70	Bq	42	LYS
70	Bq	44	MET
70	Bq	54	LYS
70	Bq	92	ILE
71	Br	41	ILE
71	Br	43	LYS
71	Br	46	LYS
71	Br	69	ARG
71	Br	97	ASN
71	Br	128	ARG
71	Br	146	ILE
71	Br	153	LYS
72	Bs	94	ASN
72	Bs	127	LEU
73	Bt	16	LYS
73	Bt	63	LYS
73	Bt	106	ILE
74	Bu	43	LYS
75	Bv	43	LYS
75	Bv	44	LEU
75	Bv	47	ILE
77	Bw	111	LEU
77	Bw	133	LEU
77	Bw	135	ARG
77	Bw	157	ILE
77	Bw	186	LYS
77	Bw	191	LEU
77	Bw	196	LEU
77	Bw	203	LYS
77	Bw	207	ILE
77	Bw	214	HIS
77	Bw	223	PHE
77	Bw	228	ASN
77	Bw	230	LEU
77	Bw	231	TRP
77	Bw	242	MET
77	Bw	245	LYS
78	Bx	27	ILE

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Mol	Chain	Res	Type
78	Bx	33	ILE
78	Bx	70	LYS
78	Bx	83	ARG
78	Bx	84	ILE
79	By	9	LYS
79	By	11	LYS
79	By	12	ILE
79	By	18	LYS
79	By	19	LYS
79	By	24	GLN
79	By	27	ARG
79	By	30	LYS
79	By	50	LYS
80	B9	106	LYS
80	B9	109	LYS
81	Bz	48	LYS
81	Bz	62	LYS
82	B2	10	LYS
82	B2	20	ARG
82	B2	31	LYS
82	B2	46	LYS
83	B3	23	ILE
84	B4	14	LYS
84	B4	39	ARG
84	B4	45	GLN
84	B4	57	ARG
84	B4	64	LYS
85	B5	11	ARG
85	B5	69	LEU
86	B6	44	LYS
86	B6	72	HIS
86	B6	79	ILE
86	B6	109	PRO
86	B6	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
9	Aa	56	GLN
9	Aa	117	ASN
9	Aa	178	ASN
9	Aa	191	HIS

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Mol	Chain	Res	Type
9	Aa	226	HIS
9	Aa	305	ASN
12	Ad	61	GLN
12	Ad	118	GLN
12	Ad	122	HIS
17	Aj	47	ASN
17	Aj	100	GLN
21	An	41	GLN
22	Ao	8	GLN
22	Ao	45	HIS
54	Bb	244	HIS
54	Bb	275	HIS
62	Bj	13	HIS
62	Bj	25	GLN
62	Bj	95	GLN
64	Bl	14	HIS
64	Bl	17	HIS
64	Bl	19	HIS
64	Bl	25	HIS
64	Bl	28	HIS
64	Bl	34	ASN
64	Bl	39	HIS
64	Bl	41	HIS
64	Bl	85	GLN
66	Bn	16	GLN
66	Bn	44	ASN
66	Bn	228	ASN
66	Bn	243	HIS
68	Bp	30	ASN
70	Bq	69	HIS
70	Bq	76	ASN
70	Bq	97	HIS
77	Bw	173	ASN
77	Bw	214	HIS
77	Bw	228	ASN
77	Bw	248	HIS
77	Bw	261	GLN
79	By	23	HIS
79	By	43	ASN
80	B9	81	ASN
80	B9	92	ASN
80	B9	107	ASN

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Mol	Chain	Res	Type
81	Bz	33	GLN
82	B2	16	HIS
83	B3	4	HIS
83	B3	25	GLN
83	B3	43	HIS
84	B4	76	ASN
84	B4	90	HIS
85	B5	7	ASN
85	B5	30	ASN
85	B5	41	ASN
85	B5	150	GLN
85	B5	185	HIS
86	B6	33	GLN
86	B6	40	GLN
86	B6	78	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	0/1563	-	-
2	AB	0/35	-	-
25	B1	0/123	-	-
26	B0	0/2903	-	-
27	BA	0/21	-	-
28	BB	0/27	-	-
29	BC	0/17	-	-
3	AC	0/32	-	-
30	BD	0/16	-	-
31	BE	0/54	-	-
32	BF	0/120	-	-
33	BG	0/48	-	-
34	BH	0/25	-	-
35	BI	0/72	-	-
36	BJ	0/30	-	-
37	BK	0/26	-	-
38	BL	0/20	-	-
39	BM	0/19	-	-
4	AD	0/42	-	-
40	BN	0/78	-	-
41	BO	0/20	-	-
42	BP	0/15	-	-

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
43	BQ	0/30	-	-
44	BR	0/30	-	-
45	BS	0/38	-	-
46	BT	0/30	-	-
47	BU	0/16	-	-
48	BV	0/22	-	-
49	BW	0/16	-	-
5	AE	0/32	-	-
50	BX	0/113	-	-
51	BY	0/115	-	-
52	BZ	0/72	-	-
6	AF	0/31	-	-
7	AG	0/14	-	-
8	AH	0/41	-	-
All	All	0/5906	-	-

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](#)

There are no ligands in this entry.

