



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:41 AM UTC

PDB ID : 7ASE / pdb_00007ase
EMDB ID : EMD-11893
Title : 43S preinitiation complex from Trypanosoma cruzi with the kDDX60 helicase
Authors : Bochler, A.; Brito Querido, J.; Prilepskaja, T.; Soufari, H.; Del Cistia, M.L.; Kuhn, L.; Rimoldi Ribeiro, A.; Valasek, L.S.; Hashem, Y.
Deposited on : 2020-10-27
Resolution : 3.33 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

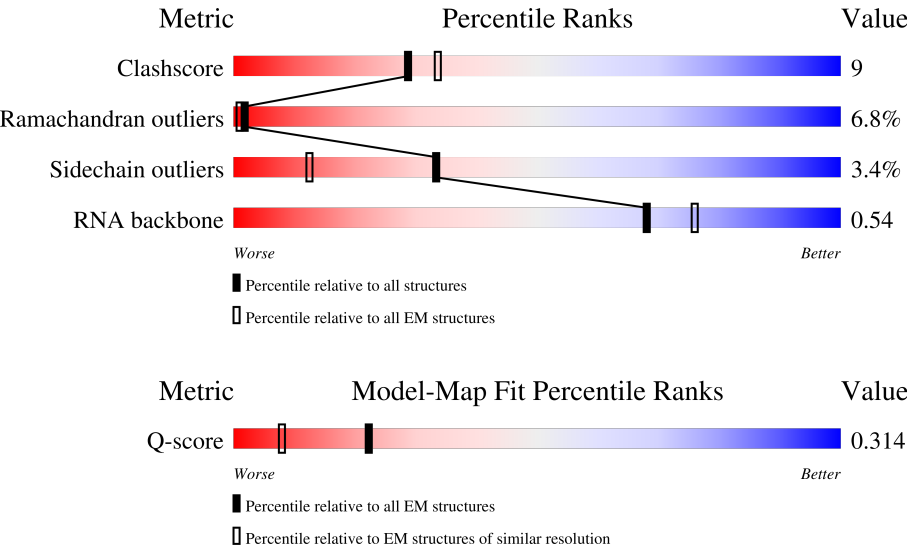
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.33 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14484 (2.83 - 3.83)

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

Mol	Chain	Length	Quality of chain
1	f	2174	54% 46% 16% 5% 30%
2	1	75	13% 83% 11%
3	0	2319	18% 72% 18% 7%

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Mol	Chain	Length	Quality of chain
4	y	137	
5	s	418	
6	j	150	
7	n	343	
8	p	318	
9	r	149	
10	u	153	
11	m	143	
12	Z	221	
13	o	190	
14	q	211	
15	R	151	
16	S	86	
17	t	112	
18	U	91	
19	v	144	
20	X	173	
21	B	190	
22	F	245	
23	d	263	
24	g	247	
25	a	110	
26	J	257	
27	h	141	
28	5	477	

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Mol	Chain	Length	Quality of chain
29	P	250	
30	i	141	
31	L	117	
32	M	214	
33	N	161	
34	O	167	
35	b	145	
36	c	66	
37	V	109	
38	w	166	
39	E	407	
40	Y	379	
41	Q	57	
42	D	34	
43	G	345	
44	K	203	
45	T	152	
46	C	716	
47	8	762	
48	W	254	
49	I	489	
50	H	334	
51	A	502	
52	l	273	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	GNP	5	502	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 136847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called kDDX60.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	1523	Total	C	N	O	S	0	0
			12257	7734	2165	2292	66		

- Molecule 2 is a RNA chain called initiator tRNA-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	75	Total	C	N	O	P	0	0
			1606	718	300	514	74		

- Molecule 3 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	2150	Total	C	N	O	P	0	0
			45795	20471	8144	15037	2143		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	143	C	A	conflict	GB 320364483
0	805	C	U	conflict	GB 320364483
0	2321	U	-	insertion	GB 320364483
0	2322	U	-	insertion	GB 320364483
0	2323	U	-	insertion	GB 320364483

- Molecule 4 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	y	123	Total	C	N	O	S	0	0
			989	628	194	165	2		

- Molecule 5 is a protein called Elongation initiation factor 2 alpha subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	s	295	Total	C	N	O	S	0	0
			2365	1489	436	427	13		

- Molecule 6 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	79	Total	C	N	O	S	0	0
			644	409	123	106	6		

- Molecule 7 is a protein called Translation initiation factor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	225	Total	C	N	O	S	0	0
			1796	1111	335	339	11		

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	310	Total	C	N	O	S	0	0
			2405	1505	424	463	13		

- Molecule 9 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	r	140	Total	C	N	O	S	0	0
			1113	706	212	192	3		

- Molecule 10 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	u	136	Total	C	N	O	S	0	0
			1108	689	224	190	5		

- Molecule 11 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	142	Total	C	N	O	S	0	0
			1116	706	220	188	2		

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	175	Total	C	N	O	S	0	0
			1404	885	283	233	3		

- Molecule 13 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	o	190	Total	C	N	O	S	0	0
			1493	932	286	269	6		

- Molecule 14 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	200	Total	C	N	O	S	0	0
			1670	1063	324	277	6		

- Molecule 15 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	141	Total	C	N	O	S	0	0
			1143	724	221	190	8		

- Molecule 16 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	82	Total	C	N	O	S	0	0
			630	384	121	116	9		

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	104	Total	C	N	O	S	0	0
			829	510	177	132	10		

- Molecule 18 is a protein called 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	68	Total	C	N	O	S	0	0
			526	315	107	100	4		

- Molecule 19 is a protein called 40S ribosomal protein S14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	135	Total	C	N	O	S	0	0
			1011	620	195	187	9		

- Molecule 20 is a protein called 40S ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	148	Total	C	N	O	S	0	0
			1212	760	239	207	6		

- Molecule 21 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	179	Total	C	N	O	S	0	0
			1483	935	297	243	8		

- Molecule 22 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	207	Total	C	N	O	S	0	0
			1658	1060	299	288	11		

- Molecule 23 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	223	Total	C	N	O	S	0	0
			1726	1098	304	314	10		

- Molecule 24 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	83	Total	C	N	O	S	0	0
			635	395	116	122	2		

- Molecule 25 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	70	Total	C	N	O	S	0	0
			553	356	97	97	3		

- Molecule 26 is a protein called RNA-binding protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	J	173	Total	C	N	O	S	0	0
			1358	862	259	234	3		

- Molecule 27 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	121	Total	C	N	O	S	0	0
			958	594	174	185	5		

- Molecule 28 is a protein called Eukaryotic translation initiation factor 2 subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	421	Total	C	N	O	S	0	0
			3245	2049	581	596	19		

- Molecule 29 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	249	Total	C	N	O	S	0	0
			1983	1244	402	333	4		

- Molecule 30 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	121	Total	C	N	O	S	0	0
			992	623	190	174	5		

- Molecule 31 is a protein called Ribosomal protein S20, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	99	Total	C	N	O	S	0	0
			784	497	144	140	3		

- Molecule 32 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	200	Total	C	N	O	S	0	0
			1587	995	302	279	11		

- Molecule 33 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N	93	Total	C	N	O	S	0	0
			780	508	136	132	4		

- Molecule 34 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	140	Total	C	N	O	S	0	0
			1116	702	221	185	8		

- Molecule 35 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	129	Total	C	N	O	S	0	0
			1019	647	188	176	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	83	THR	ALA	conflict	UNP Q4CXX2

- Molecule 36 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	60	Total	C	N	O	S	0	0
			480	303	98	78	1		

- Molecule 37 is a protein called Protein translation factor SUI1 homolog, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	V	97	Total	C	N	O	S	0	0
			789	490	152	145	2		

- Molecule 38 is a protein called Putative eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	147	Total	C	N	O	S	0	0
			1162	716	209	236	1		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	E	391	Total	C	N	O	S	0	0
			3119	1977	536	593	13		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Y	174	Total	C	N	O	S	0	0
			1387	872	243	260	12		

- Molecule 41 is a protein called Ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Q	57	Total	C	N	O	S	0	0
			462	283	96	77	6		

- Molecule 42 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	D	33	Total	C	N	O	S	0	0
			294	178	76	38	2		

- Molecule 43 is a protein called JAB_MPN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	G	308	Total	C	N	O	S	0	0
			2414	1492	442	466	14		

- Molecule 44 is a protein called CSN8_PSD8_EIF3K domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	K	201	Total	C	N	O	S	0	0
			1566	1001	256	304	5		

- Molecule 45 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	132	Total	C	N	O	S	0	0
			1057	670	204	179	4		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit 8, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	C	696	Total	C	N	O	S	0	0
			5630	3542	973	1092	23		

- Molecule 47 is a protein called eIF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	8	576	Total	C	N	O	S	0	0
			4596	2882	845	847	22		

- Molecule 48 is a protein called 40S ribosomal protein S3a-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	217	Total	C	N	O	S	0	0
			1781	1124	337	313	7		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 (EIF-3) interacting protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	I	344	Total	C	N	O	S	0	0
			2770	1771	479	503	17		

- Molecule 50 is a protein called eIF3H.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	H	297	Total	C	N	O	S	0	0
			2388	1498	421	451	18		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit 7-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A	483	Total	C	N	O	S	0	0
			3891	2446	691	729	25		

- Molecule 52 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	258	Total	C	N	O	S	0	0
			2038	1290	383	354	11		

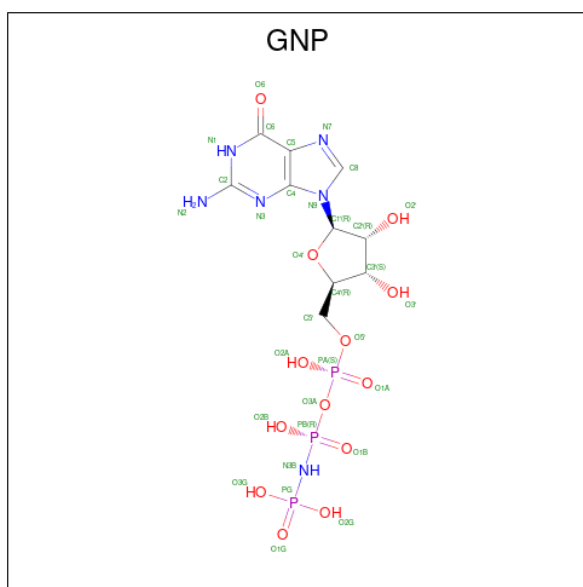
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	n	1	Total	Zn	0
			1	1	

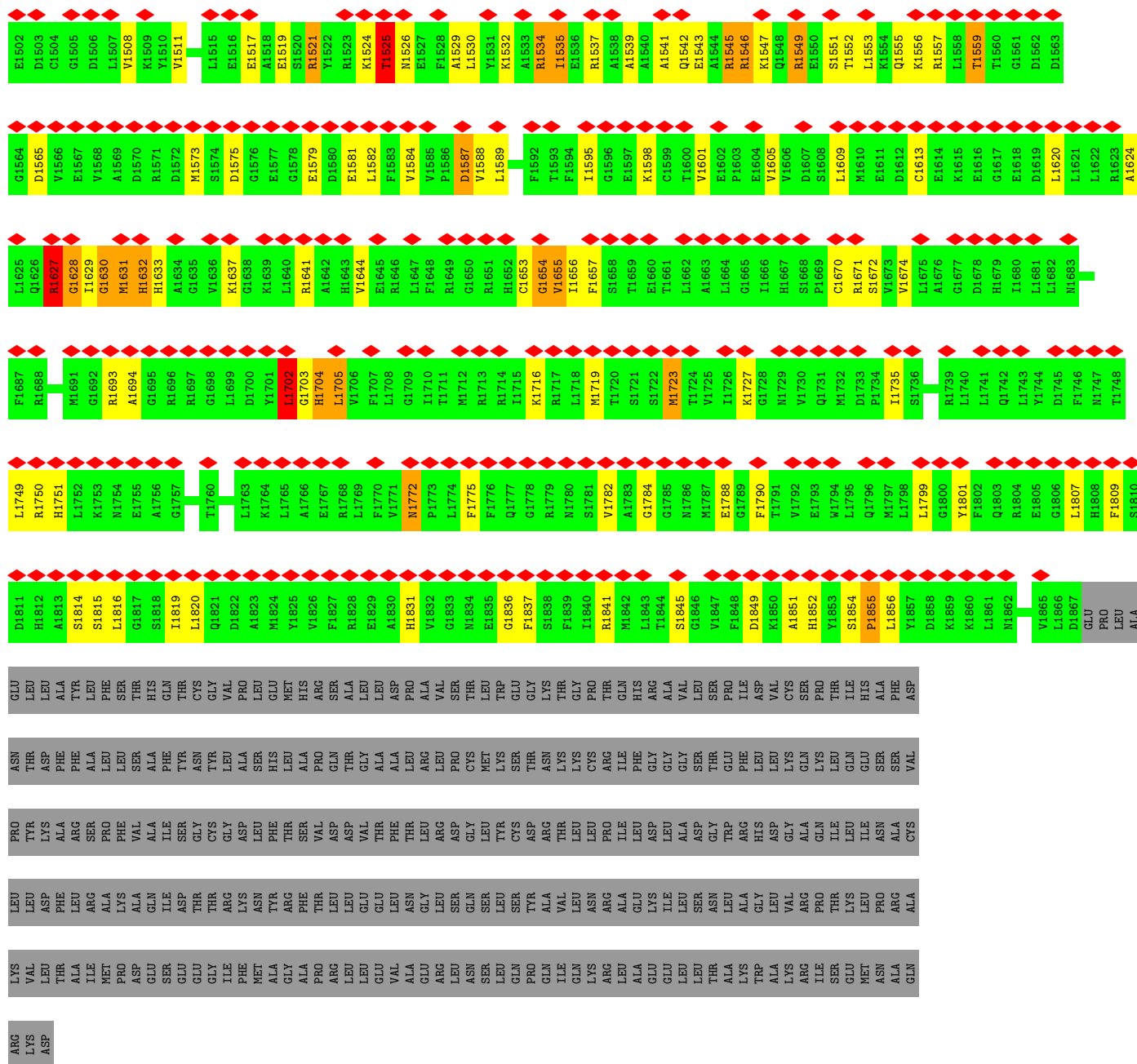
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	5	1	Total	Mg	0
			1	1	

- Molecule 55 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

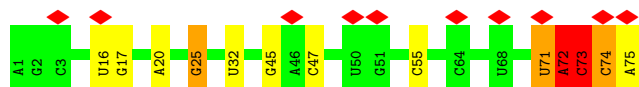


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H728	L729	L730	H731	A732	V733	D734	M735	S736	H737	G738	R739	T740	N741	R742	D744	R745	D746	I749	M753	A754	A755	I756	R758	L759	E762	K763	F764	G765	K766	N767	F768	D769	L831	Y832	G771	Y772	T773	L774	G775	G776	S777	T778	N779	T780	A781	R782	G783	L784	K785	L786	E787	M788	W789	R790	L791				
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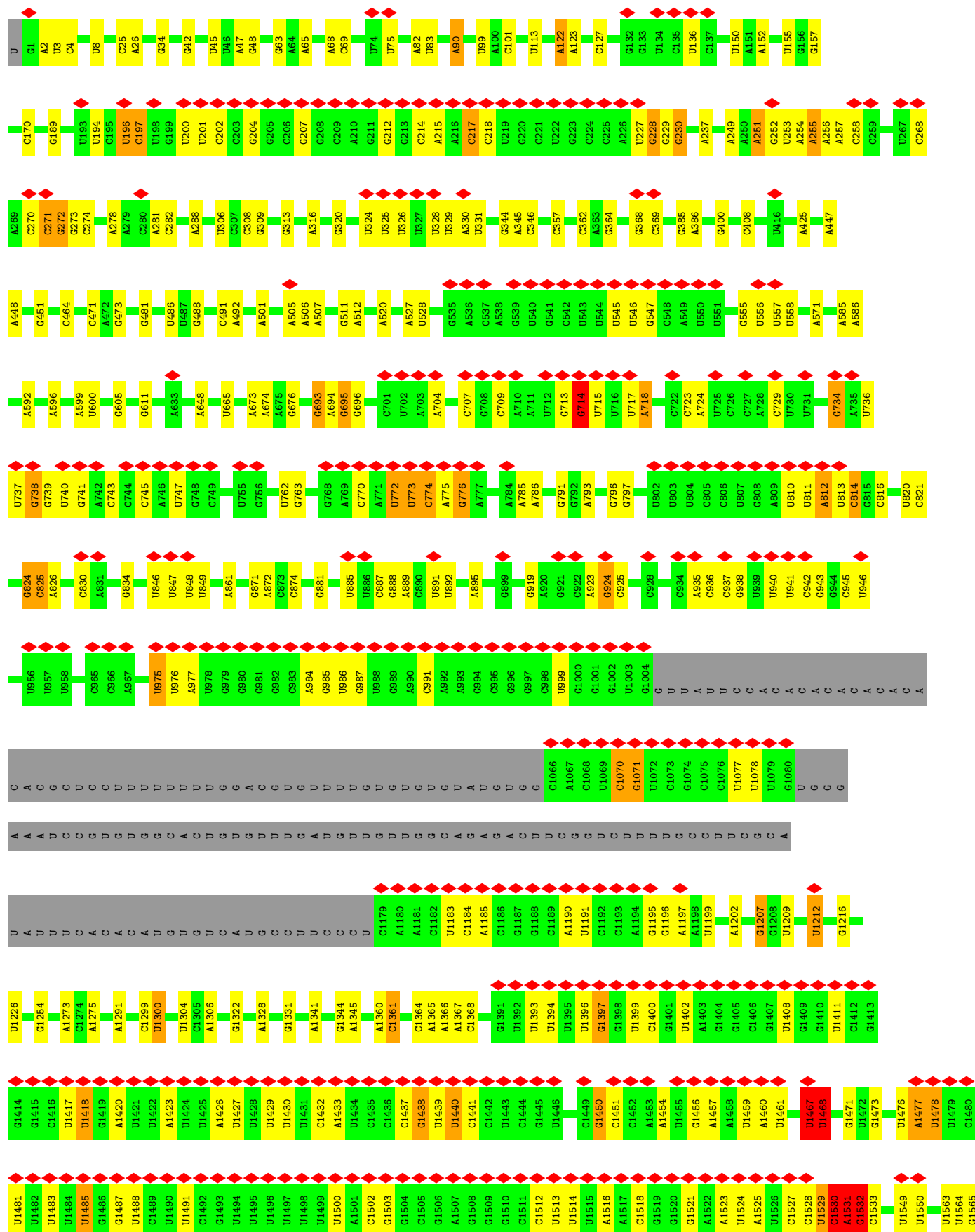
- Molecule 2: initiator tRNA-Met

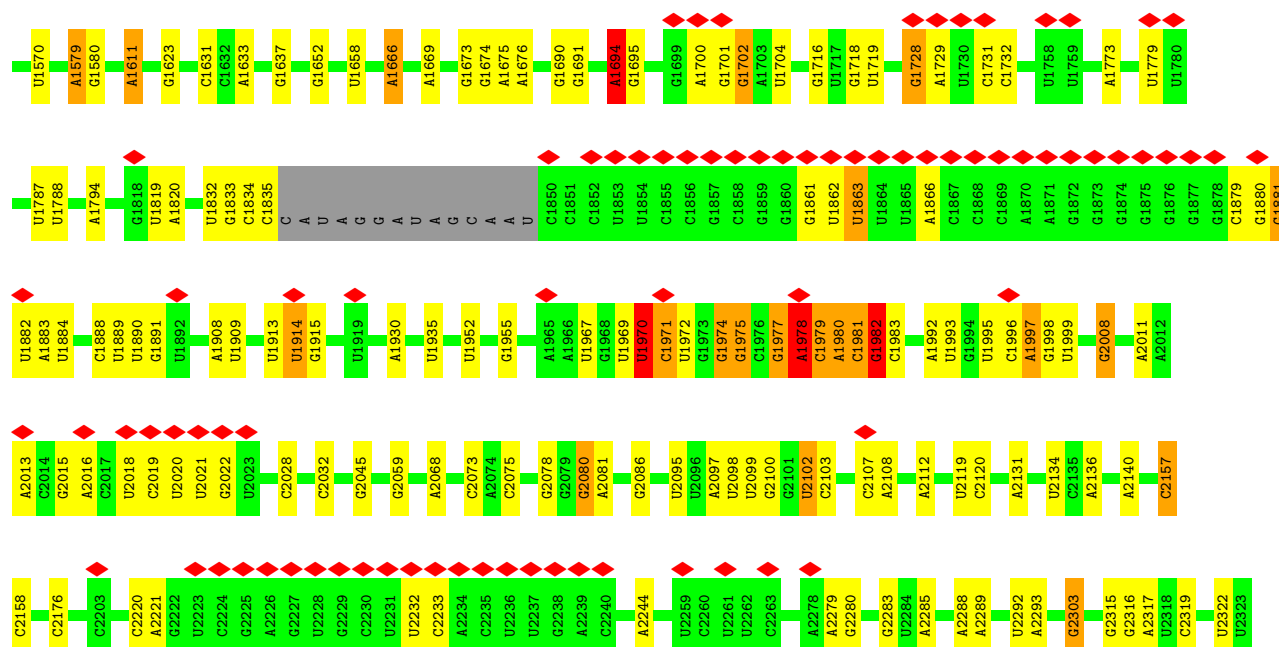
Chain 1: 13% 83% 11% . .



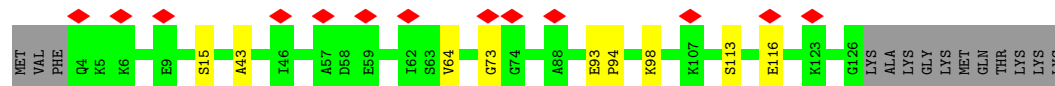
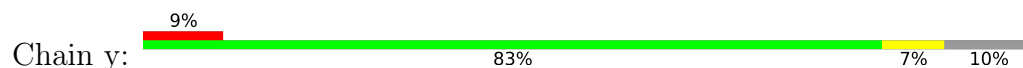
- Molecule 3: 18S

Chain 0: 18% 72% 18% . 7%

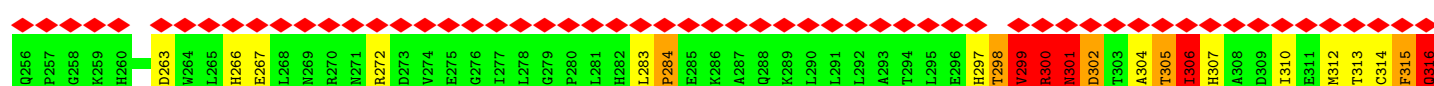
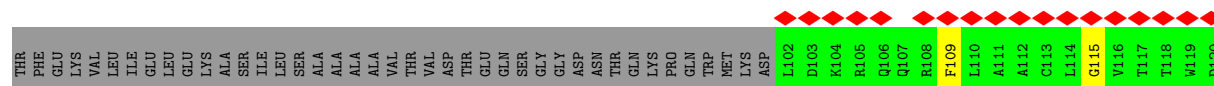
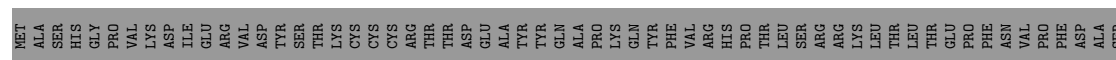


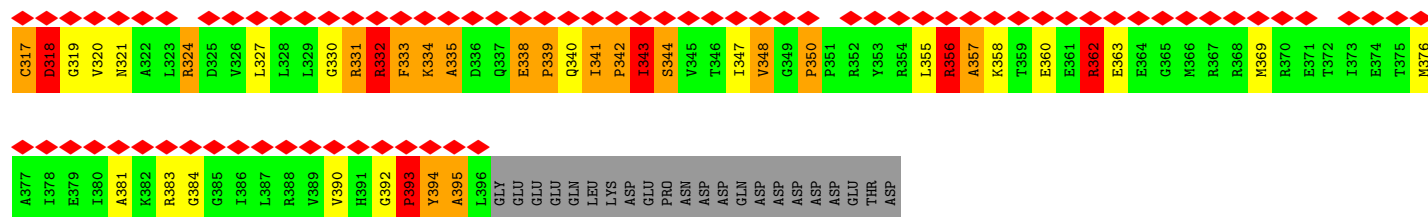


• Molecule 4: 40S ribosomal protein S24

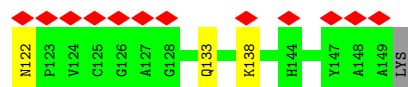
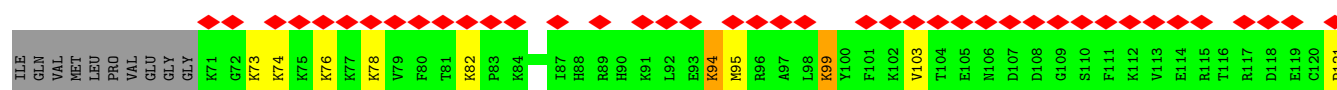
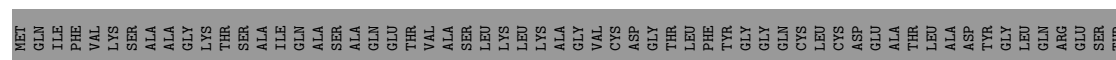


• Molecule 5: Elongation initiation factor 2 alpha subunit, putative

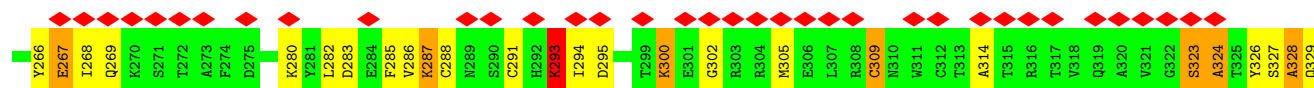
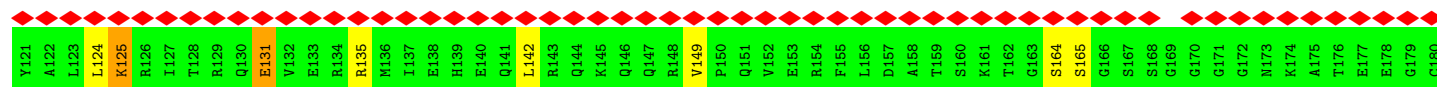
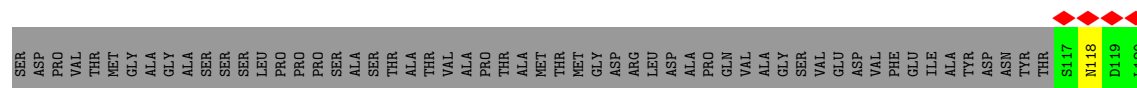
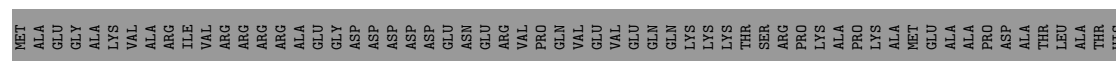
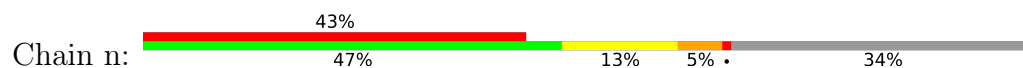




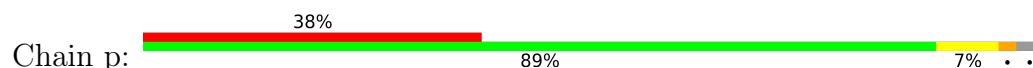
• Molecule 6: 60S ribosomal protein L40

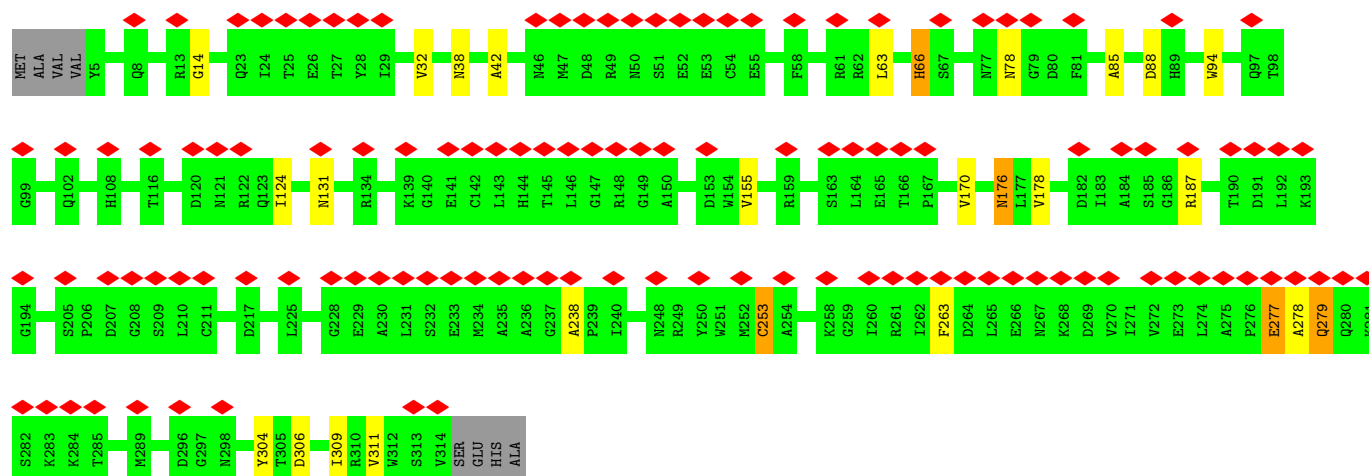


• Molecule 7: Translation initiation factor, putative

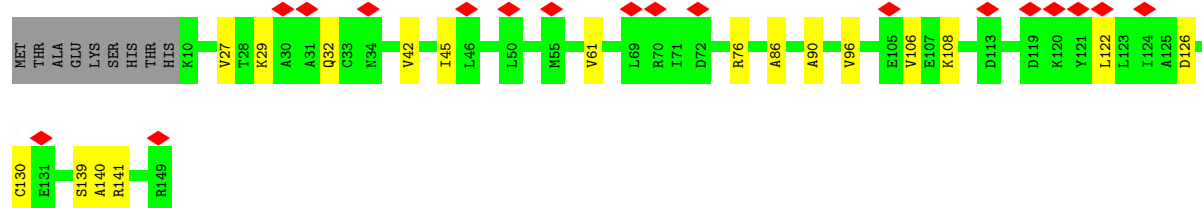
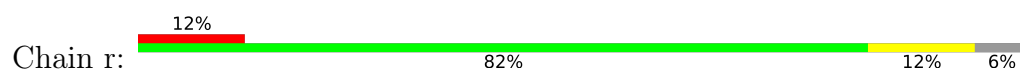


• Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein

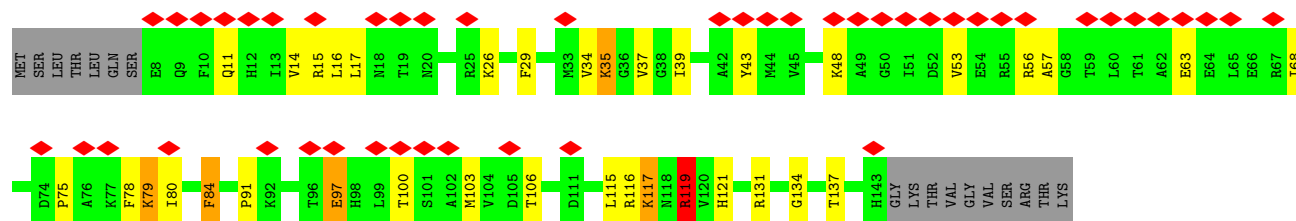




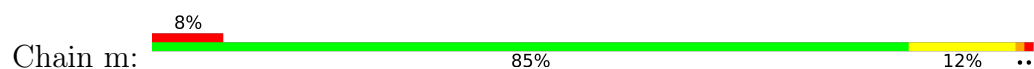
- Molecule 9: 40S ribosomal protein S16, putative



- Molecule 10: 40S ribosomal protein S18, putative

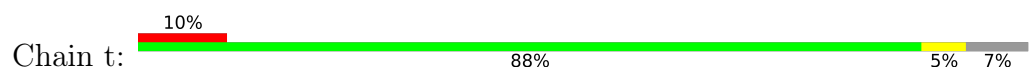


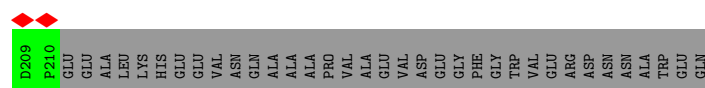
- Molecule 11: 40S ribosomal protein S23, putative



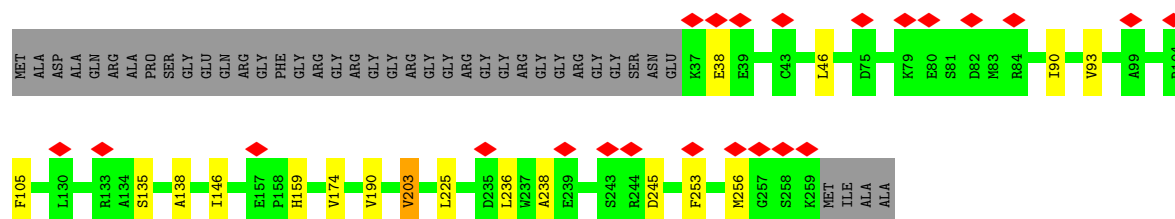
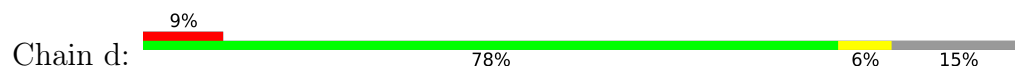
- Molecule 12: 40S ribosomal protein S8



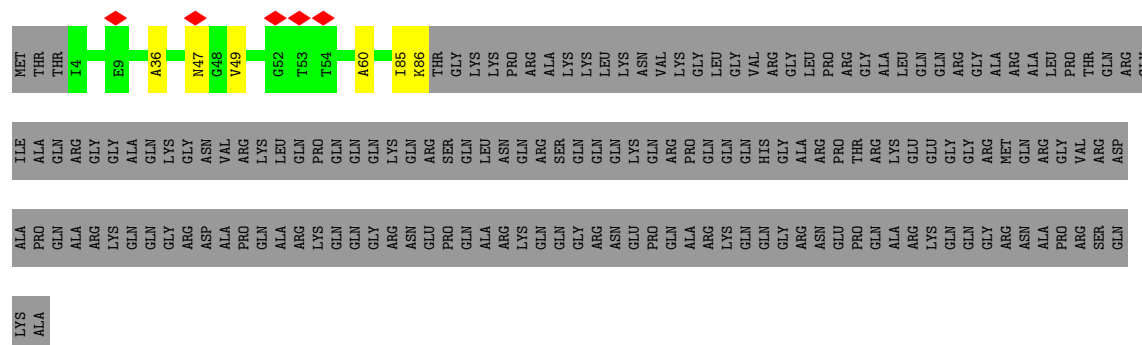




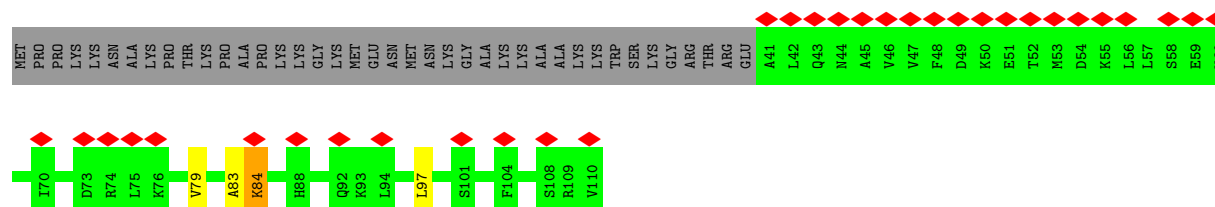
- Molecule 23: 40S ribosomal protein S2, putative



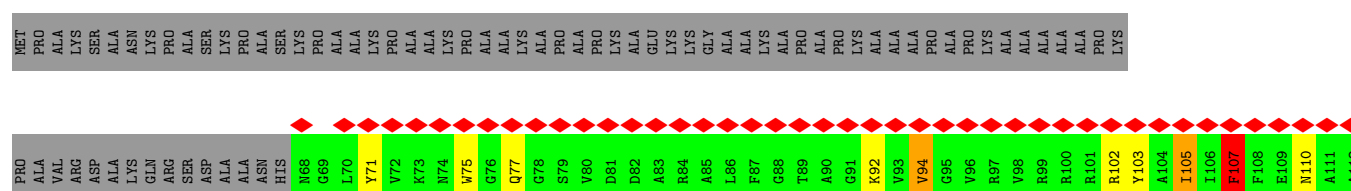
- Molecule 24: Putative 40S ribosomal protein S21

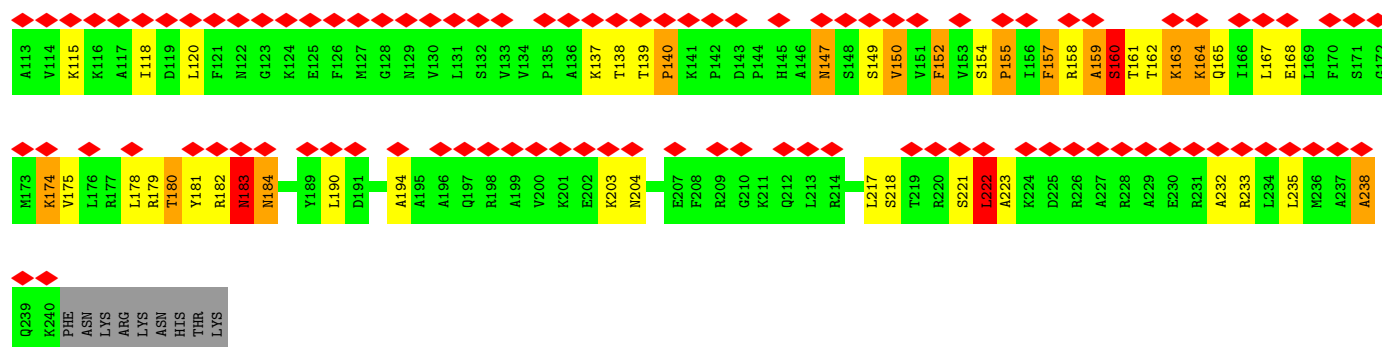


- Molecule 25: 40S ribosomal protein S25

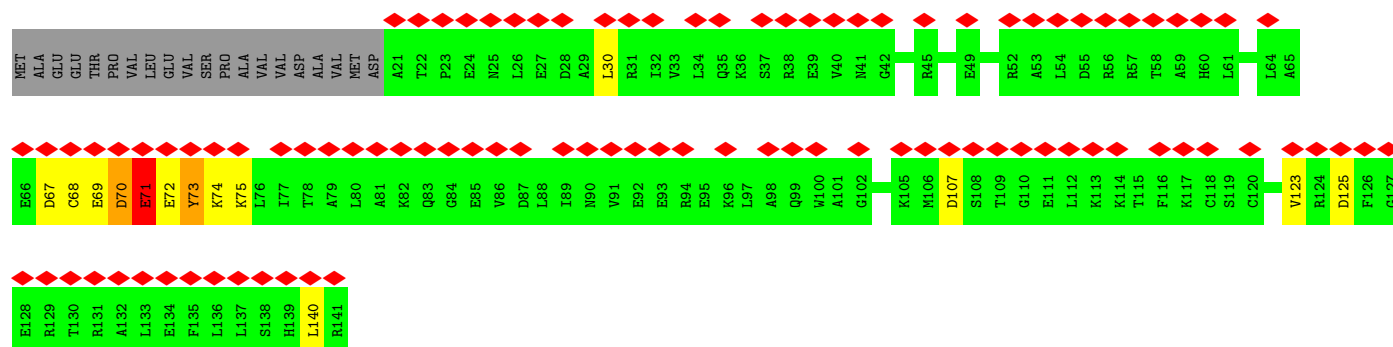
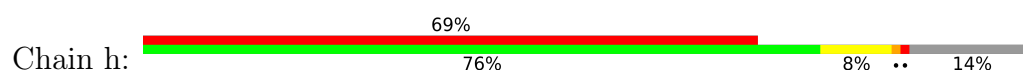


- Molecule 26: RNA-binding protein, putative

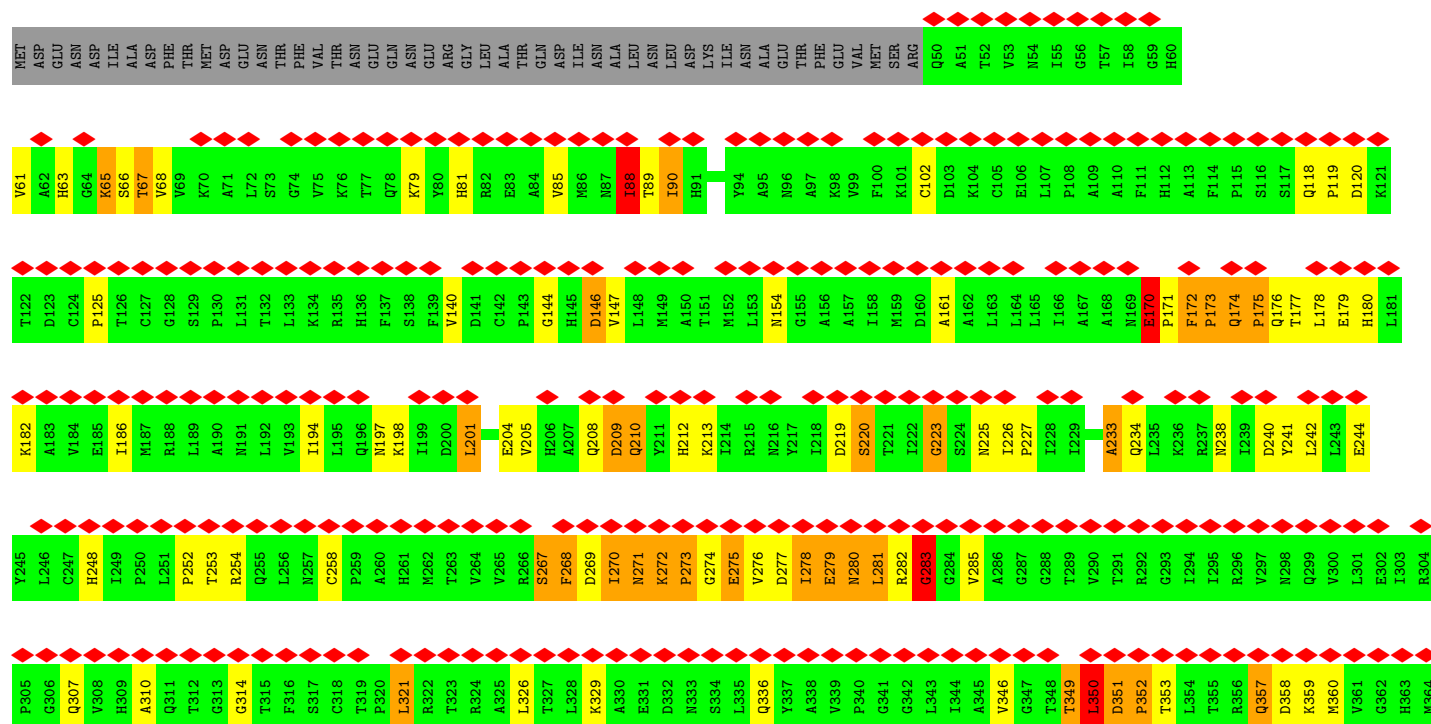
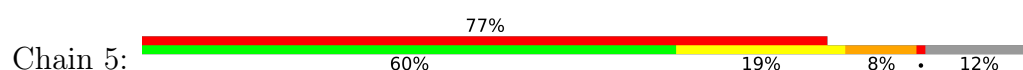


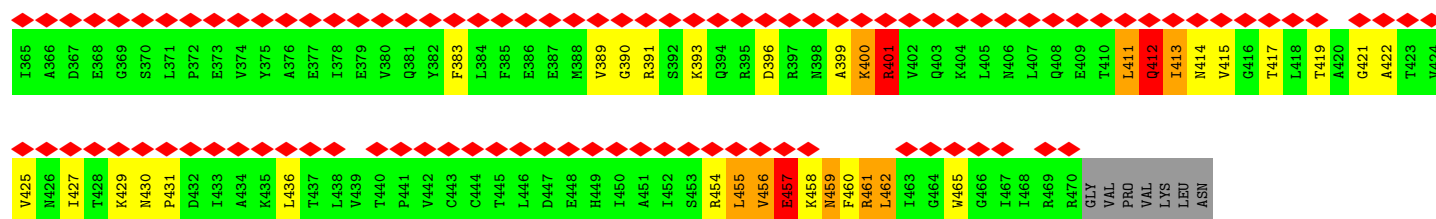


• Molecule 27: 40S ribosomal protein S12

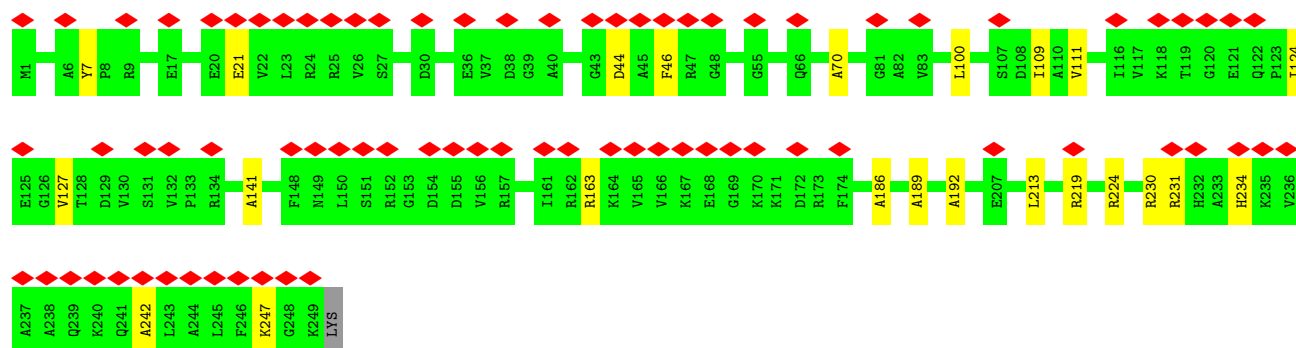
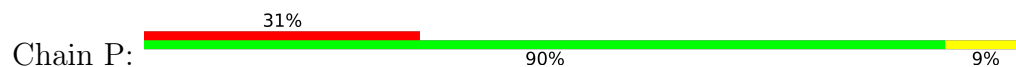


• Molecule 28: Eukaryotic translation initiation factor 2 subunit, putative

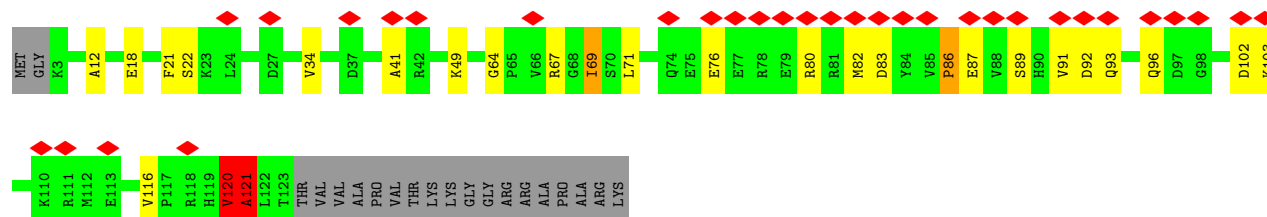




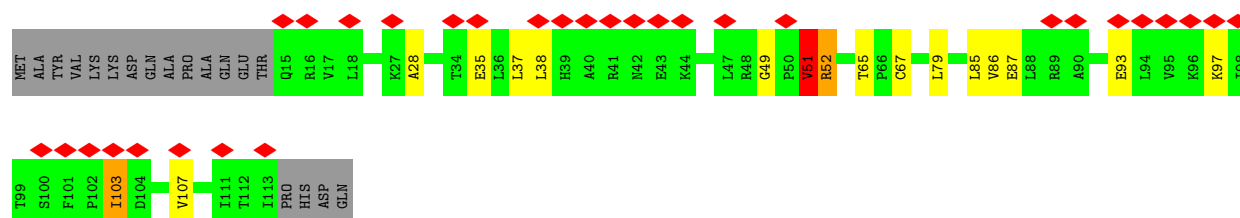
• Molecule 29: 40S ribosomal protein S6



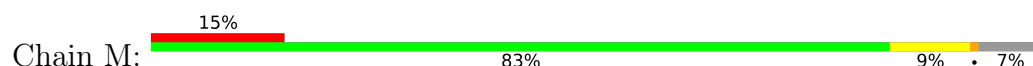
• Molecule 30: 40S ribosomal protein S17, putative



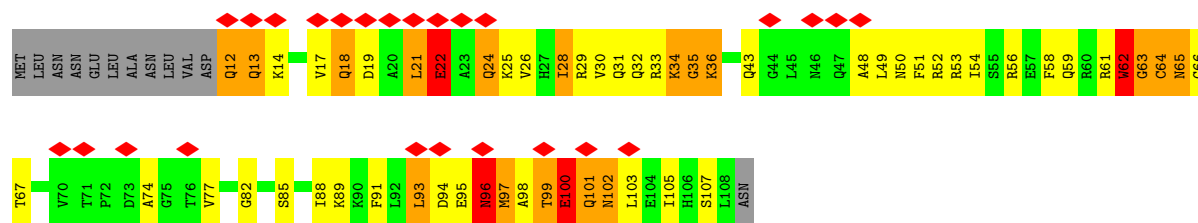
• Molecule 31: Ribosomal protein S20, putative



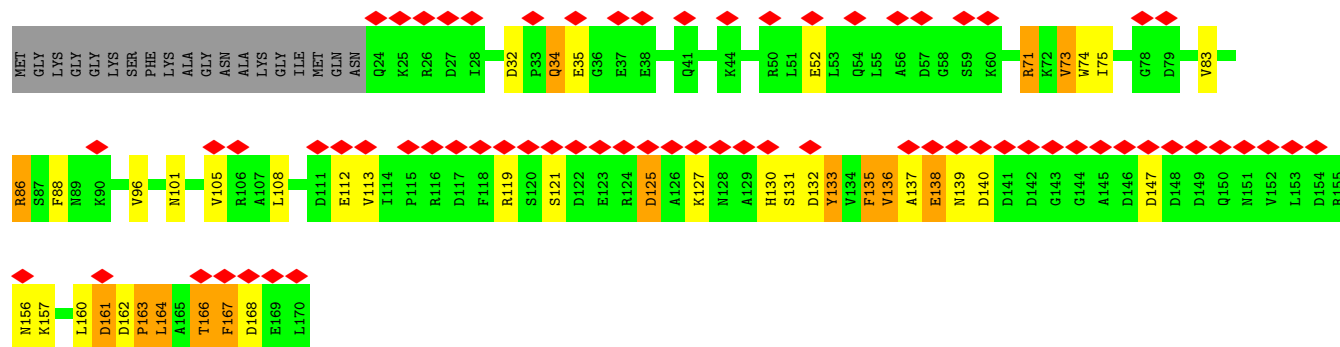
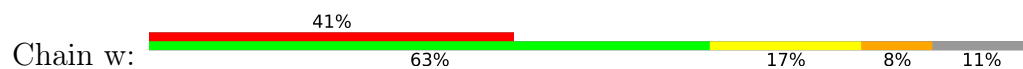
• Molecule 32: 40S ribosomal protein S3, putative



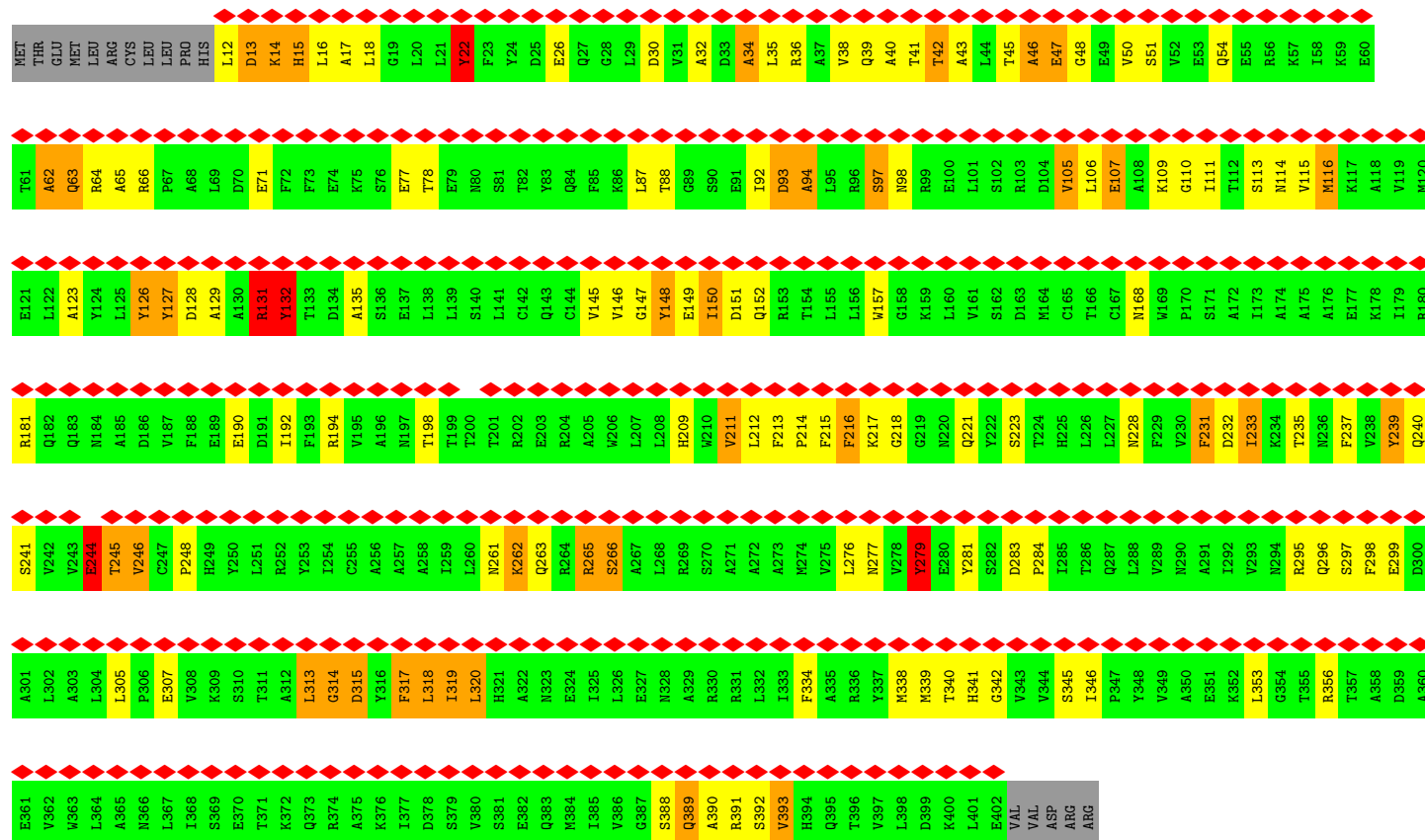




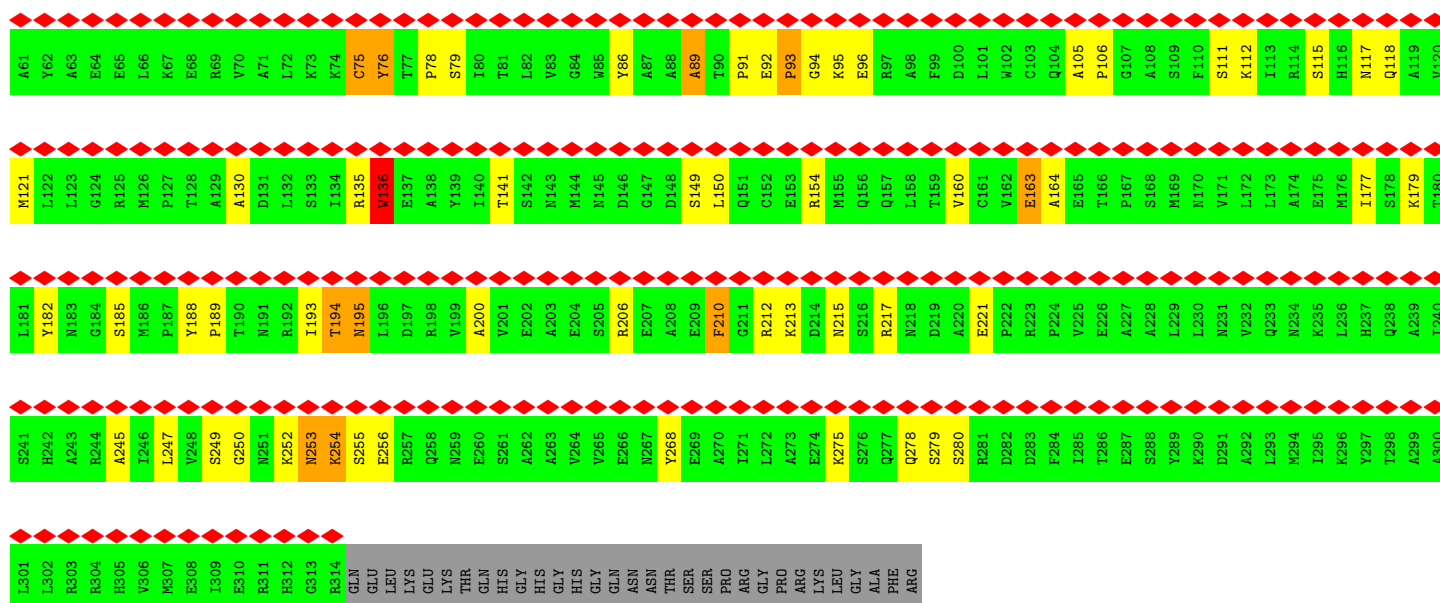
• Molecule 38: Putative eukaryotic translation initiation factor 1A



