



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:10 pm GMT

PDB ID : 4V5Z
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 PDB ID : 1J5E,1Vi6,1fjg,1iGV,1i6U,2AVY,1G1X,1RQ6,1K7K

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

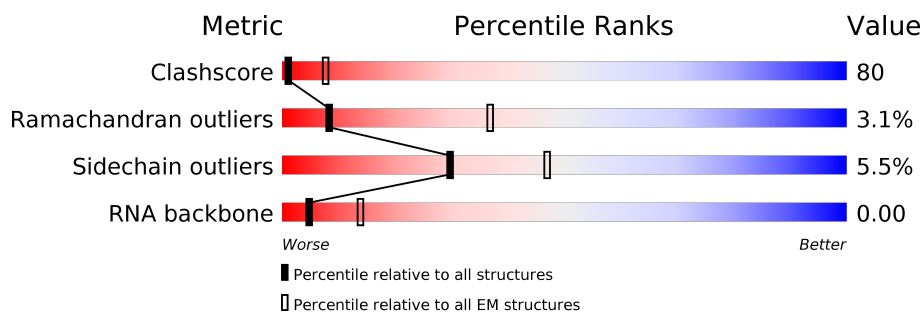
1 Overall quality at a glance

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.









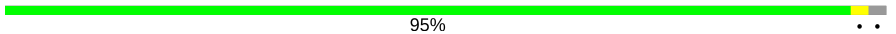











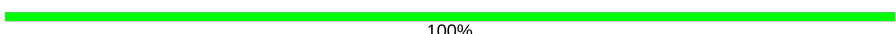
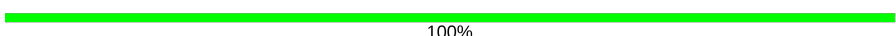

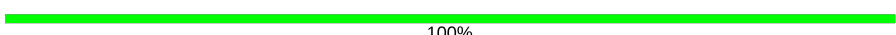
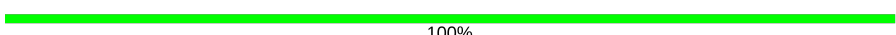
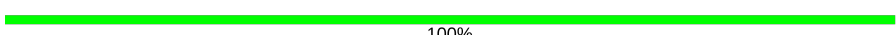

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AA	1563	89% 11%
2	AB	35	91% 9%
3	AC	32	91% 9%
4	AD	42	100%
5	AE	32	100%
6	AF	31	100%
7	AG	14	100%
8	AH	41	100%

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Mol	Chain	Length	Quality of chain
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	
29	BC	17	
30	BD	16	
31	BE	54	
32	BF	120	
33	BG	48	









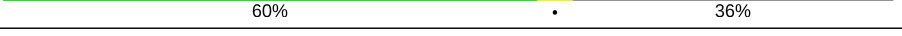


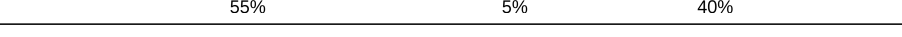

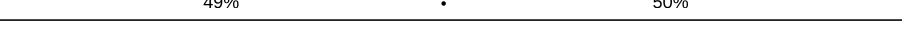


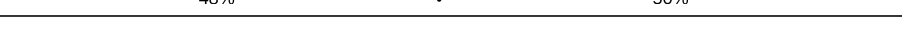
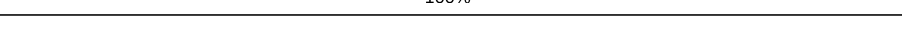
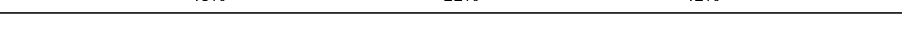
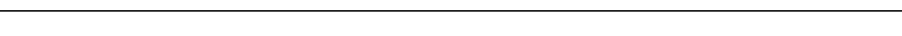

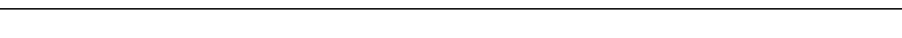

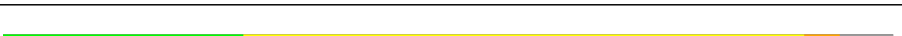

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Mol	Chain	Length	Quality of chain
34	BH	25	100%
35	BI	72	100%
36	BJ	30	100%
37	BK	26	96% .
38	BL	20	100%
39	BM	19	100%
40	BN	78	100%
41	BO	20	100%
42	BP	15	100%
43	BQ	30	100%
44	BR	30	100%
45	BS	38	100%
46	BT	30	100%
47	BU	16	100%
48	BV	22	100%
49	BW	16	100%
50	BX	113	100%
51	BY	115	100%
52	BZ	72	99% .
53	Ba	257	88% 6% . 5%
54	Bb	403	64% 20% . 14%
55	Bc	421	51% 9% . 39%
56	Bd	178	75% 15% . 7%
57	Be	192	78% 11% . 9%
58	Bf	266	34% 9% . 55%

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Mol	Chain	Length	Quality of chain
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	
79	By	135	
80	B9	58	
81	Bz	92	
82	B2	97	
83	B3	51	

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Mol	Chain	Length	Quality of chain
84	B4	106	<div><div></div><div>26%56%5%13%</div></div>
85	B5	212	<div><div></div><div>36%62%..</div></div>
86	B6	115	<div><div></div><div>26%69%..</div></div>

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		

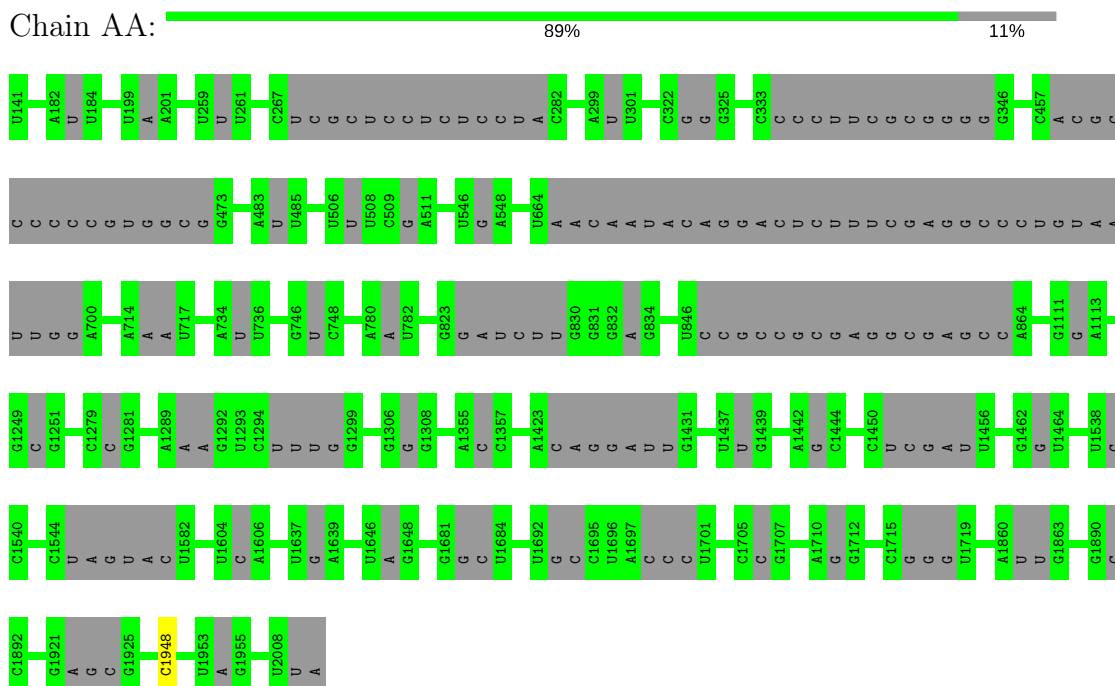
- Molecule 86 is a protein called 60S Ribosomal protein L30e.

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

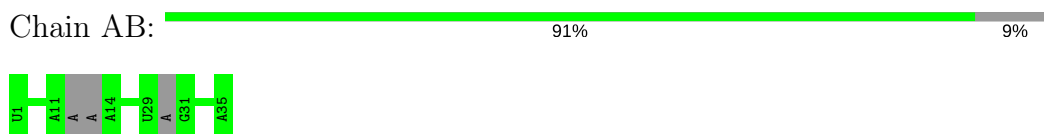
3 Residue-property plots [i](#)

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

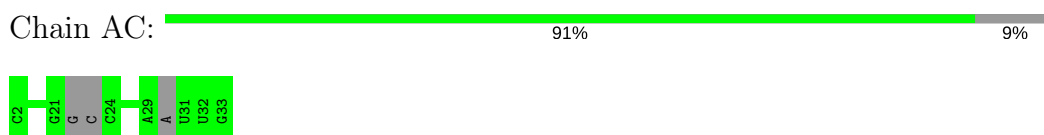
- Molecule 1: 18S Ribosomal RNA



- Molecule 2: RNA Expansion segment ES3



- Molecule 3: RNA Expansion segment ES4



- Molecule 4: RNA Expansion segment ES6 part I



There are no outlier residues recorded for this chain.

- Molecule 5: RNA Expansion segment ES6 part II

Chain AE:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: RNA Expansion segment ES9

Chain AF:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: RNA helix

Chain AG:  100%

There are no outlier residues recorded for this chain.

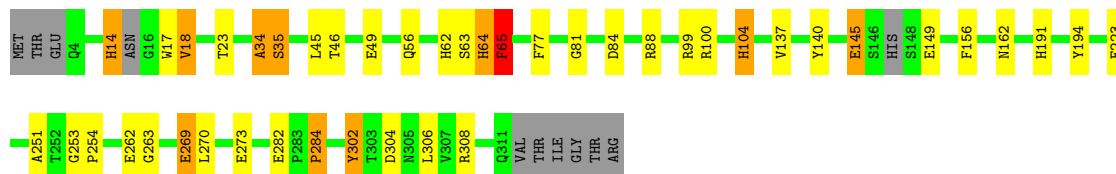
- Molecule 8: RNA helix

Chain AH:  100%


There are no outlier residues recorded for this chain.

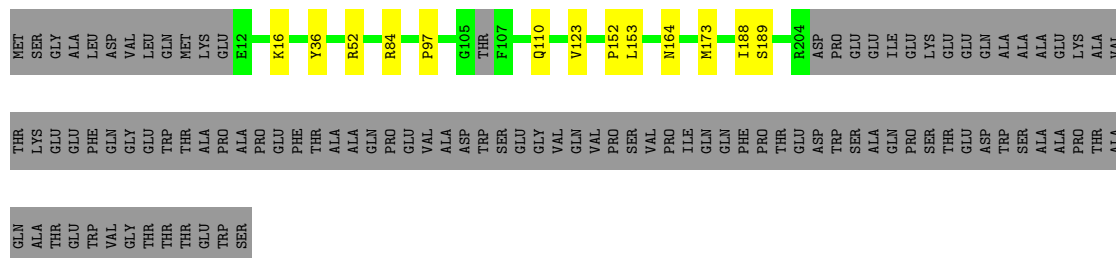
- Molecule 9: 40S Ribosomal protein RACK1

Chain Aa:  83% 10% • •



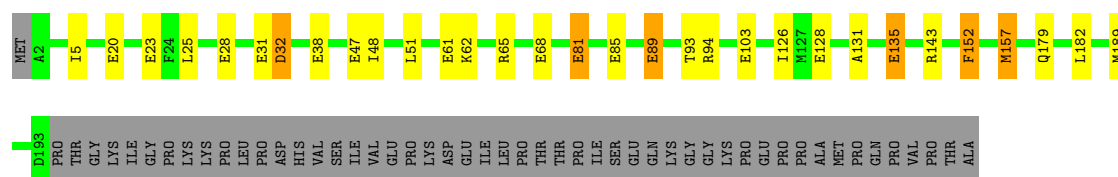
- Molecule 10: 40S Ribosomal protein SA

Chain Ab:  61% 35%

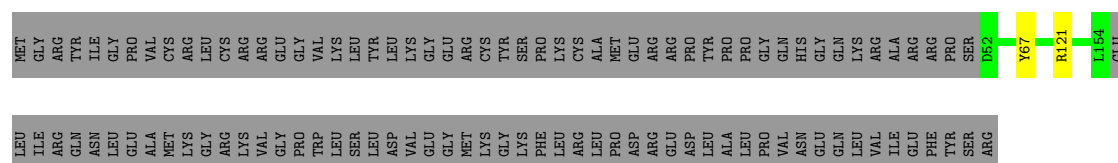


- Molecule 11: 40S Ribosomal protein S3e

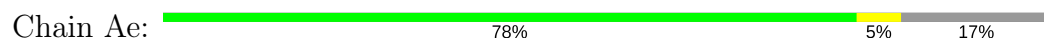
Chain Ac:  66% 10% 21%



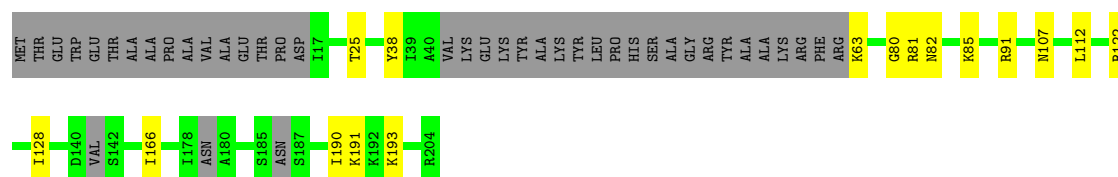
- Molecule 12: 40S Ribosomal protein S9e



- Molecule 13: 40S Ribosomal protein S2e



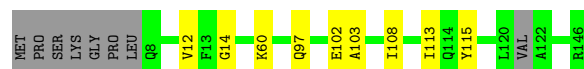
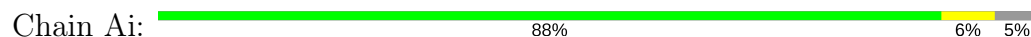
- Molecule 14: 40S Ribosomal protein S5e



- Molecule 15: 40S Ribosomal protein S15ae



- Molecule 16: 40S Ribosomal protein S16e

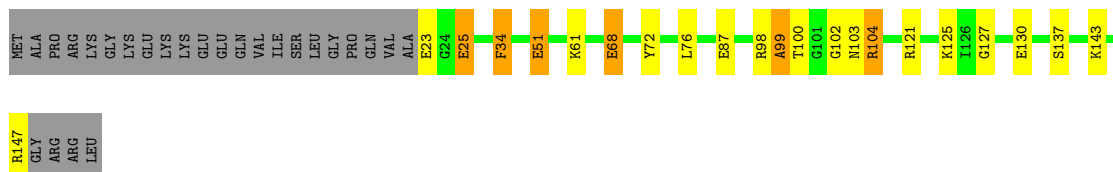


- Molecule 17: 40S Ribosomal protein S20e

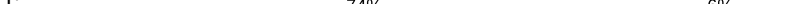


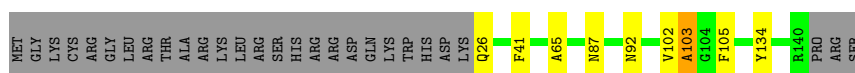
- Molecule 18: 40S Ribosomal protein S14e

Chain Ak: 68% 11% • 17%

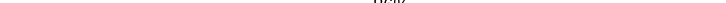


- Molecule 19: 40S Ribosomal protein S23e

Chain AI:  74% 6% 20%



- Molecule 20: 40S Ribosomal protein S18e

Chain Am: 

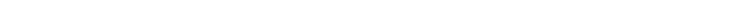


- Molecule 21: 40S Ribosomal protein S29e

Chain An:



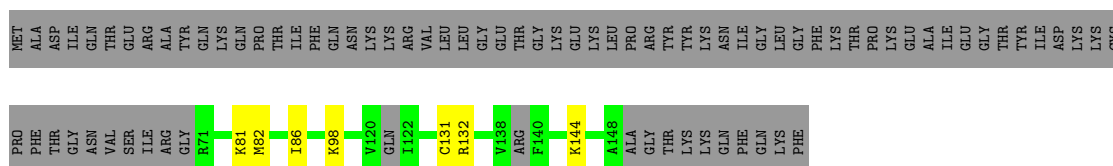
- Molecule 22: 40S Ribosomal protein S13e

Chain Ao:  78% 13% . .