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.

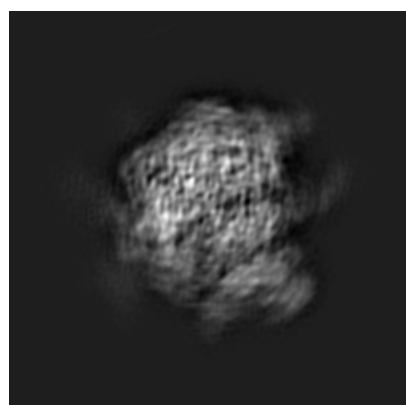
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1480. These allow visual inspection of the internal detail of the map and identification of artifacts.

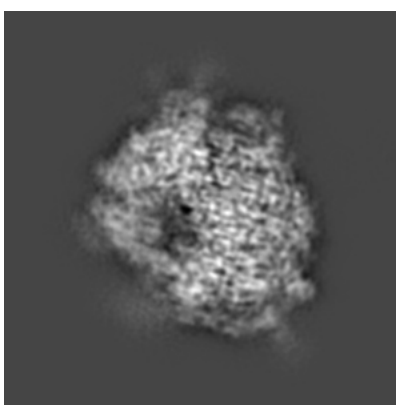
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

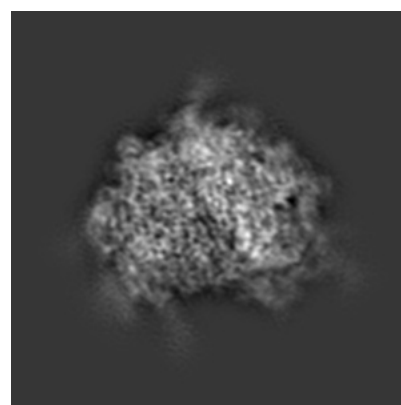
6.1.1 Primary map



X



Y



Z

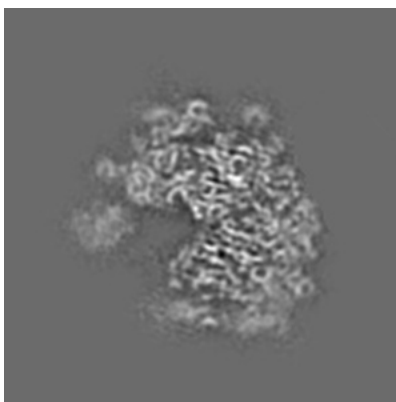
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

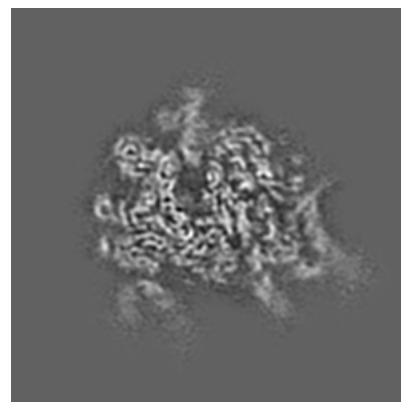
6.2.1 Primary map



X Index: 84



Y Index: 84

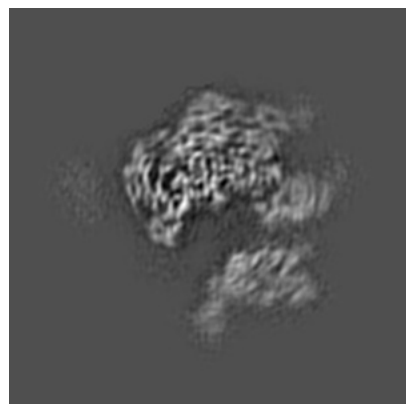


Z Index: 84

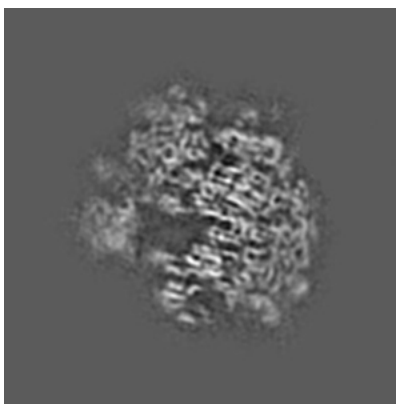
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