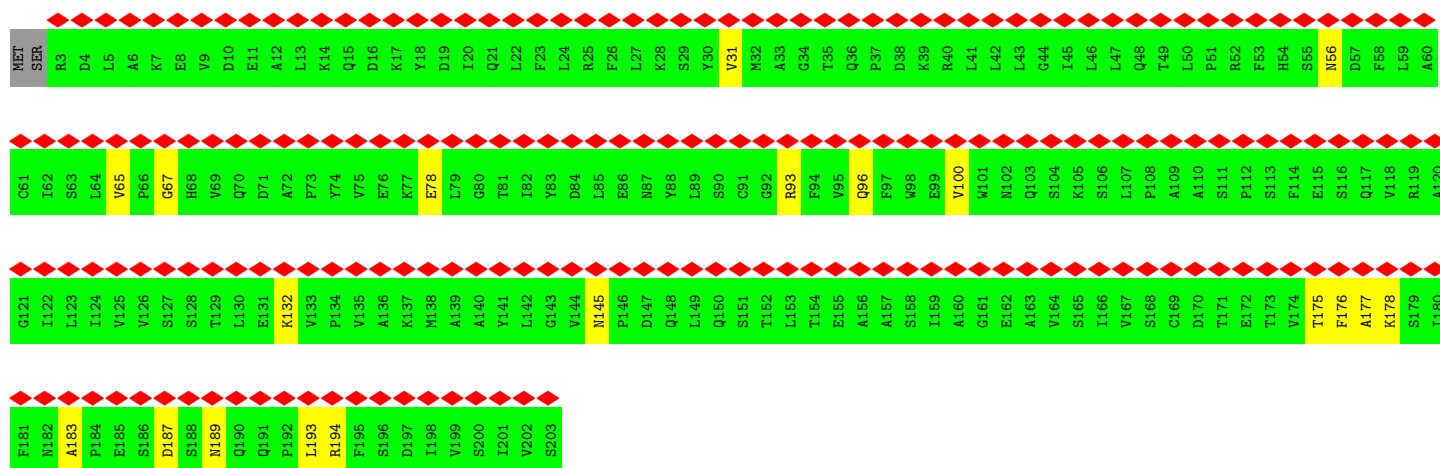
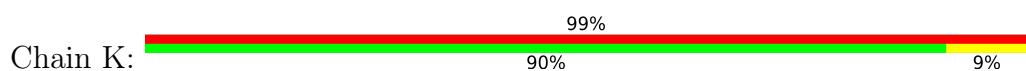
• Molecule 39: Eukaryotic translation initiation factor 3 subunit E



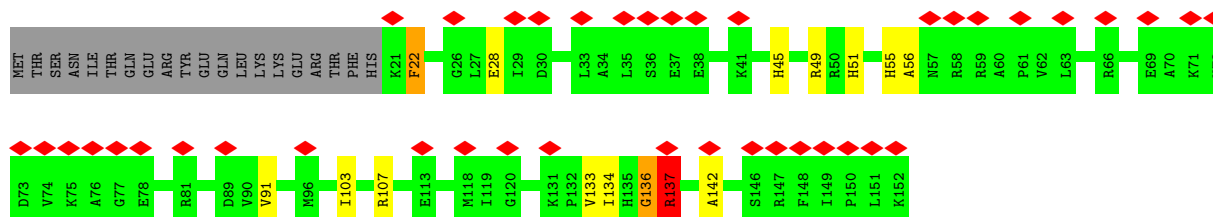
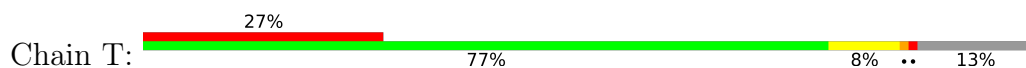
- [illegible]



• Molecule 44: CSN8_PSD8_EIF3K domain-containing protein

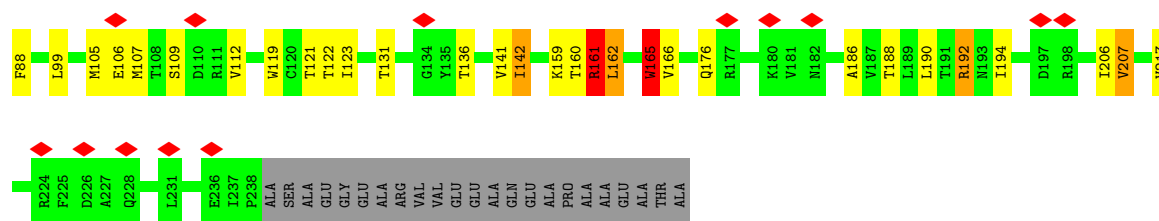


• Molecule 45: 40S ribosomal protein S15, putative

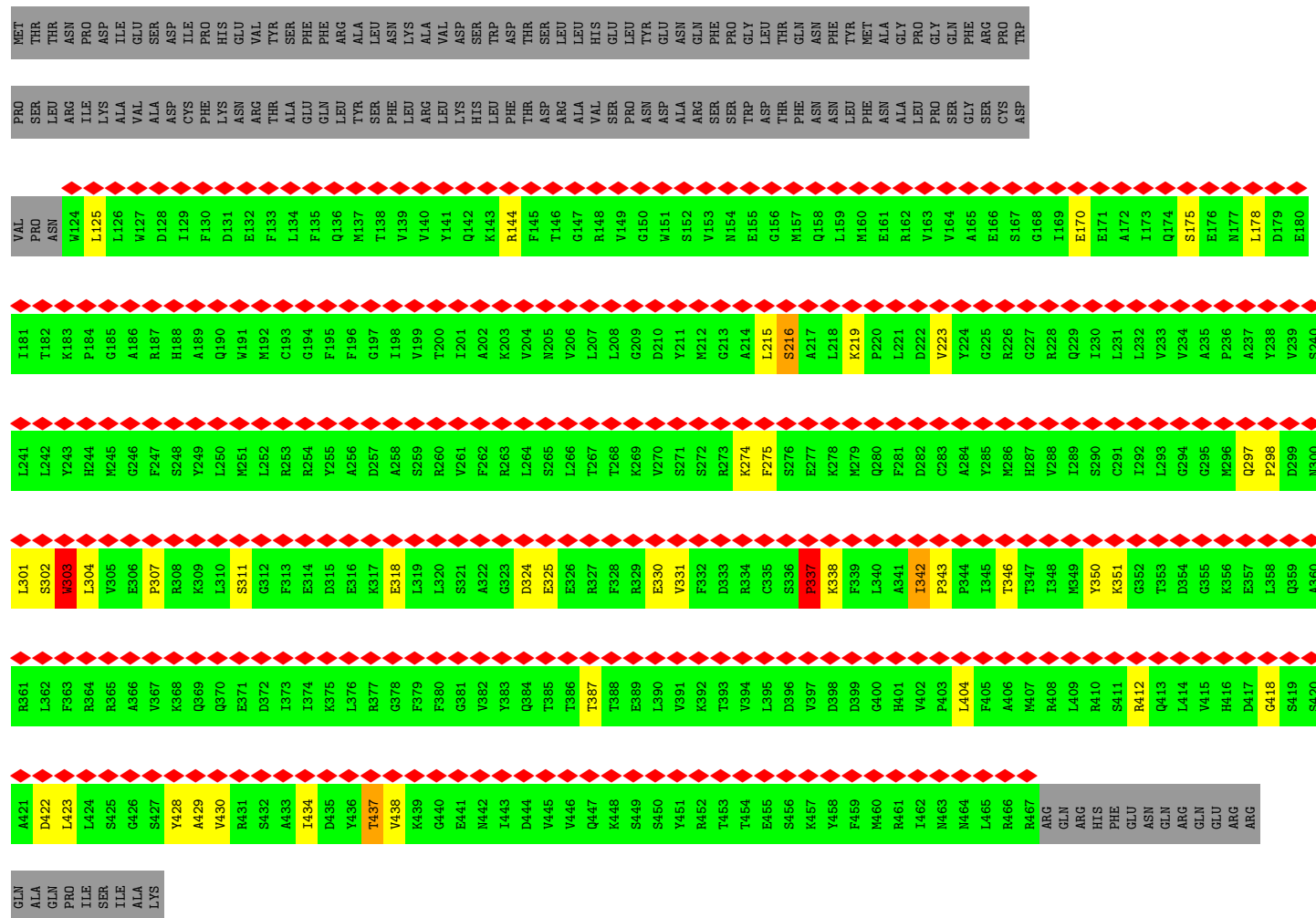


• Molecule 46: Eukaryotic translation initiation factor 3 subunit 8, putative

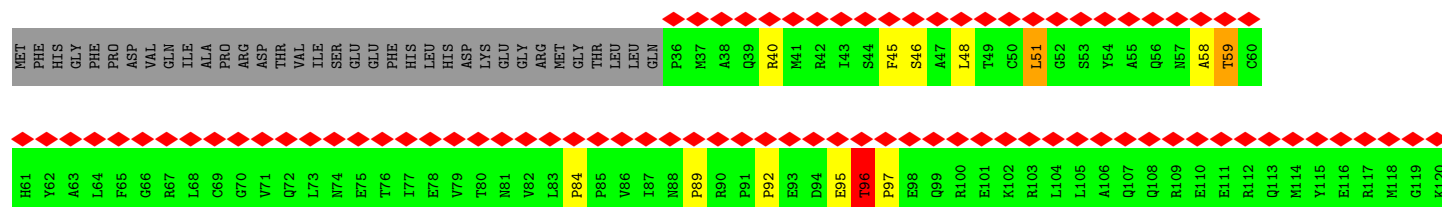


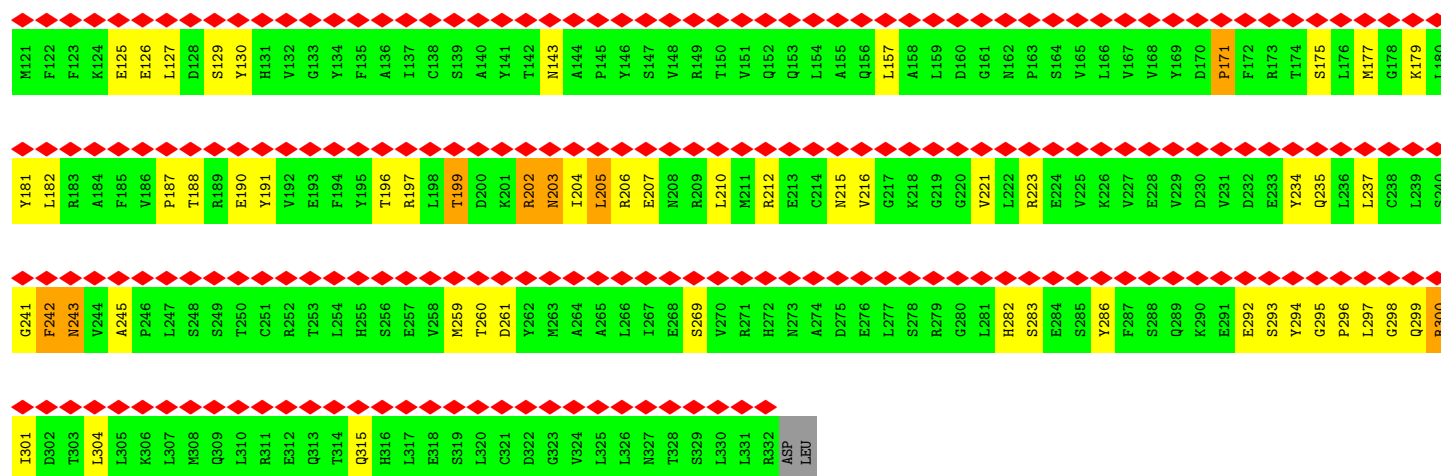


- Molecule 49: Eukaryotic translation initiation factor 3 (EIF-3) interacting protein, putative

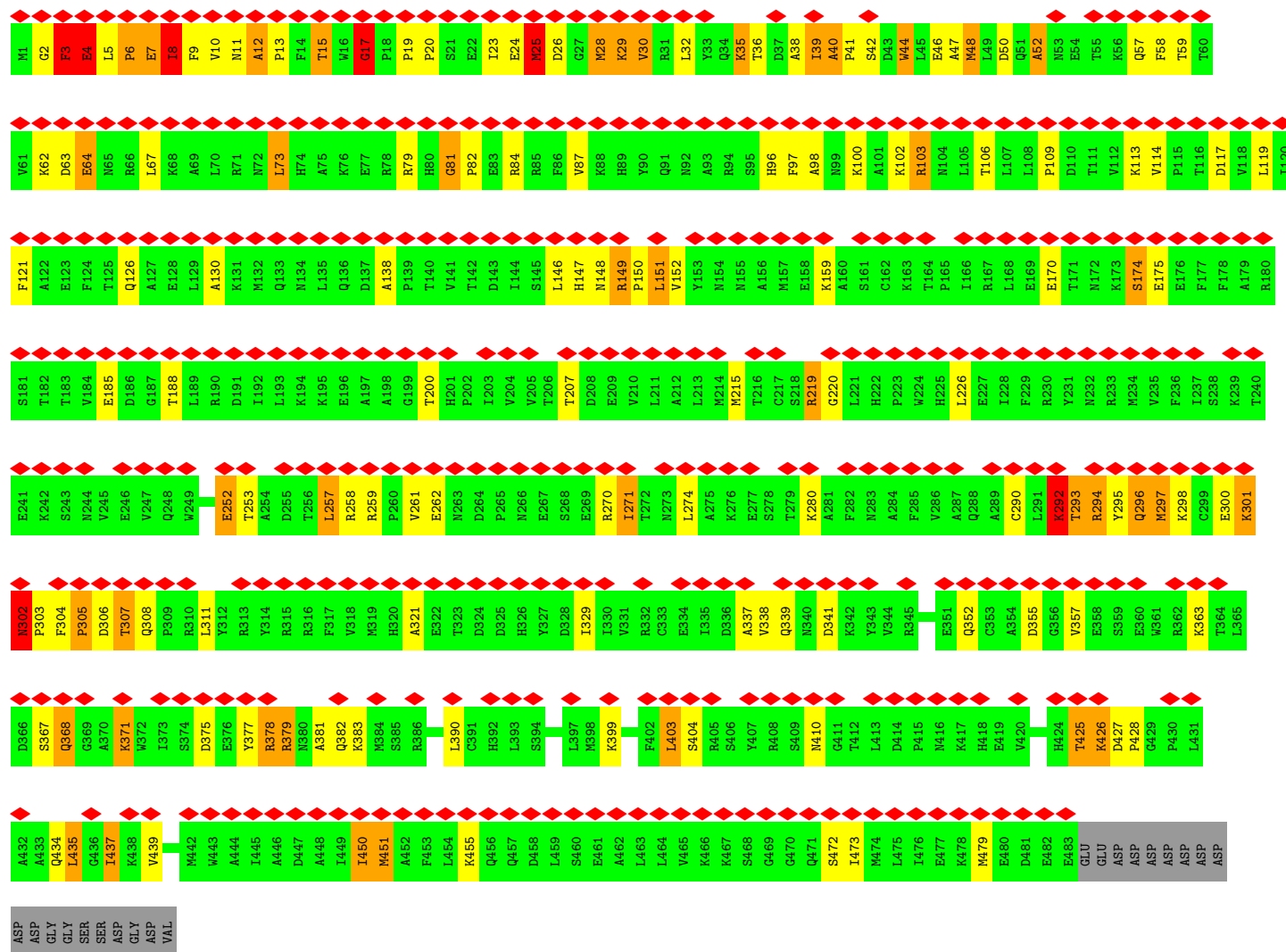


- Molecule 50: eIF3H

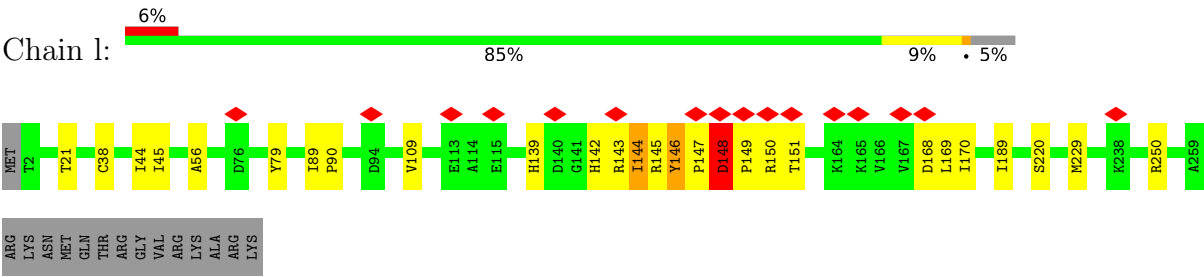




- Molecule 51: Eukaryotic translation initiation factor 3 subunit 7-like protein, putative



● Molecule 52: 40S ribosomal protein S4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0193	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	f	1.78	106/12510 (0.8%)	2.20	379/16884 (2.2%)
2	l	0.89	0/1798	1.06	5/2803 (0.2%)
3	o	0.89	2/51207 (0.0%)	1.03	53/79792 (0.1%)
4	y	1.30	1/1004 (0.1%)	1.52	10/1335 (0.7%)
5	s	1.21	1/2405 (0.0%)	1.63	34/3247 (1.0%)
6	j	1.23	0/658	1.38	4/871 (0.5%)
7	n	1.15	1/1818 (0.1%)	1.44	9/2433 (0.4%)
8	p	1.24	0/2461	1.45	21/3347 (0.6%)
9	r	1.28	0/1131	1.61	8/1520 (0.5%)
10	u	1.35	0/1126	1.72	19/1508 (1.3%)
11	m	1.25	0/1137	1.48	8/1520 (0.5%)
12	Z	1.35	0/1424	1.47	9/1904 (0.5%)
13	o	1.23	0/1515	1.60	20/2034 (1.0%)
14	q	1.33	0/1703	1.58	15/2290 (0.7%)
15	R	1.29	0/1164	1.72	19/1559 (1.2%)
16	S	1.24	0/641	1.38	4/858 (0.5%)
17	t	1.42	0/845	1.51	5/1129 (0.4%)
18	U	1.35	0/527	1.32	2/702 (0.3%)
19	v	1.33	0/1026	1.53	9/1376 (0.7%)
20	X	1.36	2/1238 (0.2%)	1.47	12/1662 (0.7%)
21	B	1.33	0/1513	1.67	19/2030 (0.9%)
22	F	1.26	0/1693	1.60	15/2290 (0.7%)
23	d	1.23	0/1760	1.55	16/2376 (0.7%)
24	g	1.24	0/644	1.46	2/875 (0.2%)
25	a	1.21	0/559	1.52	5/748 (0.7%)
26	J	1.32	0/1381	1.75	29/1857 (1.6%)
27	h	1.25	0/966	1.49	5/1295 (0.4%)
28	5	1.32	4/3302 (0.1%)	2.06	45/4483 (1.0%)
29	P	1.35	0/2008	1.57	23/2678 (0.9%)
30	i	1.28	0/1005	1.85	23/1341 (1.7%)
31	L	1.30	0/794	1.46	10/1076 (0.9%)
32	M	1.33	0/1606	1.56	17/2141 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	N	1.22	0/804	1.68	12/1082 (1.1%)
34	O	1.29	0/1140	1.64	14/1524 (0.9%)
35	b	1.26	0/1037	1.55	11/1391 (0.8%)
36	c	1.15	0/488	1.53	4/644 (0.6%)
37	V	0.96	0/799	1.26	6/1072 (0.6%)
38	w	1.16	0/1177	1.31	6/1588 (0.4%)
39	E	1.40	6/3174 (0.2%)	1.82	74/4304 (1.7%)
40	Y	1.16	0/1406	1.56	12/1890 (0.6%)
41	Q	1.37	0/468	1.60	4/618 (0.6%)
42	D	1.56	0/298	1.65	8/385 (2.1%)
43	G	1.28	0/2455	1.68	28/3323 (0.8%)
44	K	1.14	0/1597	1.67	23/2170 (1.1%)
45	T	1.27	0/1079	1.58	4/1447 (0.3%)
46	C	2.10	4/5724 (0.1%)	1.72	90/7724 (1.2%)
47	8	1.24	0/4685	1.79	91/6327 (1.4%)
48	W	1.35	5/1809 (0.3%)	1.67	30/2437 (1.2%)
49	I	1.22	0/2826	1.67	32/3809 (0.8%)
50	H	1.28	0/2431	1.69	40/3285 (1.2%)
51	A	1.24	3/3971 (0.1%)	1.58	30/5366 (0.6%)
52	l	1.31	0/2073	1.46	14/2787 (0.5%)
All	All	1.25	135/144010 (0.1%)	1.48	1387/205137 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	f	3	200
3	0	2	52
4	y	0	1
5	s	0	17
6	j	0	2
7	n	0	1
8	p	0	2
9	r	0	4
10	u	0	2
11	m	0	2
12	Z	0	2
13	o	0	1
17	t	0	1
19	v	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	X	0	10
21	B	0	4
22	F	0	3
23	d	0	3
24	g	0	1
26	J	0	21
28	5	0	12
29	P	0	4
31	L	0	7
32	M	0	2
33	N	0	1
34	O	0	6
35	b	0	1
36	c	0	3
38	w	0	6
39	E	1	73
40	Y	0	4
41	Q	0	3
42	D	0	1
43	G	0	36
44	K	0	2
45	T	0	1
46	C	1	137
47	8	0	69
48	W	0	2
49	I	2	6
50	H	0	26
51	A	0	16
52	l	0	10
All	All	9	759

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	C	411	ARG	CD-NE	128.69	3.26	1.46
1	f	301	GLU	CA-C	-37.30	1.02	1.52
1	f	1149	TYR	C-N	30.50	1.72	1.33
1	f	301	GLU	C-O	-30.05	0.86	1.24
1	f	304	PRO	CA-C	-28.52	1.19	1.52
28	5	283	GLY	N-CA	-27.68	1.05	1.45
46	C	53	ARG	C-N	24.92	1.67	1.33
1	f	1254	ALA	C-N	24.34	1.68	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	305	TYR	CA-C	-23.97	1.20	1.52
1	f	774	LEU	C-N	23.36	1.66	1.33
1	f	259	PHE	CA-C	23.33	1.81	1.52
1	f	1235	LYS	C-O	-22.07	0.98	1.24
1	f	296	TYR	N-CA	-20.67	1.19	1.46
1	f	301	GLU	C-N	20.35	1.62	1.33
1	f	234	GLY	C-N	-19.35	1.06	1.33
1	f	303	ASN	C-N	18.88	1.55	1.33
1	f	256	GLU	N-CA	-18.85	1.19	1.46
1	f	194	PHE	C-N	-18.00	1.08	1.33
1	f	306	ARG	N-CA	17.92	1.69	1.46
51	A	6	PRO	N-CA	17.79	1.70	1.47
1	f	139	MET	N-CA	-17.70	1.12	1.46
1	f	1653	CYS	C-N	17.68	1.59	1.33
1	f	307	LEU	C-N	17.66	1.65	1.33
1	f	1038	GLY	C-N	17.48	1.58	1.33
39	E	279	TYR	CG-CD1	17.27	1.75	1.39
39	E	279	TYR	CG-CD2	16.79	1.74	1.39
1	f	200	ASP	N-CA	-16.77	1.24	1.46
1	f	1703	GLY	N-CA	-16.06	1.28	1.45
1	f	1221	LEU	C-N	15.87	1.71	1.33
1	f	195	HIS	C-N	-15.71	1.12	1.33
1	f	305	TYR	C-O	15.66	1.43	1.24
39	E	279	TYR	CE1-CZ	15.51	1.75	1.38
1	f	1044	VAL	C-N	15.51	1.54	1.33
39	E	279	TYR	CE2-CZ	15.39	1.75	1.38
1	f	257	PRO	C-N	15.14	1.54	1.33
1	f	139	MET	C-N	-14.96	1.11	1.33
1	f	259	PHE	C-N	14.93	1.56	1.33
48	W	165	TRP	C-N	-14.83	1.15	1.33
1	f	1110	GLY	N-CA	-14.53	1.25	1.45
1	f	1214	ARG	C-N	-14.52	1.13	1.33
1	f	1121	CYS	C-N	14.24	1.53	1.33
1	f	131	THR	C-N	-14.18	1.13	1.33
1	f	1149	TYR	N-CA	14.16	1.64	1.46
1	f	1127	VAL	C-N	13.99	1.66	1.33
1	f	302	ALA	N-CA	13.97	1.64	1.46
1	f	197	VAL	N-CA	13.76	1.61	1.46
1	f	199	PHE	C-N	-13.71	1.14	1.33
1	f	1122	GLN	C-N	13.51	1.54	1.33
1	f	153	GLY	N-CA	-13.50	1.25	1.45
1	f	198	PHE	C-N	-13.28	1.14	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	307	LEU	CA-C	-13.18	1.35	1.52
1	f	239	ASN	C-N	13.02	1.49	1.33
1	f	1219	HIS	C-N	12.95	1.51	1.33
1	f	1655	VAL	N-CA	-12.95	1.31	1.46
1	f	772	TYR	N-CA	-12.81	1.22	1.46
1	f	229	ASN	C-N	12.73	1.51	1.33
1	f	1108	ALA	N-CA	-12.71	1.29	1.46
1	f	304	PRO	C-N	-12.69	1.16	1.33
1	f	1264	LEU	C-N	12.63	1.59	1.33
1	f	264	ASP	C-N	12.59	1.47	1.32
1	f	298	ASP	C-N	12.56	1.51	1.33
1	f	1153	ASP	C-N	12.47	1.51	1.33
1	f	132	ALA	C-N	-11.73	1.19	1.33
1	f	1492	GLY	C-N	11.70	1.61	1.33
1	f	239	ASN	CA-C	-11.46	1.38	1.52
1	f	292	ARG	N-CA	-11.42	1.32	1.45
39	E	279	TYR	CD1-CE1	11.40	1.72	1.38
39	E	279	TYR	CD2-CE2	11.28	1.72	1.38
1	f	263	SER	C-N	-11.23	1.18	1.33
1	f	134	PRO	CA-C	11.20	1.65	1.52
1	f	1147	ILE	C-N	11.05	1.49	1.33
28	5	253	THR	C-N	-10.80	1.19	1.33
1	f	296	TYR	C-N	-10.42	1.19	1.33
1	f	199	PHE	N-CA	9.95	1.58	1.46
1	f	772	TYR	C-N	9.93	1.46	1.33
1	f	792	LEU	C-N	-9.78	1.23	1.34
1	f	1655	VAL	C-O	9.53	1.33	1.24
1	f	292	ARG	C-N	9.42	1.47	1.33
1	f	264	ASP	N-CA	-9.42	1.33	1.45
1	f	1627	ARG	C-N	9.39	1.47	1.33
1	f	136	LEU	C-N	9.24	1.47	1.33
1	f	305	TYR	N-CA	-9.14	1.34	1.46
1	f	294	ALA	C-N	-9.09	1.21	1.33
1	f	1633	HIS	N-CA	8.66	1.58	1.46
48	W	165	TRP	CA-CB	-8.59	1.37	1.53
1	f	153	GLY	C-N	8.51	1.44	1.33
48	W	166	VAL	N-CA	-8.51	1.36	1.46
1	f	138	ASP	C-N	-8.23	1.21	1.33
1	f	294	ALA	N-CA	-8.18	1.35	1.45
1	f	1267	LEU	N-CA	-8.00	1.35	1.46
1	f	1148	ASP	C-N	-8.00	1.22	1.33
1	f	303	ASN	C-O	7.81	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	1042	ALA	C-N	-7.73	1.23	1.33
1	f	1042	ALA	N-CA	-7.59	1.36	1.46
1	f	1040	GLY	N-CA	-7.54	1.35	1.45
28	5	412	GLN	C-N	7.50	1.43	1.33
5	s	302	ASP	C-N	7.32	1.43	1.33
1	f	1259	CYS	C-N	7.26	1.43	1.33
1	f	305	TYR	C-N	7.25	1.43	1.33
3	0	1531	A	O3'-P	7.20	1.72	1.61
51	A	302	ASN	C-N	7.18	1.50	1.33
1	f	293	LYS	C-N	7.17	1.42	1.33
28	5	412	GLN	CA-C	-7.10	1.49	1.53
48	W	165	TRP	N-CA	-7.10	1.36	1.46
1	f	236	SER	C-N	-6.98	1.23	1.33
1	f	198	PHE	CA-C	-6.93	1.43	1.53
1	f	195	HIS	C-O	-6.79	1.15	1.24
1	f	192	ALA	C-N	6.77	1.50	1.32
1	f	1109	LEU	C-O	-6.64	1.15	1.24
1	f	292	ARG	C-O	-6.54	1.15	1.23
1	f	293	LYS	C-O	6.33	1.31	1.23
1	f	1704	HIS	C-O	-6.33	1.16	1.23
1	f	244	TYR	N-CA	-6.27	1.37	1.45
1	f	1654	GLY	C-N	6.26	1.43	1.33
1	f	259	PHE	N-CA	-6.26	1.37	1.45
4	y	15	SER	CA-C	-6.22	1.50	1.53
1	f	1670	CYS	C-N	6.21	1.42	1.33
1	f	1263	ASP	C-N	6.10	1.42	1.33
46	C	411	ARG	NE-CZ	5.98	1.39	1.33
48	W	165	TRP	CA-C	-5.93	1.44	1.52
1	f	293	LYS	N-CA	-5.90	1.38	1.45
1	f	256	GLU	C-N	-5.66	1.20	1.33
1	f	295	ASN	C-N	5.66	1.41	1.33
3	0	1532	G	O3'-P	-5.64	1.52	1.61
1	f	262	MET	C-N	5.58	1.41	1.33
1	f	262	MET	C-O	5.53	1.29	1.24
1	f	297	THR	C-N	5.53	1.41	1.33
1	f	241	SER	C-N	5.50	1.41	1.33
20	X	34	HIS	N-CA	5.46	1.56	1.46
1	f	240	PHE	C-N	5.39	1.41	1.33
46	C	214	LEU	CA-CB	5.24	1.57	1.53
20	X	33	SER	C-N	-5.18	1.26	1.33
51	A	5	LEU	C-N	5.12	1.45	1.33
1	f	242	SER	C-N	5.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	n	210	LEU	C-N	5.03	1.39	1.33