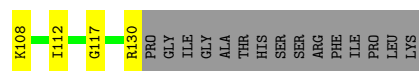
- Molecule 23: 40S Ribosomal protein S11e

Chain Aq:



- Molecule 24: 40S Ribosomal protein S15e

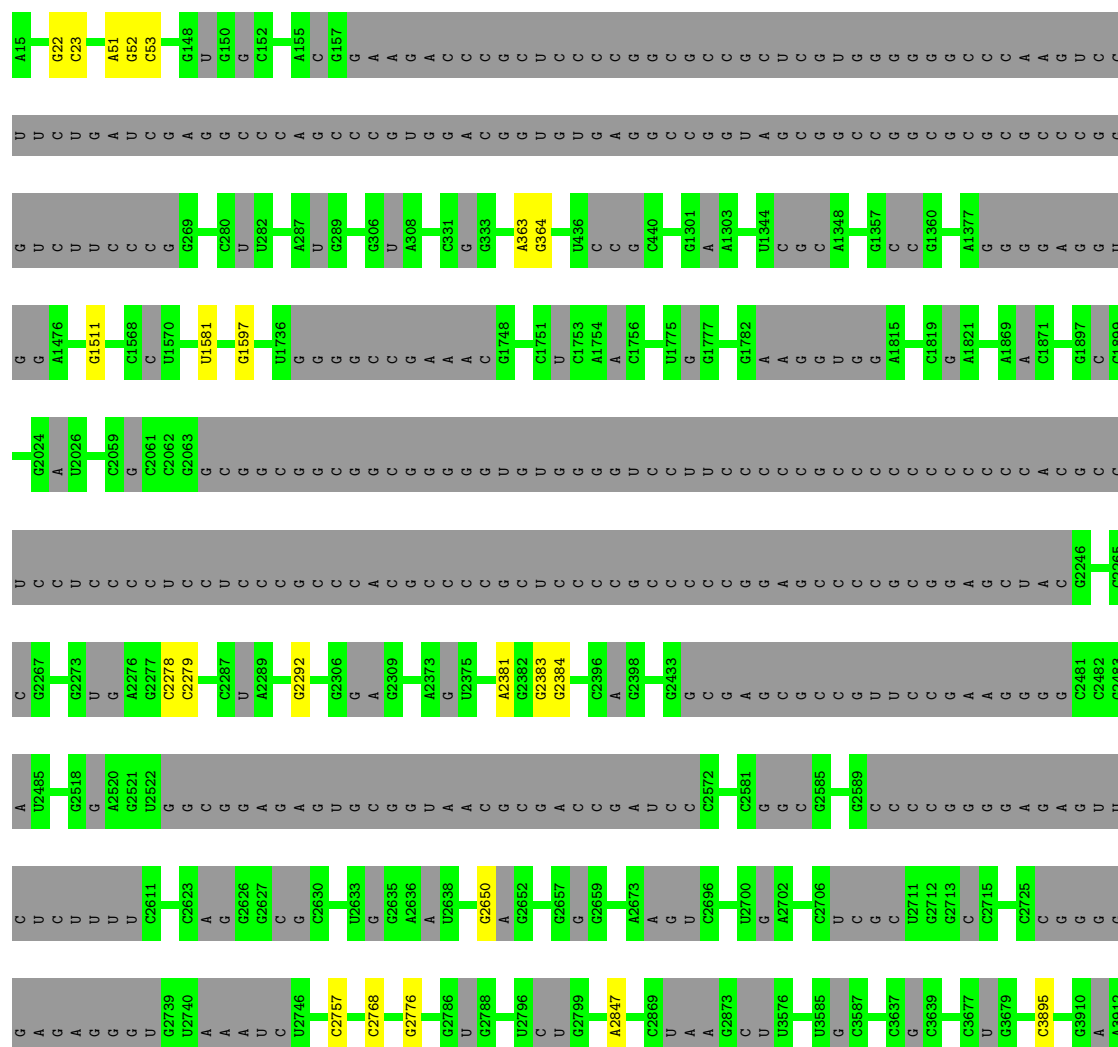
Digital Tool Type	Percentage
Digital tools	51%
Digital tools (e.g., video conferencing)	10%
Digital tools (e.g., social media)	39%

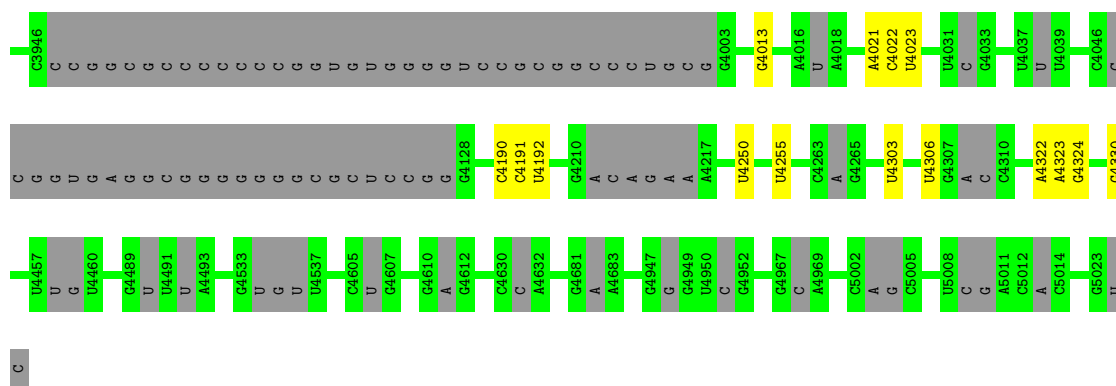


Chain B1:



Chain B0:





- Molecule 27: RNA Expansion segment ES3

Chain BA: 100%

There are no outlier residues recorded for this chain.

- Molecule 28: RNA Expansion segment ES4

Chain BB: 100%

There are no outlier residues recorded for this chain.

- Molecule 29: RNA Expansion segment ES5

Chain BC: 100%

There are no outlier residues recorded for this chain.

- Molecule 30: RNA Expansion segment ES7 part I

Chain BD: 100%

There are no outlier residues recorded for this chain.

- Molecule 31: RNA Expansion segment ES7 part II

Chain BE: 100%

There are no outlier residues recorded for this chain.

- Molecule 32: RNA Expansion segment ES7 part III

Chain BF: 100%

There are no outlier residues recorded for this chain.

- Molecule 33: RNA Expansion segment ES9

Chain BG: 100%

There are no outlier residues recorded for this chain.

- Molecule 34: RNA Expansion segment ES12

Chain BH:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: RNA Expansion segment ES15 part I

Chain BI:  100%

There are no outlier residues recorded for this chain.

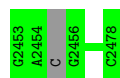
- Molecule 36: RNA Expansion segment ES15 part II

Chain BJ:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: RNA Expansion segment ES19

Chain BK:  96%



- Molecule 38: RNA Expansion segment ES20

Chain BL:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: RNA Expansion segment ES24

Chain BM:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: RNA Expansion segment ES27

Chain BN:  100%

There are no outlier residues recorded for this chain.

- Molecule 41: RNA Expansion segment ES30

Chain BO:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: RNA Expansion segment ES31 part I

Chain BP:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: RNA Expansion segment ES31 part II

Chain BQ:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: RNA Expansion segment ES39 part I

Chain BR:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: RNA Expansion segment ES39 part II

Chain BS:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: RNA Expansion segment ES39 part III

Chain BT:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: RNA Expansion segment ES41

Chain BU:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: RNA Expansion segment ES9 part2

Chain BV:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: RNA Expansion segment ES10

Chain BW:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: RNA helices

Chain BX:  100%

There are no outlier residues recorded for this chain.

- Molecule 51: 5S Ribosomal RNA

Chain BY:  100%

There are no outlier residues recorded for this chain.

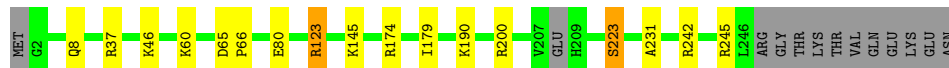
- Molecule 52: E site t-RNA

Chain BZ:  99%



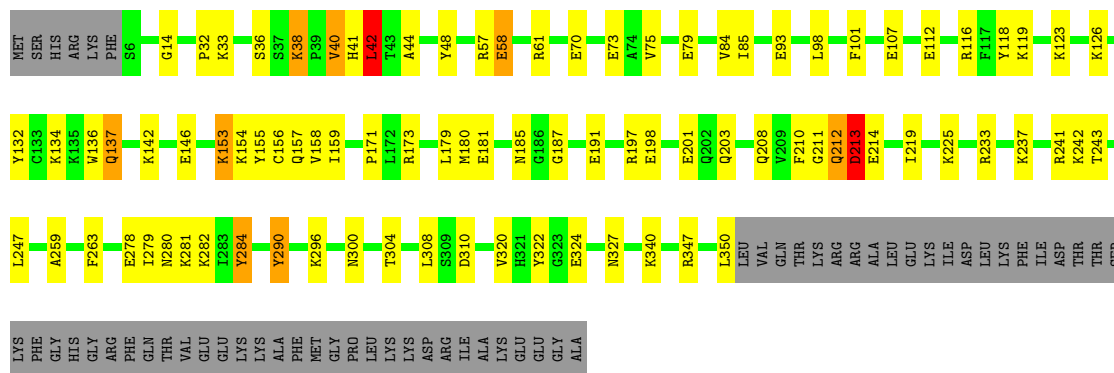
- Molecule 53: 60S Ribosomal protein L8

Chain Ba:  88% 6% 5%



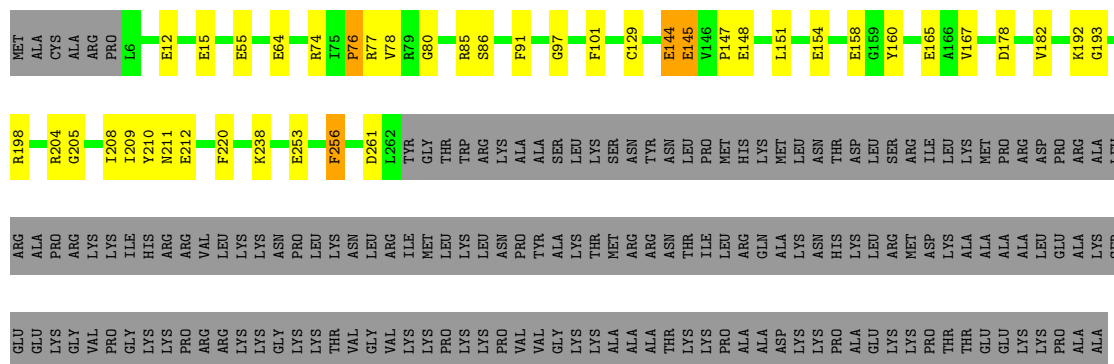
- Molecule 54: 60S Ribosomal protein L3

Chain Bb:  64% 20% 14%




- Molecule 55: 60S Ribosomal protein L4

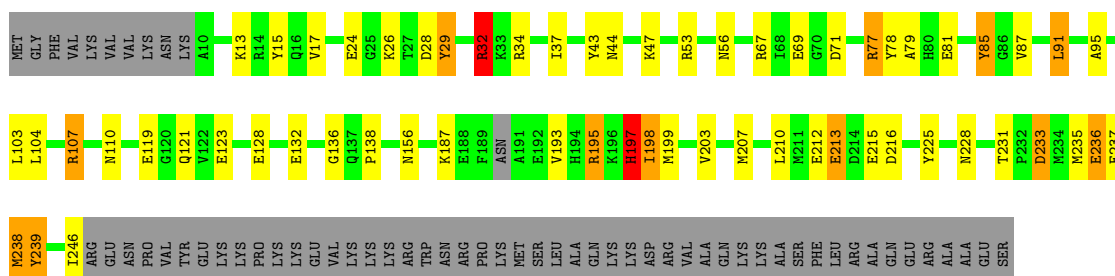
Chain Bc:  51% 9% 39%



- Molecule 56: 60S Ribosomal protein L11

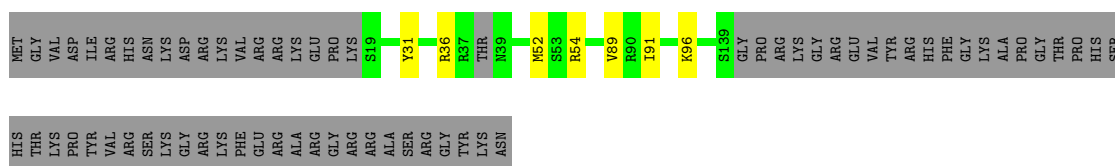
Chain Bd:  75% 15% 7%





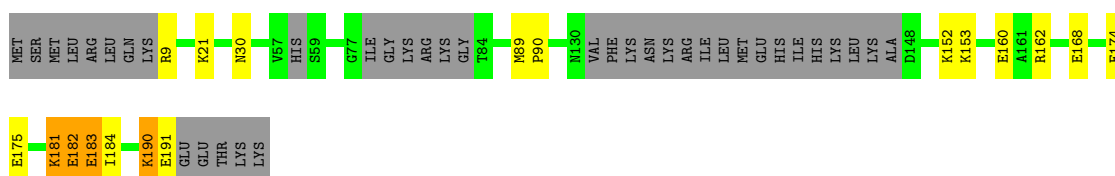
• Molecule 67: 60S Ribosomal protein L18

Chain Bo: 60% 36%



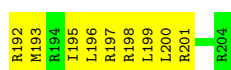
• Molecule 68: 60S Ribosomal protein L19

Chain Bp: 72% 7% 19%



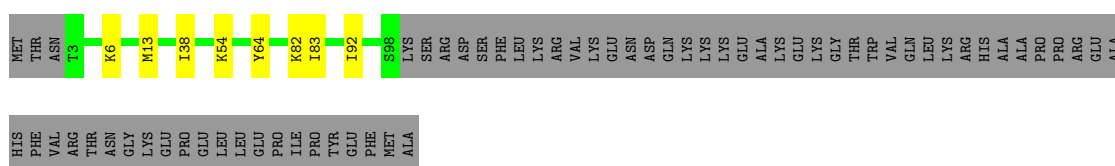
• Molecule 69: 60S Ribosomal protein L19

Chain B7: 31% 69%



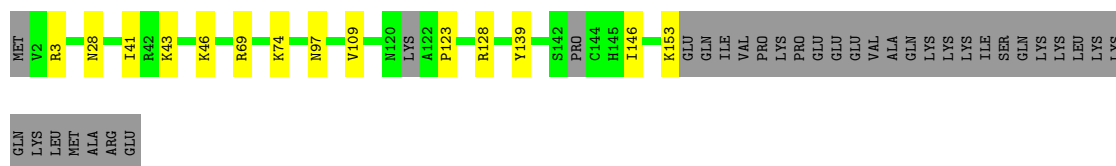
• Molecule 70: 60S Ribosomal protein L21

Chain Bq: 55% 5% 40%

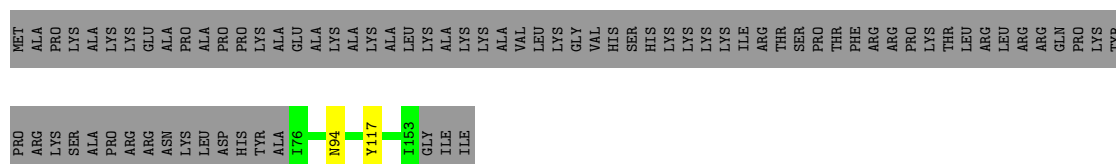


• Molecule 71: 60S Ribosomal protein L17

Chain Br: 74% 8% 18%



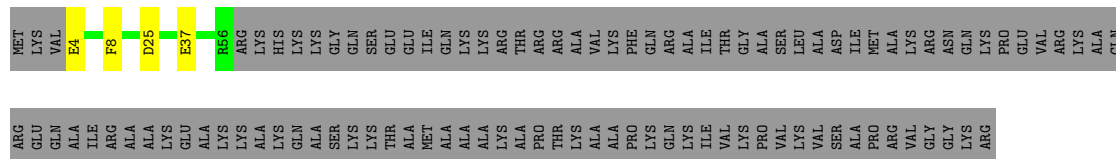
- Molecule 72: 60S Ribosomal protein L23a



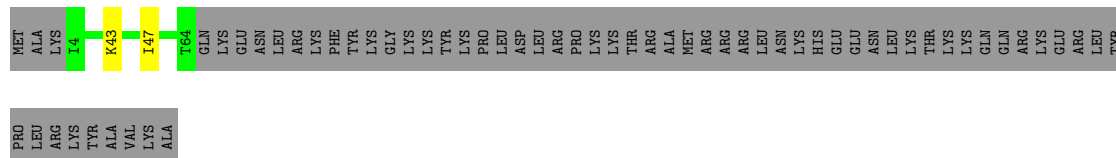
- Molecule 73: 60S Ribosomal protein L26



- Molecule 74: 60S Ribosomal protein L24



- Molecule 75: 60S Ribosomal protein L35



- Molecule 76: 60S Ribosomal protein L35



There are no outlier residues recorded for this chain.