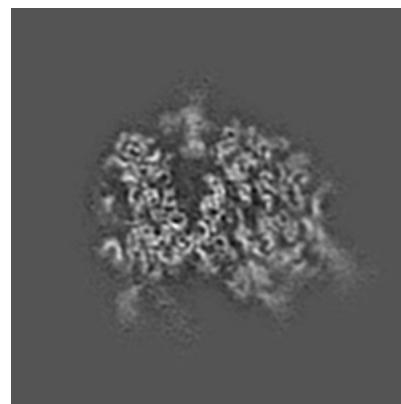
6.3.1 Primary map



X Index: 75



Y Index: 89

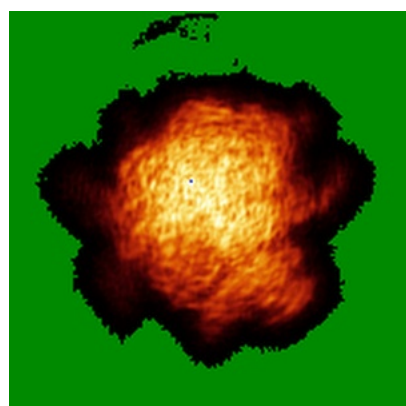


Z Index: 81

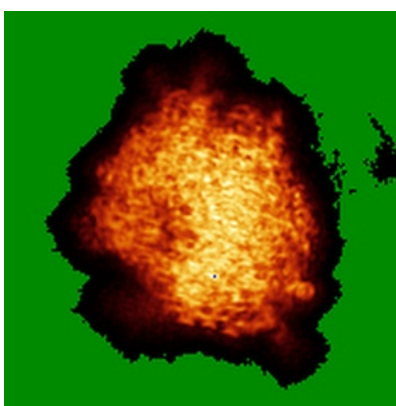
The images above show the largest variance slices of the map in three orthogonal directions.