All (1387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5	412	GLN	O-C-N	-66.91	66.11	121.65
1	f	234	GLY	O-C-N	-39.58	66.87	122.68
28	5	411	LEU	CA-C-N	-38.02	82.45	123.13
28	5	411	LEU	C-N-CA	-38.02	82.45	123.13
1	f	1147	ILE	O-C-N	32.67	160.84	122.62
1	f	307	LEU	O-C-N	-31.88	80.19	122.59
3	0	1531	A	O3'-P-O5'	23.81	139.71	104.00
1	f	131	THR	O-C-N	23.55	147.09	122.12
1	f	1127	VAL	CA-C-N	23.41	149.11	119.84
1	f	1127	VAL	C-N-CA	23.41	149.11	119.84
1	f	1147	ILE	CA-C-N	-23.08	88.27	123.13
1	f	1147	ILE	C-N-CA	-23.08	88.27	123.13
26	J	107	PHE	CA-CB-CG	22.04	135.84	113.80
1	f	152	ASP	O-C-N	-21.93	97.91	123.13
1	f	305	TYR	N-CA-CB	21.15	146.23	110.49
1	f	1654	GLY	CA-C-N	20.84	155.83	122.69
1	f	1654	GLY	C-N-CA	20.84	155.83	122.69
1	f	1070	LYS	CA-C-N	20.43	158.75	121.97
1	f	1070	LYS	C-N-CA	20.43	158.75	121.97
1	f	296	TYR	N-CA-C	20.33	154.11	110.80
1	f	134	PRO	CA-C-O	-20.04	97.53	120.97
1	f	239	ASN	CA-C-O	-19.91	99.92	120.82
1	f	262	MET	O-C-N	-19.36	102.91	123.04
1	f	1070	LYS	O-C-N	-19.34	101.18	123.22
1	f	308	ARG	CA-C-N	19.04	162.18	121.45
1	f	308	ARG	C-N-CA	19.04	162.18	121.45
28	5	267	SER	O-C-N	-18.54	103.58	123.42
1	f	306	ARG	N-CA-CB	18.42	141.62	110.49
48	W	166	VAL	N-CA-C	-18.24	94.14	110.74
1	f	1039	ARG	O-C-N	-17.90	98.78	122.59
1	f	296	TYR	CA-C-N	17.73	155.41	121.54
1	f	296	TYR	C-N-CA	17.73	155.41	121.54
1	f	263	SER	O-C-N	-17.46	100.19	123.24
1	f	238	SER	CA-C-N	17.37	143.02	120.44
1	f	238	SER	C-N-CA	17.37	143.02	120.44
1	f	239	ASN	O-C-N	-17.37	104.18	122.07
1	f	198	PHE	O-C-N	-17.10	103.01	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	1259	CYS	O-C-N	-17.03	99.94	122.59
1	f	792	LEU	CA-C-N	16.99	149.24	120.86
1	f	792	LEU	C-N-CA	16.99	149.24	120.86
1	f	259	PHE	N-CA-CB	-16.95	85.63	111.05
1	f	304	PRO	CA-C-O	-16.81	101.87	121.03
51	A	5	LEU	CA-C-N	16.75	140.77	119.84
51	A	5	LEU	C-N-CA	16.75	140.77	119.84
28	5	411	LEU	O-C-N	16.69	145.78	122.74
1	f	198	PHE	N-CA-C	-16.66	85.80	110.46
1	f	1121	CYS	CA-C-N	16.55	153.14	121.54
1	f	1121	CYS	C-N-CA	16.55	153.14	121.54
1	f	1221	LEU	O-C-N	-16.55	102.29	121.32
1	f	1254	ALA	CA-C-N	-16.50	96.91	122.81
1	f	1254	ALA	C-N-CA	-16.50	96.91	122.81
5	s	300	ARG	N-CA-C	16.48	145.91	110.80
1	f	132	ALA	O-C-N	16.06	143.95	122.59
1	f	1122	GLN	CA-C-O	-16.00	97.63	120.51
1	f	1266	PRO	CA-C-N	15.83	151.77	121.54
1	f	1266	PRO	C-N-CA	15.83	151.77	121.54
1	f	1125	LEU	CB-CA-C	-15.80	90.72	110.94
1	f	1220	LEU	O-C-N	15.40	141.05	123.04
3	0	1531	A	C2'-C3'-O3'	15.05	132.07	109.50
51	A	302	ASN	CA-C-N	14.92	138.49	119.84
51	A	302	ASN	C-N-CA	14.92	138.49	119.84
1	f	243	TYR	CA-C-N	14.52	147.40	120.97
1	f	243	TYR	C-N-CA	14.52	147.40	120.97
1	f	305	TYR	O-C-N	-14.01	103.95	122.59
1	f	236	SER	O-C-N	-13.90	109.39	123.29
1	f	1177	PRO	CB-CA-C	13.84	129.07	111.64
46	C	411	ARG	CD-NE-CZ	13.68	143.55	124.40
1	f	772	TYR	N-CA-CB	13.40	133.29	110.50
1	f	138	ASP	CA-C-N	-13.36	97.66	121.70
1	f	138	ASP	C-N-CA	-13.36	97.66	121.70
1	f	152	ASP	CA-C-N	13.35	147.58	121.41
1	f	152	ASP	C-N-CA	13.35	147.58	121.41
1	f	259	PHE	CA-C-O	-13.29	106.00	121.68
1	f	304	PRO	N-CA-C	13.11	130.59	110.80
48	W	165	TRP	CA-CB-CG	13.08	138.46	113.60
1	f	1670	CYS	O-C-N	-12.97	106.29	123.15
1	f	255	TRP	O-C-N	12.82	135.71	122.12
1	f	1264	LEU	O-C-N	-12.78	105.59	122.59
1	f	1175	PRO	O-C-N	-12.76	105.41	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	W	165	TRP	N-CA-C	12.62	128.02	112.87
1	f	1175	PRO	CA-C-N	-12.53	99.76	122.06
1	f	1175	PRO	C-N-CA	-12.53	99.76	122.06
48	W	165	TRP	CB-CG-CD2	-12.33	109.54	126.80
1	f	238	SER	CB-CA-C	-12.29	84.59	109.79
3	0	1531	A	P-O3'-C3'	12.28	138.62	120.20
3	0	1070	C	P-O3'-C3'	12.24	138.57	120.20
48	W	165	TRP	CB-CA-C	-12.22	83.45	110.21
1	f	236	SER	CA-C-N	12.19	139.88	122.94
1	f	236	SER	C-N-CA	12.19	139.88	122.94
1	f	1670	CYS	CA-C-N	12.09	140.78	122.17
1	f	1670	CYS	C-N-CA	12.09	140.78	122.17
1	f	1218	VAL	O-C-N	-12.05	110.31	122.97
1	f	1109	LEU	N-CA-C	12.05	136.47	110.80
1	f	772	TYR	O-C-N	-11.91	103.95	123.00
1	f	1121	CYS	O-C-N	11.80	138.28	122.59
1	f	1265	HIS	O-C-N	-11.71	107.86	121.32
1	f	258	GLU	O-C-N	-11.57	107.20	122.59
1	f	193	ARG	CA-C-N	11.52	143.54	121.54
1	f	193	ARG	C-N-CA	11.52	143.54	121.54
48	W	165	TRP	CB-CG-CD1	11.40	144.00	126.90
1	f	259	PHE	CB-CA-C	-11.31	88.98	110.24
3	0	1982	G	P-O5'-C5'	11.24	137.76	120.90
48	W	165	TRP	N-CA-CB	11.23	130.76	110.32
1	f	131	THR	CA-C-N	11.21	142.94	121.54
1	f	131	THR	C-N-CA	11.21	142.94	121.54
1	f	304	PRO	O-C-N	11.21	135.65	123.10
1	f	303	ASN	CA-C-O	11.16	135.45	120.16
5	s	300	ARG	CB-CA-C	-11.06	88.40	110.42
1	f	136	LEU	N-CA-CB	-10.97	91.94	110.49
1	f	258	GLU	CA-C-N	-10.95	103.43	123.03
1	f	258	GLU	C-N-CA	-10.95	103.43	123.03
3	0	217	C	P-O3'-C3'	10.94	136.60	120.20
1	f	137	CYS	O-C-N	-10.89	108.23	122.72
1	f	192	ALA	CA-C-N	-10.86	91.42	122.15
1	f	192	ALA	C-N-CA	-10.86	91.42	122.15
34	O	140	ILE	N-CA-C	-10.85	103.40	113.71
1	f	1627	ARG	O-C-N	-10.85	108.31	122.20
1	f	256	GLU	N-CA-C	10.82	133.72	109.81
1	f	301	GLU	CA-C-O	-10.76	105.12	120.51
1	f	1128	PRO	O-C-N	-10.69	108.21	122.64
1	f	293	LYS	O-C-N	-10.62	110.18	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	239	ASN	CB-CA-C	10.59	127.50	110.88
1	f	1152	LEU	CA-C-N	-10.50	106.10	122.59
1	f	1152	LEU	C-N-CA	-10.50	106.10	122.59
51	A	6	PRO	CA-N-CD	-10.47	97.34	112.00
39	E	334	PHE	CA-CB-CG	-10.38	103.42	113.80
1	f	234	GLY	CA-C-N	-10.36	101.76	121.54
1	f	234	GLY	C-N-CA	-10.36	101.76	121.54
1	f	297	THR	CA-C-N	10.34	141.29	121.54
1	f	297	THR	C-N-CA	10.34	141.29	121.54
1	f	193	ARG	O-C-N	-10.32	110.07	122.25
1	f	137	CYS	N-CA-C	-10.24	93.68	109.65
1	f	289	ASP	CA-C-N	10.19	140.03	121.70
1	f	289	ASP	C-N-CA	10.19	140.03	121.70
35	b	33	VAL	N-CA-C	-10.13	101.96	111.48
1	f	303	ASN	CA-C-N	9.97	130.37	119.90
1	f	303	ASN	C-N-CA	9.97	130.37	119.90
1	f	239	ASN	CA-C-N	9.90	137.61	121.58
1	f	239	ASN	C-N-CA	9.90	137.61	121.58
1	f	233	VAL	CA-C-O	-9.86	109.41	120.26
1	f	136	LEU	CA-C-O	-9.82	106.47	120.51
1	f	256	GLU	CA-C-N	9.73	132.00	119.84
1	f	256	GLU	C-N-CA	9.73	132.00	119.84
3	0	1579	A	P-O3'-C3'	9.71	134.77	120.20
1	f	292	ARG	CA-C-N	9.70	137.76	122.62
1	f	292	ARG	C-N-CA	9.70	137.76	122.62
41	Q	51	ILE	N-CA-C	-9.60	104.59	113.71
1	f	1267	LEU	N-CA-C	-9.59	90.37	110.80
1	f	1038	GLY	CA-C-N	9.58	139.83	121.54
1	f	1038	GLY	C-N-CA	9.58	139.83	121.54
10	u	35	LYS	N-CA-C	9.55	131.15	110.80
1	f	1254	ALA	O-C-N	9.50	135.22	122.59
47	8	452	VAL	N-CA-C	9.48	120.29	110.72
1	f	1370	LEU	N-CA-C	-9.47	103.82	114.62
47	8	39	GLN	N-CA-C	9.37	121.50	111.28
1	f	259	PHE	N-CA-C	9.23	123.94	109.81
1	f	135	GLU	CA-C-O	-9.20	110.91	121.58
1	f	1703	GLY	CA-C-N	-9.14	105.94	121.75
1	f	1703	GLY	C-N-CA	-9.14	105.94	121.75
1	f	240	PHE	O-C-N	9.08	134.51	123.26
47	8	453	ARG	CA-C-N	9.07	138.03	121.70
47	8	453	ARG	C-N-CA	9.07	138.03	121.70
28	5	427	ILE	N-CA-C	-9.06	103.56	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	C	215	ARG	N-CA-C	8.99	126.20	111.37
1	f	1653	CYS	O-C-N	8.97	133.02	122.79
1	f	1149	TYR	N-CA-C	-8.97	91.69	110.80
3	0	1530	C	OP2-P-O3'	-8.96	81.12	108.00
1	f	47	GLU	N-CA-C	-8.91	104.47	114.62
1	f	196	VAL	CA-C-N	-8.90	110.78	123.06
1	f	196	VAL	C-N-CA	-8.90	110.78	123.06
1	f	295	ASN	N-CA-C	8.87	129.69	110.80
1	f	301	GLU	O-C-N	8.84	134.35	122.59
2	1	73	C	P-O3'-C3'	8.84	133.46	120.20
3	0	1530	C	O3'-P-O5'	8.83	117.25	104.00
3	0	1531	A	C4'-C3'-O3'	8.82	122.63	109.40
3	0	2157	C	P-O3'-C3'	8.81	133.42	120.20
49	I	404	LEU	N-CA-C	-8.80	104.59	114.62
46	C	580	LYS	N-CA-C	8.74	123.50	113.01
3	0	1980	A	P-O3'-C3'	8.71	133.27	120.20
47	8	453	ARG	N-CA-C	8.71	124.04	113.41
1	f	1633	HIS	N-CA-CB	-8.71	97.39	110.97
20	X	32	ASN	CA-C-N	8.70	138.16	121.54
20	X	32	ASN	C-N-CA	8.70	138.16	121.54
1	f	266	GLU	CA-C-N	8.66	137.29	121.70
1	f	266	GLU	C-N-CA	8.66	137.29	121.70
1	f	1494	THR	CA-C-N	8.63	134.99	122.99
1	f	1494	THR	C-N-CA	8.63	134.99	122.99
46	C	333	ARG	N-CA-C	-8.56	103.97	114.75
33	N	44	VAL	N-CA-C	-8.54	102.18	109.19
1	f	1259	CYS	CA-C-N	-8.52	106.36	121.70
1	f	1259	CYS	C-N-CA	-8.52	106.36	121.70
1	f	816	LYS	CA-C-N	8.49	129.37	119.94
1	f	816	LYS	C-N-CA	8.49	129.37	119.94
1	f	293	LYS	CA-C-N	8.49	136.87	121.85
1	f	293	LYS	C-N-CA	8.49	136.87	121.85
46	C	331	ARG	CA-C-N	8.46	136.93	121.70
46	C	331	ARG	C-N-CA	8.46	136.93	121.70
33	N	93	ALA	CA-C-N	8.43	125.55	120.24
33	N	93	ALA	C-N-CA	8.43	125.55	120.24
1	f	237	ILE	CA-C-N	8.42	135.81	122.59
1	f	237	ILE	C-N-CA	8.42	135.81	122.59
1	f	238	SER	N-CA-C	8.42	122.58	109.52
1	f	302	ALA	CA-C-O	-8.40	108.50	120.51
1	f	1177	PRO	N-CA-C	-8.37	98.15	111.03
44	K	175	THR	CA-C-N	8.36	135.72	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	K	175	THR	C-N-CA	8.36	135.72	122.34
3	0	2081	A	O3'-P-O5'	8.26	116.39	104.00
1	f	1654	GLY	N-CA-C	8.25	132.74	113.18
3	0	122	A	P-O3'-C3'	8.24	132.56	120.20
1	f	1492	GLY	CA-C-N	-8.18	109.61	119.84
1	f	1492	GLY	C-N-CA	-8.18	109.61	119.84
46	C	53	ARG	O-C-N	-8.18	112.20	122.27
28	5	267	SER	CA-C-N	8.18	137.16	121.54
28	5	267	SER	C-N-CA	8.18	137.16	121.54
39	E	276	LEU	CA-C-N	8.17	136.41	121.70
39	E	276	LEU	C-N-CA	8.17	136.41	121.70
1	f	143	LEU	CA-C-N	8.12	136.32	121.70
1	f	143	LEU	C-N-CA	8.12	136.32	121.70
1	f	1153	ASP	CA-C-N	8.10	137.00	121.54
1	f	1153	ASP	C-N-CA	8.10	137.00	121.54
3	0	1468	U	P-O5'-C5'	8.09	133.04	120.90
1	f	199	PHE	N-CA-CB	-8.08	97.89	110.65
1	f	1214	ARG	O-C-N	-8.08	113.74	123.19
47	8	179	ILE	N-CA-C	-8.04	104.89	111.81
30	i	86	PRO	CA-C-N	8.04	136.18	121.70
30	i	86	PRO	C-N-CA	8.04	136.18	121.70
39	E	318	LEU	CA-C-N	8.04	136.18	121.70
39	E	318	LEU	C-N-CA	8.04	136.18	121.70
1	f	303	ASN	CB-CA-C	8.04	126.01	110.17
5	s	394	TYR	CA-C-N	8.00	136.09	121.70
5	s	394	TYR	C-N-CA	8.00	136.09	121.70
1	f	297	THR	O-C-N	7.99	133.22	122.59
51	A	3	PHE	CA-C-N	7.97	136.04	121.70
51	A	3	PHE	C-N-CA	7.97	136.04	121.70
3	0	1450	G	P-O3'-C3'	7.95	132.13	120.20
48	W	160	THR	N-CA-C	-7.94	102.56	112.72
46	C	17	VAL	N-CA-C	-7.93	105.41	113.10
1	f	294	ALA	O-C-N	7.89	132.25	123.33
1	f	243	TYR	CB-CA-C	-7.86	107.51	116.63
3	0	1532	G	O3'-P-O5'	-7.85	92.22	104.00
1	f	1110	GLY	CA-C-N	7.85	136.79	121.41
1	f	1110	GLY	C-N-CA	7.85	136.79	121.41
1	f	192	ALA	O-C-N	7.83	132.25	123.16
1	f	262	MET	CA-C-N	7.83	133.58	121.76
1	f	262	MET	C-N-CA	7.83	133.58	121.76
3	0	1531	A	O5'-C5'-C4'	7.80	123.39	111.70
1	f	306	ARG	CA-C-N	7.76	136.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	306	ARG	C-N-CA	7.76	136.37	121.54
39	E	215	PHE	CA-C-N	7.74	135.64	121.70
39	E	215	PHE	C-N-CA	7.74	135.64	121.70
39	E	77	GLU	CA-C-N	7.74	135.63	121.70
39	E	77	GLU	C-N-CA	7.74	135.63	121.70
1	f	772	TYR	CA-C-N	7.73	136.89	123.05
1	f	772	TYR	C-N-CA	7.73	136.89	123.05
26	J	149	SER	CA-C-N	7.71	135.58	121.70
26	J	149	SER	C-N-CA	7.71	135.58	121.70
1	f	195	HIS	CA-C-N	7.71	133.70	122.99
1	f	195	HIS	C-N-CA	7.71	133.70	122.99
28	5	88	ILE	N-CA-C	-7.69	97.05	108.12
1	f	194	PHE	O-C-N	7.66	132.78	122.59
1	f	308	ARG	O-C-N	-7.66	113.74	122.09
50	H	212	ARG	N-CA-CB	7.66	121.11	110.01
46	C	411	ARG	NE-CZ-NH2	7.64	126.08	119.20
3	0	1467	U	P-O3'-C3'	7.64	131.66	120.20
43	G	194	THR	CA-C-N	7.63	131.40	120.79
43	G	194	THR	C-N-CA	7.63	131.40	120.79
1	f	1702	LEU	CA-C-N	-7.63	107.67	121.93
1	f	1702	LEU	C-N-CA	-7.63	107.67	121.93
46	C	214	LEU	CA-C-N	7.62	132.25	120.82
46	C	214	LEU	C-N-CA	7.62	132.25	120.82
1	f	134	PRO	CB-CA-C	-7.61	102.21	111.11
1	f	1148	ASP	O-C-N	7.60	134.52	122.96
3	0	714	G	P-O5'-C5'	7.60	132.29	120.90
50	H	235	GLN	CA-C-N	7.56	130.74	120.54
50	H	235	GLN	C-N-CA	7.56	130.74	120.54
46	C	411	ARG	CG-CD-NE	7.55	128.62	112.00
31	L	37	LEU	CA-C-N	7.50	130.66	120.38
31	L	37	LEU	C-N-CA	7.50	130.66	120.38
10	u	35	LYS	CB-CA-C	-7.44	95.61	110.42
1	f	264	ASP	CA-C-N	7.44	134.44	122.69
1	f	264	ASP	C-N-CA	7.44	134.44	122.69
47	8	134	GLN	CA-C-N	7.40	130.50	120.44
47	8	134	GLN	C-N-CA	7.40	130.50	120.44
39	E	313	LEU	CA-C-N	7.39	135.00	121.70
39	E	313	LEU	C-N-CA	7.39	135.00	121.70
46	C	471	VAL	N-CA-C	-7.38	105.64	112.43
30	i	82	MET	CA-C-N	7.37	134.97	121.70
30	i	82	MET	C-N-CA	7.37	134.97	121.70
1	f	1219	HIS	O-C-N	-7.37	112.79	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	G	13	PHE	CA-C-N	7.34	130.07	120.60
43	G	13	PHE	C-N-CA	7.34	130.07	120.60
1	f	775	GLY	CA-C-N	7.29	135.69	121.41
1	f	775	GLY	C-N-CA	7.29	135.69	121.41
50	H	210	LEU	N-CA-C	7.28	118.86	111.07
1	f	1555	GLN	CA-C-N	7.26	134.77	121.70
1	f	1555	GLN	C-N-CA	7.26	134.77	121.70
47	8	296	ALA	CA-C-N	7.24	130.48	120.63
47	8	296	ALA	C-N-CA	7.24	130.48	120.63
10	u	100	THR	CA-C-N	7.22	134.69	121.70
10	u	100	THR	C-N-CA	7.22	134.69	121.70
22	F	82	THR	N-CA-C	-7.21	105.66	114.75
1	f	197	VAL	N-CA-CB	-7.20	98.86	111.39
1	f	1235	LYS	CA-C-O	-7.17	112.88	120.40
47	8	390	PHE	N-CA-C	-7.13	105.50	114.56
47	8	41	GLY	C-N-CD	7.13	136.28	120.60
50	H	181	TYR	CA-C-N	7.12	134.53	121.70
50	H	181	TYR	C-N-CA	7.12	134.53	121.70
1	f	1153	ASP	O-C-N	-7.11	113.91	123.15
46	C	373	VAL	CA-C-N	7.09	134.47	121.70
46	C	373	VAL	C-N-CA	7.09	134.47	121.70
39	E	209	HIS	CA-CB-CG	7.06	120.86	113.80
10	u	35	LYS	N-CA-CB	-7.06	98.56	110.49
1	f	198	PHE	CA-C-O	-7.04	112.95	121.89
46	C	468	ASN	CA-C-N	7.04	134.38	121.70
46	C	468	ASN	C-N-CA	7.04	134.38	121.70
1	f	305	TYR	CA-C-N	7.04	134.99	121.54
1	f	305	TYR	C-N-CA	7.04	134.99	121.54
1	f	240	PHE	CA-C-N	7.04	134.98	121.54
1	f	240	PHE	C-N-CA	7.04	134.98	121.54
1	f	292	ARG	O-C-N	-7.03	114.03	123.10
46	C	475	GLN	CA-C-N	7.03	134.35	121.70
46	C	475	GLN	C-N-CA	7.03	134.35	121.70
13	o	51	ARG	N-CA-C	-7.03	103.28	112.41
46	C	480	TYR	CA-C-N	7.01	134.32	121.70
46	C	480	TYR	C-N-CA	7.01	134.32	121.70
1	f	242	SER	CA-C-N	7.01	134.78	122.66
1	f	242	SER	C-N-CA	7.01	134.78	122.66
51	A	121	PHE	N-CA-C	-7.01	105.35	114.04
28	5	412	GLN	N-CA-C	-7.00	102.03	108.75
47	8	309	PHE	CA-CB-CG	-6.99	106.81	113.80
47	8	460	SER	N-CA-C	6.99	119.50	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	1630	GLY	N-CA-C	6.96	123.36	111.04
47	8	198	TYR	N-CA-C	-6.96	102.02	112.04
47	8	198	TYR	CA-C-N	6.96	129.33	120.56
47	8	198	TYR	C-N-CA	6.96	129.33	120.56
32	M	166	PHE	N-CA-C	-6.95	106.70	114.62
1	f	1655	VAL	O-C-N	-6.95	115.57	123.00
34	O	117	LEU	N-CA-C	-6.94	104.70	113.72
3	0	1694	A	P-O3'-C3'	6.90	130.55	120.20
1	f	153	GLY	CA-C-N	-6.89	111.21	120.79
1	f	153	GLY	C-N-CA	-6.89	111.21	120.79
47	8	211	PRO	CA-C-N	6.89	134.10	121.70
47	8	211	PRO	C-N-CA	6.89	134.10	121.70
52	l	148	ASP	N-CA-C	-6.88	101.44	110.39
49	I	303	TRP	CA-C-N	6.88	129.38	120.44
49	I	303	TRP	C-N-CA	6.88	129.38	120.44
1	f	264	ASP	N-CA-CB	6.87	120.72	110.29
1	f	257	PRO	O-C-N	-6.86	113.38	122.64
1	f	265	GLY	N-CA-C	-6.83	105.07	112.04
2	1	71	U	O3'-P-O5'	6.83	114.24	104.00
47	8	154	GLU	N-CA-C	-6.83	103.85	112.93
1	f	774	LEU	O-C-N	-6.82	113.52	122.59
37	V	51	PHE	CA-CB-CG	-6.82	106.98	113.80
8	p	124	ILE	N-CA-C	-6.82	98.67	108.42
3	0	1971	C	P-O3'-C3'	6.82	130.43	120.20
1	f	1845	SER	CA-C-N	6.82	127.69	119.99
1	f	1845	SER	C-N-CA	6.82	127.69	119.99
1	f	1311	SER	CA-C-N	6.81	133.95	121.70
1	f	1311	SER	C-N-CA	6.81	133.95	121.70
46	C	646	SER	CA-C-N	6.79	133.93	121.70
46	C	646	SER	C-N-CA	6.79	133.93	121.70
5	s	284	PRO	CA-C-N	6.78	129.67	120.38
5	s	284	PRO	C-N-CA	6.78	129.67	120.38
5	s	266	HIS	N-CA-C	-6.78	104.56	114.39
36	c	8	LEU	N-CA-C	-6.76	104.72	114.12
19	v	51	GLY	CA-C-N	6.76	127.48	119.98
19	v	51	GLY	C-N-CA	6.76	127.48	119.98
1	f	1257	ASN	CA-C-N	6.76	133.86	121.70
1	f	1257	ASN	C-N-CA	6.76	133.86	121.70
11	m	25	LYS	CA-C-N	6.75	127.59	120.03
11	m	25	LYS	C-N-CA	6.75	127.59	120.03
46	C	330	GLN	O-C-N	6.75	131.57	122.59
31	L	38	LEU	CA-C-N	6.74	129.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	38	LEU	C-N-CA	6.74	129.31	120.28
33	N	19	THR	N-CA-CB	6.74	121.88	110.49
10	u	29	PHE	CA-CB-CG	-6.73	107.07	113.80
1	f	199	PHE	N-CA-C	-6.73	96.25	108.02
1	f	28	ASP	N-CA-C	-6.71	105.72	114.04
1	f	278	PHE	CA-CB-CG	-6.71	107.09	113.80
17	t	55	VAL	N-CA-C	-6.68	105.20	111.48
39	E	18	LEU	CA-C-N	6.68	127.36	119.94
39	E	18	LEU	C-N-CA	6.68	127.36	119.94
51	A	439	VAL	CA-C-N	6.68	127.36	119.94
51	A	439	VAL	C-N-CA	6.68	127.36	119.94
47	8	549	HIS	N-CA-C	-6.68	105.01	113.43
1	f	296	TYR	O-C-N	-6.68	113.71	122.59
48	W	39	GLU	N-CA-C	6.68	118.56	111.28
3	0	1524	U	P-O3'-C3'	6.67	130.21	120.20
46	C	98	PHE	N-CA-C	-6.67	105.02	113.43
39	E	181	ARG	N-CA-C	6.67	118.63	111.36
7	n	149	VAL	N-CA-CB	6.67	114.99	110.52
1	f	1025	PRO	CA-C-N	6.66	133.69	121.70
1	f	1025	PRO	C-N-CA	6.66	133.69	121.70
1	f	799	ARG	N-CA-C	-6.65	104.33	113.18
1	f	204	TRP	CA-C-N	6.64	133.65	121.70
1	f	204	TRP	C-N-CA	6.64	133.65	121.70
28	5	283	GLY	CA-C-N	6.63	129.85	122.55
28	5	283	GLY	C-N-CA	6.63	129.85	122.55
23	d	90	ILE	N-CA-C	-6.62	98.08	108.81
47	8	394	PHE	CA-C-N	6.60	126.10	119.24
47	8	394	PHE	C-N-CA	6.60	126.10	119.24
39	E	342	GLY	CA-C-N	6.59	133.56	121.70
39	E	342	GLY	C-N-CA	6.59	133.56	121.70
46	C	454	ILE	CA-C-N	6.59	133.56	121.70
46	C	454	ILE	C-N-CA	6.59	133.56	121.70
35	b	62	VAL	N-CA-C	-6.56	98.28	108.44
1	f	256	GLU	O-C-N	-6.55	113.79	121.32
28	5	283	GLY	N-CA-C	6.55	128.70	113.18
1	f	1108	ALA	N-CA-C	6.55	124.74	110.80
1	f	1002	LEU	N-CA-C	-6.54	104.44	112.88
39	E	298	PHE	N-CA-C	-6.54	105.84	113.88
3	0	1982	G	C5'-C4'-C3'	-6.53	106.21	116.00
39	E	129	ALA	CA-C-N	6.53	133.45	121.70
39	E	129	ALA	C-N-CA	6.53	133.45	121.70
47	8	369	PHE	CA-C-N	6.52	133.44	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	8	369	PHE	C-N-CA	6.52	133.44	121.70
28	5	140	VAL	N-CA-C	-6.51	99.10	108.42
47	8	179	ILE	CA-C-N	6.51	129.01	120.28
47	8	179	ILE	C-N-CA	6.51	129.01	120.28
3	0	812	A	P-O3'-C3'	6.51	129.97	120.20
47	8	401	ASP	CA-C-N	6.50	127.34	119.99
47	8	401	ASP	C-N-CA	6.50	127.34	119.99
39	E	248	PRO	CA-C-N	6.50	128.89	120.44
39	E	248	PRO	C-N-CA	6.50	128.89	120.44
1	f	829	LYS	CB-CA-C	-6.50	109.09	116.63
44	K	193	LEU	CA-C-N	6.48	128.97	120.28
44	K	193	LEU	C-N-CA	6.48	128.97	120.28
39	E	123	ALA	CA-C-N	6.48	128.96	120.28
39	E	123	ALA	C-N-CA	6.48	128.96	120.28
3	0	150	U	P-O3'-C3'	6.48	129.92	120.20
46	C	53	ARG	CA-C-N	-6.48	110.49	122.09
46	C	53	ARG	C-N-CA	-6.48	110.49	122.09
1	f	1267	LEU	N-CA-CB	6.47	121.43	110.49
1	f	139	MET	N-CA-CB	-6.47	99.51	110.50
47	8	23	TYR	N-CA-C	-6.46	105.02	114.39
47	8	465	GLY	CA-C-N	6.46	128.83	120.44
47	8	465	GLY	C-N-CA	6.46	128.83	120.44
40	Y	229	ARG	N-CA-C	6.44	118.84	111.11
21	B	93	ASP	N-CA-C	-6.44	104.62	113.18
34	O	130	ILE	N-CA-C	-6.42	106.87	113.10
3	0	1983	C	P-O5'-C5'	6.42	130.53	120.90
3	0	1531	A	OP2-P-O3'	-6.42	88.75	108.00
34	O	53	ILE	N-CA-C	-6.42	106.53	112.43
46	C	580	LYS	CA-C-N	6.40	133.76	121.54
46	C	580	LYS	C-N-CA	6.40	133.76	121.54
47	8	551	LEU	CA-C-N	6.40	128.76	120.44
47	8	551	LEU	C-N-CA	6.40	128.76	120.44
34	O	136	SER	CA-C-N	6.39	127.08	119.98
34	O	136	SER	C-N-CA	6.39	127.08	119.98
1	f	1221	LEU	CA-C-N	6.36	127.79	119.84
1	f	1221	LEU	C-N-CA	6.36	127.79	119.84
46	C	630	TYR	N-CA-C	6.36	124.34	110.80
46	C	636	GLU	CA-C-N	6.36	133.15	121.70
46	C	636	GLU	C-N-CA	6.36	133.15	121.70
1	f	229	ASN	O-C-N	6.33	130.20	123.42
51	A	87	VAL	N-CA-C	-6.33	106.96	113.10
28	5	170	GLU	CA-C-N	-6.32	114.22	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5	170	GLU	C-N-CA	-6.32	114.22	120.98
47	8	534	ARG	CA-C-N	6.32	125.54	118.97