- Molecule 77: 60S Ribosomal protein L7



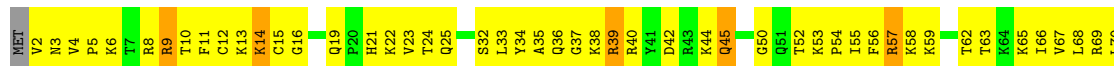
- Molecule 83: 60S Ribosomal protein L39e

Chain B3:  27% 63% 6%



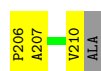
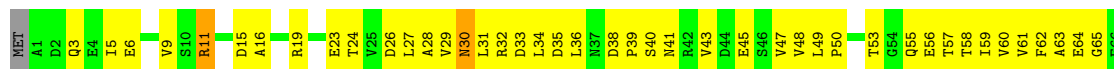
- Molecule 84: 60S Ribosomal protein L44e

Chain B4:  26% 56% 5% 13%



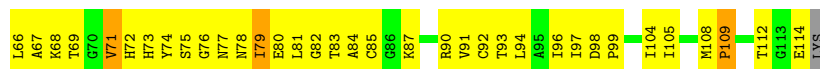
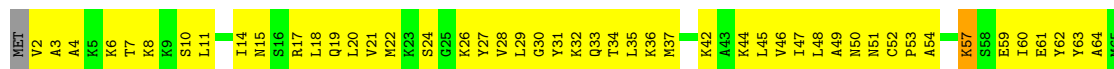
- Molecule 85: 60S Ribosomal protein L10a

Chain B5:  36% 62%



- Molecule 86: 60S Ribosomal protein L30e

Chain B6:  26% 69%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction using phase flipping and setsf in EMAN to correct the amplitudes	Depositor
Microscope	TF20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1500	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	4400	Depositor
Magnification	51000	Depositor
Image detector	Not provided	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	$\# Z > 2$	RMSZ	$\# Z > 2$
10	Ab	0.98	0/1556	1.11	2/2115 (0.1%)
11	Ac	1.13	14/1518 (0.9%)	1.08	3/2038 (0.1%)
12	Ad	1.09	0/856	1.01	1/1144 (0.1%)
13	Ae	1.00	0/1115	1.17	1/1505 (0.1%)
14	Ag	1.04	1/1288 (0.1%)	1.22	8/1725 (0.5%)
15	Ah	0.96	0/1033	1.10	1/1382 (0.1%)
16	Ai	1.08	1/1118 (0.1%)	1.20	3/1493 (0.2%)
17	Aj	1.04	0/781	1.17	0/1048
18	Ak	1.14	6/947 (0.6%)	1.24	3/1271 (0.2%)
19	Al	0.98	0/884	1.16	1/1184 (0.1%)
20	Am	1.10	0/1165	1.16	0/1555
21	An	1.14	0/420	1.22	1/557 (0.2%)
22	Ao	1.30	8/721 (1.1%)	1.25	3/962 (0.3%)
23	Aq	1.09	0/637	1.23	0/849
24	As	1.06	0/735	1.20	2/980 (0.2%)
53	Ba	1.05	0/1904	1.15	2/2552 (0.1%)
54	Bb	1.13	15/2824 (0.5%)	1.26	13/3786 (0.3%)
55	Bc	1.04	12/2076 (0.6%)	1.13	5/2790 (0.2%)
56	Bd	1.22	14/1347 (1.0%)	1.37	16/1801 (0.9%)
57	Be	1.05	10/1426 (0.7%)	1.13	4/1916 (0.2%)
58	Bf	1.11	7/932 (0.8%)	1.48	12/1256 (1.0%)
59	Bg	1.42	6/332 (1.8%)	1.10	1/454 (0.2%)
60	Bh	1.00	7/1358 (0.5%)	1.21	9/1811 (0.5%)
61	Bi	1.00	0/578	1.05	0/775
62	Bj	1.10	0/1118	1.13	0/1502
63	Bk	0.92	4/940 (0.4%)	1.07	4/1264 (0.3%)
64	Bl	1.04	0/972	1.22	2/1299 (0.2%)
65	Bm	1.10	0/1491	1.13	4/1999 (0.2%)
66	Bn	1.19	14/1949 (0.7%)	1.55	33/2615 (1.3%)
67	Bo	1.11	1/965 (0.1%)	1.17	1/1292 (0.1%)
68	Bp	1.22	6/1338 (0.4%)	1.19	4/1766 (0.2%)
69	B7	1.44	0/129	1.14	0/167
70	Bq	1.05	0/788	1.14	1/1049 (0.1%)
71	Br	1.03	0/1240	1.17	3/1660 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
72	Bs	0.88	0/630	1.09	1/850 (0.1%)
73	Bt	1.06	0/924	1.16	1/1223 (0.1%)
74	Bu	1.01	2/455 (0.4%)	1.03	1/610 (0.2%)
75	Bv	1.01	0/476	1.02	0/632
76	B8	1.09	0/77	1.08	0/103
77	Bw	1.07	0/1301	1.31	2/1737 (0.1%)
78	Bx	1.22	5/681 (0.7%)	1.50	10/908 (1.1%)
79	By	1.19	0/519	1.21	1/680 (0.1%)
80	B9	0.98	0/467	1.05	0/626
81	Bz	0.96	0/558	1.17	0/745
82	B2	1.13	0/415	1.36	3/547 (0.5%)
83	B3	1.11	0/439	1.03	0/580
84	B4	1.06	0/773	1.13	0/1022
85	B5	0.98	0/1638	1.13	0/2222
86	B6	0.97	0/885	1.11	0/1186
9	Aa	1.00	8/2434 (0.3%)	1.29	19/3309 (0.6%)
All	All	1.08	141/51153 (0.3%)	1.20	181/68542 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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
9	Aa	0	17
All	All	6	93

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	Bn	81	GLU	CD-OE2	10.45	1.37	1.25
55	Bc	55	GLU	CD-OE2	9.63	1.36	1.25
14	Ag	122	ARG	C-N	9.62	1.56	1.34
68	Bp	183	GLU	CD-OE2	9.38	1.35	1.25
9	Aa	282	GLU	CD-OE2	9.37	1.35	1.25
54	Bb	198	GLU	CD-OE2	9.16	1.35	1.25
78	Bx	94	GLU	CD-OE2	9.13	1.35	1.25
68	Bp	160	GLU	CD-OE2	9.13	1.35	1.25
60	Bh	55	GLU	CD-OE2	9.13	1.35	1.25
54	Bb	58	GLU	CD-OE2	9.12	1.35	1.25
55	Bc	12	GLU	CD-OE2	9.10	1.35	1.25
22	Ao	5	GLU	CD-OE2	9.10	1.35	1.25
54	Bb	73	GLU	CD-OE2	9.10	1.35	1.25
22	Ao	82	GLU	CD-OE2	9.08	1.35	1.25
54	Bb	324	GLU	CD-OE2	9.08	1.35	1.25
54	Bb	112	GLU	CD-OE2	9.06	1.35	1.25
22	Ao	25	GLU	CD-OE2	9.06	1.35	1.25
54	Bb	201	GLU	CD-OE2	9.04	1.35	1.25
55	Bc	15	GLU	CD-OE2	9.04	1.35	1.25
22	Ao	75	GLU	CD-OE2	9.02	1.35	1.25
54	Bb	93	GLU	CD-OE2	9.02	1.35	1.25
57	Be	147	GLU	CD-OE2	9.02	1.35	1.25
22	Ao	13	GLU	CD-OE2	9.01	1.35	1.25
11	Ac	85	GLU	CD-OE2	9.00	1.35	1.25
56	Bd	81	GLU	CD-OE2	9.00	1.35	1.25
57	Be	183	GLU	CD-OE2	8.98	1.35	1.25
18	Ak	25	GLU	CD-OE2	8.98	1.35	1.25
55	Bc	148	GLU	CD-OE2	8.98	1.35	1.25
78	Bx	56	GLU	CD-OE2	8.97	1.35	1.25
18	Ak	68	GLU	CD-OE2	8.97	1.35	1.25
54	Bb	79	GLU	CD-OE2	8.96	1.35	1.25
18	Ak	130	GLU	CD-OE2	8.96	1.35	1.25
55	Bc	158	GLU	CD-OE2	8.95	1.35	1.25
56	Bd	66	GLU	CD-OE2	8.95	1.35	1.25
54	Bb	107	GLU	CD-OE2	8.93	1.35	1.25
9	Aa	145	GLU	CD-OE2	8.93	1.35	1.25
11	Ac	28	GLU	CD-OE2	8.93	1.35	1.25
54	Bb	70	GLU	CD-OE2	8.91	1.35	1.25
68	Bp	174	GLU	CD-OE2	8.91	1.35	1.25
78	Bx	96	GLU	CD-OE2	8.91	1.35	1.25
60	Bh	57	GLU	CD-OE2	8.90	1.35	1.25
22	Ao	40	GLU	CD-OE2	8.90	1.35	1.25
57	Be	113	GLU	CD-OE2	8.90	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Ak	23	GLU	CD-OE2	8.89	1.35	1.25
54	Bb	191	GLU	CD-OE2	8.89	1.35	1.25
54	Bb	278	GLU	CD-OE2	8.89	1.35	1.25
56	Bd	80	GLU	CD-OE2	8.89	1.35	1.25
55	Bc	253	GLU	CD-OE2	8.89	1.35	1.25
11	Ac	89	GLU	CD-OE2	8.88	1.35	1.25
58	Bf	105	GLU	CD-OE2	8.88	1.35	1.25
22	Ao	72	GLU	CD-OE2	8.88	1.35	1.25
54	Bb	214	GLU	CD-OE2	8.88	1.35	1.25
18	Ak	51	GLU	CD-OE2	8.88	1.35	1.25
78	Bx	48	GLU	CD-OE2	8.88	1.35	1.25
55	Bc	212	GLU	CD-OE2	8.87	1.35	1.25
59	Bg	299	GLU	CD-OE2	8.87	1.35	1.25
68	Bp	168	GLU	CD-OE2	8.87	1.35	1.25
66	Bn	119	GLU	CD-OE2	8.86	1.35	1.25
59	Bg	306	GLU	CD-OE2	8.86	1.35	1.25
60	Bh	62	GLU	CD-OE2	8.86	1.35	1.25
66	Bn	213	GLU	CD-OE2	8.86	1.35	1.25
68	Bp	175	GLU	CD-OE2	8.86	1.35	1.25
55	Bc	144	GLU	CD-OE2	8.85	1.35	1.25
66	Bn	69	GLU	CD-OE2	8.85	1.35	1.25
9	Aa	149	GLU	CD-OE2	8.84	1.35	1.25
58	Bf	165	GLU	CD-OE2	8.84	1.35	1.25
18	Ak	87	GLU	CD-OE2	8.83	1.35	1.25
63	Bk	99	GLU	CD-OE2	8.83	1.35	1.25
56	Bd	14	GLU	CD-OE2	8.82	1.35	1.25
22	Ao	6	GLU	CD-OE2	8.82	1.35	1.25
59	Bg	263	GLU	CD-OE2	8.81	1.35	1.25
63	Bk	111	GLU	CD-OE2	8.80	1.35	1.25
60	Bh	65	GLU	CD-OE2	8.80	1.35	1.25
78	Bx	24	GLU	CD-OE2	8.80	1.35	1.25
9	Aa	223	GLU	CD-OE2	8.79	1.35	1.25
54	Bb	146	GLU	CD-OE2	8.79	1.35	1.25
56	Bd	28	GLU	CD-OE2	8.79	1.35	1.25
55	Bc	154	GLU	CD-OE2	8.78	1.35	1.25
59	Bg	302	GLU	CD-OE2	8.77	1.35	1.25
56	Bd	41	GLU	CD-OE2	8.75	1.35	1.25
74	Bu	4	GLU	CD-OE2	8.75	1.35	1.25
11	Ac	38	GLU	CD-OE2	8.74	1.35	1.25
11	Ac	61	GLU	CD-OE2	8.74	1.35	1.25
60	Bh	44	GLU	CD-OE2	8.73	1.35	1.25
56	Bd	111	GLU	CD-OE2	8.72	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	Bn	215	GLU	CD-OE2	8.71	1.35	1.25
9	Aa	269	GLU	CD-OE2	8.71	1.35	1.25
57	Be	143	GLU	CD-OE2	8.71	1.35	1.25
11	Ac	103	GLU	CD-OE2	8.70	1.35	1.25
9	Aa	49	GLU	CD-OE2	8.70	1.35	1.25
57	Be	66	GLU	CD-OE2	8.70	1.35	1.25
11	Ac	20	GLU	CD-OE2	8.70	1.35	1.25
55	Bc	145	GLU	CD-OE2	8.70	1.35	1.25
59	Bg	305	GLU	CD-OE2	8.70	1.35	1.25
57	Be	14	GLU	CD-OE2	8.69	1.35	1.25
58	Bf	220	GLU	CD-OE2	8.68	1.35	1.25
55	Bc	64	GLU	CD-OE2	8.68	1.35	1.25
66	Bn	24	GLU	CD-OE2	8.68	1.35	1.25
56	Bd	161	GLU	CD-OE2	8.66	1.35	1.25
58	Bf	210	GLU	CD-OE2	8.66	1.35	1.25
68	Bp	182	GLU	CD-OE2	8.66	1.35	1.25
58	Bf	109	GLU	CD-OE2	8.66	1.35	1.25
60	Bh	149	GLU	CD-OE2	8.64	1.35	1.25
9	Aa	273	GLU	CD-OE2	8.63	1.35	1.25
56	Bd	160	GLU	CD-OE2	8.62	1.35	1.25
11	Ac	23	GLU	CD-OE2	8.62	1.35	1.25
56	Bd	93	GLU	CD-OE2	8.62	1.35	1.25
58	Bf	148	GLU	CD-OE2	8.60	1.35	1.25
66	Bn	123	GLU	CD-OE2	8.59	1.35	1.25
57	Be	107	GLU	CD-OE2	8.58	1.35	1.25
11	Ac	47	GLU	CD-OE2	8.57	1.35	1.25
63	Bk	71	GLU	CD-OE2	8.56	1.35	1.25
11	Ac	68	GLU	CD-OE2	8.53	1.35	1.25
66	Bn	212	GLU	CD-OE2	8.53	1.35	1.25
11	Ac	128	GLU	CD-OE2	8.50	1.35	1.25
11	Ac	81	GLU	CD-OE2	8.50	1.34	1.25
66	Bn	132	GLU	CD-OE2	8.49	1.34	1.25
56	Bd	84	GLU	CD-OE2	8.48	1.34	1.25
59	Bg	303	GLU	CD-OE2	8.44	1.34	1.25
66	Bn	128	GLU	CD-OE2	8.43	1.34	1.25
11	Ac	135	GLU	CD-OE2	8.42	1.34	1.25
74	Bu	37	GLU	CD-OE2	8.42	1.34	1.25
55	Bc	165	GLU	CD-OE2	8.41	1.34	1.25
56	Bd	115	LEU	CB-CG	8.33	1.76	1.52
11	Ac	31	GLU	CD-OE2	8.32	1.34	1.25
56	Bd	91	GLU	CD-OE2	8.29	1.34	1.25
60	Bh	145	GLU	CD-OE2	8.29	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	Bn	237	GLU	CD-OE2	8.21	1.34	1.25
57	Be	44	GLU	CD-OE2	8.14	1.34	1.25
9	Aa	262	GLU	CD-OE2	8.10	1.34	1.25
66	Bn	198	ILE	N-CA	8.09	1.62	1.46
63	Bk	124	GLU	CD-OE2	7.84	1.34	1.25
58	Bf	119	GLU	CD-OE2	7.78	1.34	1.25
54	Bb	181	GLU	CD-OE2	7.72	1.34	1.25
57	Be	120	GLU	CD-OE2	7.60	1.34	1.25
57	Be	152	GLU	CD-OE2	7.18	1.33	1.25
16	Ai	12	VAL	CA-CB	-6.67	1.40	1.54
66	Bn	197	HIS	CA-C	6.55	1.70	1.52
56	Bd	115	LEU	CA-CB	6.42	1.68	1.53
67	Bo	52	MET	C-N	6.18	1.48	1.34
66	Bn	236	GLU	CD-OE2	5.30	1.31	1.25