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

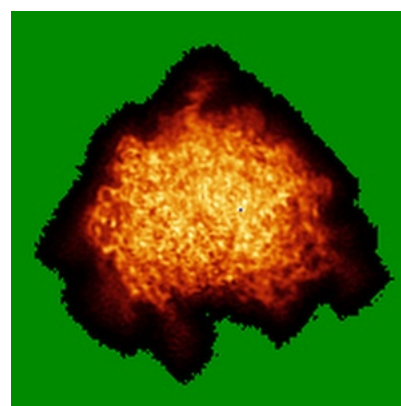
6.4.1 Primary map



X



Y

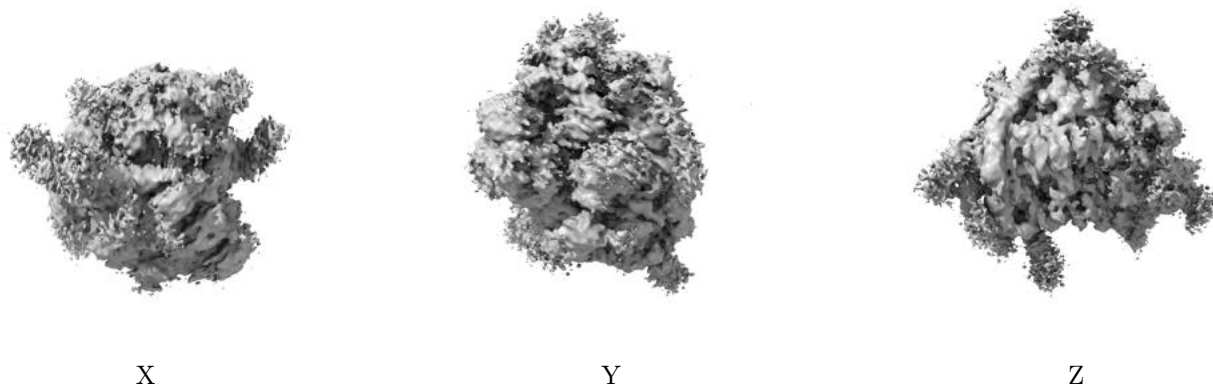


Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

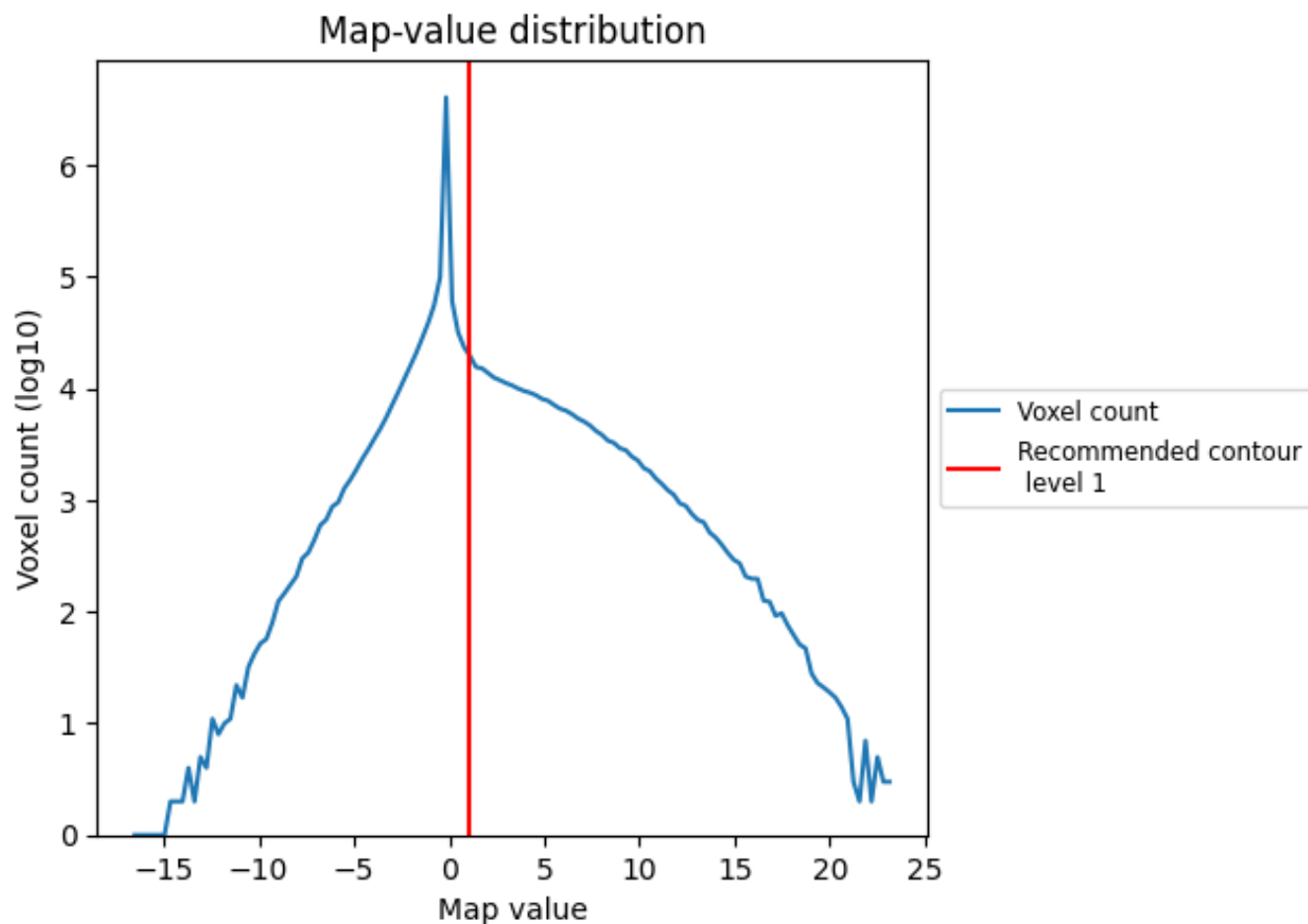
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