47	8	534	ARG	C-N-CA	6.32	125.54	118.97
1	f	289	ASP	N-CA-C	6.31	117.82	111.07
1	f	1493	PRO	O-C-N	6.31	131.16	122.64
1	f	1125	LEU	CA-C-N	6.28	133.63	122.08
1	f	1125	LEU	C-N-CA	6.28	133.63	122.08
47	8	518	GLU	CA-C-N	6.28	133.00	121.70
47	8	518	GLU	C-N-CA	6.28	133.00	121.70
48	W	217	VAL	N-CA-C	-6.27	100.08	108.35
51	A	450	ILE	CA-C-N	6.26	133.50	121.54
51	A	450	ILE	C-N-CA	6.26	133.50	121.54
22	F	88	ARG	N-CA-C	-6.26	103.13	111.96
40	Y	208	PRO	CA-C-O	-6.26	111.48	120.56
50	H	286	TYR	CA-C-N	6.26	128.58	120.44
50	H	286	TYR	C-N-CA	6.26	128.58	120.44
3	0	1979	C	P-O3'-C3'	6.26	129.58	120.20
8	p	309	ILE	N-CA-C	-6.26	98.66	108.86
1	f	1100	ASN	CA-C-N	6.25	127.66	119.84
1	f	1100	ASN	C-N-CA	6.25	127.66	119.84
46	C	138	ILE	CB-CA-C	-6.25	103.97	111.97
30	i	41	ALA	N-CA-C	-6.25	107.50	114.62
46	C	488	GLU	CA-C-N	6.23	133.44	121.54
46	C	488	GLU	C-N-CA	6.23	133.44	121.54
1	f	829	LYS	CA-C-N	6.22	128.62	120.28
1	f	829	LYS	C-N-CA	6.22	128.62	120.28
21	B	71	GLU	CA-C-N	6.21	127.00	119.99
21	B	71	GLU	C-N-CA	6.21	127.00	119.99
50	H	215	ASN	CA-C-N	6.20	128.37	120.56
50	H	215	ASN	C-N-CA	6.20	128.37	120.56
30	i	102	ASP	CA-C-N	6.20	129.40	120.79
30	i	102	ASP	C-N-CA	6.20	129.40	120.79
13	o	114	VAL	N-CA-C	-6.19	107.22	113.47
33	N	23	ILE	N-CA-C	-6.19	99.57	108.42
1	f	913	GLU	N-CA-C	-6.19	104.55	113.21
47	8	294	ASN	N-CA-C	-6.18	105.89	113.50
50	H	234	TYR	N-CA-C	-6.18	105.53	114.12
5	s	342	PRO	CA-C-N	6.17	132.81	121.70
5	s	342	PRO	C-N-CA	6.17	132.81	121.70
39	E	42	THR	N-CA-CB	6.17	120.92	110.49
22	F	171	ARG	CA-C-N	6.15	128.43	120.44
22	F	171	ARG	C-N-CA	6.15	128.43	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	E	88	THR	N-CA-C	-6.15	104.95	112.88
46	C	346	LEU	CA-C-N	6.14	132.76	121.70
46	C	346	LEU	C-N-CA	6.14	132.76	121.70
26	J	235	LEU	CA-C-N	6.14	128.42	120.44
26	J	235	LEU	C-N-CA	6.14	128.42	120.44
16	S	26	VAL	N-CA-C	-6.14	106.77	111.62
47	8	351	PHE	CA-C-N	6.14	133.26	121.54
47	8	351	PHE	C-N-CA	6.14	133.26	121.54
50	H	143	ASN	CA-C-N	6.14	127.76	120.09
50	H	143	ASN	C-N-CA	6.14	127.76	120.09
39	E	131	ARG	CA-C-N	6.13	133.25	121.54
39	E	131	ARG	C-N-CA	6.13	133.25	121.54
5	s	241	ALA	CA-C-N	6.12	128.77	120.38
5	s	241	ALA	C-N-CA	6.12	128.77	120.38
46	C	244	SER	N-CA-C	-6.12	105.04	113.18
1	f	1039	ARG	CB-CA-C	6.12	122.60	110.42
47	8	295	SER	CA-C-N	6.12	128.48	120.28
47	8	295	SER	C-N-CA	6.12	128.48	120.28
44	K	65	VAL	CA-C-N	6.12	126.13	119.89
44	K	65	VAL	C-N-CA	6.12	126.13	119.89
47	8	438	LEU	CA-C-N	6.10	128.46	120.28
47	8	438	LEU	C-N-CA	6.10	128.46	120.28
38	w	105	VAL	N-CA-C	-6.10	105.19	110.74
51	A	119	LEU	CA-C-N	6.10	129.28	120.98
51	A	119	LEU	C-N-CA	6.10	129.28	120.98
1	f	1856	LEU	CA-C-N	6.09	128.73	120.38
1	f	1856	LEU	C-N-CA	6.09	128.73	120.38
35	b	41	MET	CA-C-N	6.09	129.05	120.28
35	b	41	MET	C-N-CA	6.09	129.05	120.28
39	E	98	ASN	CA-C-N	6.09	128.36	120.44
39	E	98	ASN	C-N-CA	6.09	128.36	120.44
17	t	80	ALA	CA-C-N	6.09	129.05	120.28
17	t	80	ALA	C-N-CA	6.09	129.05	120.28
1	f	1440	GLU	N-CA-CB	6.08	120.77	110.49
3	0	1728	G	P-O3'-C3'	6.08	129.32	120.20
48	W	165	TRP	CA-C-N	-6.08	113.47	120.88
48	W	165	TRP	C-N-CA	-6.08	113.47	120.88
1	f	705	GLU	N-CA-C	-6.08	106.03	113.50
31	L	103	ILE	N-CA-C	-6.05	106.86	112.43
41	Q	33	ARG	N-CA-CB	6.04	120.70	110.49
1	f	1362	GLU	CA-C-N	6.04	125.72	119.92
1	f	1362	GLU	C-N-CA	6.04	125.72	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	s	298	THR	CA-C-N	6.04	132.57	121.70
5	s	298	THR	C-N-CA	6.04	132.57	121.70
13	o	114	VAL	CA-C-N	6.03	125.83	120.10
13	o	114	VAL	C-N-CA	6.03	125.83	120.10
3	0	251	A	P-O3'-C3'	6.02	129.23	120.20
43	G	136	TRP	CA-CB-CG	6.02	125.03	113.60
23	d	105	PHE	CA-CB-CG	-6.01	107.79	113.80
28	5	242	LEU	CA-C-N	6.00	128.64	120.54
28	5	242	LEU	C-N-CA	6.00	128.64	120.54
3	0	718	A	P-O5'-C5'	6.00	129.90	120.90
16	S	67	PRO	N-CA-C	-6.00	107.79	114.92
1	f	241	SER	O-C-N	-5.99	114.62	122.59
46	C	143	GLU	CA-C-N	5.98	128.22	120.44
46	C	143	GLU	C-N-CA	5.98	128.22	120.44
1	f	146	SER	N-CA-C	-5.98	100.69	109.18
40	Y	352	SER	N-CA-C	-5.98	105.31	114.16
46	C	77	TRP	N-CA-C	-5.96	105.67	113.12
1	f	1263	ASP	CA-C-N	5.96	132.92	121.54
1	f	1263	ASP	C-N-CA	5.96	132.92	121.54
23	d	174	VAL	N-CA-C	-5.95	99.91	108.42
25	a	84	LYS	CA-C-N	5.95	126.55	119.94
25	a	84	LYS	C-N-CA	5.95	126.55	119.94
47	8	464	ILE	CA-C-N	5.94	126.54	119.94
47	8	464	ILE	C-N-CA	5.94	126.54	119.94
50	H	212	ARG	CB-CA-C	5.94	120.20	110.88
1	f	1044	VAL	CA-C-N	-5.93	114.53	122.72
1	f	1044	VAL	C-N-CA	-5.93	114.53	122.72
3	0	2018	U	P-O3'-C3'	5.92	129.07	120.20
48	W	72	ASP	N-CA-C	-5.92	105.06	112.93
43	G	206	ARG	CA-C-N	5.91	128.12	120.44
43	G	206	ARG	C-N-CA	5.91	128.12	120.44
1	f	1229	GLN	CA-C-N	5.91	128.47	120.38
1	f	1229	GLN	C-N-CA	5.91	128.47	120.38
20	X	54	GLY	N-CA-C	-5.90	104.22	112.13
32	M	8	ARG	N-CA-C	-5.89	105.09	112.93
5	s	174	ILE	N-CA-C	-5.89	108.11	113.71
1	f	1269	ILE	N-CA-C	-5.88	99.07	107.77
23	d	93	VAL	N-CA-C	-5.88	100.59	108.35
7	n	302	GLY	N-CA-C	-5.88	105.74	112.79
46	C	173	GLU	CA-C-N	5.87	132.27	121.70
46	C	173	GLU	C-N-CA	5.87	132.27	121.70
47	8	353	ARG	CA-C-N	5.87	126.46	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	8	353	ARG	C-N-CA	5.87	126.46	119.94
3	0	2220	C	P-O3'-C3'	5.86	128.99	120.20
52	l	170	ILE	N-CA-C	-5.86	99.36	108.44
19	v	50	THR	CA-C-N	5.85	126.58	120.03
19	v	50	THR	C-N-CA	5.85	126.58	120.03
29	P	231	ARG	CA-C-N	5.85	128.44	120.54
29	P	231	ARG	C-N-CA	5.85	128.44	120.54
44	K	176	PHE	CA-C-N	5.85	132.23	121.70
44	K	176	PHE	C-N-CA	5.85	132.23	121.70
50	H	242	PHE	CA-CB-CG	-5.84	107.95	113.80
1	f	134	PRO	N-CA-C	5.84	120.07	110.55
3	0	1974	G	C4'-C3'-C2'	-5.84	96.76	102.60
10	u	63	GLU	N-CA-C	-5.83	101.72	110.06
5	s	390	VAL	CA-C-N	5.82	132.18	121.70
5	s	390	VAL	C-N-CA	5.82	132.18	121.70
35	b	40	VAL	CA-C-N	5.82	128.39	120.54
35	b	40	VAL	C-N-CA	5.82	128.39	120.54
47	8	338	THR	CA-C-N	5.82	128.00	120.44
47	8	338	THR	C-N-CA	5.82	128.00	120.44
1	f	1400	ASP	CA-C-N	5.81	129.54	120.82
1	f	1400	ASP	C-N-CA	5.81	129.54	120.82
34	O	71	TYR	CA-C-N	5.81	128.41	120.46
34	O	71	TYR	C-N-CA	5.81	128.41	120.46
1	f	262	MET	CA-C-O	-5.80	114.92	121.25
2	1	74	C	O3'-P-O5'	-5.80	95.29	104.00
42	D	29	MET	CA-C-N	5.80	128.32	120.38
42	D	29	MET	C-N-CA	5.80	128.32	120.38
1	f	296	TYR	N-CA-CB	-5.79	100.70	110.49
1	f	256	GLU	N-CA-CB	-5.79	100.07	110.37
1	f	1831	HIS	CA-C-N	5.79	128.35	120.77
1	f	1831	HIS	C-N-CA	5.79	128.35	120.77
1	f	1308	ASN	N-CA-C	-5.78	100.63	109.65
3	0	1978	A	P-O5'-C5'	5.78	129.57	120.90
43	G	150	LEU	N-CA-C	-5.78	105.12	113.21
46	C	320	LEU	CA-C-N	5.78	128.03	120.28
46	C	320	LEU	C-N-CA	5.78	128.03	120.28
46	C	490	LYS	N-CA-C	-5.78	105.32	112.72
8	p	178	VAL	N-CA-C	-5.78	99.90	108.45
50	H	125	GLU	N-CA-C	-5.77	100.17	108.60
10	u	119	ARG	N-CA-C	5.77	119.20	111.24
46	C	375	GLU	CA-C-N	5.77	127.94	120.44
46	C	375	GLU	C-N-CA	5.77	127.94	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5	346	VAL	CA-C-N	5.77	126.17	120.98
28	5	346	VAL	C-N-CA	5.77	126.17	120.98
1	f	1727	LYS	CA-C-N	5.77	126.72	120.44
1	f	1727	LYS	C-N-CA	5.77	126.72	120.44
17	t	50	ALA	CA-C-N	5.76	128.28	120.38
17	t	50	ALA	C-N-CA	5.76	128.28	120.38
5	s	360	GLU	N-CA-C	-5.76	106.23	113.72
8	p	238	ALA	CA-C-N	5.76	125.78	119.90
8	p	238	ALA	C-N-CA	5.76	125.78	119.90
50	H	96	THR	O-C-N	-5.75	114.70	121.32
1	f	1127	VAL	C-N-CD	-5.75	101.42	125.00
1	f	291	ARG	CA-C-N	-5.75	112.80	122.92
1	f	291	ARG	C-N-CA	-5.75	112.80	122.92
43	G	86	TYR	N-CA-C	-5.75	100.52	109.72
48	W	112	VAL	N-CA-CB	5.75	116.89	110.51
50	H	45	PHE	CA-C-N	5.75	132.52	121.54
50	H	45	PHE	C-N-CA	5.75	132.52	121.54
52	l	90	PRO	CA-C-N	5.74	128.76	120.38
52	l	90	PRO	C-N-CA	5.74	128.76	120.38
45	T	103	ILE	N-CA-C	-5.74	100.21	108.42
1	f	1306	TRP	CA-CB-CG	5.73	124.49	113.60
46	C	579	ILE	N-CA-C	5.73	116.38	110.82
35	b	61	ILE	N-CA-C	-5.72	99.58	108.44
50	H	59	THR	CA-C-N	5.71	131.99	121.70
50	H	59	THR	C-N-CA	5.71	131.99	121.70
1	f	1032	LEU	CA-C-N	5.71	128.20	120.38
1	f	1032	LEU	C-N-CA	5.71	128.20	120.38
8	p	304	TYR	CA-C-N	5.71	127.93	120.28
8	p	304	TYR	C-N-CA	5.71	127.93	120.28
20	X	63	ALA	CA-C-N	5.71	127.75	120.56
20	X	63	ALA	C-N-CA	5.71	127.75	120.56
47	8	125	ALA	CA-C-N	5.71	127.86	120.44
47	8	125	ALA	C-N-CA	5.71	127.86	120.44
1	f	1107	GLY	N-CA-C	5.70	121.59	112.58
26	J	165	GLN	CA-C-N	5.70	128.24	120.77
26	J	165	GLN	C-N-CA	5.70	128.24	120.77
51	A	4	GLU	N-CA-CB	5.70	120.20	110.50
6	j	122	ASN	CA-C-N	5.70	125.17	119.24
6	j	122	ASN	C-N-CA	5.70	125.17	119.24
45	T	22	PHE	N-CA-CB	5.70	120.12	110.49
48	W	65	VAL	N-CA-C	-5.70	99.66	107.75
49	I	342	ILE	CA-C-O	5.70	122.90	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	u	115	LEU	CA-C-N	5.70	128.23	120.54
10	u	115	LEU	C-N-CA	5.70	128.23	120.54
10	u	34	VAL	CA-C-N	5.70	132.42	121.54
10	u	34	VAL	C-N-CA	5.70	132.42	121.54
40	Y	320	PRO	CA-C-N	5.69	127.84	120.44
40	Y	320	PRO	C-N-CA	5.69	127.84	120.44
43	G	96	GLU	N-CA-C	5.69	119.33	112.38
1	f	288	HIS	CA-C-N	5.69	127.84	120.44
1	f	288	HIS	C-N-CA	5.69	127.84	120.44
5	s	155	LEU	N-CA-C	-5.69	107.58	114.75
10	u	97	GLU	N-CA-C	-5.69	102.37	111.02
46	C	685	VAL	N-CA-CB	5.69	117.20	110.55
50	H	283	SER	N-CA-C	5.69	117.15	111.07
30	i	103	LYS	CA-C-N	5.68	128.20	120.54
30	i	103	LYS	C-N-CA	5.68	128.20	120.54
1	f	288	HIS	CA-C-O	5.67	121.23	117.94
15	R	46	THR	CA-C-N	5.67	125.78	119.32
15	R	46	THR	C-N-CA	5.67	125.78	119.32
52	l	229	MET	N-CA-C	-5.67	106.03	113.17
1	f	812	LEU	CA-C-N	5.66	128.19	120.54
1	f	812	LEU	C-N-CA	5.66	128.19	120.54
1	f	1579	GLU	CA-C-N	5.66	131.89	121.70
1	f	1579	GLU	C-N-CA	5.66	131.89	121.70
8	p	14	GLY	CA-C-N	5.66	129.29	120.75
8	p	14	GLY	C-N-CA	5.66	129.29	120.75
1	f	1425	LEU	N-CA-C	-5.66	103.99	111.96
39	E	50	VAL	CA-C-N	5.65	127.79	120.44
39	E	50	VAL	C-N-CA	5.65	127.79	120.44
51	A	175	GLU	CA-C-N	5.65	127.85	120.28
51	A	175	GLU	C-N-CA	5.65	127.85	120.28
3	0	1397	G	O5'-C5'-C4'	5.65	119.97	111.50
46	C	640	ILE	N-CA-CB	5.65	117.16	110.55
28	5	360	MET	N-CA-C	-5.64	104.81	112.26
50	H	171	PRO	CA-C-N	5.64	129.63	120.60
50	H	171	PRO	C-N-CA	5.64	129.63	120.60
1	f	1371	VAL	N-CA-C	-5.64	100.22	108.11
1	f	1654	GLY	O-C-N	-5.64	115.37	122.70
26	J	157	PHE	CA-CB-CG	-5.64	108.16	113.80
28	5	253	THR	O-C-N	5.63	130.51	123.19
3	0	924	G	O4'-C1'-N9	5.63	116.95	108.50
47	8	505	THR	CA-C-N	5.63	127.76	120.44
47	8	505	THR	C-N-CA	5.63	127.76	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	8	515	ALA	CA-C-N	5.63	127.76	120.44
47	8	515	ALA	C-N-CA	5.63	127.76	120.44
1	f	235	LEU	CA-C-N	-5.63	111.62	122.09
1	f	235	LEU	C-N-CA	-5.63	111.62	122.09
1	f	1312	LEU	CA-C-N	5.63	132.29	121.54
1	f	1312	LEU	C-N-CA	5.63	132.29	121.54
52	l	250	ARG	CA-C-N	5.63	128.09	120.38
52	l	250	ARG	C-N-CA	5.63	128.09	120.38
39	E	307	GLU	CA-C-N	5.63	127.65	120.56
39	E	307	GLU	C-N-CA	5.63	127.65	120.56
48	W	190	LEU	CA-C-N	5.63	128.09	120.38
48	W	190	LEU	C-N-CA	5.63	128.09	120.38
49	I	302	SER	CA-C-N	5.63	132.29	121.54
49	I	302	SER	C-N-CA	5.63	132.29	121.54
42	D	30	ARG	CA-C-N	5.62	127.81	120.28
42	D	30	ARG	C-N-CA	5.62	127.81	120.28
23	d	190	VAL	CA-C-N	5.62	125.29	119.05
23	d	190	VAL	C-N-CA	5.62	125.29	119.05
28	5	146	ASP	CA-C-N	5.61	128.44	120.53
28	5	146	ASP	C-N-CA	5.61	128.44	120.53
5	s	225	GLU	CA-C-N	5.60	127.83	120.60
5	s	225	GLU	C-N-CA	5.60	127.83	120.60
46	C	304	THR	CA-C-N	5.60	132.23	121.54
46	C	304	THR	C-N-CA	5.60	132.23	121.54
28	5	425	VAL	N-CA-C	-5.59	107.36	112.96
12	Z	103	VAL	N-CA-C	-5.59	99.75	108.86
39	E	305	LEU	CA-C-N	5.59	124.78	118.97
39	E	305	LEU	C-N-CA	5.59	124.78	118.97
1	f	1415	LYS	CA-C-N	5.58	127.70	120.44
1	f	1415	LYS	C-N-CA	5.58	127.70	120.44
52	l	189	ILE	N-CA-C	-5.58	100.44	108.42
5	s	109	PHE	CA-C-N	5.57	128.06	120.54
5	s	109	PHE	C-N-CA	5.57	128.06	120.54
47	8	292	ILE	CA-C-N	5.57	128.20	120.29
47	8	292	ILE	C-N-CA	5.57	128.20	120.29
46	C	78	SER	CA-C-N	5.57	127.68	120.44
46	C	78	SER	C-N-CA	5.57	127.68	120.44
1	f	1519	GLU	CA-C-N	5.57	127.68	120.44
1	f	1519	GLU	C-N-CA	5.57	127.68	120.44
1	f	1110	GLY	N-CA-C	5.57	120.67	111.59
26	J	181	TYR	N-CA-C	-5.57	104.91	112.26
46	C	238	THR	CA-C-N	5.57	128.53	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	C	238	THR	C-N-CA	5.57	128.53	120.79
47	8	459	ALA	N-CA-C	5.57	118.19	111.40
1	f	1260	TYR	N-CA-CB	5.57	119.96	110.50
25	a	97	LEU	N-CA-C	-5.57	101.06	109.85
1	f	307	LEU	CB-CA-C	-5.56	99.35	110.42
1	f	1637	LYS	CA-C-N	5.56	126.16	119.98
1	f	1637	LYS	C-N-CA	5.56	126.16	119.98
28	5	258	CYS	CA-C-N	5.56	125.58	119.90
28	5	258	CYS	C-N-CA	5.56	125.58	119.90
39	E	315	ASP	CA-C-N	5.56	131.24	122.78
39	E	315	ASP	C-N-CA	5.56	131.24	122.78
3	0	272	G	C2'-C3'-O3'	5.56	117.84	109.50
43	G	135	ARG	N-CA-C	5.56	117.14	111.14
1	f	57	ILE	N-CA-C	-5.56	107.56	112.90
23	d	253	PHE	CA-CB-CG	-5.56	108.24	113.80
34	O	66	ASN	CA-C-O	-5.56	113.80	119.08
45	T	49	ARG	CA-C-N	5.56	127.99	120.38
45	T	49	ARG	C-N-CA	5.56	127.99	120.38
46	C	612	TYR	N-CA-CB	5.55	119.88	110.49
22	F	133	ASP	CA-C-N	5.55	129.15	120.82
22	F	133	ASP	C-N-CA	5.55	129.15	120.82
1	f	1214	ARG	CA-C-N	-5.55	110.94	121.54
1	f	1214	ARG	C-N-CA	-5.55	110.94	121.54
28	5	201	LEU	N-CA-C	-5.55	106.64	113.41
13	o	134	ASN	CA-C-N	5.54	127.97	120.38
13	o	134	ASN	C-N-CA	5.54	127.97	120.38
1	f	136	LEU	O-C-N	-5.54	115.22	122.59
24	g	60	ALA	CA-C-N	5.54	125.98	119.94
24	g	60	ALA	C-N-CA	5.54	125.98	119.94
27	h	67	ASP	N-CA-C	-5.54	104.07	112.99
1	f	836	VAL	CA-C-N	5.54	127.54	120.56
1	f	836	VAL	C-N-CA	5.54	127.54	120.56
26	J	238	ALA	CA-C-N	5.54	128.02	120.54
26	J	238	ALA	C-N-CA	5.54	128.02	120.54
29	P	189	ALA	CA-C-N	5.54	128.02	120.54
29	P	189	ALA	C-N-CA	5.54	128.02	120.54
48	W	162	LEU	CA-C-N	5.54	128.03	120.77
48	W	162	LEU	C-N-CA	5.54	128.03	120.77
5	s	222	LYS	CA-C-N	5.54	126.09	119.94
5	s	222	LYS	C-N-CA	5.54	126.09	119.94
47	8	291	ILE	CA-C-N	5.54	128.04	120.46
47	8	291	ILE	C-N-CA	5.54	128.04	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	1217	GLU	CA-C-N	5.53	130.46	122.77
1	f	1217	GLU	C-N-CA	5.53	130.46	122.77
39	E	212	LEU	N-CA-C	-5.53	99.03	110.80
47	8	221	LEU	CA-C-N	5.53	127.52	120.56
47	8	221	LEU	C-N-CA	5.53	127.52	120.56
34	O	135	SER	N-CA-C	-5.53	104.56	112.13
21	B	108	LEU	CA-C-N	5.52	127.95	120.38
21	B	108	LEU	C-N-CA	5.52	127.95	120.38
31	L	51	VAL	CB-CA-C	5.52	120.35	111.29
39	E	157	TRP	CA-C-N	5.51	126.06	119.94
39	E	157	TRP	C-N-CA	5.51	126.06	119.94
13	o	128	SER	CA-C-N	5.51	125.17	119.05
13	o	128	SER	C-N-CA	5.51	125.17	119.05
26	J	221	SER	CA-C-N	5.51	131.62	121.70
26	J	221	SER	C-N-CA	5.51	131.62	121.70
28	5	401	ARG	CA-C-N	5.51	127.88	120.50
28	5	401	ARG	C-N-CA	5.51	127.88	120.50
48	W	109	SER	CA-C-N	5.51	127.98	120.54
48	W	109	SER	C-N-CA	5.51	127.98	120.54
49	I	330	GLU	CA-C-N	5.51	127.50	120.56
49	I	330	GLU	C-N-CA	5.51	127.50	120.56
1	f	1440	GLU	N-CA-C	-5.50	99.07	110.80
29	P	224	ARG	CA-C-N	5.50	127.97	120.54
29	P	224	ARG	C-N-CA	5.50	127.97	120.54
8	p	88	ASP	CA-CB-CG	5.50	118.10	112.60
46	C	331	ARG	N-CA-C	-5.50	99.08	110.80
28	5	357	GLN	N-CA-C	-5.50	108.35	114.62
49	I	216	SER	N-CA-CB	5.50	119.78	110.49
30	i	121	ALA	N-CA-CB	5.50	118.64	110.40
20	X	33	SER	CA-C-N	5.49	131.58	121.70
20	X	33	SER	C-N-CA	5.49	131.58	121.70
14	q	169	SER	CA-C-N	5.49	128.19	120.28
14	q	169	SER	C-N-CA	5.49	128.19	120.28
9	r	140	ALA	N-CA-C	5.49	117.33	110.91
43	G	105	ALA	N-CA-C	5.48	120.21	112.75
48	W	161	ARG	CA-C-N	5.48	128.41	120.79
48	W	161	ARG	C-N-CA	5.48	128.41	120.79
43	G	59	THR	CA-C-N	5.48	131.56	121.70
43	G	59	THR	C-N-CA	5.48	131.56	121.70
3	0	2102	U	C2'-C3'-O3'	5.47	117.71	109.50
50	H	179	LYS	N-CA-C	-5.46	107.87	114.75
1	f	284	ALA	CA-C-N	5.45	127.90	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	284	ALA	C-N-CA	5.45	127.90	120.54
1	f	237	ILE	CA-C-O	-5.45	114.57	120.67
1	f	882	GLU	CA-C-N	5.45	127.90	120.54
1	f	882	GLU	C-N-CA	5.45	127.90	120.54
10	u	79	LYS	N-CA-CB	5.45	119.70	110.49
46	C	342	LEU	CA-C-N	5.45	127.42	120.56
46	C	342	LEU	C-N-CA	5.45	127.42	120.56
51	A	270	ARG	CA-C-N	5.45	131.77	121.97
51	A	270	ARG	C-N-CA	5.45	131.77	121.97
7	n	210	LEU	CA-C-N	-5.44	114.11	119.93
7	n	210	LEU	C-N-CA	-5.44	114.11	119.93
8	p	66	HIS	N-CA-CB	5.44	119.69	110.49
26	J	222	LEU	CA-C-N	5.44	131.50	121.70
26	J	222	LEU	C-N-CA	5.44	131.50	121.70
33	N	81	GLU	CA-C-N	5.44	127.84	120.38
33	N	81	GLU	C-N-CA	5.44	127.84	120.38
3	0	2303	G	P-O5'-C5'	-5.44	112.74	120.90
7	n	263	ILE	N-CA-C	-5.44	100.00	108.81
21	B	100	VAL	CA-C-N	5.44	124.89	119.24
21	B	100	VAL	C-N-CA	5.44	124.89	119.24
44	K	56	ASN	CA-C-N	5.44	127.56	120.28
44	K	56	ASN	C-N-CA	5.44	127.56	120.28
43	G	195	ASN	N-CA-C	5.43	117.65	111.02
12	Z	32	LEU	CA-C-N	5.43	125.44	119.90
12	Z	32	LEU	C-N-CA	5.43	125.44	119.90
15	R	31	ARG	CA-C-N	5.43	127.87	120.54
15	R	31	ARG	C-N-CA	5.43	127.87	120.54
21	B	38	LYS	CA-C-N	5.43	128.09	120.28
21	B	38	LYS	C-N-CA	5.43	128.09	120.28
27	h	107	ASP	CA-C-N	5.43	127.55	120.28
27	h	107	ASP	C-N-CA	5.43	127.55	120.28
1	f	264	ASP	O-C-N	-5.42	116.83	122.96
21	B	171	VAL	CA-C-N	5.42	128.33	120.79
21	B	171	VAL	C-N-CA	5.42	128.33	120.79
26	J	167	LEU	CA-C-N	5.42	127.86	120.54
26	J	167	LEU	C-N-CA	5.42	127.86	120.54
25	a	83	ALA	CA-C-N	5.42	127.81	120.38
25	a	83	ALA	C-N-CA	5.42	127.81	120.38
32	M	137	VAL	N-CA-C	-5.42	101.19	108.35
1	f	136	LEU	N-CA-C	-5.42	99.26	110.80
8	p	253	CYS	N-CA-CB	5.42	119.65	110.49
43	G	256	GLU	CA-C-N	5.42	127.48	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	G	256	GLU	C-N-CA	5.42	127.48	120.44
46	C	581	ASN	N-CA-CB	5.42	119.65	110.49
1	f	1027	ASN	CA-C-N	5.42	127.80	120.38
1	f	1027	ASN	C-N-CA	5.42	127.80	120.38
13	o	174	TYR	CA-C-N	5.42	127.85	120.54
13	o	174	TYR	C-N-CA	5.42	127.85	120.54
13	o	159	LEU	CA-C-N	5.42	127.80	120.38
13	o	159	LEU	C-N-CA	5.42	127.80	120.38
33	N	78	GLU	CA-C-N	5.42	126.11	119.99
33	N	78	GLU	C-N-CA	5.42	126.11	119.99
1	f	102	ILE	N-CA-CB	5.41	116.52	110.51
8	p	170	VAL	N-CA-C	-5.41	100.27	108.17
1	f	1609	LEU	CA-C-N	5.41	127.85	120.54
1	f	1609	LEU	C-N-CA	5.41	127.85	120.54
4	y	43	ALA	CA-C-N	5.41	127.84	120.54
4	y	43	ALA	C-N-CA	5.41	127.84	120.54
14	q	50	THR	N-CA-C	-5.41	104.34	111.96
28	5	81	HIS	CA-C-N	5.41	127.52	120.28
28	5	81	HIS	C-N-CA	5.41	127.52	120.28
29	P	234	HIS	CA-C-N	5.40	128.29	120.79
29	P	234	HIS	C-N-CA	5.40	128.29	120.79
43	G	249	SER	N-CA-C	-5.40	106.61	114.12
1	f	1102	GLY	N-CA-C	-5.40	100.39	113.18
30	i	64	GLY	CA-C-N	5.40	125.70	119.93
30	i	64	GLY	C-N-CA	5.40	125.70	119.93
39	E	66	ARG	CA-C-N	5.39	124.58	118.97
39	E	66	ARG	C-N-CA	5.39	124.58	118.97
39	E	45	THR	CA-C-N	5.39	131.84	121.54
39	E	45	THR	C-N-CA	5.39	131.84	121.54
36	c	33	ARG	CA-C-N	5.39	129.76	121.19
36	c	33	ARG	C-N-CA	5.39	129.76	121.19
8	p	63	LEU	N-CA-C	-5.39	101.50	110.17
1	f	1166	VAL	CA-C-N	5.38	127.81	120.54
1	f	1166	VAL	C-N-CA	5.38	127.81	120.54
43	G	253	ASN	N-CA-C	-5.38	107.36	114.04
1	f	1705	LEU	N-CA-CB	-5.38	102.48	111.20
1	f	771	GLY	N-CA-C	-5.38	102.37	112.64
32	M	135	VAL	N-CA-C	-5.38	100.73	108.42
43	G	210	PHE	N-CA-C	-5.38	106.20	114.16
46	C	96	GLU	N-CA-CB	5.38	119.58	110.49
39	E	239	TYR	CA-C-N	5.37	127.42	120.44
39	E	239	TYR	C-N-CA	5.37	127.42	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Y	319	GLU	CA-C-N	5.37	125.44	119.32
40	Y	319	GLU	C-N-CA	5.37	125.44	119.32
49	I	297	GLN	CA-C-N	5.37	126.56	119.84