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Bf	196	ARG	CA-CB-CG	16.48	149.66	113.40
56	Bd	115	LEU	CB-CG-CD1	15.28	136.98	111.00
54	Bb	211	GLY	C-N-CA	13.91	156.47	121.70
78	Bx	38	PHE	CB-CA-C	13.85	138.10	110.40
18	Ak	99	ALA	N-CA-CB	13.56	129.09	110.10
60	Bh	20	ARG	CA-C-N	-12.35	90.04	117.20
56	Bd	115	LEU	CA-CB-CG	11.99	142.88	115.30
60	Bh	20	ARG	N-CA-C	-11.71	79.39	111.00
58	Bf	197	LYS	CB-CA-C	11.17	132.73	110.40
60	Bh	8	TYR	CB-CG-CD1	-10.98	114.41	121.00
9	Aa	14	HIS	CA-CB-CG	10.32	131.14	113.60
66	Bn	236	GLU	CA-CB-CG	10.32	136.09	113.40
78	Bx	41	ARG	NE-CZ-NH1	9.85	125.23	120.30
66	Bn	78	TYR	CB-CG-CD1	-9.80	115.12	121.00
66	Bn	199	MET	CA-CB-CG	9.39	129.26	113.30
56	Bd	115	LEU	CD1-CG-CD2	-9.38	82.36	110.50
66	Bn	237	GLU	CA-CB-CG	9.29	133.85	113.40
9	Aa	64	HIS	N-CA-CB	-9.18	94.08	110.60
14	Ag	122	ARG	O-C-N	-8.98	108.33	122.70
66	Bn	71	ASP	CB-CG-OD1	8.90	126.31	118.30
66	Bn	78	TYR	CB-CG-CD2	8.84	126.31	121.00
82	B2	17	THR	C-N-CA	-8.71	99.93	121.70
56	Bd	130	PHE	CA-C-O	-8.48	102.29	120.10
66	Bn	107	ARG	NE-CZ-NH1	-8.46	116.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Bb	211	GLY	O-C-N	-8.45	109.18	122.70
54	Bb	211	GLY	CA-C-N	8.40	135.69	117.20
66	Bn	29	TYR	CB-CG-CD1	-8.36	115.98	121.00
78	Bx	38	PHE	CB-CG-CD1	-8.28	115.00	120.80
9	Aa	306	LEU	CB-CG-CD1	8.26	125.04	111.00
58	Bf	137	ARG	NE-CZ-NH1	8.20	124.40	120.30
9	Aa	63	SER	C-N-CA	8.11	141.99	121.70
56	Bd	115	LEU	CB-CG-CD2	8.11	124.79	111.00
68	Bp	90	PRO	N-CA-C	8.07	133.09	112.10
66	Bn	238	MET	CG-SD-CE	8.06	113.10	100.20
68	Bp	191	GLU	CB-CA-C	7.94	126.28	110.40
65	Bm	81	TYR	CB-CG-CD2	-7.84	116.30	121.00
66	Bn	107	ARG	NE-CZ-NH2	-7.81	116.40	120.30
60	Bh	20	ARG	O-C-N	7.77	135.13	122.70
56	Bd	115	LEU	N-CA-CB	7.53	125.45	110.40
54	Bb	212	GLN	N-CA-CB	7.42	123.96	110.60
65	Bm	106	ALA	CB-CA-C	-7.25	99.22	110.10
66	Bn	203	VAL	CG1-CB-CG2	7.25	122.50	110.90
66	Bn	81	GLU	CB-CA-C	7.24	124.89	110.40
66	Bn	198	ILE	N-CA-CB	7.22	127.41	110.80
60	Bh	31	ARG	NE-CZ-NH1	7.18	123.89	120.30
56	Bd	13	ARG	NE-CZ-NH1	7.18	123.89	120.30
9	Aa	18	VAL	CA-CB-CG2	7.11	121.57	110.90
66	Bn	107	ARG	NH1-CZ-NH2	7.06	127.17	119.40
16	Ai	12	VAL	CA-CB-CG1	-7.04	100.34	110.90
66	Bn	198	ILE	CA-CB-CG2	7.04	124.97	110.90
57	Be	88	PHE	CB-CG-CD2	-6.98	115.91	120.80
60	Bh	20	ARG	CA-C-O	6.96	134.71	120.10
78	Bx	41	ARG	CB-CG-CD	6.92	129.59	111.60
54	Bb	284	TYR	CB-CG-CD1	-6.90	116.86	121.00
58	Bf	196	ARG	CD-NE-CZ	6.74	133.03	123.60
66	Bn	197	HIS	CA-C-N	6.74	132.03	117.20
56	Bd	130	PHE	CA-C-N	6.73	132.01	117.20
9	Aa	302	TYR	CB-CG-CD1	-6.69	116.99	121.00
11	Ac	25	LEU	CB-CG-CD1	-6.69	99.63	111.00
59	Bg	295	PRO	N-CA-CB	6.67	111.31	103.30
56	Bd	132	VAL	CG1-CB-CG2	-6.65	100.26	110.90
58	Bf	197	LYS	N-CA-CB	6.64	122.55	110.60
66	Bn	103	LEU	CB-CG-CD1	6.62	122.25	111.00
55	Bc	178	ASP	CB-CG-OD1	6.60	124.24	118.30
66	Bn	198	ILE	CG1-CB-CG2	-6.58	96.93	111.40
66	Bn	197	HIS	CB-CA-C	6.57	123.53	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	Bn	235	MET	CB-CA-C	6.55	123.49	110.40
9	Aa	64	HIS	C-N-CA	6.51	137.98	121.70
56	Bd	166	PHE	CB-CG-CD2	-6.51	116.24	120.80
18	Ak	98	ARG	C-N-CA	6.47	137.88	121.70
58	Bf	137	ARG	NE-CZ-NH2	-6.47	117.06	120.30
66	Bn	239	TYR	CB-CG-CD2	-6.46	117.12	121.00
73	Bt	78	TYR	CA-CB-CG	-6.45	101.14	113.40
66	Bn	246	ILE	CG1-CB-CG2	-6.33	97.47	111.40
9	Aa	65	PHE	N-CA-CB	6.26	121.87	110.60
66	Bn	87	VAL	N-CA-C	6.25	127.89	111.00
16	Ai	12	VAL	CG1-CB-CG2	6.23	120.86	110.90
9	Aa	308	ARG	NE-CZ-NH2	-6.19	117.21	120.30
53	Ba	123	ARG	CB-CA-C	-6.18	98.04	110.40
78	Bx	38	PHE	O-C-N	-6.12	112.90	122.70
9	Aa	84	ASP	CA-CB-CG	-6.12	99.93	113.40
65	Bm	62	TYR	CA-CB-CG	-6.08	101.84	113.40
60	Bh	59	LEU	CB-CG-CD1	-6.07	100.68	111.00
55	Bc	261	ASP	CB-CG-OD1	6.06	123.76	118.30
58	Bf	207	VAL	CG1-CB-CG2	-6.06	101.20	110.90
66	Bn	85	TYR	CB-CG-CD1	-6.04	117.38	121.00
13	Ae	124	MET	CG-SD-CE	-6.03	90.56	100.20
21	An	21	CYS	N-CA-CB	6.02	121.43	110.60
58	Bf	156	VAL	CG1-CB-CG2	-6.01	101.29	110.90
66	Bn	32	ARG	NE-CZ-NH1	5.97	123.29	120.30
82	B2	8	PHE	CB-CA-C	-5.93	98.54	110.40
78	Bx	39	LYS	N-CA-C	5.92	126.98	111.00
54	Bb	233	ARG	NE-CZ-NH1	5.92	123.26	120.30
66	Bn	199	MET	CA-C-N	5.91	128.03	116.20
54	Bb	210	PHE	C-N-CA	5.89	134.68	122.30
11	Ac	32	ASP	CB-CG-OD1	5.89	123.60	118.30
24	As	98	ASN	C-N-CA	-5.88	109.94	122.30
78	Bx	38	PHE	CA-C-N	5.88	130.15	117.20
57	Be	10	VAL	O-C-N	-5.87	113.30	122.70
56	Bd	163	MET	CG-SD-CE	-5.87	90.81	100.20
19	Al	103	ALA	N-CA-CB	5.83	118.27	110.10
56	Bd	120	ASP	CB-CG-OD1	5.83	123.55	118.30
64	Bl	91	ALA	N-CA-C	-5.82	95.28	111.00
63	Bk	59	ASP	CB-CG-OD1	5.82	123.53	118.30
58	Bf	190	LEU	CB-CG-CD2	5.79	120.84	111.00
78	Bx	38	PHE	CA-CB-CG	5.78	127.77	113.90
58	Bf	196	ARG	CB-CG-CD	5.78	126.62	111.60
14	Ag	38	TYR	CA-CB-CG	-5.74	102.49	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Ag	122	ARG	CA-C-N	5.73	129.81	117.20
71	Br	139	TYR	CA-CB-CG	-5.67	102.62	113.40
14	Ag	25	THR	CA-CB-CG2	-5.66	104.48	112.40
71	Br	109	VAL	CB-CA-C	-5.64	100.68	111.40
57	Be	31	ARG	CA-CB-CG	5.64	125.80	113.40
55	Bc	167	VAL	CA-CB-CG2	5.63	119.35	110.90
77	Bw	127	VAL	N-CA-C	-5.62	95.83	111.00
63	Bk	21	PRO	CA-N-CD	-5.58	103.69	111.50
53	Ba	223	SER	N-CA-CB	5.55	118.83	110.50
66	Bn	77	ARG	CD-NE-CZ	5.55	131.37	123.60
9	Aa	100	ARG	NE-CZ-NH1	5.54	123.07	120.30
64	Bl	104	VAL	CB-CA-C	-5.54	100.87	111.40
63	Bk	54	ALA	CB-CA-C	5.53	118.39	110.10
55	Bc	129	CYS	CA-CB-SG	-5.53	104.06	114.00
24	As	117	GLY	N-CA-C	-5.52	99.30	113.10
54	Bb	282	LYS	N-CA-CB	-5.51	100.69	110.60
78	Bx	36	VAL	CA-CB-CG2	-5.48	102.68	110.90
22	Ao	77	TYR	CG-CD2-CE2	-5.48	116.92	121.30
74	Bu	25	ASP	CB-CG-OD1	5.46	123.21	118.30
22	Ao	37	ARG	NE-CZ-NH1	5.43	123.02	120.30
16	Ai	115	TYR	C-N-CA	5.43	135.27	121.70
77	Bw	246	THR	C-N-CA	-5.42	108.14	121.70
66	Bn	199	MET	CB-CA-C	-5.41	99.58	110.40
68	Bp	191	GLU	N-CA-CB	5.41	120.33	110.60
65	Bm	81	TYR	CB-CG-CD1	5.39	124.23	121.00
12	Ad	67	TYR	CA-CB-CG	-5.37	103.20	113.40
9	Aa	35	SER	N-CA-CB	-5.36	102.46	110.50
18	Ak	34	PHE	CB-CA-C	5.35	121.10	110.40
14	Ag	81	ARG	N-CA-C	-5.35	96.57	111.00
70	Bq	64	TYR	CA-CB-CG	-5.34	103.25	113.40
15	Ah	46	TYR	CA-CB-CG	-5.32	103.30	113.40
72	Bs	117	TYR	CA-CB-CG	-5.31	103.31	113.40
56	Bd	131	TYR	N-CA-CB	5.29	120.13	110.60
57	Be	132	VAL	CG1-CB-CG2	5.27	119.34	110.90
9	Aa	34	ALA	CB-CA-C	-5.26	102.20	110.10
54	Bb	279	ILE	CB-CA-C	5.26	122.13	111.60
9	Aa	306	LEU	CB-CA-C	5.26	120.20	110.20
14	Ag	107	ASN	CA-CB-CG	-5.25	101.86	113.40
56	Bd	136	ARG	NE-CZ-NH2	5.22	122.91	120.30
14	Ag	112	LEU	CB-CA-C	-5.21	100.29	110.20
11	Ac	65	ARG	NE-CZ-NH2	5.20	122.90	120.30
63	Bk	127	ASP	CB-CG-OD1	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Bb	57	ARG	NE-CZ-NH1	5.20	122.90	120.30
10	Ab	164	ASN	CB-CA-C	-5.17	100.06	110.40
54	Bb	241	ARG	NE-CZ-NH1	5.16	122.88	120.30
66	Bn	198	ILE	N-CA-C	5.14	124.88	111.00
66	Bn	91	LEU	N-CA-CB	-5.13	100.14	110.40
66	Bn	95	ALA	CB-CA-C	5.13	117.79	110.10
9	Aa	84	ASP	CB-CG-OD2	-5.12	113.69	118.30
67	Bo	31	TYR	CB-CA-C	-5.10	100.20	110.40
10	Ab	36	TYR	CA-CB-CG	-5.09	103.73	113.40
9	Aa	17	TRP	C-N-CA	5.09	134.42	121.70
56	Bd	132	VAL	CA-CB-CG2	5.09	118.53	110.90
78	Bx	41	ARG	CD-NE-CZ	5.08	130.72	123.60
66	Bn	195	ARG	NE-CZ-NH2	5.08	122.84	120.30
9	Aa	100	ARG	CD-NE-CZ	5.08	130.71	123.60
14	Ag	80	GLY	C-N-CA	-5.07	109.02	121.70
54	Bb	281	LYS	CB-CA-C	-5.06	100.28	110.40
82	B2	18	LEU	C-N-CA	5.05	134.34	121.70
60	Bh	118	PHE	CB-CG-CD1	-5.05	117.27	120.80
56	Bd	107	PHE	CB-CG-CD2	5.04	124.33	120.80
71	Br	109	VAL	CG1-CB-CG2	5.04	118.96	110.90
66	Bn	198	ILE	CB-CA-C	-5.03	101.53	111.60
54	Bb	213	ASP	N-CA-C	5.03	124.57	111.00
68	Bp	190	LYS	CA-C-O	-5.02	109.55	120.10
9	Aa	62	HIS	CA-CB-CG	5.02	122.13	113.60
58	Bf	204	PHE	CB-CA-C	5.02	120.44	110.40
55	Bc	55	GLU	CB-CA-C	5.02	120.43	110.40
9	Aa	56	GLN	CB-CA-C	5.01	120.43	110.40
22	Ao	77	TYR	CB-CG-CD1	-5.01	117.99	121.00
79	By	59	GLY	N-CA-C	-5.01	100.57	113.10
60	Bh	133	VAL	CA-CB-CG2	-5.01	103.39	110.90
58	Bf	119	GLU	OE1-CD-OE2	-5.01	117.29	123.30

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	Mainchain,Peptide
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	Mainchain,Peptide
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	Sidechain,Mainchain,Peptide

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	1	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	0	0
9	Aa	2380	0	2337	0	0
10	Ab	1521	0	1531	0	0
11	Ac	1498	0	1575	0	0
12	Ad	845	0	879	0	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	0	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	0	0
22	Ao	710	0	743	0	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	102	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	0	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	0	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	0	0
49	BW	16	0	0	0	0
50	BX	113	0	0	0	0
51	BY	115	0	0	0	0
52	BZ	72	0	0	4	0
53	Ba	1867	0	1961	0	0
54	Bb	2765	0	2877	0	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	0	0
63	Bk	927	0	986	0	0
64	Bl	951	0	985	0	0
65	Bm	1454	0	1498	0	0
66	Bn	1912	0	1887	0	0
67	Bo	956	0	1057	0	0
68	Bp	1329	0	1449	0	0
69	B7	129	0	152	9	0
70	Bq	773	0	829	0	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	0	0
78	Bx	670	0	710	0	0
79	By	514	0	578	0	0
80	B9	460	0	481	80	0
81	Bz	548	0	567	0	0
82	B2	407	0	423	148	0
83	B3	429	0	466	84	0
84	B4	760	0	820	143	0
85	B5	1621	0	1559	330	0
86	B6	874	0	920	191	0
All	All	55531	0	52502	984	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 80.