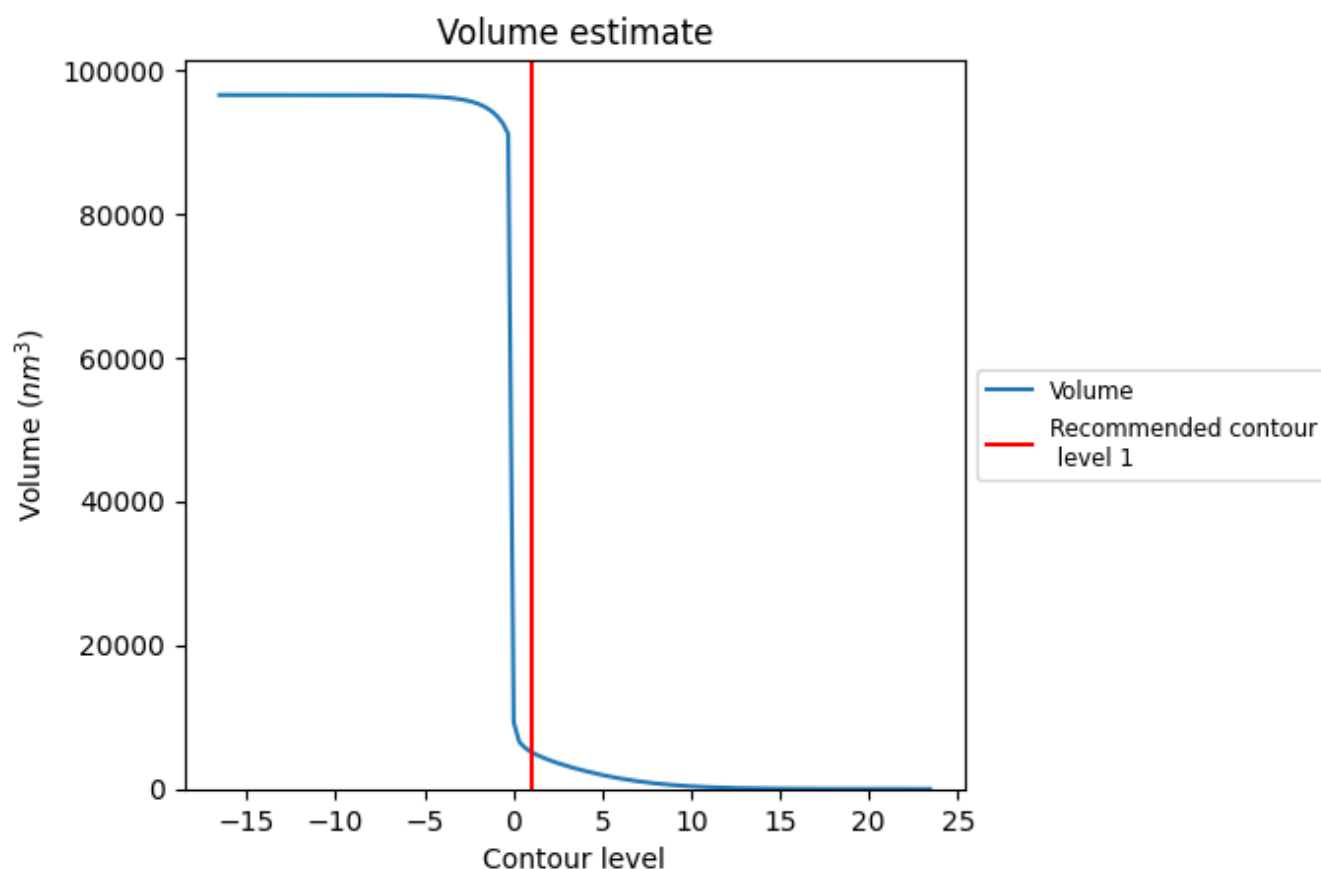
This section contains the results of statistical analysis of the map.

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.