49	I	297	GLN	C-N-CA	5.37	126.56	119.84
1	f	237	ILE	O-C-N	-5.37	117.35	123.10
1	f	1589	LEU	CA-C-N	5.37	124.55	118.97
1	f	1589	LEU	C-N-CA	5.37	124.55	118.97
30	i	49	LYS	CA-C-N	5.37	127.41	120.70
30	i	49	LYS	C-N-CA	5.37	127.41	120.70
39	E	16	LEU	N-CA-C	-5.37	105.55	112.68
1	f	1040	GLY	N-CA-C	5.36	121.95	112.83
18	U	109	ARG	N-CA-C	-5.36	108.51	114.62
3	0	693	G	P-O3'-C3'	5.35	128.23	120.20
30	i	21	PHE	CA-CB-CG	-5.35	108.45	113.80
1	f	1704	HIS	CA-C-O	-5.35	115.55	121.33
11	m	77	ASN	N-CA-C	-5.35	108.52	114.62
14	q	26	ALA	CA-C-N	5.35	127.76	120.54
14	q	26	ALA	C-N-CA	5.35	127.76	120.54
1	f	1082	ILE	N-CA-C	5.35	116.72	110.62
7	n	131	GLU	CA-C-N	5.35	127.50	120.60
7	n	131	GLU	C-N-CA	5.35	127.50	120.60
12	Z	196	THR	N-CA-C	-5.35	108.01	114.75
1	f	1311	SER	O-C-N	-5.34	115.48	122.59
11	m	12	LYS	CA-C-N	5.34	127.70	120.38
11	m	12	LYS	C-N-CA	5.34	127.70	120.38
50	H	89	PRO	N-CA-C	-5.34	108.56	114.92
28	5	210	GLN	CA-C-N	5.34	127.44	120.28
28	5	210	GLN	C-N-CA	5.34	127.44	120.28
35	b	112	ASP	CA-C-N	5.34	127.69	120.38
35	b	112	ASP	C-N-CA	5.34	127.69	120.38
26	J	218	SER	N-CA-C	-5.34	100.81	108.60
15	R	113	PHE	CA-C-N	5.34	127.89	120.63
15	R	113	PHE	C-N-CA	5.34	127.89	120.63
28	5	359	LYS	N-CA-C	-5.34	105.47	112.41
2	1	72	A	O5'-C5'-C4'	5.33	119.50	111.50
29	P	141	ALA	CA-C-N	5.33	127.69	120.38
29	P	141	ALA	C-N-CA	5.33	127.69	120.38
46	C	624	ASP	N-CA-C	-5.33	106.83	113.55
1	f	1003	ILE	N-CA-C	-5.33	107.53	112.43
49	I	387	THR	CA-C-N	5.33	127.68	120.38
49	I	387	THR	C-N-CA	5.33	127.68	120.38
30	i	34	VAL	CA-C-N	5.33	127.47	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	34	VAL	C-N-CA	5.33	127.47	120.60
50	H	48	LEU	CA-C-N	5.33	127.42	120.28
50	H	48	LEU	C-N-CA	5.33	127.42	120.28
34	O	83	MET	CA-C-N	5.33	126.75	120.09
34	O	83	MET	C-N-CA	5.33	126.75	120.09
5	s	390	VAL	N-CA-C	5.33	115.77	110.23
28	5	240	ASP	CA-CB-CG	5.33	117.93	112.60
3	0	986	U	P-O5'-C5'	5.32	128.88	120.90
41	Q	12	LYS	N-CA-C	-5.32	106.17	113.30
3	0	713	G	P-O3'-C3'	-5.32	112.22	120.20
12	Z	109	PHE	CA-CB-CG	-5.32	108.48	113.80
1	f	1052	LYS	CA-C-N	5.32	129.10	120.60
1	f	1052	LYS	C-N-CA	5.32	129.10	120.60
8	p	38	ASN	N-CA-C	5.32	118.53	111.30
39	E	132	TYR	N-CA-C	-5.32	99.48	110.80
14	q	173	ILE	CA-C-N	5.31	127.45	120.60
14	q	173	ILE	C-N-CA	5.31	127.45	120.60
43	G	115	SER	N-CA-C	-5.31	106.30	114.16
1	f	784	LEU	CA-C-N	5.31	128.17	120.79
1	f	784	LEU	C-N-CA	5.31	128.17	120.79
6	j	95	MET	CA-C-N	5.31	127.40	120.28
6	j	95	MET	C-N-CA	5.31	127.40	120.28
39	E	393	VAL	CA-C-N	5.31	127.35	120.44
39	E	393	VAL	C-N-CA	5.31	127.35	120.44
50	H	292	GLU	N-CA-C	-5.31	104.74	113.50
3	0	2157	C	C2'-C3'-O3'	5.31	121.66	113.70
49	I	331	VAL	CA-C-N	5.31	127.34	120.44
49	I	331	VAL	C-N-CA	5.31	127.34	120.44
1	f	1727	LYS	N-CA-C	-5.31	105.26	112.26
3	0	2081	A	P-O3'-C3'	5.30	128.16	120.20
30	i	120	VAL	CA-C-N	5.30	131.25	121.70
30	i	120	VAL	C-N-CA	5.30	131.25	121.70
18	U	105	GLU	N-CA-CB	5.30	119.45	110.49
29	P	192	ALA	CA-C-N	5.30	127.39	120.28
29	P	192	ALA	C-N-CA	5.30	127.39	120.28
22	F	18	VAL	CA-C-N	5.29	127.69	120.54
22	F	18	VAL	C-N-CA	5.29	127.69	120.54
50	H	96	THR	CA-C-O	-5.29	112.92	120.16
1	f	685	LYS	CA-C-N	5.29	127.80	120.29
1	f	685	LYS	C-N-CA	5.29	127.80	120.29
5	s	394	TYR	O-C-N	-5.29	117.34	122.99
8	p	277	GLU	N-CA-CB	5.29	119.42	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	46	LEU	CA-C-N	5.28	125.95	120.03
23	d	46	LEU	C-N-CA	5.28	125.95	120.03
47	8	233	GLU	CA-C-N	5.28	127.30	120.44
47	8	233	GLU	C-N-CA	5.28	127.30	120.44
44	K	96	GLN	CA-C-N	5.28	127.30	120.44
44	K	96	GLN	C-N-CA	5.28	127.30	120.44
48	W	70	LEU	N-CA-C	-5.28	101.10	109.76
12	Z	175	ALA	CA-C-N	5.28	127.97	120.53
12	Z	175	ALA	C-N-CA	5.28	127.97	120.53
28	5	220	SER	N-CA-C	-5.28	104.80	113.50
43	G	78	PRO	N-CA-C	-5.28	108.64	114.92
46	C	506	GLN	N-CA-C	5.28	117.71	111.33
44	K	78	GLU	CA-C-N	5.27	127.35	120.28
44	K	78	GLU	C-N-CA	5.27	127.35	120.28
46	C	46	GLU	N-CA-C	-5.27	106.35	114.16
1	f	792	LEU	O-C-N	-5.27	115.38	122.23
13	o	43	GLN	N-CA-C	-5.27	105.56	112.41
26	J	168	GLU	CA-C-N	5.27	127.59	120.38
26	J	168	GLU	C-N-CA	5.27	127.59	120.38
1	f	1170	ILE	N-CA-C	-5.27	107.62	112.83
1	f	1587	ASP	CA-CB-CG	5.26	117.86	112.60
49	I	223	VAL	CA-C-N	5.26	127.33	120.28
49	I	223	VAL	C-N-CA	5.26	127.33	120.28
51	A	280	LYS	CA-C-N	5.26	127.65	120.54
51	A	280	LYS	C-N-CA	5.26	127.65	120.54
32	M	69	THR	CA-C-N	5.26	127.64	120.54
32	M	69	THR	C-N-CA	5.26	127.64	120.54
50	H	203	ASN	N-CA-CB	5.26	119.38	110.49
11	m	131	TYR	N-CA-C	-5.26	106.25	113.30
19	v	66	ALA	CA-C-N	5.26	128.10	120.79
19	v	66	ALA	C-N-CA	5.26	128.10	120.79
44	K	145	ASN	CA-C-N	5.26	125.06	119.28
44	K	145	ASN	C-N-CA	5.26	125.06	119.28
38	w	73	VAL	N-CA-C	-5.25	101.41	108.35
15	R	62	GLN	CA-C-N	5.25	127.65	120.46
15	R	62	GLN	C-N-CA	5.25	127.65	120.46
46	C	472	LEU	N-CA-C	-5.25	106.92	113.38
51	A	219	ARG	CB-CA-C	-5.25	110.54	116.63
1	f	288	HIS	CB-CA-C	-5.25	109.51	117.07
1	f	305	TYR	CB-CA-C	-5.25	99.97	110.42
43	G	154	ARG	N-CA-C	-5.25	101.31	109.24
49	I	418	GLY	CA-C-N	5.25	127.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	I	418	GLY	C-N-CA	5.25	127.31	120.28
3	0	1970	U	O4'-C1'-N1	5.25	116.07	108.20
33	N	74	PHE	N-CA-C	-5.24	101.57	109.85
48	W	123	ILE	N-CA-C	-5.24	100.32	108.81
1	f	705	GLU	CA-C-N	5.24	131.40	121.97
1	f	705	GLU	C-N-CA	5.24	131.40	121.97
26	J	138	THR	N-CA-C	-5.24	106.57	113.17
28	5	241	TYR	CA-C-N	5.24	129.52	121.19
28	5	241	TYR	C-N-CA	5.24	129.52	121.19
22	F	63	LEU	CA-C-N	5.23	127.60	120.54
22	F	63	LEU	C-N-CA	5.23	127.60	120.54
39	E	22	TYR	CA-C-N	5.23	127.72	120.29
39	E	22	TYR	C-N-CA	5.23	127.72	120.29
21	B	88	GLU	N-CA-C	-5.22	106.22	112.59
30	i	22	SER	N-CA-C	-5.22	106.49	112.92
46	C	112	THR	CA-C-N	5.22	126.37	119.84
46	C	112	THR	C-N-CA	5.22	126.37	119.84
49	I	311	SER	CA-C-N	5.22	125.74	119.94
49	I	311	SER	C-N-CA	5.22	125.74	119.94
46	C	305	ASP	N-CA-C	5.22	121.92	110.80
47	8	242	THR	CA-C-N	5.22	127.23	120.44
47	8	242	THR	C-N-CA	5.22	127.23	120.44
48	W	45	LYS	N-CA-C	-5.22	100.79	108.99
32	M	71	CYS	CA-C-N	5.22	128.05	120.79
32	M	71	CYS	C-N-CA	5.22	128.05	120.79
50	H	207	GLU	CA-C-N	5.22	127.22	120.44
50	H	207	GLU	C-N-CA	5.22	127.22	120.44
32	M	117	ALA	CA-C-N	5.22	128.04	120.79
32	M	117	ALA	C-N-CA	5.22	128.04	120.79
50	H	315	GLN	N-CA-C	5.22	116.97	111.28
1	f	20	ASP	CA-C-N	5.21	127.27	120.28
1	f	20	ASP	C-N-CA	5.21	127.27	120.28
8	p	176	ASN	N-CA-CB	5.21	119.30	110.49
23	d	135	SER	N-CA-CB	5.21	117.52	109.91
29	P	127	VAL	N-CA-C	-5.21	108.76	113.71
37	V	85	SER	CA-C-N	5.21	127.58	120.54
37	V	85	SER	C-N-CA	5.21	127.58	120.54
15	R	63	VAL	CA-C-N	5.21	127.52	120.38
15	R	63	VAL	C-N-CA	5.21	127.52	120.38
28	5	336	GLN	N-CA-C	-5.21	107.30	113.97
46	C	411	ARG	NE-CZ-NH1	-5.21	116.30	121.50
4	y	113	SER	CA-C-N	5.20	127.31	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	y	113	SER	C-N-CA	5.20	127.31	120.60
48	W	176	GLN	N-CA-C	-5.20	107.48	113.88
4	y	116	GLU	CA-C-N	5.20	127.20	120.44
4	y	116	GLU	C-N-CA	5.20	127.20	120.44
20	X	128	PRO	CA-C-N	5.20	127.25	120.28
20	X	128	PRO	C-N-CA	5.20	127.25	120.28
44	K	65	VAL	CA-C-O	-5.20	117.24	119.94
46	C	467	ARG	CA-C-N	5.20	131.47	121.54
46	C	467	ARG	C-N-CA	5.20	131.47	121.54
49	I	178	LEU	CA-C-N	5.20	127.25	120.28
49	I	178	LEU	C-N-CA	5.20	127.25	120.28
20	X	125	HIS	N-CA-C	-5.20	101.69	109.95
1	f	20	ASP	N-CA-C	-5.20	106.18	112.88
50	H	157	LEU	N-CA-C	-5.19	106.97	113.72
47	8	324	GLY	CA-C-N	5.19	125.70	119.94
47	8	324	GLY	C-N-CA	5.19	125.70	119.94
35	b	35	VAL	CA-C-N	5.19	127.55	120.54
35	b	35	VAL	C-N-CA	5.19	127.55	120.54
1	f	1841	ARG	N-CA-C	5.19	117.61	111.33
15	R	38	CYS	CA-C-N	5.19	127.23	120.28
15	R	38	CYS	C-N-CA	5.19	127.23	120.28
32	M	21	PHE	CA-C-N	5.19	128.00	120.79
32	M	21	PHE	C-N-CA	5.19	128.00	120.79
1	f	838	ASN	CA-CB-CG	5.18	117.78	112.60
1	f	1162	GLY	CA-C-N	5.18	131.03	121.70
1	f	1162	GLY	C-N-CA	5.18	131.03	121.70
37	V	82	GLY	N-CA-C	-5.18	106.48	112.29
47	8	414	ALA	CA-C-N	5.18	127.18	120.44
47	8	414	ALA	C-N-CA	5.18	127.18	120.44
49	I	170	GLU	CA-C-N	5.18	127.23	120.28
49	I	170	GLU	C-N-CA	5.18	127.23	120.28
52	l	109	VAL	N-CA-C	-5.18	102.31	109.46
8	p	85	ALA	N-CA-C	-5.18	101.50	109.52
40	Y	267	HIS	CA-C-N	5.18	127.98	120.79
40	Y	267	HIS	C-N-CA	5.18	127.98	120.79
47	8	284	ASP	CA-C-N	5.18	124.35	118.97
47	8	284	ASP	C-N-CA	5.18	124.35	118.97
50	H	199	THR	N-CA-CB	5.18	119.24	110.49
9	r	108	LYS	CA-C-N	5.17	127.47	120.38
9	r	108	LYS	C-N-CA	5.17	127.47	120.38
13	o	177	LYS	N-CA-C	-5.17	105.29	111.03
1	f	64	ASP	CA-C-N	5.17	127.52	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	64	ASP	C-N-CA	5.17	127.52	120.54
46	C	106	LEU	CA-C-N	5.17	127.16	120.44
46	C	106	LEU	C-N-CA	5.17	127.16	120.44
1	f	1304	VAL	CA-C-N	5.17	131.28	121.97
1	f	1304	VAL	C-N-CA	5.17	131.28	121.97
42	D	16	LYS	CA-C-N	5.17	127.52	120.54
42	D	16	LYS	C-N-CA	5.17	127.52	120.54
7	n	285	PHE	CA-CB-CG	-5.17	108.64	113.80
49	I	337	PRO	N-CA-C	5.16	123.11	112.47
29	P	230	ARG	CA-C-N	5.16	127.97	120.79
29	P	230	ARG	C-N-CA	5.16	127.97	120.79
34	O	84	ARG	CA-C-N	5.16	125.46	119.47
34	O	84	ARG	C-N-CA	5.16	125.46	119.47
46	C	312	HIS	CA-C-N	5.16	127.20	120.28
46	C	312	HIS	C-N-CA	5.16	127.20	120.28
28	5	177	THR	CA-C-N	5.16	127.51	120.54
28	5	177	THR	C-N-CA	5.16	127.51	120.54
47	8	325	GLY	CA-C-N	5.16	127.15	120.44
47	8	325	GLY	C-N-CA	5.16	127.15	120.44
23	d	245	ASP	CA-C-N	5.16	125.20	119.32
23	d	245	ASP	C-N-CA	5.16	125.20	119.32
1	f	686	LYS	CA-C-N	5.16	127.53	120.77
1	f	686	LYS	C-N-CA	5.16	127.53	120.77
7	n	124	LEU	N-CA-C	-5.16	101.46	109.14
1	f	32	GLU	CA-C-N	5.15	127.25	120.60
1	f	32	GLU	C-N-CA	5.15	127.25	120.60
8	p	187	ARG	CA-C-N	5.15	128.53	120.75
8	p	187	ARG	C-N-CA	5.15	128.53	120.75
49	I	307	PRO	CA-C-N	5.15	127.14	120.44
49	I	307	PRO	C-N-CA	5.15	127.14	120.44
12	Z	179	GLN	CA-C-N	5.15	127.49	120.54
12	Z	179	GLN	C-N-CA	5.15	127.49	120.54
29	P	21	GLU	CA-C-N	5.15	127.79	120.53
29	P	21	GLU	C-N-CA	5.15	127.79	120.53
38	w	108	LEU	CA-C-N	5.15	127.79	120.53
38	w	108	LEU	C-N-CA	5.15	127.79	120.53
39	E	168	ASN	CA-C-N	5.14	127.37	120.58
39	E	168	ASN	C-N-CA	5.14	127.37	120.58
3	0	1071	G	O5'-C5'-C4'	5.14	119.21	111.50
5	s	356	ARG	CA-C-N	-5.14	111.72	121.54
5	s	356	ARG	C-N-CA	-5.14	111.72	121.54
39	E	228	ASN	CA-C-N	5.14	127.12	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	E	228	ASN	C-N-CA	5.14	127.12	120.44
49	I	318	GLU	CA-C-N	5.14	127.12	120.44
49	I	318	GLU	C-N-CA	5.14	127.12	120.44
40	Y	208	PRO	N-CA-CB	5.14	108.07	103.08
1	f	797	GLN	N-CA-C	-5.14	99.86	110.80
1	f	1799	LEU	CA-C-N	5.14	125.64	119.94
1	f	1799	LEU	C-N-CA	5.14	125.64	119.94
1	f	909	ARG	N-CA-C	-5.13	105.68	111.28
1	f	1122	GLN	CA-C-N	-5.13	114.04	122.67
1	f	1122	GLN	C-N-CA	-5.13	114.04	122.67
27	h	30	LEU	CA-C-N	5.13	127.41	120.38
27	h	30	LEU	C-N-CA	5.13	127.41	120.38
48	W	122	THR	N-CA-C	-5.13	101.26	109.07
5	s	350	PRO	CA-C-O	-5.13	113.12	120.56
15	R	94	ARG	CA-C-N	5.13	127.47	120.54
15	R	94	ARG	C-N-CA	5.13	127.47	120.54
28	5	177	THR	N-CA-CB	5.13	117.40	109.91
39	E	299	GLU	CA-C-N	5.13	127.11	120.44
39	E	299	GLU	C-N-CA	5.13	127.11	120.44
3	0	1579	A	C4'-C3'-C2'	-5.13	97.47	102.60
39	E	34	ALA	CA-C-N	5.13	130.94	121.70
39	E	34	ALA	C-N-CA	5.13	130.94	121.70
19	v	58	ASP	CA-C-N	5.13	127.15	120.28
19	v	58	ASP	C-N-CA	5.13	127.15	120.28
13	o	162	GLU	CA-C-N	5.13	127.21	120.60
13	o	162	GLU	C-N-CA	5.13	127.21	120.60
11	m	71	ARG	N-CA-C	-5.12	99.99	108.75
1	f	1693	ARG	N-CA-C	-5.12	101.40	109.50
40	Y	213	LEU	CA-C-N	5.12	127.56	120.29
40	Y	213	LEU	C-N-CA	5.12	127.56	120.29
50	H	216	VAL	CA-C-N	5.12	125.63	119.94
50	H	216	VAL	C-N-CA	5.12	125.63	119.94
46	C	203	ALA	CA-C-N	5.12	127.10	120.44
46	C	203	ALA	C-N-CA	5.12	127.10	120.44
14	q	27	LYS	CA-C-N	5.12	127.14	120.28
14	q	27	LYS	C-N-CA	5.12	127.14	120.28
43	G	164	ALA	N-CA-CB	5.12	121.93	111.08
29	P	186	ALA	CA-C-N	5.12	127.47	120.77
29	P	186	ALA	C-N-CA	5.12	127.47	120.77
47	8	177	GLU	CA-C-N	5.12	127.14	120.28
47	8	177	GLU	C-N-CA	5.12	127.14	120.28
1	f	921	ILE	CA-C-N	5.12	124.56	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	921	ILE	C-N-CA	5.12	124.56	119.24
3	0	1981	C	P-O3'-C3'	5.11	127.87	120.20
4	y	98	LYS	CA-C-N	5.11	127.39	120.38
4	y	98	LYS	C-N-CA	5.11	127.39	120.38
51	A	174	SER	CA-C-N	5.11	127.13	120.28
51	A	174	SER	C-N-CA	5.11	127.13	120.28
13	o	100	ASP	N-CA-C	-5.11	106.18	112.72
46	C	430	VAL	CA-C-N	5.11	127.08	120.44
46	C	430	VAL	C-N-CA	5.11	127.08	120.44
26	J	232	ALA	CA-C-N	5.11	127.38	120.38
26	J	232	ALA	C-N-CA	5.11	127.38	120.38
39	E	17	ALA	CA-C-N	5.11	127.08	120.44
39	E	17	ALA	C-N-CA	5.11	127.08	120.44
46	C	630	TYR	CA-C-N	5.11	130.89	121.70
46	C	630	TYR	C-N-CA	5.11	130.89	121.70
9	r	27	VAL	N-CA-C	-5.11	100.72	108.17
11	m	80	LYS	N-CA-C	-5.10	101.53	109.24
14	q	40	ARG	N-CA-C	-5.10	105.36	112.30
21	B	82	TYR	N-CA-CB	5.10	119.11	110.49
44	K	93	ARG	CA-C-N	5.10	127.11	120.28
44	K	93	ARG	C-N-CA	5.10	127.11	120.28
10	u	106	THR	N-CA-C	-5.09	106.16	112.93
5	s	244	ALA	CA-C-N	5.09	127.86	120.79
5	s	244	ALA	C-N-CA	5.09	127.86	120.79
52	l	89	ILE	CA-C-N	5.09	124.26	118.97
52	l	89	ILE	C-N-CA	5.09	124.26	118.97
9	r	86	ALA	CA-C-N	5.09	127.41	120.54
9	r	86	ALA	C-N-CA	5.09	127.41	120.54
47	8	451	ALA	CA-C-N	5.09	127.64	120.42
47	8	451	ALA	C-N-CA	5.09	127.64	120.42
19	v	46	PHE	N-CA-C	-5.08	108.82	114.62
37	V	28	ILE	N-CA-C	-5.08	100.56	108.95
38	w	101	ASN	CA-C-N	5.08	124.87	119.28
38	w	101	ASN	C-N-CA	5.08	124.87	119.28
51	A	35	LYS	N-CA-C	-5.08	101.41	109.59
15	R	70	LYS	CA-C-N	5.08	127.69	120.53
15	R	70	LYS	C-N-CA	5.08	127.69	120.53
31	L	28	ALA	CA-C-N	5.08	127.42	120.46
31	L	28	ALA	C-N-CA	5.08	127.42	120.46
50	H	202	ARG	CA-C-N	5.08	131.24	121.54
50	H	202	ARG	C-N-CA	5.08	131.24	121.54
32	M	49	ILE	N-CA-C	-5.08	100.93	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	13	VAL	CA-C-N	5.08	127.33	120.38
16	S	13	VAL	C-N-CA	5.08	127.33	120.38
22	F	134	HIS	CA-C-N	5.08	127.08	120.28
22	F	134	HIS	C-N-CA	5.08	127.08	120.28
10	u	78	PHE	N-CA-C	-5.07	107.07	114.12
10	u	121	HIS	CA-C-N	5.07	127.59	120.28
10	u	121	HIS	C-N-CA	5.07	127.59	120.28
48	W	186	ALA	CA-C-N	5.07	127.69	120.53
48	W	186	ALA	C-N-CA	5.07	127.69	120.53
28	5	238	ASN	N-CA-C	-5.07	105.94	113.40
29	P	7	TYR	CA-C-N	5.07	124.73	119.56
29	P	7	TYR	C-N-CA	5.07	124.73	119.56
20	X	90	VAL	N-CA-C	-5.07	101.18	108.89
39	E	317	PHE	N-CA-C	-5.07	101.49	109.50
47	8	142	VAL	CA-C-N	5.07	124.24	118.97
47	8	142	VAL	C-N-CA	5.07	124.24	118.97
1	f	1283	ILE	N-CA-C	-5.07	100.95	108.45
46	C	201	LYS	CA-C-N	5.07	127.38	120.54
46	C	201	LYS	C-N-CA	5.07	127.38	120.54
47	8	395	PRO	CA-C-N	5.07	127.07	120.28
47	8	395	PRO	C-N-CA	5.07	127.07	120.28
51	A	215	MET	N-CA-C	-5.07	105.94	112.68
32	M	9	MET	CA-C-N	5.07	127.41	120.77
32	M	9	MET	C-N-CA	5.07	127.41	120.77
1	f	1251	LYS	CA-C-N	5.06	131.09	121.97
1	f	1251	LYS	C-N-CA	5.06	131.09	121.97
14	q	172	PRO	CA-C-N	5.06	127.40	120.77
14	q	172	PRO	C-N-CA	5.06	127.40	120.77
15	R	84	ILE	N-CA-C	-5.06	102.37	107.89
32	M	119	MET	CA-C-N	5.06	125.70	120.03
32	M	119	MET	C-N-CA	5.06	125.70	120.03
8	p	155	VAL	N-CA-C	-5.06	104.53	110.05
13	o	75	ALA	CA-C-N	5.06	127.40	120.77
13	o	75	ALA	C-N-CA	5.06	127.40	120.77
23	d	138	ALA	CA-C-N	5.06	127.32	120.38
23	d	138	ALA	C-N-CA	5.06	127.32	120.38
1	f	1613	CYS	CA-C-N	5.06	127.31	120.38
1	f	1613	CYS	C-N-CA	5.06	127.31	120.38
47	8	342	PRO	N-CA-C	-5.06	108.20	114.68
1	f	839	GLN	CA-C-N	5.06	127.31	120.38
1	f	839	GLN	C-N-CA	5.06	127.31	120.38
15	R	89	TYR	CA-C-N	5.06	127.82	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	89	TYR	C-N-CA	5.06	127.82	120.79
21	B	110	THR	CA-C-N	5.06	127.12	120.60
21	B	110	THR	C-N-CA	5.06	127.12	120.60
43	G	200	ALA	CA-C-N	5.05	126.93	120.56
43	G	200	ALA	C-N-CA	5.05	126.93	120.56
4	y	93	GLU	CA-C-N	5.05	126.16	119.84
4	y	93	GLU	C-N-CA	5.05	126.16	119.84
1	f	1559	THR	N-CA-CB	5.05	119.03	110.49
5	s	250	TYR	CA-C-N	5.05	124.22	118.97
5	s	250	TYR	C-N-CA	5.05	124.22	118.97
20	X	15	LEU	N-CA-C	-5.05	105.21	113.19
36	c	9	ALA	N-CA-C	-5.05	107.14	113.15
37	V	30	VAL	N-CA-C	-5.05	100.63	108.81
22	F	170	GLY	CA-C-N	5.05	127.36	120.54
22	F	170	GLY	C-N-CA	5.05	127.36	120.54
26	J	164	LYS	N-CA-C	5.04	121.55	110.80
1	f	1655	VAL	CA-C-O	5.04	127.13	121.28
2	1	71	U	C4'-C3'-C2'	-5.04	97.56	102.60
3	0	1071	G	P-O5'-C5'	5.04	128.47	120.90
3	0	1477	A	P-O3'-C3'	5.04	127.77	120.20
14	q	158	PHE	CA-CB-CG	-5.04	108.76	113.80
26	J	163	LYS	CA-C-N	5.04	131.17	121.54
26	J	163	LYS	C-N-CA	5.04	131.17	121.54
30	i	12	ALA	CA-C-N	5.04	127.29	120.38
30	i	12	ALA	C-N-CA	5.04	127.29	120.38
49	I	125	LEU	CA-C-N	5.04	127.00	120.44
49	I	125	LEU	C-N-CA	5.04	127.00	120.44
30	i	21	PHE	N-CA-C	-5.04	104.39	110.44
39	E	246	VAL	N-CA-C	-5.04	98.86	109.34
46	C	318	VAL	CA-C-N	5.04	131.16	121.54
46	C	318	VAL	C-N-CA	5.04	131.16	121.54
46	C	214	LEU	N-CA-C	-5.04	99.72	109.24
1	f	1331	PHE	CA-CB-CG	-5.04	108.77	113.80
39	E	16	LEU	CA-C-N	5.04	126.99	120.44
39	E	16	LEU	C-N-CA	5.04	126.99	120.44
26	J	140	PRO	CA-C-N	5.03	127.22	120.58
26	J	140	PRO	C-N-CA	5.03	127.22	120.58
51	A	35	LYS	CA-C-O	-5.03	115.38	120.71
3	0	1832	U	P-O3'-C3'	5.03	127.75	120.20
22	F	107	ILE	N-CA-C	-5.03	102.57	107.55
33	N	18	PHE	CA-C-N	5.03	131.15	121.54
33	N	18	PHE	C-N-CA	5.03	131.15	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	E	356	ARG	CA-C-N	5.03	127.02	120.28
39	E	356	ARG	C-N-CA	5.03	127.02	120.28
47	8	252	LEU	CA-C-N	5.03	126.98	120.44
47	8	252	LEU	C-N-CA	5.03	126.98	120.44
21	B	70	LEU	CA-C-N	5.03	127.02	120.28
21	B	70	LEU	C-N-CA	5.03	127.02	120.28
26	J	178	LEU	N-CA-C	-5.03	101.95	109.95
39	E	51	SER	CA-C-N	5.03	126.90	120.56
39	E	51	SER	C-N-CA	5.03	126.90	120.56
47	8	160	ALA	CA-C-N	5.03	130.75	121.70
47	8	160	ALA	C-N-CA	5.03	130.75	121.70
52	l	56	ALA	CA-C-N	5.03	127.33	120.54
52	l	56	ALA	C-N-CA	5.03	127.33	120.54
1	f	135	GLU	CA-C-N	5.03	131.14	121.54
1	f	135	GLU	C-N-CA	5.03	131.14	121.54
1	f	1179	VAL	N-CA-C	-5.03	101.25	108.89
21	B	93	ASP	CA-C-N	5.03	127.52	120.28
21	B	93	ASP	C-N-CA	5.03	127.52	120.28
29	P	213	LEU	CA-C-N	5.02	127.32	120.54
29	P	213	LEU	C-N-CA	5.02	127.32	120.54
13	o	166	ALA	N-CA-C	-5.02	103.88	111.56
14	q	31	GLU	CA-C-N	5.02	127.71	120.38
14	q	31	GLU	C-N-CA	5.02	127.71	120.38
41	Q	43	CYS	N-CA-C	-5.02	100.55	108.73
42	D	25	ARG	CA-C-N	5.02	126.97	120.44
42	D	25	ARG	C-N-CA	5.02	126.97	120.44
23	d	256	MET	CA-C-N	5.02	126.45	120.13
23	d	256	MET	C-N-CA	5.02	126.45	120.13
44	K	67	GLY	CA-C-N	5.02	127.00	120.28
44	K	67	GLY	C-N-CA	5.02	127.00	120.28
51	A	17	GLY	CA-C-N	5.02	125.55	120.38
51	A	17	GLY	C-N-CA	5.02	125.55	120.38
39	E	26	GLU	CA-C-N	5.02	126.96	120.44
39	E	26	GLU	C-N-CA	5.02	126.96	120.44
9	r	90	ALA	CA-C-N	5.01	127.34	120.77
9	r	90	ALA	C-N-CA	5.01	127.34	120.77
10	u	34	VAL	N-CA-C	-5.01	108.09	112.90
44	K	100	VAL	CA-C-N	5.01	127.83	120.71
44	K	100	VAL	C-N-CA	5.01	127.83	120.71
5	s	213	ALA	N-CA-C	5.01	118.50	112.38
31	L	97	LYS	CA-C-N	5.01	127.06	120.60
31	L	97	LYS	C-N-CA	5.01	127.06	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	E	116	MET	N-CA-CB	5.01	118.96	110.49
43	G	105	ALA	CA-C-N	5.01	124.18	118.97
43	G	105	ALA	C-N-CA	5.01	124.18	118.97
47	8	532	ASP	CA-C-N	5.00	126.86	120.56
47	8	532	ASP	C-N-CA	5.00	126.86	120.56
52	1	220	SER	N-CA-C	-5.00	106.42	112.88