All (984) 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:B0:4255: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
26:B0:4192:U:P	84:B4:2:VAL:HG21	1.53	1.48
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
26:B0:4322:A:P	84:B4:34:TYR:CG	2.14	1.37
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
25:B1:54:A:P	83:B3:21:ARG:CG	2.16	1.33
26:B0:4323:A:P	84:B4:36:GLN:N	2.01	1.33
26:B0:2768:C:P	82:B2:11:ARG:HH22	1.53	1.30
26:B0:364:G:P	82:B2:36:LYS:HE2	1.72	1.29
26:B0:4021:A:P	85:B5:199:TYR:CZ	2.25	1.28
26:B0:4255:U:P	84:B4:13:LYS:CE	2.20	1.27
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B0:4023:U:P	85:B5:31:LEU:O	1.98	1.20
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
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
26:B0:1581:U:P	82:B2:3:LYS:HG2	1.87	1.14
26:B0:1511:G:P	82:B2:16:HIS:CE1	2.41	1.13
86:B6:96:ILE:HD13	86:B6:105:ILE:HD11	1.26	1.13
86:B6:81:LEU:HD22	86:B6:91:VAL:HB	1.33	1.11
84:B4:70:LEU:HD11	84:B4:83:LEU:HD11	1.28	1.10
80:B9:87:VAL:HG12	80:B9:89:LEU:H	1.17	1.08
26:B0:4330:G:P	84:B4:85:ILE:HD13	1.93	1.08
85:B5:106:ALA:HB1	85:B5:110:LEU:HD12	1.35	1.08
85:B5:74:VAL:HG21	85:B5:142:ILE:HD12	1.36	1.07
84:B4:34:TYR:HA	84:B4:38:LYS:HD2	1.32	1.07
26:B0:2292:G:P	80:B9:71:PRO:HG3	1.96	1.06
83:B3:23:ILE:HG21	83:B3:35:ILE:HG22	1.32	1.06
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
85:B5:103:PHE:HB3	85:B5:145:MET:HE2	1.36	1.06
26:B0:4323:A:P	84:B4:36:GLN:CA	2.44	1.05
82:B2:18:LEU:HB2	82:B2:25:LYS:HA	1.34	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
84:B4:40:ARG:HA	84:B4:44:LYS:HB3	1.38	1.03
26:B0:4330:G:P	84:B4:85:ILE:CD1	2.47	1.03
85:B5:202:THR:HG23	85:B5:205:GLY:H	1.24	1.00
85:B5:84:LEU:HD23	85:B5:110:LEU:HD21	1.42	0.99
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
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
83:B3:27:ILE:HG12	83:B3:35:ILE:HD12	1.43	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
86:B6:51:ASN:HB3	86:B6:78:ASN:HD21	1.30	0.96
85:B5:159:PHE:CZ	85:B5:161:THR:HB	2.00	0.95
26:B0:4324:G:P	84:B4:36:GLN:OE1	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
86:B6:79:ILE:HG22	86:B6:90:ARG:HG2	1.50	0.94
26:B0:2650:G:P	86:B6:91:VAL:HA	2.09	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
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
85:B5:84:LEU:CD2	85:B5:110:LEU:HD21	1.98	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
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
85:B5:5:ILE:CD1	85:B5:177:ILE:HG21	1.99	0.91
85:B5:159:PHE:CE2	85:B5:161:THR:HB	2.05	0.91
82:B2:18:LEU:HD23	82:B2:24:SER:H	1.34	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
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
82:B2:18:LEU:HD12	82:B2:19:CYS:H	1.33	0.90
86:B6:26:LYS:HB3	86:B6:97:ILE:HG12	1.53	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
86:B6:77:ASN:HB3	86:B6:79:ILE:CD1	2.01	0.90
85:B5:59:ILE:CD1	85:B5:145:MET:HB3	2.00	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
84:B4:69:ARG:CG	84:B4:80:LYS:HD3	2.02	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
26:B0:4322:A:P	84:B4:34:TYR:C	2.49	0.89
85:B5:87:LEU:HB3	85:B5:117:TYR:CZ	2.05	0.89
25:B1:105:A:P	82:B2:39:TYR:HE2	1.94	0.89
85:B5:62:PHE:CZ	85:B5:81:GLU:HA	2.07	0.89
85:B5:74:VAL:CG2	85:B5:139:VAL:HA	2.03	0.89
82:B2:18:LEU:HD12	82:B2:27:TYR:HB2	1.52	0.89
26:B0:1581:U:P	82:B2:3:LYS:CG	2.62	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:74:VAL:HG11	85:B5:142:ILE:CG2	2.03	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
85:B5:74:VAL:HG11	85:B5:142:ILE:HB	1.56	0.87
85:B5:151:LEU:HA	85:B5:159:PHE:CE1	2.10	0.87
26:B0:4322:A:P	84:B4:34:TYR:CB	0.97	0.87
80:B9:82:VAL:HG23	80:B9:83:LYS:HD2	1.55	0.87
86:B6:77:ASN:HB3	86:B6:79:ILE:HD13	1.55	0.86
86:B6:96:ILE:HD13	86:B6:105:ILE:CD1	2.05	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
85:B5:60:VAL:HG21	85:B5:104:PHE:CD2	2.10	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
85:B5:34:LEU:HD21	85:B5:40:SER:HB3	1.58	0.85
69:B7:198:ARG:HA	69:B7:201:ARG:HE	1.42	0.85
86:B6:44:LYS:HD3	86:B6:98:ASP:HA	1.58	0.85
82:B2:28:HIS:C	82:B2:31:LYS:HE2	1.96	0.85
85:B5:59:ILE:HD13	85:B5:145:MET:HB3	1.59	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
86:B6:50:ASN:HD22	86:B6:76:GLY:HA2	1.42	0.84
85:B5:62:PHE:CD1	85:B5:110:LEU:HG	2.12	0.84
85:B5:103:PHE:CZ	85:B5:148:THR:HG23	2.12	0.84
80:B9:92:ASN:HB3	80:B9:119:ALA:O	1.78	0.84
82:B2:27:TYR:CE1	82:B2:29:LEU:HD13	2.13	0.84
86:B6:37:MET:HE1	86:B6:97:ILE:HA	1.58	0.84
26:B0:4250:U:P	84:B4:9:ARG:HH12	2.00	0.84
85:B5:62:PHE:CZ	85:B5:81:GLU:HG2	2.12	0.84
86:B6:81:LEU:HD21	86:B6:94:LEU:HG	1.59	0.84
85:B5:84:LEU:HD11	85:B5:118:LEU:CD2	2.07	0.83
85:B5:74:VAL:HG11	85:B5:142:ILE:CB	2.09	0.83
26:B0:4322:A:P	84:B4:34:TYR:HB2	0.29	0.83
86:B6:4:ALA:HB3	86:B6:73:HIS:CD2	2.13	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
84:B4:23:VAL:HG23	84:B4:70:LEU:HD23	1.61	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
26:B0:2384:G:P	83:B3:44:TRP:HB3	2.20	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B6:45:LEU:HD12	86:B6:71:VAL:CB	2.09	0.82
80:B9:114:ARG:O	80:B9:118:LEU:HD13	1.78	0.82
83:B3:24:PRO:O	83:B3:27:ILE:HG22	1.78	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
84:B4:69:ARG:CD	84:B4:80:LYS:HD3	2.10	0.81
85:B5:74:VAL:CG2	85:B5:142:ILE:HD12	2.10	0.81
83:B3:23:ILE:CG2	83:B3:35:ILE:HG22	2.10	0.81
25:B1:54:A:P	83:B3:21:ARG:CD	2.69	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
85:B5:5:ILE:CD1	85:B5:177:ILE:HD13	2.09	0.81
85:B5:62:PHE:CD2	85:B5:110:LEU:HG	2.14	0.81
80:B9:87:VAL:HG12	80:B9:89:LEU:N	1.96	0.81
85:B5:143:GLU:CA	85:B5:146:LYS:HE2	2.10	0.80
85:B5:117:TYR:CD2	85:B5:118:LEU:HD22	2.16	0.80
86:B6:17:ARG:HH12	86:B6:108:MET:HB2	1.45	0.80
85:B5:78:VAL:C	85:B5:79:LEU:HD12	2.02	0.80
26:B0:4323:A:P	84:B4:36:GLN:HA	2.20	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
26:B0:364:G:P	82:B2:36:LYS:CE	2.66	0.80
25:B1:105:A:P	82:B2:39:TYR:CE2	2.74	0.80
85:B5:58:THR:HG23	85:B5:101:THR:HA	1.64	0.80
85:B5:111:MET:CE	85:B5:131:PRO:HG3	2.12	0.80
82:B2:27:TYR:HE1	82:B2:29:LEU:HD13	1.46	0.80
84:B4:14:LYS:HE3	84:B4:14:LYS:HA	1.63	0.80
69:B7:195:ILE:O	69:B7:199:LEU:HD13	1.82	0.80
85:B5:105:ILE:HG21	85:B5:132:LEU:HD23	1.62	0.79
26:B0:4323:A:P	84:B4:35:ALA:C	2.60	0.79
26:B0:1597:G:P	82:B2:10:LYS:CG	2.71	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
85:B5:45:GLU:OE2	85:B5:188:LEU:HD11	1.83	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
85:B5:138:VAL:O	85:B5:141:VAL:HG22	1.83	0.78
84:B4:65:LYS:CB	84:B4:85:ILE:HG12	2.12	0.78
80:B9:78:LEU:HD23	80:B9:79:VAL:N	1.97	0.78
26:B0:1511:G:P	82:B2:16:HIS:HE1	2.01	0.78
86:B6:31:TYR:O	86:B6:34:THR:HG22	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:48:VAL:HG21	85:B5:144:ARG:HE	1.49	0.78
86:B6:45:LEU:HB2	86:B6:71:VAL:HB	1.64	0.78
86:B6:44:LYS:HB2	86:B6:96:ILE:HG23	1.64	0.78
85:B5:190:LYS:H	85:B5:190:LYS:HD3	1.49	0.78
85:B5:192:PRO:O	85:B5:195:ILE:HG22	1.83	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
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
26:B0:2383:G:P	83:B3:48:LYS:HD2	2.23	0.77
82:B2:31:LYS:CD	82:B2:33:THR:H	1.96	0.77
26:B0:4322:A:P	84:B4:34:TYR:HB3	1.37	0.77
86:B6:21:VAL:HG21	86:B6:96:ILE:CD1	2.14	0.77
85:B5:58:THR:HG21	85:B5:100:ASP:O	1.84	0.77
80:B9:75:ARG:HB3	80:B9:95:TYR:CD2	2.18	0.77
84:B4:2:VAL:HA	84:B4:90:HIS:CE1	2.18	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
80:B9:87:VAL:CG1	80:B9:89:LEU:HD23	2.15	0.77
85:B5:58:THR:HG21	85:B5:101:THR:HA	1.67	0.77
85:B5:104:PHE:CZ	85:B5:122:LEU:HD21	2.20	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
82:B2:18:LEU:HD22	82:B2:26:ALA:H	1.48	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
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
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
80:B9:100:ALA:O	80:B9:103:VAL:HG22	1.86	0.76
26:B0:2384:G:P	83:B3:44:TRP:CB	2.73	0.76
85:B5:198:VAL:HG22	85:B5:210:VAL:HG22	1.68	0.76
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
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
85:B5:163:VAL:CG1	85:B5:173:ILE:HG23	2.15	0.75
86:B6:21:VAL:HG21	86:B6:96:ILE:HD12	1.68	0.75
26:B0:2278:C:P	80:B9:103:VAL:HA	2.26	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:B2:28:HIS:O	82:B2:31:LYS:HG3	1.87	0.75
82:B2:15:THR:HG22	82:B2:16:HIS:H	1.51	0.75
82:B2:31:LYS:HE3	82:B2:32:SER:HA	1.68	0.75
80:B9:79:VAL:HG23	80:B9:84:GLU:CB	2.17	0.75
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
85:B5:202:THR:HG23	85:B5:205:GLY:N	2.00	0.74
80:B9:81:ASN:HD22	80:B9:83:LYS:H	1.34	0.74
26:B0:4250:U:P	84:B4:9:ARG:NH2	2.60	0.74
83:B3:27:ILE:HD12	83:B3:30:LYS:HD2	1.69	0.74
26:B0:2757:C:P	83:B3:7:PHE:CE1	2.77	0.74
86:B6:44:LYS:HB2	86:B6:96:ILE:CG2	2.18	0.74
82:B2:24:SER:C	82:B2:25:LYS:HD2	2.08	0.74
86:B6:79:ILE:HD13	86:B6:79:ILE:H	1.52	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
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
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
84:B4:34:TYR:CA	84:B4:38:LYS:HD2	2.16	0.73
86:B6:45:LEU:HD12	86:B6:71:VAL:CG1	2.18	0.73
26:B0:4255:U:P	84:B4:13:LYS:NZ	2.61	0.73
80:B9:81:ASN:HD21	80:B9:83:LYS:HB2	1.54	0.73
26:B0:4191:C:P	84:B4:2:VAL:HG12	2.29	0.73
26:B0:22:G:P	82:B2:44:LYS:NZ	2.61	0.73
85:B5:87:LEU:HB3	85:B5:117:TYR:CE2	2.23	0.73
25:B1:54:A:P	83:B3:21:ARG:CB	2.76	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
80:B9:99:ILE:CG2	80:B9:103:VAL:HG21	2.18	0.73
86:B6:29:LEU:HD21	86:B6:87:LYS:HE3	1.68	0.73
86:B6:81:LEU:O	86:B6:81:LEU:HD23	1.88	0.73
86:B6:26:LYS:HB3	86:B6:97:ILE:CG1	2.19	0.73
83:B3:41:ARG:HB3	83:B3:41:ARG:NH1	2.03	0.73
85:B5:36:LEU:O	85:B5:36:LEU:HD23	1.89	0.73
86:B6:18:LEU:HD13	86:B6:18:LEU:O	1.88	0.73
86:B6:81:LEU:HD21	86:B6:94:LEU:CG	2.18	0.73
86:B6:49:ALA:HB3	86:B6:52:CYS:SG	2.29	0.72
86:B6:6:LYS:HD2	86:B6:14:ILE:HD13	1.71	0.72
26:B0:53:C:P	82:B2:47:TYR:HE1	2.11	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:60:VAL:HG13	85:B5:101:THR:CG2	2.19	0.72
85:B5:27:LEU:CD1	85:B5:29:VAL:HG23	2.19	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
80:B9:70:LEU:HD11	80:B9:76:LYS:HB3	1.71	0.72
85:B5:60:VAL:HG22	85:B5:103:PHE:O	1.89	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
84:B4:14:LYS:CE	84:B4:14:LYS:HA	2.19	0.72
82:B2:4:GLY:HA3	82:B2:8:PHE:CZ	2.23	0.72
85:B5:43:VAL:HG12	85:B5:151:LEU:O	1.90	0.72
26:B0:2650:G:P	86:B6:92:CYS:N	2.60	0.72
86:B6:91:VAL:HG11	86:B6:94:LEU:CD2	2.20	0.71
85:B5:60:VAL:HG23	85:B5:104:PHE:HA	1.72	0.71
26:B0:4330:G:P	84:B4:85:ILE:HD11	2.27	0.71
83:B3:5:LYS:HB2	83:B3:9:ILE:CG2	2.20	0.71
85:B5:29:VAL:HG22	85:B5:198:VAL:HG12	1.73	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
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
84:B4:75:PRO:HG2	84:B4:77:CYS:H	1.55	0.71
84:B4:69:ARG:HB3	84:B4:80:LYS:CD	2.21	0.71
86:B6:48:LEU:HD12	86:B6:74:TYR:CZ	2.25	0.71
84:B4:35:ALA:O	84:B4:38:LYS:HG2	1.91	0.71
84:B4:91:PHE:CE2	84:B4:93:LEU:HD21	2.26	0.71
85:B5:151:LEU:HD12	85:B5:159:PHE:CZ	2.26	0.71
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
82:B2:18:LEU:HD23	82:B2:24:SER:CA	2.21	0.70
85:B5:195:ILE:HD11	85:B5:198:VAL:CG1	2.21	0.70
86:B6:32:LYS:HG2	86:B6:36:LYS:HE3	1.73	0.70
85:B5:34:LEU:HD13	85:B5:35:ASP:N	2.06	0.70
82:B2:18:LEU:HD13	82:B2:26:ALA:C	2.12	0.70
80:B9:70:LEU:HD11	80:B9:76:LYS:CB	2.22	0.70
85:B5:74:VAL:HG21	85:B5:142:ILE:CD1	2.20	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
25:B1:55:G:P	83:B3:21:ARG:NH2	2.65	0.70
85:B5:151:LEU:HA	85:B5:159:PHE:CZ	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:27:LEU:HG	85:B5:180:ILE:HD11	1.74	0.70
26:B0:4022:C:P	85:B5:197:THR:H	2.15	0.69
85:B5:43:VAL:HG13	85:B5:188:LEU:HD12	1.72	0.69
83:B3:13:LEU:HD23	83:B3:49:LEU:CD2	2.22	0.69
26:B0:4021:A:P	85:B5:199:TYR:CE1	2.84	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:B0:2292:G:P	80:B9:71:PRO:CG	2.78	0.69
26:B0:53:C:P	82:B2:47:TYR:CE1	2.85	0.69
86:B6:71:VAL:HG22	86:B6:112:THR:OG1	1.92	0.69
80:B9:76:LYS:O	80:B9:76:LYS:HD2	1.91	0.69
82:B2:10:LYS:HE3	82:B2:12:ARG:N	2.07	0.69
69:B7:196:LEU:O	69:B7:200:LEU:HG	1.93	0.69
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
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
85:B5:34:LEU:CD2	85:B5:41:ASN:HD22	2.06	0.68
84:B4:19:GLN:OE1	84:B4:74:GLU:HB3	1.92	0.68
85:B5:38:ASP:HB3	85:B5:39:PRO:HD2	1.76	0.68
80:B9:88:LEU:O	80:B9:88:LEU:HD13	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
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
82:B2:28:HIS:O	82:B2:31:LYS:HE2	1.94	0.68
85:B5:103:PHE:CB	85:B5:145:MET:HE2	2.19	0.68
86:B6:44:LYS:HD3	86:B6:98:ASP:OD1	1.94	0.67
80:B9:92:ASN:HD22	80:B9:120:ILE:HG12	1.59	0.67
86:B6:77:ASN:HB3	86:B6:79:ILE:HD11	1.76	0.67
85:B5:34:LEU:HB3	85:B5:157:ARG:HD3	1.76	0.67
84:B4:68:LEU:HD11	84:B4:91:PHE:CE1	2.30	0.67
85:B5:161:THR:HG21	85:B5:180:ILE:HD13	1.76	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
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
85:B5:111:MET:HE1	85:B5:131:PRO:HG3	1.76	0.67
85:B5:111:MET:HE3	85:B5:131:PRO:HG3	1.76	0.67
25:B1:55:G:P	83:B3:21:ARG:CZ	2.82	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:62:PHE:CE2	85:B5:110:LEU:HG	2.31	0.66
85:B5:43:VAL:HG11	85:B5:151:LEU:CD2	2.25	0.66
80:B9:83:LYS:HD2	80:B9:83:LYS:H	1.60	0.66
86:B6:17:ARG:HD3	86:B6:105:ILE:CD1	2.25	0.66
85:B5:23:GLU:OE1	85:B5:204:MET:HB2	1.96	0.66
85:B5:151:LEU:HD12	85:B5:159:PHE:CG	2.31	0.66
84:B4:66:ILE:HG22	84:B4:68:LEU:HG	1.76	0.66
82:B2:52:LYS:HD3	82:B2:52:LYS:H	1.60	0.66
26:B0:4022:C:P	85:B5:30:ASN:HB3	2.36	0.66
85:B5:59:ILE:HD11	85:B5:145:MET:HB3	1.77	0.66
85:B5:59:ILE:HD11	85:B5:145:MET:C	2.16	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
85:B5:105:ILE:HG21	85:B5:132:LEU:CD2	2.25	0.65
52:BZ:75:C:P	84:B4:54:PRO:HD2	2.37	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
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
84:B4:69:ARG:CB	84:B4:80:LYS:HD3	2.26	0.65
85:B5:62:PHE:CE1	85:B5:110:LEU:HG	2.31	0.65
84:B4:34:TYR:HA	84:B4:38:LYS:CD	2.19	0.65
26:B0:4306:U:P	84:B4:80:LYS:NZ	2.70	0.65
84:B4:65:LYS:HB3	84:B4:85:ILE:CG1	2.20	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
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
85:B5:57:THR:HG22	85:B5:146:LYS:O	1.97	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
84:B4:69:ARG:HB3	84:B4:80:LYS:HD3	1.76	0.64
86:B6:45:LEU:CD1	86:B6:71:VAL:HB	2.26	0.64
26:B0:22:G:P	82:B2:44:LYS:HZ3	2.20	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
85:B5:56:GLU:OE1	85:B5:146:LYS:HD2	1.95	0.64
85:B5:110:LEU:HD13	85:B5:110:LEU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
82:B2:19:CYS:SG	82:B2:20:ARG:HD3	2.38	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
86:B6:79:ILE:HG22	86:B6:90:ARG:CG	2.25	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
80:B9:83:LYS:HD2	80:B9:83:LYS:N	2.13	0.64
85:B5:98:ALA:O	85:B5:127:LYS:HE3	1.98	0.64
80:B9:87:VAL:HG11	80:B9:89:LEU:HB2	1.79	0.64
86:B6:7:THR:HG22	86:B6:8:LYS:N	2.14	0.63
85:B5:150:GLN:NE2	85:B5:152:ARG:HD3	2.12	0.63
85:B5:43:VAL:HG22	85:B5:188:LEU:CD1	2.28	0.63
86:B6:104:ILE:HG13	86:B6:105:ILE:N	2.13	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
86:B6:29:LEU:HD12	86:B6:29:LEU:O	1.99	0.63
84:B4:75:PRO:HG2	84:B4:77:CYS:HB3	1.81	0.63
83:B3:15:LYS:HD2	83:B3:15:LYS:C	2.19	0.63
83:B3:35:ILE:HG23	83:B3:37:TYR:N	2.13	0.63
86:B6:79:ILE:CG2	86:B6:90:ARG:HG2	2.27	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
82:B2:18:LEU:HD22	82:B2:24:SER:HB3	1.81	0.63
85:B5:143:GLU:HG2	85:B5:146:LYS:HE2	1.81	0.63
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
85:B5:195:ILE:HD11	85:B5:198:VAL:HG13	1.79	0.62
86:B6:11:LEU:HD12	86:B6:14:ILE:HD11	1.81	0.62
82:B2:20:ARG:HG2	82:B2:21:ARG:N	2.15	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
26:B0:2384:G:P	83:B3:44:TRP:HB2	2.39	0.62
82:B2:31:LYS:HE3	82:B2:31:LYS:O	1.99	0.62
85:B5:122:LEU:HD12	85:B5:129:PRO:HD3	1.81	0.62
25:B1:45:C:P	83:B3:15:LYS:CE	2.75	0.62
84:B4:39:ARG:H	84:B4:39:ARG:HD3	1.65	0.62
85:B5:43:VAL:HG11	85:B5:151:LEU:CG	2.29	0.62
83:B3:17:GLN:O	83:B3:20:ASN:HB2	1.99	0.61
80:B9:96:CYS:SG	80:B9:121:ARG:HB3	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:B2:31:LYS:HD2	82:B2:33:THR:N	2.09	0.61
85:B5:34:LEU:HD21	85:B5:41:ASN:HD22	1.64	0.61
80:B9:75:ARG:HB3	80:B9:95:TYR:HD2	1.65	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
86:B6:6:LYS:CD	86:B6:14:ILE:HG21	2.31	0.61
85:B5:62:PHE:CZ	85:B5:110:LEU:HG	2.36	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
85:B5:190:LYS:HG2	85:B5:191:GLY:H	1.66	0.61
85:B5:5:ILE:O	85:B5:9:VAL:HG23	2.01	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
86:B6:45:LEU:HD23	86:B6:96:ILE:HG22	1.82	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
80:B9:82:VAL:HG12	80:B9:111:ILE:HA	1.83	0.60
1:AA:1948:C:P	26:B0:2847:A:P	2.99	0.60
84:B4:38:LYS:HG3	84:B4:39:ARG:N	2.16	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
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
85:B5:57:THR:HG22	85:B5:146:LYS:C	2.22	0.60
86:B6:44:LYS:CG	86:B6:98:ASP:HA	2.31	0.60
82:B2:31:LYS:HE3	82:B2:31:LYS:C	2.21	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
80:B9:82:VAL:CG2	80:B9:83:LYS:HD2	2.29	0.60
85:B5:74:VAL:CG1	85:B5:142:ILE:HB	2.31	0.60
85:B5:50:PRO:CG	85:B5:179:VAL:HG21	2.31	0.60
86:B6:4:ALA:HB3	86:B6:73:HIS:NE2	2.17	0.60
85:B5:43:VAL:HG22	85:B5:188:LEU:HD12	1.83	0.59
85:B5:27:LEU:HD13	85:B5:28:ALA:N	2.17	0.59
86:B6:50:ASN:OD1	86:B6:74:TYR:HB3	2.02	0.59
26:B0:2279:C:P	80:B9:104:SER:HB3	2.43	0.59
84:B4:55:ILE:HG22	84:B4:56:PHE:O	2.02	0.59
85:B5:103:PHE:CD1	85:B5:145:MET:HE3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:47:VAL:CG1	85:B5:179:VAL:HG12	2.32	0.59
85:B5:69:LEU:N	85:B5:69:LEU:HD22	2.16	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
26:B0:1597:G:P	82:B2:10:LYS:HG3	2.41	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
82:B2:31:LYS:CE	82:B2:33:THR:H	2.16	0.59
85:B5:149:VAL:HG21	85:B5:161:THR:OG1	2.03	0.59
85:B5:62:PHE:CZ	85:B5:110:LEU:HD23	2.37	0.59
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
82:B2:46:LYS:H	82:B2:46:LYS:HD3	1.68	0.58
82:B2:46:LYS:N	82:B2:46:LYS:HD3	2.18	0.58
85:B5:156:ARG:HG2	85:B5:157:ARG:N	2.16	0.58
85:B5:24:THR:HG22	85:B5:203:THR:OG1	2.03	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
82:B2:43:ARG:HG2	82:B2:44:LYS:N	2.17	0.58
86:B6:15:ASN:ND2	86:B6:80:GLU:HG3	2.18	0.58
80:B9:109:LYS:HA	80:B9:109:LYS:HE3	1.86	0.58
82:B2:19:CYS:HB2	82:B2:27:TYR:HD2	1.68	0.58
82:B2:18:LEU:HD13	82:B2:27:TYR:N	2.17	0.58
86:B6:14:ILE:CG2	86:B6:108:MET:HE2	2.34	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
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
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
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
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
80:B9:81:ASN:HA	80:B9:111:ILE:HD11	1.86	0.57
85:B5:5:ILE:HD13	85:B5:177:ILE:CD1	2.33	0.57
82:B2:3:LYS:C	82:B2:8:PHE:HZ	2.07	0.57
85:B5:122:LEU:CD1	85:B5:129:PRO:HD3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B6:22:MET:HA	86:B6:27:TYR:HD2	1.65	0.57