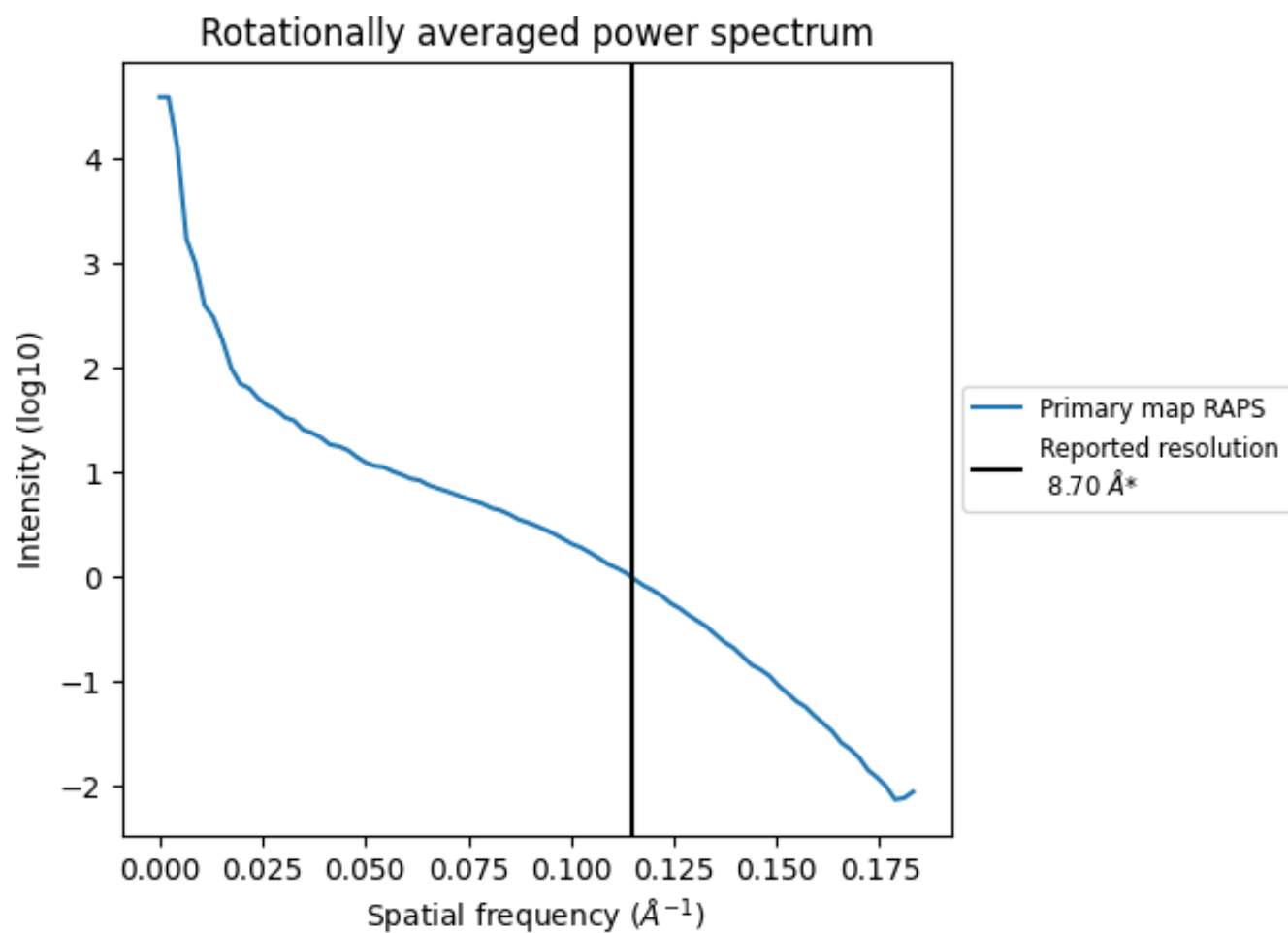
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5149 nm^3 ; this corresponds to an approximate mass of 4651 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 0.115 Å⁻¹

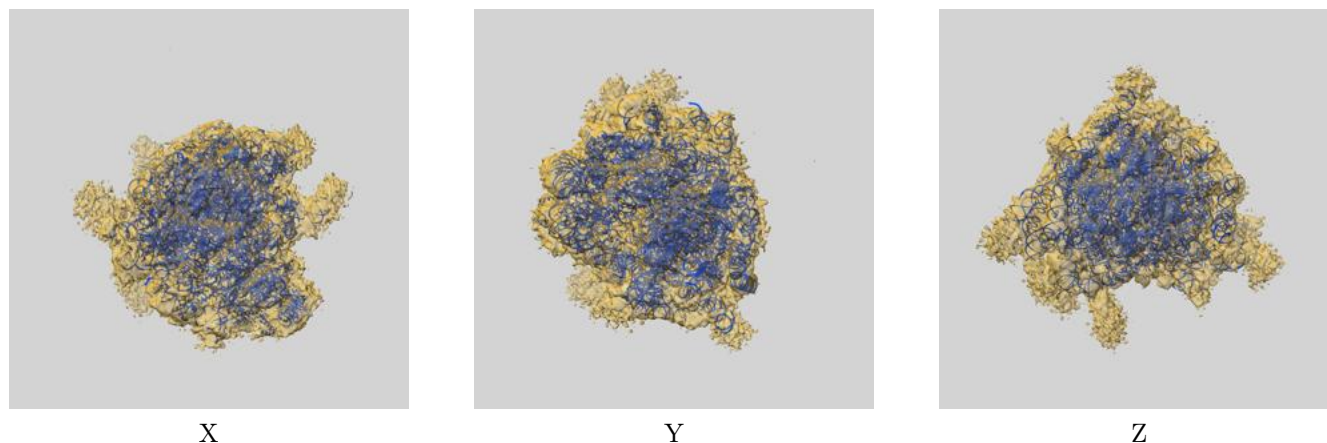
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