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	f	296	TYR	CA
1	f	305	TYR	CA
1	f	772	TYR	CA
3	0	974	A	C1'
3	0	1833	G	C1'
39	E	281	TYR	CA
46	C	429	SER	CA
49	I	337	PRO	CA
49	I	350	TYR	CA

All (759) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	0	1185	A	Sidechain
3	0	1207	G	Sidechain
3	0	1254	G	Sidechain
3	0	1331	G	Sidechain
3	0	1418	U	Sidechain
3	0	1473	G	Sidechain
3	0	1485	U	Sidechain
3	0	1488	U	Sidechain
3	0	1518	C	Sidechain
3	0	152	A	Sidechain
3	0	1611	A	Sidechain
3	0	1666	A	Sidechain
3	0	1694	A	Sidechain
3	0	1702	G	Sidechain
3	0	1704	U	Sidechain
3	0	1779	U	Sidechain
3	0	1930	A	Sidechain
3	0	1970	U	Sidechain
3	0	1978	A	Sidechain

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Mol	Chain	Res	Type	Group
3	0	1997	A	Sidechain
3	0	2008	G	Sidechain
3	0	2011	A	Sidechain
3	0	2020	U	Sidechain
3	0	2078	G	Sidechain
3	0	2080	G	Sidechain
3	0	2086	G	Sidechain
3	0	2098	U	Sidechain
3	0	2102	U	Sidechain
3	0	2119	U	Sidechain
3	0	212	G	Sidechain
3	0	2120	C	Sidechain
3	0	2134	U	Sidechain
3	0	2136	A	Sidechain
3	0	2244	A	Sidechain
3	0	229	G	Sidechain
3	0	237	A	Sidechain
3	0	255	A	Sidechain
3	0	271	C	Sidechain
3	0	313	G	Sidechain
3	0	324	U	Sidechain
3	0	481	G	Sidechain
3	0	695	G	Sidechain
3	0	714	G	Sidechain
3	0	736	U	Sidechain
3	0	738	G	Sidechain
3	0	773	U	Sidechain
3	0	776	G	Sidechain
3	0	8	U	Sidechain
3	0	824	G	Sidechain
3	0	90	A	Sidechain
3	0	936	C	Sidechain
3	0	975	U	Sidechain
28	5	102	CYS	Peptide
28	5	233	ALA	Peptide
28	5	267	SER	Mainchain
28	5	271	ASN	Peptide
28	5	273	PRO	Peptide
28	5	278	ILE	Peptide
28	5	283	GLY	Peptide
28	5	411	LEU	Mainchain
28	5	412	GLN	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
28	5	89	THR	Peptide,Mainchain
47	8	114	GLY	Peptide
47	8	115	GLU	Peptide
47	8	116	THR	Peptide
47	8	117	PRO	Peptide
47	8	118	SER	Peptide
47	8	127	LEU	Peptide
47	8	128	SER	Peptide
47	8	130	VAL	Peptide
47	8	132	PRO	Peptide
47	8	157	SER	Peptide
47	8	158	PHE	Peptide
47	8	161	ILE	Peptide
47	8	162	GLY	Peptide
47	8	186	ASN	Peptide
47	8	187	LEU	Peptide
47	8	189	ARG	Peptide
47	8	197	ALA	Mainchain
47	8	204	ARG	Peptide
47	8	207	LEU	Peptide
47	8	209	PRO	Peptide
47	8	210	ILE	Peptide
47	8	214	VAL	Peptide
47	8	22	ASN	Peptide
47	8	238	GLU	Peptide
47	8	240	PRO	Peptide
47	8	241	ASN	Peptide
47	8	256	LEU	Peptide
47	8	257	THR	Peptide
47	8	258	GLU	Peptide
47	8	259	MET	Peptide
47	8	261	SER	Peptide
47	8	262	TRP	Peptide
47	8	277	GLN	Peptide
47	8	279	ILE	Peptide
47	8	305	SER	Peptide
47	8	306	HIS	Peptide
47	8	322	GLY	Peptide
47	8	340	CYS	Peptide
47	8	345	ASN	Peptide
47	8	347	GLU	Peptide
47	8	349	ARG	Peptide

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Mol	Chain	Res	Type	Group
47	8	350	ASN	Peptide
47	8	368	LEU	Peptide,Mainchain
47	8	376	ALA	Peptide
47	8	388	GLN	Peptide
47	8	392	LYS	Peptide
47	8	393	ALA	Peptide
47	8	405	ARG	Peptide
47	8	424	ILE	Peptide
47	8	425	VAL	Peptide
47	8	435	GLU	Mainchain
47	8	467	ASN	Peptide
47	8	469	ALA	Peptide
47	8	470	SER	Peptide
47	8	473	VAL	Peptide
47	8	475	ILE	Peptide
47	8	492	ILE	Peptide
47	8	500	SER	Peptide
47	8	520	VAL	Peptide
47	8	521	ASP	Peptide
47	8	547	ILE	Peptide
47	8	56	PHE	Peptide
47	8	59	GLU	Peptide
47	8	60	GLN	Peptide
47	8	61	GLY	Peptide
47	8	62	ILE	Peptide
47	8	67	PHE	Peptide
47	8	74	ASN	Peptide
51	A	103	ARG	Peptide
51	A	17	GLY	Peptide
51	A	19	PRO	Peptide
51	A	2	GLY	Peptide
51	A	23	ILE	Peptide
51	A	24	GLU	Peptide
51	A	25	MET	Peptide
51	A	3	PHE	Peptide
51	A	4	GLU	Peptide
51	A	40	ALA	Peptide
51	A	57	GLN	Peptide
51	A	59	THR	Peptide
51	A	62	LYS	Peptide
51	A	64	GLU	Peptide
51	A	81	GLY	Peptide

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Mol	Chain	Res	Type	Group
51	A	97	PHE	Peptide
21	B	130	GLN	Peptide
21	B	159	ASP	Peptide
21	B	166	GLY	Peptide
21	B	81	ASP	Peptide
46	C	102	PRO	Peptide
46	C	108	CYS	Peptide
46	C	11	ASP	Peptide
46	C	113	PRO	Peptide
46	C	114	ASP	Peptide
46	C	12	GLU	Peptide
46	C	122	LYS	Peptide
46	C	123	GLU	Peptide
46	C	124	THR	Peptide
46	C	125	PHE	Peptide
46	C	126	LYS	Peptide
46	C	128	PRO	Peptide
46	C	14	LEU	Peptide
46	C	147	ILE	Peptide
46	C	157	ASP	Peptide
46	C	158	GLU	Peptide
46	C	159	GLU	Peptide
46	C	16	GLU	Peptide
46	C	160	SER	Peptide
46	C	162	GLU	Peptide
46	C	164	GLY	Peptide
46	C	166	ASP	Peptide
46	C	168	GLY	Peptide
46	C	169	GLN	Peptide
46	C	17	VAL	Peptide
46	C	170	GLY	Peptide
46	C	172	GLU	Peptide
46	C	175	GLU	Peptide
46	C	178	GLU	Peptide
46	C	179	GLU	Peptide
46	C	19	HIS	Peptide
46	C	194	LYS	Peptide
46	C	195	ARG	Peptide
46	C	196	ALA	Peptide
46	C	214	LEU	Peptide
46	C	22	GLU	Peptide
46	C	237	ALA	Peptide

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Mol	Chain	Res	Type	Group
46	C	256	THR	Peptide
46	C	258	ASN	Peptide
46	C	259	PRO	Peptide
46	C	260	ALA	Peptide
46	C	267	PHE	Peptide
46	C	268	SER	Peptide
46	C	271	LEU	Peptide
46	C	274	LYS	Peptide
46	C	281	GLY	Peptide
46	C	282	LEU	Peptide
46	C	283	CYS	Peptide
46	C	327	TYR	Peptide
46	C	328	TYR	Peptide
46	C	329	GLN	Peptide
46	C	332	LYS	Peptide
46	C	333	ARG	Peptide
46	C	344	GLU	Peptide
46	C	345	ILE	Peptide
46	C	348	SER	Peptide
46	C	350	ARG	Peptide
46	C	351	GLN	Peptide
46	C	352	GLN	Peptide
46	C	358	TYR	Peptide
46	C	361	MET	Peptide
46	C	362	THR	Peptide
46	C	363	ARG	Peptide
46	C	364	LEU	Peptide
46	C	365	THR	Peptide
46	C	374	ILE	Peptide
46	C	382	GLN	Peptide
46	C	386	VAL	Peptide
46	C	387	ILE	Peptide
46	C	388	GLY	Peptide
46	C	391	GLU	Peptide
46	C	394	CYS	Peptide
46	C	395	SER	Peptide
46	C	429	SER	Peptide
46	C	450	ALA	Peptide
46	C	453	VAL	Peptide
46	C	46	GLU	Peptide
46	C	464	TRP	Peptide,Mainchain
46	C	465	SER	Peptide

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Mol	Chain	Res	Type	Group
46	C	466	ASN	Peptide
46	C	467	ARG	Peptide
46	C	469	HIS	Peptide
46	C	471	VAL	Peptide
46	C	495	LEU	Peptide
46	C	501	TYR	Peptide
46	C	502	ILE	Peptide
46	C	504	HIS	Peptide,Mainchain
46	C	51	LEU	Peptide
46	C	522	LYS	Peptide
46	C	523	GLU	Peptide
46	C	524	ALA	Peptide
46	C	525	LYS	Peptide
46	C	526	LYS	Peptide
46	C	527	PRO	Peptide
46	C	528	TYR	Peptide
46	C	542	ASN	Peptide
46	C	544	MET	Peptide
46	C	545	ALA	Peptide
46	C	547	GLN	Peptide
46	C	548	PRO	Peptide
46	C	549	LEU	Peptide
46	C	553	PRO	Peptide
46	C	555	GLU	Peptide
46	C	568	LYS	Peptide
46	C	570	GLY	Peptide
46	C	571	ASP	Peptide
46	C	580	LYS	Peptide
46	C	581	ASN	Peptide
46	C	582	MET	Peptide
46	C	584	ALA	Peptide
46	C	585	TRP	Peptide
46	C	586	SER	Peptide
46	C	590	ASN	Peptide
46	C	591	GLY	Peptide
46	C	610	PHE	Peptide
46	C	612	TYR	Peptide
46	C	616	CYS	Peptide
46	C	617	ASN	Peptide
46	C	619	ALA	Peptide
46	C	621	ILE	Peptide
46	C	622	SER	Peptide

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Mol	Chain	Res	Type	Group
46	C	630	TYR	Sidechain
46	C	633	ASN	Peptide
46	C	634	GLU	Peptide
46	C	636	GLU	Peptide
46	C	647	GLU	Peptide
46	C	653	ILE	Peptide
46	C	654	ALA	Peptide
46	C	73	ASP	Peptide
46	C	75	GLU	Peptide
46	C	76	SER	Peptide
46	C	94	HIS	Peptide
46	C	95	LYS	Peptide
46	C	97	LYS	Peptide
46	C	99	LYS	Peptide
42	D	7	PRO	Peptide
39	E	105	VAL	Peptide
39	E	106	LEU	Peptide
39	E	107	GLU	Peptide
39	E	109	LYS	Peptide
39	E	111	ILE	Peptide
39	E	113	SER	Peptide
39	E	114	ASN	Peptide
39	E	115	VAL	Peptide
39	E	12	LEU	Peptide
39	E	126	TYR	Peptide,Sidechain
39	E	127	TYR	Peptide
39	E	128	ASP	Peptide
39	E	13	ASP	Peptide
39	E	131	ARG	Peptide
39	E	14	LYS	Peptide
39	E	147	GLY	Peptide
39	E	148	TYR	Peptide
39	E	15	HIS	Peptide
39	E	150	ILE	Peptide
39	E	190	GLU	Peptide
39	E	192	ILE	Peptide
39	E	194	ARG	Peptide
39	E	211	VAL	Peptide
39	E	216	PHE	Peptide
39	E	218	GLY	Peptide
39	E	221	GLN	Peptide
39	E	223	SER	Peptide

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Mol	Chain	Res	Type	Group
39	E	231	PHE	Peptide
39	E	233	ILE	Peptide
39	E	235	THR	Peptide
39	E	237	PHE	Peptide
39	E	244	GLU	Peptide
39	E	245	THR	Peptide
39	E	262	LYS	Peptide
39	E	263	GLN	Peptide
39	E	265	ARG	Peptide
39	E	266	SER	Peptide
39	E	283	ASP	Peptide
39	E	295	ARG	Peptide
39	E	297	SER	Peptide
39	E	30	ASP	Peptide
39	E	314	GLY	Peptide
39	E	315	ASP	Peptide
39	E	317	PHE	Peptide
39	E	318	LEU	Peptide
39	E	319	ILE	Peptide
39	E	32	ALA	Peptide
39	E	338	MET	Peptide
39	E	339	MET	Peptide
39	E	34	ALA	Peptide
39	E	340	THR	Peptide
39	E	345	SER	Peptide
39	E	35	LEU	Peptide
39	E	353	LEU	Peptide
39	E	38	VAL	Peptide
39	E	388	SER	Peptide
39	E	389	GLN	Peptide
39	E	390	ALA	Peptide
39	E	392	SER	Peptide
39	E	40	ALA	Peptide
39	E	41	THR	Peptide
39	E	42	THR	Peptide
39	E	43	ALA	Peptide
39	E	46	ALA	Peptide
39	E	47	GLU	Peptide
39	E	48	GLY	Peptide
39	E	62	ALA	Peptide
39	E	63	GLN	Peptide
39	E	64	ARG	Peptide

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Mol	Chain	Res	Type	Group
39	E	93	ASP	Peptide
39	E	94	ALA	Peptide
39	E	97	SER	Peptide
22	F	155	ALA	Peptide
22	F	191	THR	Peptide
22	F	198	TRP	Peptide
43	G	106	PRO	Peptide
43	G	111	SER	Peptide
43	G	112	LYS	Peptide
43	G	117	ASN	Peptide
43	G	118	GLN	Peptide
43	G	163	GLU	Peptide
43	G	179	LYS	Peptide
43	G	182	TYR	Peptide
43	G	185	SER	Peptide
43	G	188	TYR	Peptide
43	G	189	PRO	Peptide
43	G	194	THR	Peptide
43	G	195	ASN	Peptide
43	G	210	PHE	Peptide
43	G	212	ARG	Peptide
43	G	215	ASN	Peptide
43	G	217	ARG	Peptide
43	G	24	ARG	Peptide
43	G	250	GLY	Peptide
43	G	253	ASN	Peptide
43	G	254	LYS	Peptide
43	G	255	SER	Peptide
43	G	26	ARG	Peptide
43	G	268	TYR	Sidechain
43	G	278	GLN	Peptide
43	G	280	SER	Peptide
43	G	46	TYR	Sidechain
43	G	60	ARG	Peptide
43	G	75	CYS	Peptide
43	G	76	TYR	Peptide
43	G	79	SER	Peptide
43	G	89	ALA	Peptide
43	G	92	GLU	Peptide
43	G	93	PRO	Peptide
43	G	94	GLY	Peptide
43	G	95	LYS	Peptide

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Mol	Chain	Res	Type	Group
50	H	126	GLU	Peptide
50	H	127	LEU	Peptide
50	H	129	SER	Peptide,Mainchain
50	H	187	PRO	Peptide
50	H	188	THR	Peptide
50	H	190	GLU	Peptide
50	H	196	THR	Peptide
50	H	197	ARG	Peptide
50	H	202	ARG	Peptide
50	H	205	LEU	Peptide
50	H	221	VAL	Peptide
50	H	223	ARG	Peptide
50	H	241	GLY	Peptide
50	H	242	PHE	Peptide
50	H	243	ASN	Peptide
50	H	260	THR	Peptide
50	H	261	ASP	Peptide
50	H	269	SER	Peptide
50	H	293	SER	Peptide
50	H	294	TYR	Peptide
50	H	295	GLY	Peptide
50	H	299	GLN	Peptide
50	H	300	ARG	Peptide
50	H	92	PRO	Peptide
50	H	96	THR	Peptide
49	I	324	ASP	Peptide
49	I	342	ILE	Peptide
49	I	422	ASP	Peptide
49	I	429	ALA	Peptide
49	I	437	THR	Peptide
49	I	438	VAL	Peptide
26	J	107	PHE	Peptide
26	J	120	LEU	Peptide
26	J	139	THR	Peptide
26	J	147	ASN	Peptide
26	J	150	VAL	Peptide
26	J	154	SER	Peptide
26	J	155	PRO	Peptide
26	J	158	ARG	Peptide
26	J	159	ALA	Peptide
26	J	160	SER	Peptide
26	J	174	LYS	Peptide

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Mol	Chain	Res	Type	Group
26	J	179	ARG	Peptide
26	J	180	THR	Peptide
26	J	182	ARG	Peptide
26	J	183	ASN	Peptide
26	J	184	ASN	Peptide
26	J	203	LYS	Peptide
26	J	217	LEU	Peptide
26	J	71	TYR	Sidechain
26	J	77	GLN	Peptide
26	J	92	LYS	Peptide
44	K	178	LYS	Peptide
44	K	189	ASN	Peptide
31	L	103	ILE	Peptide
31	L	107	VAL	Peptide
31	L	35	GLU	Peptide
31	L	49	GLY	Peptide
31	L	51	VAL	Peptide
31	L	52	ARG	Peptide
31	L	93	GLU	Peptide
32	M	36	VAL	Peptide
32	M	7	LYS	Peptide
33	N	34	THR	Peptide
34	O	13	ARG	Sidechain
34	O	148	ALA	Peptide
34	O	49	ASN	Peptide
34	O	50	CYS	Peptide
34	O	70	TYR	Sidechain
34	O	95	ARG	Peptide
29	P	124	ILE	Peptide
29	P	163	ARG	Sidechain
29	P	219	ARG	Sidechain
29	P	44	ASP	Peptide
41	Q	11	GLN	Peptide
41	Q	42	GLN	Peptide
41	Q	48	ALA	Peptide
45	T	142	ALA	Peptide
48	W	136	THR	Peptide
48	W	99	LEU	Peptide
20	X	32	ASN	Peptide
20	X	33	SER	Peptide,Mainchain
20	X	35	ASN	Peptide
20	X	37	ASN	Peptide