80:B9:87:VAL:CG1	80:B9:89:LEU:HB2	2.34	0.57
85:B5:98:ALA:CB	85:B5:121:VAL:HG12	2.35	0.57
85:B5:15:ASP:O	85:B5:206:PRO:HD2	2.04	0.57
82:B2:28:HIS:ND1	82:B2:30:GLN:HB3	2.20	0.57
82:B2:18:LEU:HD11	82:B2:34:CYS:SG	2.45	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
80:B9:123:THR:HG23	80:B9:124:ASN:N	2.20	0.57
80:B9:87:VAL:HG12	80:B9:88:LEU:N	2.20	0.57
26:B0:22:G:P	82:B2:44:LYS:HZ1	2.26	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
83:B3:24:PRO:HB2	83:B3:26:TRP:CD1	2.40	0.57
86:B6:66:LEU:C	86:B6:66:LEU:HD13	2.25	0.57
86:B6:31:TYR:CA	86:B6:93:THR:HG21	2.28	0.57
82:B2:19:CYS:HB2	82:B2:27:TYR:CD2	2.39	0.57
82:B2:27:TYR:HD2	82:B2:34:CYS:HG	1.51	0.57
69:B7:193:MET:O	69:B7:197:ARG:HG3	2.04	0.57
83:B3:23:ILE:HD13	83:B3:23:ILE:H	1.69	0.56
84:B4:85:ILE:O	84:B4:85:ILE:HG23	2.05	0.56
85:B5:57:THR:HG22	85:B5:146:LYS:HA	1.87	0.56
80:B9:70:LEU:HD12	80:B9:70:LEU:H	1.69	0.56
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:B6:45:LEU:CB	86:B6:71:VAL:HB	2.33	0.56
86:B6:11:LEU:CD1	86:B6:75:SER:HB3	2.35	0.56
83:B3:27:ILE:HG13	83:B3:31:THR:CG2	2.36	0.56
84:B4:52:THR:HG23	84:B4:52:THR:O	2.06	0.56
85:B5:43:VAL:O	85:B5:152:ARG:HA	2.05	0.56
86:B6:29:LEU:C	86:B6:29:LEU:HD12	2.26	0.56
86:B6:7:THR:HG22	86:B6:8:LYS:H	1.71	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
86:B6:31:TYR:HA	86:B6:93:THR:CG2	2.29	0.56
82:B2:45:ARG:HD2	82:B2:45:ARG:C	2.27	0.56
83:B3:49:LEU:HD12	83:B3:49:LEU:N	2.21	0.56
83:B3:35:ILE:HG23	83:B3:37:TYR:H	1.70	0.56
86:B6:6:LYS:HG2	86:B6:112:THR:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B6:79:ILE:CD1	86:B6:79:ILE:H	2.17	0.56
86:B6:14:ILE:HG13	86:B6:15:ASN:N	2.20	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
84:B4:23:VAL:HG23	84:B4:70:LEU:CD2	2.34	0.55
85:B5:121:VAL:HG13	85:B5:125:ARG:NH1	2.21	0.55
85:B5:34:LEU:HD13	85:B5:40:SER:HB2	1.87	0.55
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
86:B6:29:LEU:HA	86:B6:94:LEU:CD2	2.36	0.55
80:B9:81:ASN:ND2	80:B9:83:LYS:HB2	2.20	0.55
26:B0:52:G:P	82:B2:49:TRP:CG	3.00	0.55
85:B5:31:LEU:HB2	85:B5:157:ARG:HB3	1.87	0.55
80:B9:89:LEU:HD22	80:B9:89:LEU:N	2.21	0.55
85:B5:125:ARG:HB3	85:B5:127:LYS:HE2	1.89	0.55
85:B5:173:ILE:O	85:B5:177:ILE:HG13	2.06	0.55
85:B5:16:ALA:HB1	85:B5:202:THR:HG21	1.88	0.55
80:B9:80:HIS:H	80:B9:84:GLU:HG3	1.72	0.55
86:B6:21:VAL:CG2	86:B6:96:ILE:HD11	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
84:B4:69:ARG:HG3	84:B4:80:LYS:HD3	1.86	0.55
85:B5:74:VAL:HG11	85:B5:142:ILE:HG22	1.87	0.54
82:B2:29:LEU:HD22	82:B2:29:LEU:H	1.73	0.54
84:B4:57:ARG:HD2	84:B4:57:ARG:H	1.72	0.54
84:B4:6:LYS:HG3	84:B4:93:LEU:HB3	1.88	0.54
85:B5:45:GLU:HB3	85:B5:183:ARG:HG2	1.89	0.54
85:B5:34:LEU:H	85:B5:157:ARG:HH11	1.55	0.54
86:B6:14:ILE:HG22	86:B6:108:MET:HE2	1.89	0.54
86:B6:19:GLN:O	86:B6:22:MET:HG3	2.08	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
85:B5:57:THR:HG22	85:B5:146:LYS:CA	2.37	0.54
86:B6:93:THR:O	86:B6:94:LEU:HD23	2.07	0.54
80:B9:79:VAL:CG2	80:B9:84:GLU:HB2	2.24	0.54
83:B3:13:LEU:C	83:B3:13:LEU:HD13	2.27	0.54
84:B4:75:PRO:O	84:B4:76:ASN:HB2	2.06	0.54
85:B5:58:THR:O	85:B5:58:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
80:B9:104:SER:O	80:B9:108:ARG:HG3	2.07	0.54
82:B2:33:THR:HG23	82:B2:33:THR:O	2.07	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
82:B2:29:LEU:HD22	82:B2:29:LEU:N	2.23	0.54
80:B9:99:ILE:HG22	80:B9:103:VAL:HG21	1.88	0.54
85:B5:64:GLU:HG2	85:B5:65:GLY:N	2.23	0.53
85:B5:5:ILE:HD11	85:B5:177:ILE:HD13	1.88	0.53
69:B7:198:ARG:HB2	69:B7:201:ARG:HH21	1.73	0.53
80:B9:98:GLU:HA	80:B9:123:THR:HG22	1.91	0.53
84:B4:58:LYS:HE2	84:B4:59:LYS:O	2.08	0.53
85:B5:27:LEU:C	85:B5:27:LEU:HD13	2.28	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
80:B9:75:ARG:HB3	80:B9:95:TYR:CE2	2.43	0.53
83:B3:35:ILE:HG12	83:B3:37:TYR:HD1	1.73	0.53
69:B7:198:ARG:HA	69:B7:201:ARG:NE	2.18	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
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
80:B9:99:ILE:HG22	80:B9:103:VAL:CG2	2.39	0.53
85:B5:60:VAL:HG22	85:B5:104:PHE:HA	1.88	0.53
86:B6:59:GLU:HB3	86:B6:63:TYR:CE1	2.43	0.53
86:B6:51:ASN:CB	86:B6:78:ASN:HD21	2.14	0.53
86:B6:7:THR:N	86:B6:10:SER:HB2	2.24	0.53
26:B0:4013:G:P	85:B5:124:PRO:CG	2.97	0.53
26:B0:4013:G:P	85:B5:124:PRO:CB	2.97	0.52
86:B6:6:LYS:CD	86:B6:14:ILE:HD13	2.39	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
26:B0:363:A:P	82:B2:24:SER:HG	2.26	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
85:B5:177:ILE:O	85:B5:180:ILE:HG12	2.10	0.52
26:B0:4022:C:P	85:B5:196:ASP:HB2	2.49	0.52
80:B9:70:LEU:HD12	80:B9:70:LEU:N	2.24	0.52
85:B5:74:VAL:HG12	85:B5:74:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:70:ARG:HD2	85:B5:137:ASP:CG	2.30	0.52
83:B3:23:ILE:CD1	83:B3:23:ILE:H	2.22	0.52
82:B2:11:ARG:HG3	82:B2:12:ARG:HG3	1.92	0.52
80:B9:122:VAL:O	80:B9:122:VAL:HG23	2.10	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
84:B4:33:LEU:O	84:B4:38:LYS:HD2	2.09	0.52
26:B0:4013:G:P	85:B5:124:PRO:HG3	2.50	0.52
86:B6:6:LYS:HB3	86:B6:10:SER:HB3	1.90	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
82:B2:18:LEU:HD12	82:B2:27:TYR:CB	2.33	0.51
86:B6:24:SER:HB2	86:B6:26:LYS:HD2	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
26:B0:2650:G:P	86:B6:91:VAL:CA	2.89	0.51
85:B5:137:ASP:OD1	85:B5:139:VAL:HG23	2.11	0.51
85:B5:34:LEU:HB3	85:B5:157:ARG:HG2	1.92	0.51
85:B5:198:VAL:HG23	85:B5:210:VAL:HG13	1.92	0.51
80:B9:84:GLU:HA	80:B9:84:GLU:OE1	2.10	0.51
26:B0:2776:G:P	82:B2:3:LYS:N	2.83	0.51
86:B6:68:LYS:HG2	86:B6:68:LYS:O	2.09	0.51
80:B9:88:LEU:HD13	80:B9:88:LEU:C	2.31	0.51
86:B6:18:LEU:CD1	86:B6:85:CYS:HA	2.40	0.51
85:B5:120:THR:HG23	85:B5:121:VAL:N	2.26	0.51
85:B5:70:ARG:CG	85:B5:137:ASP:HA	2.41	0.51
85:B5:50:PRO:HD3	85:B5:179:VAL:HG21	1.91	0.51
84:B4:2:VAL:HG23	84:B4:3:ASN:N	2.26	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
85:B5:45:GLU:CD	85:B5:188:LEU:HD11	2.30	0.51
86:B6:66:LEU:O	86:B6:66:LEU:HD13	2.10	0.51
26:B0:1511:G:P	82:B2:16:HIS:NE2	2.81	0.51
84:B4:69:ARG:HD2	84:B4:80:LYS:CD	2.36	0.51
85:B5:150:GLN:HE21	85:B5:152:ARG:CD	2.22	0.51
85:B5:34:LEU:C	85:B5:34:LEU:HD13	2.31	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:B5:62:PHE:CE2	85:B5:110:LEU:CD2	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:103:PHE:CD1	85:B5:145:MET:CE	2.94	0.50
84:B4:56:PHE:CZ	84:B4:57:ARG:HD3	2.46	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
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
83:B3:35:ILE:CD1	83:B3:37:TYR:CD1	2.95	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
85:B5:5:ILE:HD13	85:B5:177:ILE:CG2	2.35	0.50
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
86:B6:6:LYS:HD3	86:B6:14:ILE:CG2	2.43	0.49
26:B0:2278:C:P	80:B9:104:SER:N	2.83	0.49
85:B5:69:LEU:H	85:B5:69:LEU:CD2	2.24	0.49
26:B0:2381:A:P	82:B2:14:LYS:CE	3.00	0.49
82:B2:18:LEU:HB3	82:B2:24:SER:O	2.12	0.49
86:B6:81:LEU:C	86:B6:81:LEU:HD23	2.33	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
84:B4:39:ARG:N	84:B4:39:ARG:HD3	2.27	0.49
86:B6:18:LEU:C	86:B6:18:LEU:HD13	2.32	0.49
86:B6:37:MET:CE	86:B6:42:LYS:HB3	2.43	0.49
82:B2:24:SER:O	82:B2:25:LYS:HD2	2.11	0.49
80:B9:78:LEU:HD23	80:B9:78:LEU:C	2.32	0.49
26:B0:4306:U:P	84:B4:80:LYS:HZ2	2.33	0.49
85:B5:141:VAL:HG23	85:B5:142:ILE:N	2.27	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
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
82:B2:19:CYS:HB2	82:B2:34:CYS:SG	2.53	0.49
26:B0:2383:G:P	83:B3:49:LEU:HD13	2.53	0.49
82:B2:18:LEU:HD12	82:B2:19:CYS:N	2.14	0.49
86:B6:59:GLU:HB3	86:B6:63:TYR:HE1	1.78	0.49
86:B6:53:PRO:O	86:B6:54:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:B5:105:ILE:HA	85:B5:130:GLU:O	2.12	0.49
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
80:B9:83:LYS:CD	80:B9:83:LYS:H	2.24	0.48
82:B2:12:ARG:NE	83:B3:4:HIS:CD2	2.81	0.48
84:B4:62:THR:HG23	84:B4:63:THR:N	2.28	0.48
85:B5:151:LEU:CD1	85:B5:159:PHE:CZ	2.95	0.48
85:B5:58:THR:HG23	85:B5:101:THR:CA	2.41	0.48
86:B6:61:GLU:HG3	86:B6:62:TYR:N	2.28	0.48
85:B5:151:LEU:CD1	85:B5:159:PHE:CG	2.96	0.48
85:B5:43:VAL:HG22	85:B5:188:LEU:HD13	1.96	0.48
83:B3:15:LYS:HD2	83:B3:15:LYS:O	2.14	0.48
83:B3:5:LYS:HB2	83:B3:9:ILE:HG23	1.93	0.48
85:B5:31:LEU:HD23	85:B5:195:ILE:HA	1.95	0.48
86:B6:6:LYS:NZ	86:B6:71:VAL:HG11	2.29	0.48
86:B6:71:VAL:HG12	86:B6:71:VAL:O	2.12	0.48
26:B0:4303:U:P	84:B4:37:GLY:HA3	2.53	0.48
26:B0:52:G:P	82:B2:49:TRP:H	2.36	0.48
82:B2:28:HIS:CA	82:B2:31:LYS:HE2	2.43	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
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
85:B5:190:LYS:H	85:B5:190:LYS:CD	2.23	0.48
85:B5:87:LEU:CB	85:B5:117:TYR:CE2	2.97	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
85:B5:43:VAL:CG1	85:B5:188:LEU:HD12	2.43	0.47
80:B9:87:VAL:HG11	80:B9:89:LEU:HD23	1.95	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
83:B3:6:THR:HG23	83:B3:9:ILE:H	1.79	0.47
86:B6:46:VAL:CG1	86:B6:72:HIS:HB3	2.44	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
80:B9:81:ASN:HD22	80:B9:83:LYS:N	2.09	0.47
82:B2:29:LEU:CD2	82:B2:29:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
82:B2:15:THR:HG23	82:B2:28:HIS:NE2	2.30	0.47
84:B4:32:SER:O	84:B4:33:LEU:HB2	2.13	0.47
85:B5:43:VAL:HA	85:B5:188:LEU:HD13	1.97	0.47
83:B3:35:ILE:CG2	83:B3:37:TYR:HB2	2.44	0.47
84:B4:23:VAL:HG22	84:B4:68:LEU:HB3	1.97	0.47
69:B7:192:ARG:HG3	69:B7:193:MET:N	2.30	0.47
85:B5:74:VAL:HG12	85:B5:146:LYS:HD3	1.96	0.47
86:B6:44:LYS:HD3	86:B6:98:ASP:CA	2.38	0.47
80:B9:87:VAL:HG12	80:B9:89:LEU:HD23	1.94	0.47
85:B5:104:PHE:CZ	85:B5:122:LEU:CD2	2.94	0.47
85:B5:57:THR:HG21	85:B5:145:MET:O	2.15	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
82:B2:18:LEU:CG	82:B2:19:CYS:N	2.78	0.47
85:B5:60:VAL:N	85:B5:101:THR:HG21	2.29	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
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
80:B9:78:LEU:HD22	80:B9:80:HIS:NE2	2.31	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
83:B3:21:ARG:HA	83:B3:22:PRO:HD3	1.65	0.46
82:B2:18:LEU:HG	82:B2:22:CYS:HB2	1.98	0.46
84:B4:4:VAL:HG13	84:B4:5:PRO:HD2	1.97	0.46
84:B4:78:ARG:O	84:B4:78:ARG:HG2	2.16	0.46
85:B5:98:ALA:CB	85:B5:121:VAL:CG1	2.93	0.46
85:B5:16:ALA:CB	85:B5:202:THR:HG21	2.45	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
25:B1:54:A:P	83:B3:21:ARG:HD3	2.52	0.46
26:B0:3895:C:P	84:B4:50:GLY:N	2.89	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
80:B9:70:LEU:H	80:B9:70:LEU:CD1	2.29	0.46
83:B3:21:ARG:HD2	83:B3:21:ARG:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
26:B0:4323:A:P	84:B4:36:GLN:CB	3.04	0.46
82:B2:26:ALA:O	82:B2:34:CYS:HA	2.16	0.46
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:B5:105: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:B5:151:LEU:HD12	85:B5:159:PHE:CD2	2.51	0.45
85:B5:49:LEU:HD22	85:B5:176:ASN:HB3	1.98	0.45
85:B5:118:LEU:HD22	85:B5:118:LEU:N	2.31	0.45
86:B6:3:ALA:HB3	86:B6:74:TYR:CD1	2.51	0.45
85:B5:163:VAL:O	85:B5:163:VAL:HG12	2.16	0.45
86:B6:47:ILE:O	86:B6:48:LEU:HD23	2.16	0.45
86:B6:15:ASN:OD1	86:B6:84:ALA:HB2	2.16	0.45
84:B4:38:LYS:HG2	84:B4:39:ARG:CD	2.46	0.45
86:B6:81:LEU:HD22	86:B6:91:VAL:CB	2.24	0.45
86:B6:29:LEU:CB	86:B6:94:LEU:CD2	2.94	0.45
83:B3:20:ASN:HD21	83:B3:42:ARG:HB3	1.81	0.45
26:B0:4191:C:P	84:B4:2:VAL:HG13	2.55	0.45
85:B5:98:ALA:HB3	85:B5:121:VAL:HG12	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
82:B2:49:TRP:O	82:B2:50:SER:HB2	2.16	0.45
86:B6:34:THR:HG23	86:B6:35:LEU:N	2.31	0.45
83:B3:35:ILE:CG1	83:B3:37:TYR:HD1	2.30	0.45
82:B2:20:ARG:H	82:B2:20:ARG:HD3	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
86:B6:30:GLY:C	86:B6:93:THR:HG23	2.37	0.45
85:B5:47:VAL:CG1	85:B5:179:VAL:CG1	2.95	0.45
82:B2:4:GLY:CA	82:B2:8:PHE:CZ	2.96	0.45
85:B5:98:ALA:HB3	85:B5:121:VAL:CG1	2.47	0.45
80:B9:101:HIS:HA	80:B9:108:ARG:NH2	2.31	0.45
80:B9:81:ASN:ND2	80:B9:83:LYS:H	2.09	0.45
26:B0:4192:U:P	84:B4:2:VAL:CB	3.03	0.45
82:B2:18:LEU:HD23	82:B2:24:SER:CB	2.47	0.45
85:B5:47:VAL:HG11	85:B5:179:VAL:HG12	1.99	0.45
85:B5:43:VAL:HG11	85:B5:151:LEU:HD23	1.97	0.45
85:B5:61:VAL:HG13	85:B5:132:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	85:B5:190:LYS:HD3	2.26	0.44
86:B6:14:ILE:CG2	86:B6:108:MET:CE	2.95	0.44
86:B6:17:ARG:HD3	86:B6:105:ILE:HD13	1.97	0.44
86:B6:20:LEU:HD23	86:B6:20:LEU:C	2.37	0.44
80:B9:92:ASN:ND2	80:B9:120:ILE:HG12	2.29	0.44
83:B3:11:ARG:HG3	83:B3:12:PHE:N	2.32	0.44
85:B5:30:ASN:HD22	85:B5:31:LEU:N	2.14	0.44
84:B4:22:LYS:HE3	84:B4:71:GLU:OE1	2.16	0.44
85:B5:156:ARG:HD3	85:B5:158:THR:CG2	2.48	0.44
85:B5:45:GLU:CB	85:B5:183:ARG:CG	2.95	0.44
26:B0:4192:U:P	84:B4:2:VAL:HG11	2.57	0.44
25:B1:54:A:P	83:B3:21:ARG:HB2	2.57	0.44
86:B6:21:VAL:HG13	86:B6:26:LYS:HB2	1.98	0.44
80:B9:118:LEU:O	80:B9:119:ALA:HB3	2.18	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
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
85:B5:143:GLU:HG2	85:B5:146:LYS:CE	2.45	0.44
85:B5:36:LEU:C	85:B5:36:LEU:HD23	2.38	0.44
26:B0:3895:C:P	84:B4:50:GLY:H	2.41	0.44
86:B6:31:TYR:CA	86:B6:93:THR:CG2	2.94	0.44
85:B5:174:ALA:HA	85:B5:177:ILE:HD12	1.99	0.44
82:B2:28:HIS:N	82:B2:31:LYS:CE	2.81	0.44
84:B4:22:LYS:HE3	84:B4:71:GLU:CD	2.38	0.44
84:B4:55:ILE:HG22	84:B4:56:PHE:N	2.32	0.44
84:B4:19:GLN:HB2	84:B4:72:CYS:SG	2.58	0.44
86:B6:7:THR:CG2	86:B6:8:LYS:N	2.81	0.44
82:B2:18:LEU:HD23	82:B2:24:SER:HB3	2.00	0.43
83:B3:35:ILE:HG21	83:B3:37:TYR:HB2	2.00	0.43
83:B3:6:THR:H	83:B3:9:ILE:CG2	2.31	0.43
84:B4:38:LYS:HG3	84:B4:39:ARG:HD3	2.00	0.43
80:B9:70:LEU:HD11	80:B9:76:LYS:N	2.33	0.43
86:B6:52:CYS:HB2	86:B6:57:LYS:HD3	1.99	0.43
82:B2:16:HIS:HA	82:B2:27:TYR:O	2.18	0.43
82:B2:18:LEU:CD2	82:B2:24:SER:CB	2.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
26:B0:23:C:P	82:B2:44:LYS:CE	2.92	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
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
85:B5:62:PHE:CD1	85:B5:62:PHE:C	2.92	0.43
80:B9:87:VAL:HB	80:B9:90:MET:H	1.83	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
82:B2:15:THR:CG2	82:B2:16:HIS:H	2.21	0.43
82:B2:31:LYS:HZ2	82:B2:33:THR:N	2.17	0.43
86:B6:3:ALA:N	86:B6:74:TYR:CD1	2.86	0.43
80:B9:89:LEU:CD2	80:B9:89:LEU:H	2.32	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
26:B0:2279:C:P	80:B9:104:SER:CB	3.07	0.42
83:B3:35:ILE:CD1	83:B3:37:TYR:HD1	2.31	0.42
26:B0:2383:G:P	83:B3:48:LYS:NZ	2.92	0.42
80:B9:85:LEU:O	80:B9:90:MET:HG2	2.19	0.42
84:B4:38:LYS:CG	84:B4:39:ARG:N	2.81	0.42
84:B4:4:VAL:O	84:B4:93:LEU:HD13	2.19	0.42
85:B5:138:VAL:HB	85:B5:141:VAL:HG22	2.01	0.42
86:B6:28:VAL:CG2	86:B6:37:MET:SD	3.07	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
86:B6:17:ARG:HH11	86:B6:17:ARG:HG3	1.84	0.42
85:B5:185:HIS:HD2	85:B5:192:PRO:CD	2.32	0.42
84:B4:8:ARG:HG2	84:B4:9:ARG:N	2.35	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
86:B6:81:LEU:CD2	86:B6:94:LEU:HD11	2.49	0.42
86:B6:96:ILE:HG23	86:B6:96:ILE:O	2.20	0.42
82:B2:10:LYS:HE3	82:B2:11:ARG:N	2.34	0.42
86:B6:37:MET:HE3	86:B6:42:LYS:HB3	2.02	0.42
82:B2:42:LYS:HB3	82:B2:43:ARG:H	1.57	0.42
82:B2:8:PHE:HB3	82:B2:9:GLY:H	1.50	0.42
83:B3:6:THR:HG23	83:B3:8:ARG:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
85:B5:79:LEU:HD12	85:B5:79:LEU:N	2.34	0.42
86:B6:6:LYS:HZ2	86:B6:14:ILE:HG21	1.81	0.42
80:B9:99:ILE:HG21	80:B9:103:VAL:HG21	2.00	0.42
86:B6:31:TYR:N	86:B6:93:THR:CG2	2.83	0.42
26:B0:2292:G:P	80:B9:71:PRO:CB	3.08	0.42
84:B4:53:LYS:CB	84:B4:54:PRO:HD3	2.36	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
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
83:B3:15:LYS:O	83:B3:18:LYS:HB2	2.20	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
85:B5:103:PHE:HD1	85:B5:145:MET:HE3	1.82	0.41
86:B6:79:ILE:HG12	86:B6:80:GLU:N	2.35	0.41
80:B9:123:THR:CG2	80:B9:124:ASN:N	2.83	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
86:B6:31:TYR:CE2	86:B6:35:LEU:HD11	2.55	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
85:B5:120:THR:CG2	85:B5:121:VAL:N	2.83	0.41
84:B4:35:ALA:H	84:B4:38:LYS:HB3	1.85	0.41
85:B5:34:LEU:CD1	85:B5:40:SER:CB	2.95	0.41
85:B5:34:LEU:CD2	85:B5:40:SER:CB	2.93	0.41
69:B7:192:ARG:O	69:B7:196:LEU:HD13	2.20	0.41
85:B5:151:LEU:HD13	85:B5:159:PHE:CE2	2.55	0.41
85:B5:3:GLN:O	85:B5:6:GLU:HG3	2.21	0.41
85:B5:184:LEU:O	85:B5:184:LEU:HD23	2.21	0.41
86:B6:48:LEU:CD2	86:B6:60:ILE:CD1	2.98	0.41
85:B5:159:PHE:HZ	85:B5:161:THR:HB	1.71	0.41
84:B4:32:SER:O	84:B4:34:TYR:CD1	2.74	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
84:B4:69:ARG:HB3	84:B4:80:LYS:HE2	2.03	0.41
86:B6:45:LEU:HD23	86:B6:45:LEU:C	2.41	0.41
86:B6:78:ASN:H	86:B6:78:ASN:ND2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:B7:193:MET:CE	69:B7:197:ARG:HH21	2.34	0.41
84:B4:62:THR:CG2	84:B4:63:THR:N	2.83	0.41
85:B5:168:MET:HB2	85:B5:173:ILE:HD11	2.03	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:B5:185:HIS:HA	85:B5:189:GLU:O	2.21	0.41
86:B6:37:MET:HE2	86:B6:42:LYS:CB	2.51	0.41
80:B9:85:LEU:HD11	80:B9:111:ILE:HG23	2.03	0.41
80:B9:89:LEU:CD2	80:B9:89:LEU:N	2.83	0.41
26:B0:4306:U:P	84:B4:80:LYS:HZ1	2.43	0.40
80:B9:89:LEU:HD22	80:B9:89:LEU:H	1.85	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
82:B2:27:TYR:CD1	82:B2:27:TYR:C	2.95	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:B6:44:LYS:HD2	86:B6:44:LYS:HA	1.95	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:B5:111:MET:HE1	85:B5:131:PRO:CG	2.48	0.40
85:B5:196:ASP:C	85:B5:197:THR:HG23	2.42	0.40
85:B5:58:THR:HG23	85:B5:102:ASP:N	2.33	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%)	3 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	Ab	188/295 (64%)	180 (96%)	5 (3%)	3 (2%)	11	51
11	Ac	190/243 (78%)	171 (90%)	12 (6%)	7 (4%)	4	33
12	Ad	101/209 (48%)	100 (99%)	1 (1%)	0	100	100
13	Ae	144/179 (80%)	136 (94%)	6 (4%)	2 (1%)	13	54
14	Ag	153/204 (75%)	147 (96%)	4 (3%)	2 (1%)	14	56
15	Ah	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
16	Ai	134/146 (92%)	120 (90%)	11 (8%)	3 (2%)	8	44
17	Aj	95/119 (80%)	87 (92%)	3 (3%)	5 (5%)	2	26
18	Ak	123/151 (82%)	86 (70%)	31 (25%)	6 (5%)	2	27
19	Al	113/143 (79%)	88 (78%)	17 (15%)	8 (7%)	1	19
20	Am	138/152 (91%)	125 (91%)	9 (6%)	4 (3%)	5	38
21	An	47/56 (84%)	42 (89%)	4 (8%)	1 (2%)	8	45
22	Ao	83/89 (93%)	67 (81%)	15 (18%)	1 (1%)	15	57
23	Aq	70/158 (44%)	65 (93%)	4 (6%)	1 (1%)	13	54
24	As	86/145 (59%)	75 (87%)	7 (8%)	4 (5%)	3	28
53	Ba	240/257 (93%)	219 (91%)	14 (6%)	7 (3%)	5	38
54	Bb	343/403 (85%)	255 (74%)	58 (17%)	30 (9%)	1	15
55	Bc	255/421 (61%)	211 (83%)	33 (13%)	11 (4%)	3	29
56	Bd	163/178 (92%)	140 (86%)	19 (12%)	4 (2%)	6	41
57	Be	173/192 (90%)	155 (90%)	14 (8%)	4 (2%)	7	43
58	Bf	118/266 (44%)	103 (87%)	8 (7%)	7 (6%)	2	23
59	Bg	46/317 (14%)	37 (80%)	8 (17%)	1 (2%)	8	44
60	Bh	164/214 (77%)	154 (94%)	8 (5%)	2 (1%)	15	57
61	Bi	72/165 (44%)	67 (93%)	4 (6%)	1 (1%)	13	54
62	Bj	134/203 (66%)	129 (96%)	4 (3%)	1 (1%)	25	68
63	Bk	122/140 (87%)	114 (93%)	6 (5%)	2 (2%)	11	51
64	Bl	116/148 (78%)	110 (95%)	4 (3%)	2 (2%)	11	50
65	Bm	173/204 (85%)	164 (95%)	8 (5%)	1 (1%)	28	71
66	Bn	232/297 (78%)	186 (80%)	30 (13%)	16 (7%)	1	20
67	Bo	116/188 (62%)	109 (94%)	5 (4%)	2 (2%)	11	50
68	Bp	151/196 (77%)	141 (93%)	6 (4%)	4 (3%)	6	40