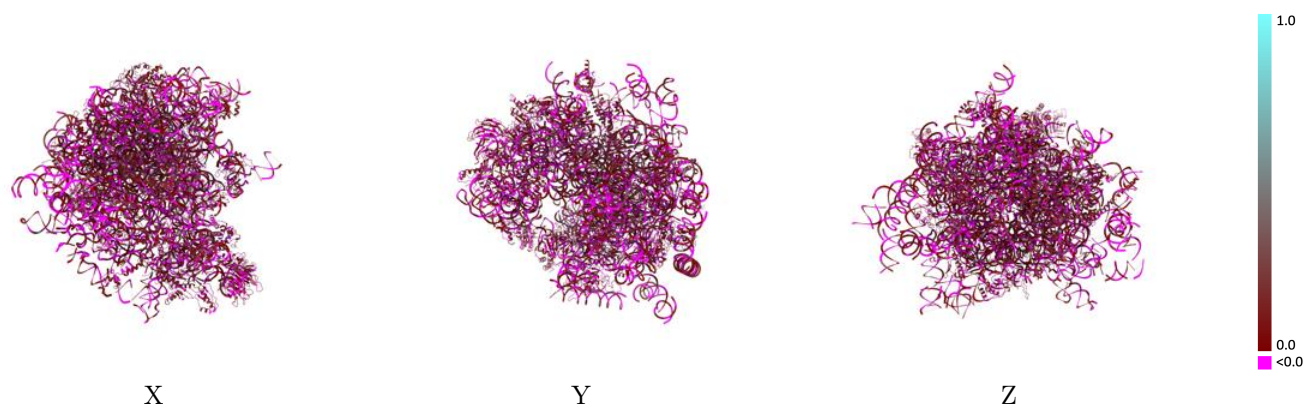
This section contains information regarding the fit between EMDB map EMD-1480 and PDB model 4V5Z. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