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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%)	17	60
71	Br	144/184 (78%)	137 (95%)	6 (4%)	1 (1%)	25	68
72	Bs	76/156 (49%)	74 (97%)	2 (3%)	0	100	100
73	Bt	100/145 (69%)	95 (95%)	3 (3%)	2 (2%)	9	46
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	19
78	Bx	78/125 (62%)	66 (85%)	7 (9%)	5 (6%)	1	22
79	By	52/135 (38%)	39 (75%)	7 (14%)	6 (12%)	0	8
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	7
83	B3	46/51 (90%)	46 (100%)	0	0	100	100
84	B4	90/106 (85%)	87 (97%)	2 (2%)	1 (1%)	17	60
85	B5	208/212 (98%)	199 (96%)	7 (3%)	2 (1%)	18	61
86	B6	111/115 (96%)	104 (94%)	5 (4%)	2 (2%)	10	49
All	All	6163/8734 (71%)	5492 (89%)	479 (8%)	192 (3%)	8	37

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%)	78	89
10	Ab	160/244 (66%)	152 (95%)	8 (5%)	28	60
11	Ac	157/202 (78%)	145 (92%)	12 (8%)	15	47
12	Ad	89/181 (49%)	88 (99%)	1 (1%)	78	89
13	Ae	117/146 (80%)	111 (95%)	6 (5%)	28	60
14	Ag	138/170 (81%)	131 (95%)	7 (5%)	28	60
15	Ah	110/113 (97%)	108 (98%)	2 (2%)	64	84
16	Ai	114/121 (94%)	110 (96%)	4 (4%)	41	69
17	Aj	90/107 (84%)	84 (93%)	6 (7%)	19	51
18	Ak	98/119 (82%)	90 (92%)	8 (8%)	13	43
19	Al	90/115 (78%)	89 (99%)	1 (1%)	78	89
20	Am	120/132 (91%)	114 (95%)	6 (5%)	28	60
21	An	43/49 (88%)	42 (98%)	1 (2%)	56	79
22	Ao	77/80 (96%)	71 (92%)	6 (8%)	15	46
23	Aq	72/142 (51%)	67 (93%)	5 (7%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	As	79/130 (61%)	71 (90%)	8 (10%)	9	33
53	Ba	187/199 (94%)	177 (95%)	10 (5%)	26	59
54	Bb	298/348 (86%)	271 (91%)	27 (9%)	11	38
55	Bc	214/351 (61%)	204 (95%)	10 (5%)	30	62
56	Bd	139/149 (93%)	134 (96%)	5 (4%)	40	68
57	Be	156/171 (91%)	147 (94%)	9 (6%)	23	56
58	Bf	100/223 (45%)	86 (86%)	14 (14%)	4	23
59	Bg	29/258 (11%)	29 (100%)	0	100	100
60	Bh	141/181 (78%)	136 (96%)	5 (4%)	41	69
61	Bi	64/137 (47%)	62 (97%)	2 (3%)	45	71
62	Bj	114/174 (66%)	110 (96%)	4 (4%)	41	69
63	Bk	97/107 (91%)	91 (94%)	6 (6%)	21	54
64	Bl	99/122 (81%)	97 (98%)	2 (2%)	60	82
65	Bm	148/172 (86%)	143 (97%)	5 (3%)	42	69
66	Bn	197/251 (78%)	177 (90%)	20 (10%)	8	33
67	Bo	108/165 (66%)	105 (97%)	3 (3%)	49	74
68	Bp	141/175 (81%)	134 (95%)	7 (5%)	28	60
69	B7	13/13 (100%)	13 (100%)	0	100	100
70	Bq	82/139 (59%)	76 (93%)	6 (7%)	16	49
71	Br	131/163 (80%)	120 (92%)	11 (8%)	13	43
72	Bs	69/133 (52%)	68 (99%)	1 (1%)	71	86
73	Bt	103/135 (76%)	101 (98%)	2 (2%)	62	82
74	Bu	46/126 (36%)	46 (100%)	0	100	100
75	Bv	53/110 (48%)	51 (96%)	2 (4%)	38	67
76	B8	9/9 (100%)	9 (100%)	0	100	100
77	Bw	137/234 (58%)	115 (84%)	22 (16%)	3	17
78	Bx	71/110 (64%)	66 (93%)	5 (7%)	18	50
79	By	56/121 (46%)	44 (79%)	12 (21%)	1	8
80	B9	51/51 (100%)	48 (94%)	3 (6%)	23	55
81	Bz	57/75 (76%)	57 (100%)	0	100	100
82	B2	42/80 (52%)	38 (90%)	4 (10%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	B3	45/48 (94%)	43 (96%)	2 (4%)	33	63
84	B4	83/94 (88%)	78 (94%)	5 (6%)	22	55
85	B5	177/178 (99%)	173 (98%)	4 (2%)	56	79
86	B6	95/97 (98%)	92 (97%)	3 (3%)	44	71
All	All	5371/7425 (72%)	5076 (94%)	295 (6%)	30	58

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Aa	35	SER
9	Aa	88	ARG
9	Aa	284	PRO
10	Ab	16	LYS
10	Ab	52	ARG
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	94	ARG
11	Ac	126	ILE
11	Ac	135	GLU
11	Ac	143	ARG
11	Ac	157	MET
11	Ac	179	GLN
11	Ac	182	LEU
11	Ac	189	MET
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	91	ARG

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Mol	Chain	Res	Type
14	Ag	128	ILE
14	Ag	166	ILE
14	Ag	190	ILE
14	Ag	191	LYS
14	Ag	193	LYS
15	Ah	61	ILE
15	Ah	126	LEU
16	Ai	60	LYS
16	Ai	97	GLN
16	Ai	108	ILE
16	Ai	113	ILE
17	Aj	19	ARG
17	Aj	47	ASN
17	Aj	84	ILE
17	Aj	91	LEU
17	Aj	101	ILE
17	Aj	104	ILE
18	Ak	25	GLU
18	Ak	51	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
20	Am	24	ARG
20	Am	55	ARG
20	Am	78	LYS
20	Am	86	ARG
20	Am	94	LYS
20	Am	114	LEU
21	An	54	LYS
22	Ao	4	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
23	Aq	98	LYS

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Mol	Chain	Res	Type
23	Aq	132	ARG
23	Aq	144	LYS
24	As	44	ARG
24	As	51	ARG
24	As	52	LYS
24	As	77	LYS
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	145	LYS
53	Ba	174	ARG
53	Ba	179	ILE
53	Ba	190	LYS
53	Ba	200	ARG
53	Ba	242	ARG
53	Ba	245	ARG
54	Bb	33	LYS
54	Bb	36	SER
54	Bb	38	LYS
54	Bb	40	VAL
54	Bb	42	LEU
54	Bb	58	GLU
54	Bb	75	VAL
54	Bb	98	LEU
54	Bb	119	LYS
54	Bb	123	LYS
54	Bb	126	LYS
54	Bb	134	LYS
54	Bb	136	TRP
54	Bb	137	GLN
54	Bb	142	LYS
54	Bb	179	LEU
54	Bb	180	MET
54	Bb	185	ASN
54	Bb	197	ARG
54	Bb	212	GLN
54	Bb	213	ASP
54	Bb	225	LYS

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Mol	Chain	Res	Type
54	Bb	237	LYS
54	Bb	280	ASN
54	Bb	300	ASN
54	Bb	340	LYS
54	Bb	350	LEU
55	Bc	74	ARG
55	Bc	144	GLU
55	Bc	151	LEU
55	Bc	192	LYS
55	Bc	198	ARG
55	Bc	208	ILE
55	Bc	209	ILE
55	Bc	211	ASN
55	Bc	238	LYS
55	Bc	256	PHE
56	Bd	15	LEU
56	Bd	63	ARG
56	Bd	107	PHE
56	Bd	109	ILE
56	Bd	118	LYS
57	Be	11	ASP
57	Be	18	ILE
57	Be	50	LYS
57	Be	51	LYS
57	Be	113	GLU
57	Be	129	ARG
57	Be	143	GLU
57	Be	168	LYS
57	Be	170	LYS
58	Bf	110	LYS
58	Bf	113	ARG
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	187	LYS
58	Bf	190	LEU
58	Bf	193	LEU
58	Bf	196	ARG

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Mol	Chain	Res	Type
58	Bf	204	PHE
60	Bh	6	ARG
60	Bh	14	LYS
60	Bh	31	ARG
60	Bh	137	ILE
60	Bh	166	ILE
61	Bi	94	LYS
61	Bi	103	ASN
62	Bj	50	LYS
62	Bj	58	ARG
62	Bj	64	ASN
62	Bj	78	ILE
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	11	LEU
64	Bl	42	ARG
65	Bm	13	LYS
65	Bm	19	MET
65	Bm	64	ILE
65	Bm	67	ARG
65	Bm	176	LYS
66	Bn	13	LYS
66	Bn	26	LYS
66	Bn	28	ASP
66	Bn	32	ARG
66	Bn	34	ARG
66	Bn	47	LYS
66	Bn	53	ARG
66	Bn	77	ARG
66	Bn	91	LEU
66	Bn	104	LEU
66	Bn	121	GLN
66	Bn	156	ASN
66	Bn	187	LYS
66	Bn	193	VAL
66	Bn	195	ARG
66	Bn	197	HIS
66	Bn	207	MET

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Mol	Chain	Res	Type
66	Bn	233	ASP
66	Bn	236	GLU
66	Bn	238	MET
67	Bo	36	ARG
67	Bo	54	ARG
67	Bo	91	ILE
68	Bp	9	ARG
68	Bp	21	LYS
68	Bp	30	ASN
68	Bp	152	LYS
68	Bp	153	LYS
68	Bp	162	ARG
68	Bp	183	GLU
70	Bq	6	LYS
70	Bq	13	MET
70	Bq	38	ILE
70	Bq	54	LYS
70	Bq	82	LYS
70	Bq	92	ILE
71	Br	3	ARG
71	Br	28	ASN
71	Br	41	ILE
71	Br	43	LYS
71	Br	46	LYS
71	Br	69	ARG
71	Br	74	LYS
71	Br	97	ASN
71	Br	128	ARG
71	Br	146	ILE
71	Br	153	LYS
72	Bs	94	ASN
73	Bt	63	LYS
73	Bt	106	ILE
75	Bv	43	LYS
75	Bv	47	ILE
77	Bw	111	LEU
77	Bw	116	ARG
77	Bw	133	LEU
77	Bw	135	ARG
77	Bw	149	LYS
77	Bw	157	ILE
77	Bw	173	ASN

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Mol	Chain	Res	Type
77	Bw	186	LYS
77	Bw	191	LEU
77	Bw	196	LEU
77	Bw	203	LYS
77	Bw	207	ILE
77	Bw	209	MET
77	Bw	214	HIS
77	Bw	221	LYS
77	Bw	222	ARG
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	33	ILE
78	Bx	44	ARG
78	Bx	57	MET
78	Bx	83	ARG
78	Bx	84	ILE
79	By	9	LYS
79	By	11	LYS
79	By	12	ILE
79	By	14	LYS
79	By	18	LYS
79	By	19	LYS
79	By	22	ARG
79	By	24	GLN
79	By	27	ARG
79	By	30	LYS
79	By	50	LYS
79	By	64	LYS
80	B9	69	MET
80	B9	76	LYS
80	B9	109	LYS
82	B2	10	LYS
82	B2	20	ARG
82	B2	31	LYS
82	B2	46	LYS
83	B3	15	LYS
83	B3	23	ILE
84	B4	9	ARG

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Mol	Chain	Res	Type
84	B4	14	LYS
84	B4	39	ARG
84	B4	45	GLN
84	B4	57	ARG
85	B5	11	ARG
85	B5	30	ASN
85	B5	108	LYS
85	B5	190	LYS
86	B6	79	ILE
86	B6	109	PRO
86	B6	114	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
9	Aa	20	GLN
9	Aa	56	GLN
9	Aa	187	ASN
9	Aa	226	HIS
12	Ad	61	GLN
17	Aj	47	ASN
17	Aj	100	GLN
21	An	41	GLN
22	Ao	8	GLN
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	39	HIS
64	Bl	85	GLN
66	Bn	16	GLN
66	Bn	228	ASN
66	Bn	243	HIS
68	Bp	30	ASN
70	Bq	48	GLN
70	Bq	69	HIS
77	Bw	173	ASN
77	Bw	214	HIS

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Mol	Chain	Res	Type
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
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	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	-	-

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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	-	-
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 carbohydrates 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.