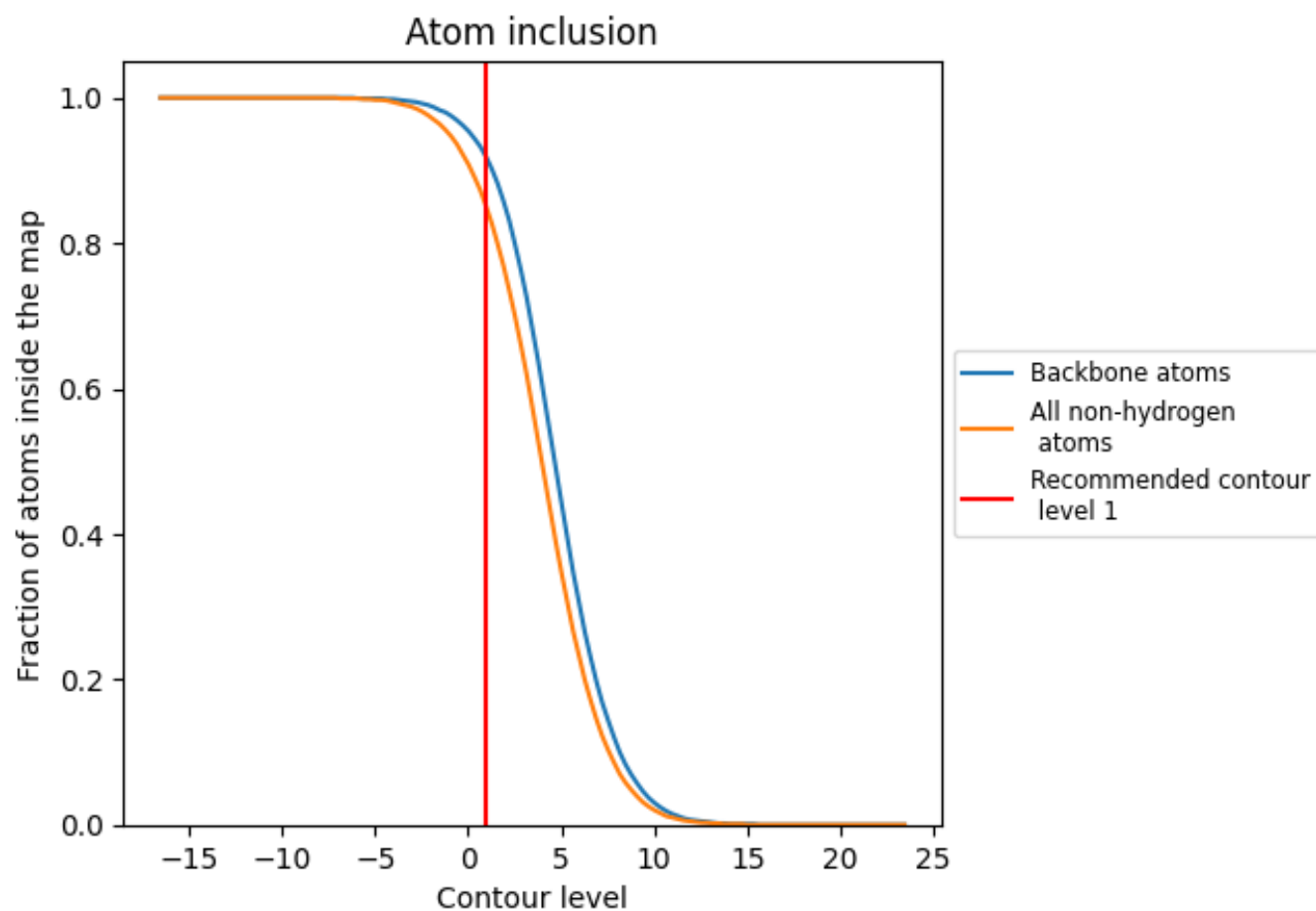


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 85% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.0750
AA	 0.8920	 0.0490
AB	 0.8440	 0.0270
AC	 0.9310	 0.0130
AD	 0.9520	 0.0480
AE	 0.9060	 -0.0110
AF	 1.0000	 0.0070
AG	 0.6430	 0.0290
AH	 0.8050	 -0.0040
Aa	 0.9250	 0.0570
Ab	 0.9260	 0.1090
Ac	 0.8790	 0.0870
Ad	 0.9520	 0.0740
Ae	 0.8850	 0.0810
Ag	 0.8940	 0.0520
Ah	 0.8890	 0.0940
Ai	 0.9430	 0.0410
Aj	 0.8920	 0.0370
Ak	 0.8710	 0.0940
Al	 0.8480	 0.0780
Am	 0.9020	 0.0670
An	 0.8470	 0.0030
Ao	 0.7740	 0.1030
Aq	 0.8290	 0.0550
As	 0.9740	 0.0510
B0	 0.9060	 0.0720
B1	 0.9170	 0.0430
B2	 0.8110	 0.0660
B3	 0.7790	 0.0890
B4	 0.7360	 0.0360
B5	 0.8870	 0.0520
B6	 0.8190	 0.0980
B7	 0.8330	 0.1100
B8	 0.9210	 0.1960
B9	 0.8510	 0.0850



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Chain	Atom inclusion	Q-score
BA	 0.8090	 0.0660
BB	 0.8890	 0.0320
BC	 0.8820	 0.0480
BD	 0.8750	 -0.0010
BE	 0.8700	 0.0470
BF	 0.9170	 0.0400
BG	 0.7710	 0.0190
BH	 0.7600	 0.0070
BI	 0.9030	 0.0510
BJ	 0.8330	 0.0430
BK	 0.5200	 0.0340
BL	 1.0000	 0.0490
BM	 0.8420	 0.0050
BN	 0.6540	 -0.0040
BO	 0.9500	 0.0230
BP	 0.7330	 0.0770
BQ	 0.8670	 0.0200
BR	 0.8330	 0.0420
BS	 0.8950	 0.0340
BT	 0.8670	 0.0260
BU	 0.8750	 0.0650
BV	 0.7270	 0.0060
BW	 0.5620	 0.0120
BX	 0.9030	 0.0560
BY	 0.7480	 0.0100
BZ	 0.8610	 0.0440
Ba	 0.7710	 0.1030
Bb	 0.7590	 0.0560
Bc	 0.8320	 0.0730
Bd	 0.8510	 0.0790
Be	 0.8900	 0.1110
Bf	 0.8990	 0.1080
Bg	 0.9850	 0.1320
Bh	 0.8090	 0.0880
Bi	 0.9340	 0.0100
Bj	 0.7050	 0.0620
Bk	 0.8320	 0.1150
Bl	 0.8240	 0.0590
Bm	 0.8270	 0.0560
Bn	 0.7120	 0.0320
Bo	 0.8530	 0.0810
Bp	 0.8690	 0.1260

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Chain	Atom inclusion	Q-score
Bq	 0.7690	 0.0770
Br	 0.8640	 0.1060
Bs	 0.8110	 0.1220
Bt	 0.8900	 0.1040
Bu	 0.8620	 0.1020
Bv	 0.8130	 0.1500
Bw	 0.7930	 0.0960
Bx	 0.8360	 0.0720
By	 0.6480	 0.0340
Bz	 0.7900	 0.0990