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Mol	Chain	Res	Type	Group
20	X	40	HIS	Peptide
20	X	41	VAL	Peptide
20	X	42	ASN	Peptide
20	X	44	SER	Peptide
20	X	81	ILE	Peptide
40	Y	278	THR	Peptide
40	Y	318	PHE	Peptide
40	Y	355	ASP	Peptide
40	Y	365	ALA	Peptide
12	Z	205	GLU	Peptide
12	Z	67	TRP	Peptide
35	b	75	ILE	Peptide
36	c	12	GLY	Peptide
36	c	22	ALA	Peptide
36	c	33	ARG	Sidechain
23	d	203	VAL	Peptide
23	d	236	LEU	Peptide
23	d	38	GLU	Peptide
1	f	1010	GLU	Peptide
1	f	1024	ASN	Peptide
1	f	1038	GLY	Mainchain
1	f	1039	ARG	Mainchain
1	f	1044	VAL	Mainchain
1	f	1070	LYS	Peptide,Mainchain
1	f	1080	ALA	Peptide
1	f	1100	ASN	Peptide
1	f	1101	PRO	Peptide
1	f	1107	GLY	Peptide
1	f	1109	LEU	Peptide
1	f	1110	GLY	Peptide,Mainchain
1	f	1116	GLN	Peptide
1	f	1118	HIS	Peptide
1	f	112	ILE	Peptide
1	f	1121	CYS	Peptide
1	f	1122	GLN	Mainchain
1	f	1126	THR	Mainchain
1	f	1128	PRO	Mainchain
1	f	1148	ASP	Peptide,Mainchain
1	f	1153	ASP	Mainchain
1	f	1172	ALA	Peptide
1	f	1175	PRO	Mainchain
1	f	1176	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	f	1212	LYS	Peptide
1	f	1214	ARG	Mainchain
1	f	1218	VAL	Mainchain
1	f	1219	HIS	Mainchain
1	f	1220	LEU	Peptide
1	f	1235	LYS	Mainchain
1	f	1250	LYS	Peptide
1	f	1251	LYS	Peptide
1	f	1258	ASN	Peptide
1	f	1259	CYS	Peptide
1	f	1264	LEU	Peptide,Mainchain
1	f	1265	HIS	Peptide,Mainchain
1	f	1266	PRO	Peptide,Mainchain
1	f	1267	LEU	Peptide
1	f	1268	SER	Peptide
1	f	1277	ARG	Peptide
1	f	1284	SER	Peptide
1	f	1306	TRP	Peptide
1	f	132	ALA	Peptide
1	f	1338	THR	Peptide
1	f	135	GLU	Peptide,Mainchain
1	f	1359	LEU	Peptide
1	f	136	LEU	Peptide
1	f	1361	HIS	Peptide
1	f	1369	ASN	Peptide
1	f	137	CYS	Peptide,Mainchain
1	f	1373	GLU	Peptide
1	f	1378	PHE	Peptide
1	f	1402	ALA	Peptide
1	f	143	LEU	Peptide
1	f	1439	GLN	Peptide
1	f	145	ALA	Peptide
1	f	1466	VAL	Peptide
1	f	1467	SER	Peptide
1	f	1470	GLY	Peptide
1	f	1474	PHE	Peptide
1	f	152	ASP	Peptide,Mainchain
1	f	1524	LYS	Peptide
1	f	1582	LEU	Peptide
1	f	1584	VAL	Peptide
1	f	1620	LEU	Peptide
1	f	1627	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	f	163	PRO	Peptide
1	f	1632	HIS	Peptide
1	f	164	GLN	Peptide
1	f	1654	GLY	Peptide
1	f	1702	LEU	Peptide
1	f	1723	MET	Peptide
1	f	1749	LEU	Peptide
1	f	1772	ASN	Peptide
1	f	1775	PHE	Peptide
1	f	1784	GLY	Peptide
1	f	1788	GLU	Peptide
1	f	1790	PHE	Peptide
1	f	1801	TYR	Peptide
1	f	1807	LEU	Peptide
1	f	1809	PHE	Peptide
1	f	1814	SER	Peptide
1	f	1815	SER	Peptide
1	f	1836	GLY	Peptide
1	f	1849	ASP	Peptide
1	f	1854	SER	Peptide
1	f	1855	PRO	Peptide
1	f	189	CYS	Peptide
1	f	193	ARG	Peptide,Mainchain
1	f	194	PHE	Mainchain
1	f	195	HIS	Mainchain
1	f	198	PHE	Peptide,Mainchain
1	f	199	PHE	Mainchain
1	f	201	SER	Peptide
1	f	202	LEU	Peptide
1	f	206	TRP	Peptide
1	f	207	GLU	Peptide
1	f	227	SER	Peptide
1	f	234	GLY	Mainchain
1	f	235	LEU	Peptide
1	f	236	SER	Peptide
1	f	237	ILE	Peptide
1	f	238	SER	Peptide
1	f	239	ASN	Peptide,Mainchain
1	f	240	PHE	Peptide,Mainchain
1	f	241	SER	Mainchain
1	f	242	SER	Peptide
1	f	243	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	f	257	PRO	Mainchain
1	f	258	GLU	Mainchain
1	f	259	PHE	Peptide,Mainchain
1	f	26	SER	Peptide
1	f	261	LEU	Peptide
1	f	262	MET	Mainchain
1	f	263	SER	Peptide,Mainchain
1	f	264	ASP	Peptide
1	f	267	GLN	Peptide
1	f	268	LEU	Peptide
1	f	269	GLY	Peptide
1	f	291	ARG	Mainchain
1	f	292	ARG	Peptide,Sidechain
1	f	294	ALA	Peptide
1	f	295	ASN	Peptide,Mainchain
1	f	296	TYR	Peptide,Sidechain,Mainchain
1	f	297	THR	Peptide
1	f	298	ASP	Peptide
1	f	300	ASP	Peptide
1	f	301	GLU	Peptide
1	f	302	ALA	Peptide,Mainchain
1	f	304	PRO	Peptide
1	f	305	TYR	Peptide
1	f	306	ARG	Peptide
1	f	307	LEU	Peptide,Mainchain
1	f	38	SER	Peptide
1	f	46	SER	Peptide
1	f	55	VAL	Peptide
1	f	56	THR	Peptide
1	f	679	ASN	Peptide
1	f	681	THR	Peptide
1	f	682	ALA	Peptide
1	f	696	ASN	Peptide
1	f	700	ARG	Peptide
1	f	705	GLU	Peptide
1	f	718	THR	Peptide
1	f	719	VAL	Peptide
1	f	720	ALA	Peptide
1	f	721	GLU	Peptide
1	f	722	TRP	Peptide
1	f	723	HIS	Peptide
1	f	736	SER	Peptide

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Mol	Chain	Res	Type	Group
1	f	772	TYR	Peptide,Mainchain
1	f	773	THR	Peptide
1	f	775	GLY	Peptide
1	f	794	ALA	Peptide
1	f	795	ALA	Peptide
1	f	796	SER	Peptide
1	f	798	LEU	Peptide
1	f	800	GLU	Peptide
1	f	801	VAL	Peptide
1	f	802	GLU	Peptide
1	f	803	PHE	Peptide
1	f	824	SER	Peptide
1	f	832	TYR	Peptide
1	f	833	GLY	Peptide
1	f	834	PHE	Peptide
1	f	849	ASN	Peptide
1	f	860	ALA	Peptide
1	f	874	ARG	Sidechain
1	f	89	VAL	Peptide
1	f	913	GLU	Peptide
1	f	934	VAL	Peptide
1	f	944	SER	Peptide
1	f	962	SER	Peptide
1	f	976	ASN	Peptide
1	f	981	THR	Peptide
1	f	987	LEU	Peptide
1	f	990	ASP	Peptide
1	f	996	THR	Peptide
24	g	36	ALA	Peptide
6	j	103	VAL	Peptide
6	j	82	LYS	Peptide
52	l	142	HIS	Peptide
52	l	143	ARG	Peptide,Sidechain
52	l	144	ILE	Peptide
52	l	145	ARG	Peptide
52	l	146	TYR	Peptide
52	l	147	PRO	Peptide
52	l	148	ASP	Peptide
52	l	149	PRO	Peptide
52	l	151	THR	Peptide
11	m	107	ARG	Peptide
11	m	124	LYS	Peptide

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Mol	Chain	Res	Type	Group
7	n	295	ASP	Peptide
13	o	151	ASN	Peptide
8	p	263	PHE	Peptide
8	p	42	ALA	Peptide
9	r	29	LYS	Peptide
9	r	42	VAL	Peptide
9	r	45	ILE	Peptide
9	r	76	ARG	Peptide
5	s	115	GLY	Peptide
5	s	272	ARG	Sidechain
5	s	299	VAL	Peptide
5	s	301	ASN	Peptide
5	s	312	MET	Peptide
5	s	333	PHE	Peptide
5	s	334	LYS	Peptide
5	s	335	ALA	Peptide
5	s	338	GLU	Peptide
5	s	339	PRO	Peptide
5	s	340	GLN	Peptide
5	s	343	ILE	Peptide
5	s	344	SER	Peptide
5	s	362	ARG	Peptide
5	s	392	GLY	Peptide
5	s	393	PRO	Peptide
5	s	395	ALA	Peptide
17	t	41	PHE	Peptide
10	u	48	LYS	Peptide
10	u	56	ARG	Sidechain
19	v	105	ALA	Peptide
19	v	92	ALA	Peptide
38	w	112	GLU	Peptide
38	w	119	ARG	Peptide
38	w	121	SER	Peptide
38	w	157	LYS	Peptide
38	w	52	GLU	Peptide
38	w	83	VAL	Peptide
4	y	73	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f	12257	0	12096	627	0
2	l	1606	0	816	23	0
3	o	45795	0	23111	114	0
4	y	989	0	1065	0	0
5	s	2365	0	2421	216	0
6	j	644	0	677	18	0
7	n	1796	0	1824	136	0
8	p	2405	0	2323	7	0
9	r	1113	0	1175	1	0
10	u	1108	0	1144	15	0
11	m	1116	0	1169	28	0
12	Z	1404	0	1503	0	0
13	o	1493	0	1562	25	0
14	q	1670	0	1778	1	0
15	R	1143	0	1226	0	0
16	S	630	0	630	51	0
17	t	829	0	866	0	0
18	U	526	0	550	34	0
19	v	1011	0	1019	0	0
20	X	1212	0	1250	23	0
21	B	1483	0	1548	1	0
22	F	1658	0	1704	0	0
23	d	1726	0	1774	2	0
24	g	635	0	631	0	0
25	a	553	0	608	1	0
26	J	1358	0	1419	38	0
27	h	958	0	981	16	0
28	5	3245	0	3326	289	0
29	P	1983	0	2131	1	0
30	i	992	0	1054	1	0
31	L	784	0	848	3	0
32	M	1587	0	1662	2	0
33	N	780	0	771	0	0
34	O	1116	0	1166	2	0
35	b	1019	0	1050	0	0
36	c	480	0	532	18	0
37	V	789	0	800	128	0
38	w	1162	0	1128	82	0
39	E	3119	0	3106	40	0
40	Y	1387	0	1429	70	0
41	Q	462	0	475	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	D	294	0	336	0	0
43	G	2414	0	2396	2	0
44	K	1566	0	1566	0	0
45	T	1057	0	1099	6	0
46	C	5630	0	5586	327	0
47	8	4596	0	4584	177	0
48	W	1781	0	1852	97	0
49	I	2770	0	2786	1	0
50	H	2388	0	2377	5	0
51	A	3891	0	3874	264	0
52	l	2038	0	2142	0	0
53	n	1	0	0	0	0
54	5	1	0	0	0	0
55	5	32	0	13	21	0
All	All	136847	0	114959	2365	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 9.

All (2365) 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)
39:E:279:TYR:CE1	39:E:279:TYR:CZ	1.75	1.69
39:E:279:TYR:CZ	39:E:279:TYR:CE2	1.75	1.69
39:E:279:TYR:CD1	39:E:279:TYR:CG	1.75	1.69
39:E:279:TYR:CG	39:E:279:TYR:CD2	1.74	1.68
7:n:326:TYR:CD2	37:V:77:VAL:HG21	1.27	1.67
51:A:253:THR:HG21	51:A:381:ALA:CB	1.24	1.56
1:f:837:ILE:CD1	46:C:9:ASP:HB2	1.31	1.55
1:f:259:PHE:CA	1:f:259:PHE:C	1.81	1.53
1:f:306:ARG:N	1:f:306:ARG:CA	1.69	1.53
51:A:253:THR:CG2	51:A:381:ALA:HB3	1.03	1.50
11:m:73:GLN:NE2	11:m:80:LYS:HE2	1.20	1.50
51:A:253:THR:CG2	51:A:381:ALA:CB	1.80	1.49
46:C:53:ARG:C	46:C:54:ASN:N	1.67	1.49
18:U:98:MET:HE1	51:A:371:LYS:CA	1.40	1.48
1:f:1221:LEU:C	1:f:1222:PRO:N	1.71	1.47
1:f:1254:ALA:C	1:f:1255:GLN:N	1.68	1.46
1:f:837:ILE:HD12	46:C:9:ASP:CB	1.45	1.46
5:s:306:ILE:CG2	5:s:393:PRO:HB2	1.45	1.46
1:f:1149:TYR:C	1:f:1150:VAL:N	1.72	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:88:ILE:CD1	28:5:90:ILE:HD11	1.46	1.44
28:5:393:LYS:HZ3	46:C:21:ASP:CB	1.31	1.42
28:5:178:LEU:CD1	28:5:396:ASP:OD1	1.65	1.42
18:U:98:MET:CE	51:A:371:LYS:HA	1.48	1.40
1:f:243:TYR:OH	1:f:323:LYS:CA	1.68	1.39
51:A:152:VAL:HG13	51:A:293:THR:CG2	1.50	1.39
28:5:219:ASP:CG	28:5:225:ASN:HD21	1.31	1.38
7:n:125:LYS:HZ1	40:Y:364:GLN:NE2	1.21	1.37
47:8:75:ARG:HA	47:8:76:ASN:CB	1.37	1.37
51:A:6:PRO:CA	51:A:6:PRO:N	1.70	1.36
1:f:297:THR:CG2	1:f:303:ASN:HB3	1.54	1.36
48:W:81:ASP:OD2	48:W:84:ARG:NH2	1.56	1.35
16:S:45:THR:HG22	16:S:58:ASN:CB	1.57	1.34
16:S:45:THR:CG2	16:S:58:ASN:HB3	1.55	1.34
28:5:197:ASN:ND2	55:5:502:GNP:N7	1.70	1.34
51:A:152:VAL:CG1	51:A:293:THR:HG21	1.55	1.34
46:C:233:LEU:N	46:C:234:PRO:O	1.61	1.33
1:f:1632:HIS:CE1	1:f:1641:ARG:HE	1.44	1.33
16:S:45:THR:CG2	16:S:58:ASN:CB	2.07	1.33
5:s:305:THR:HB	5:s:358:LYS:CB	1.58	1.32
46:C:431:HIS:O	46:C:435:LEU:CD2	1.75	1.32
28:5:271:ASN:OD1	28:5:281:LEU:HB3	1.29	1.32
7:n:125:LYS:NZ	40:Y:364:GLN:HE22	1.23	1.32
28:5:79:LYS:HZ1	28:5:357:GLN:CD	1.34	1.32
28:5:271:ASN:OD1	28:5:281:LEU:CB	1.78	1.31
47:8:30:LEU:CD1	47:8:52:ALA:HB2	1.61	1.30
7:n:118:ASN:ND2	40:Y:265:ARG:NH1	1.79	1.30
5:s:331:ARG:CD	5:s:344:SER:OG	1.78	1.29
7:n:326:TYR:CD2	37:V:77:VAL:CG2	2.14	1.29
38:w:71:ARG:HA	38:w:74:TRP:CZ3	1.66	1.29
1:f:832:TYR:CG	46:C:11:ASP:HB3	1.66	1.29
7:n:142:LEU:CD1	40:Y:332:ILE:O	1.80	1.29
1:f:1266:PRO:O	1:f:1401:GLU:HA	1.15	1.28
5:s:298:THR:HA	5:s:299:VAL:CG2	1.64	1.28
5:s:306:ILE:HD13	5:s:369:MET:SD	1.72	1.28
5:s:331:ARG:HB3	5:s:342:PRO:CG	1.63	1.27
28:5:219:ASP:OD2	28:5:225:ASN:ND2	1.68	1.27
5:s:331:ARG:CB	5:s:342:PRO:HG3	1.64	1.26
51:A:150:PRO:CG	51:A:311:LEU:HD12	1.64	1.25
1:f:297:THR:HG21	1:f:303:ASN:CB	1.67	1.25
5:s:149:SER:HB2	5:s:164:ILE:O	1.14	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:1068:ASN:CB	1:f:1122:GLN:HE22	1.49	1.25
47:8:73:TRP:O	47:8:76:ASN:HB2	1.30	1.25
51:A:151:LEU:CD2	51:A:294:ARG:HE	1.48	1.25
1:f:1108:ALA:HB2	1:f:1113:ASP:OD1	1.13	1.24
1:f:762:GLU:CG	1:f:782:VAL:HG22	1.65	1.24
37:V:53:ARG:NH2	46:C:37:GLU:HG3	1.48	1.24
38:w:34:GLN:O	38:w:35:GLU:HG2	1.26	1.24
47:8:6:LYS:N	48:W:77:GLN:NE2	1.85	1.23
7:n:118:ASN:HD21	40:Y:265:ARG:NH1	1.34	1.23
1:f:302:ALA:C	1:f:303:ASN:OD1	1.80	1.23
2:1:75:A:N6	28:5:282:ARG:NH2	1.86	1.23
5:s:306:ILE:CG2	5:s:394:TYR:CD1	2.21	1.23
1:f:1397:LEU:O	1:f:1401:GLU:HG3	1.39	1.22
3:0:1440:U:N3	46:C:387:ILE:HG22	1.55	1.21
28:5:393:LYS:NZ	46:C:21:ASP:CB	1.99	1.21
28:5:219:ASP:CG	28:5:225:ASN:ND2	1.94	1.21
1:f:1624:ALA:O	1:f:1629:ILE:O	1.59	1.21
1:f:1595:ILE:HD11	1:f:1628:GLY:N	1.54	1.21
1:f:1109:LEU:HD12	1:f:1130:THR:OG1	1.41	1.21
1:f:766:LYS:HB3	1:f:778:THR:OG1	1.36	1.20
36:c:8:LEU:CD2	38:w:86:ARG:NE	2.03	1.20
47:8:6:LYS:N	48:W:77:GLN:HE21	1.35	1.20
51:A:253:THR:HG23	51:A:381:ALA:CB	1.71	1.20
1:f:1397:LEU:O	1:f:1401:GLU:CG	1.88	1.20
1:f:137:CYS:O	1:f:302:ALA:HB1	1.39	1.19
1:f:807:MET:HE1	1:f:855:ASP:OD1	1.40	1.19
7:n:249:GLU:OE1	7:n:280:LYS:NZ	1.73	1.19
7:n:326:TYR:CE2	37:V:77:VAL:CG2	2.25	1.19
1:f:739:ARG:HA	1:f:742:ASN:ND2	1.56	1.19
1:f:739:ARG:CA	1:f:742:ASN:HD21	1.56	1.19
38:w:71:ARG:CB	38:w:74:TRP:HH2	1.55	1.19
1:f:832:TYR:CD1	46:C:11:ASP:HB3	1.76	1.19
5:s:331:ARG:CG	5:s:342:PRO:HG3	1.72	1.19
51:A:152:VAL:CG1	51:A:293:THR:CG2	2.16	1.19
28:5:147:VAL:CG1	37:V:17:VAL:HG22	1.72	1.19
46:C:234:PRO:HG3	51:A:44:TRP:NE1	1.57	1.19
1:f:832:TYR:HB3	46:C:11:ASP:HB2	1.20	1.19
1:f:295:ASN:OD1	1:f:303:ASN:ND2	1.73	1.18
38:w:71:ARG:CA	38:w:74:TRP:CZ3	2.26	1.18
39:E:245:THR:OG1	51:A:7:GLU:OE1	1.62	1.18
1:f:1109:LEU:HD23	1:f:1110:GLY:N	1.55	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:s:306:ILE:CD1	5:s:369:MET:SD	2.31	1.18
5:s:331:ARG:CB	5:s:342:PRO:CG	2.19	1.18
28:5:219:ASP:CB	28:5:225:ASN:ND2	2.06	1.18
46:C:431:HIS:O	46:C:435:LEU:HD23	1.30	1.18
11:m:73:GLN:HE22	11:m:80:LYS:CE	1.57	1.17
7:n:326:TYR:CE2	37:V:77:VAL:HG21	1.79	1.17
28:5:182:LYS:NZ	28:5:389:VAL:HG11	1.60	1.17
16:S:76:THR:CG2	51:A:41:PRO:HB3	1.74	1.17
28:5:182:LYS:HZ1	28:5:389:VAL:HG11	1.04	1.17
37:V:89:LYS:HG3	37:V:103:LEU:CD2	1.74	1.17
1:f:1624:ALA:O	1:f:1629:ILE:HG22	1.41	1.16
47:8:30:LEU:CD1	47:8:52:ALA:CB	2.22	1.16
5:s:332:ARG:HA	5:s:334:LYS:N	1.59	1.16
7:n:118:ASN:CG	40:Y:265:ARG:HH12	1.52	1.16
48:W:71:ALA:HB1	48:W:77:GLN:O	1.45	1.16
28:5:351:ASP:OD2	28:5:352:PRO:HD2	1.45	1.15
3:0:937:C:O2'	20:X:43:MET:HE1	1.47	1.15
11:m:80:LYS:O	11:m:81:ILE:HG13	1.46	1.15
28:5:85:VAL:CG1	37:V:21:LEU:HD21	1.76	1.15
28:5:88:ILE:HD12	28:5:90:ILE:CD1	1.76	1.15
46:C:234:PRO:CG	51:A:44:TRP:NE1	2.07	1.15
1:f:1397:LEU:O	1:f:1401:GLU:CD	1.88	1.15
28:5:61:VAL:HG23	55:5:502:GNP:O3G	1.47	1.14
47:8:6:LYS:N	48:W:77:GLN:CG	2.07	1.14
5:s:347:ILE:O	28:5:272:LYS:CE	1.94	1.14
8:p:279:GLN:HE22	51:A:410:ASN:HA	1.10	1.14
11:m:73:GLN:NE2	11:m:80:LYS:CE	2.09	1.14
5:s:331:ARG:HG2	5:s:342:PRO:HB3	1.24	1.14
37:V:89:LYS:CG	37:V:103:LEU:HD21	1.77	1.14
47:8:75:ARG:HA	47:8:76:ASN:HB2	1.28	1.14
1:f:832:TYR:CG	46:C:11:ASP:CB	2.29	1.13
28:5:88:ILE:HD12	28:5:90:ILE:CG1	1.79	1.13
5:s:298:THR:HA	5:s:299:VAL:HG22	1.24	1.13
48:W:40:VAL:CG2	48:W:75:LYS:HE3	1.77	1.13
48:W:162:LEU:HD22	48:W:207:VAL:HG13	1.31	1.13
51:A:151:LEU:O	51:A:338:VAL:CG2	1.97	1.13
16:S:66:ARG:HD2	46:C:194:LYS:HZ3	1.01	1.13
46:C:329:GLN:HB2	46:C:331:ARG:HD3	1.18	1.13
47:8:30:LEU:HD11	47:8:52:ALA:HB2	1.31	1.12
47:8:40:TRP:CH2	47:8:87:GLY:HA3	1.83	1.13
1:f:259:PHE:C	1:f:259:PHE:CG	2.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:45:THR:HG22	16:S:58:ASN:HB2	1.13	1.12
16:S:63:LYS:HD2	46:C:192:LYS:HG3	1.28	1.12
1:f:243:TYR:OH	1:f:323:LYS:HA	1.26	1.12
38:w:71:ARG:CB	38:w:74:TRP:CH2	2.32	1.12
39:E:198:THR:OG1	51:A:6:PRO:HG3	1.47	1.12
48:W:43:PHE:CG	48:W:73:LEU:CD1	2.31	1.12
1:f:1071:VAL:HG11	1:f:1147:ILE:HG12	1.28	1.12
5:s:331:ARG:HD2	5:s:344:SER:OG	1.44	1.12
16:S:45:THR:HG21	16:S:58:ASN:H	1.08	1.11
37:V:52:ARG:CZ	46:C:39:THR:OG1	1.97	1.11
1:f:1494:THR:OG1	1:f:1672:SER:HB2	1.48	1.11
5:s:306:ILE:CB	5:s:393:PRO:CB	2.28	1.11
1:f:837:ILE:HD11	46:C:9:ASP:HB2	1.24	1.11
51:A:152:VAL:HG13	51:A:293:THR:HG22	1.14	1.11
1:f:187:MET:HB2	1:f:193:ARG:HH21	0.97	1.10
1:f:151:ILE:HG12	1:f:261:LEU:HB3	1.27	1.10
1:f:1259:CYS:CB	1:f:1260:TYR:HA	1.79	1.10
1:f:187:MET:HB2	1:f:193:ARG:NH2	1.65	1.09
5:s:306:ILE:HG22	5:s:394:TYR:CD1	1.86	1.09
28:5:400:LYS:HD2	46:C:20:HIS:N	1.67	1.09
1:f:837:ILE:CD1	46:C:9:ASP:CB	2.12	1.09
28:5:219:ASP:HB2	28:5:225:ASN:ND2	1.64	1.09
20:X:38:LYS:HB3	20:X:39:LYS:HA	1.20	1.09
1:f:906:GLU:OE1	28:5:204:GLU:HG3	1.53	1.09
47:8:75:ARG:CA	47:8:76:ASN:CB	2.28	1.09
1:f:1632:HIS:CE1	1:f:1641:ARG:NE	2.19	1.08
7:n:142:LEU:HD11	40:Y:332:ILE:O	1.47	1.08
51:A:149:ARG:NE	51:A:295:TYR:O	1.85	1.08
51:A:427:ASP:OD1	51:A:428:PRO:HD2	1.50	1.08
28:5:88:ILE:CD1	28:5:90:ILE:CD1	2.29	1.08
51:A:12:ALA:HB1	51:A:13:PRO:CD	1.82	1.08
16:S:45:THR:HG23	16:S:58:ASN:HB3	1.29	1.08
37:V:50:ASN:HD21	37:V:52:ARG:HD3	1.06	1.08
37:V:52:ARG:NH2	37:V:53:ARG:HD3	1.67	1.08
3:0:1209:U:C4	3:0:1209:U:C6	2.41	1.08
38:w:71:ARG:C	38:w:74:TRP:HZ3	1.59	1.08
5:s:318:ASP:O	5:s:383:ARG:O	1.69	1.08
5:s:331:ARG:HB3	5:s:342:PRO:HG2	1.17	1.08
46:C:204:GLN:HA	46:C:207:LYS:HE2	1.35	1.08
47:8:40:TRP:HH2	47:8:87:GLY:HA3	0.91	1.08
1:f:261:LEU:HG	1:f:295:ASN:ND2	1.66	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:W:43:PHE:CD1	48:W:73:LEU:HD11	1.89	1.07
1:f:832:TYR:HB3	46:C:11:ASP:CB	1.84	1.07
1:f:1068:ASN:CA	1:f:1122:GLN:HE22	1.64	1.07
5:s:306:ILE:HG21	5:s:393:PRO:CB	1.83	1.07
28:5:178:LEU:HD12	28:5:396:ASP:OD1	0.91	1.07
28:5:351:ASP:CG	28:5:352:PRO:HD2	1.78	1.07
1:f:297:THR:O	1:f:299:ALA:HB2	1.52	1.07
5:s:305:THR:HB	5:s:358:LYS:CA	1.84	1.07
38:w:71:ARG:HB2	38:w:74:TRP:HH2	1.01	1.07
51:A:149:ARG:CD	51:A:295:TYR:O	2.03	1.07
1:f:261:LEU:HG	1:f:295:ASN:HD22	0.93	1.06
5:s:331:ARG:O	5:s:333:PHE:CB	2.03	1.06
8:p:279:GLN:HE22	51:A:410:ASN:CA	1.68	1.06
28:5:61:VAL:CG2	55:5:502:GNP:O3G	2.03	1.06
1:f:1044:VAL:CG1	1:f:1220:LEU:HD12	1.85	1.06
37:V:89:LYS:HG3	37:V:103:LEU:HD21	1.11	1.06
48:W:75:LYS:HB3	48:W:76:THR:HG22	1.07	1.06
47:8:62:ILE:HG23	47:8:64:VAL:H	1.16	1.06
47:8:73:TRP:O	47:8:76:ASN:CB	2.02	1.06
3:0:1440:U:H3	46:C:387:ILE:HG22	0.92	1.06
1:f:1108:ALA:CB	1:f:1113:ASP:OD1	2.03	1.06
5:s:306:ILE:HG12	5:s:369:MET:HE1	1.36	1.06
28:5:179:GLU:OE1	28:5:461:ARG:NH1	1.89	1.06
28:5:393:LYS:NZ	46:C:21:ASP:HB3	1.64	1.06
1:f:306:ARG:N	1:f:306:ARG:HA	1.71	1.05
28:5:79:LYS:NZ	28:5:357:GLN:CD	2.13	1.05
51:A:294:ARG:NH1	51:A:307:THR:HB	1.71	1.05
51:A:295:TYR:OH	51:A:341:ASP:OD1	1.74	1.05
1:f:129:TYR:O	1:f:132:ALA:HB3	1.55	1.05
1:f:1109:LEU:HD23	1:f:1110:GLY:H	0.92	1.05
5:s:356:ARG:HG2	5:s:357:ALA:H	1.19	1.05
47:8:62:ILE:HG21	47:8:64:VAL:HG22	1.36	1.05
38:w:34:GLN:O	38:w:35:GLU:CG	2.04	1.05
47:8:30:LEU:HD13	47:8:52:ALA:HB2	1.34	1.05
51:A:150:PRO:CD	51:A:311:LEU:HD12	1.86	1.05
5:s:331:ARG:CG	5:s:342:PRO:CG	2.34	1.05
5:s:347:ILE:O	28:5:272:LYS:NZ	1.87	1.05
38:w:71:ARG:HB2	38:w:74:TRP:CH2	1.89	1.05
27:h:72:GLU:O	27:h:74:LYS:N	1.90	1.05
51:A:150:PRO:HG3	51:A:311:LEU:HD12	1.09	1.05
1:f:762:GLU:HG3	1:f:782:VAL:HG22	1.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:326:TYR:HD2	37:V:77:VAL:CG2	1.61	1.04
1:f:243:TYR:OH	1:f:323:LYS:N	1.90	1.04
7:n:333:ARG:O	7:n:335:LYS:N	1.90	1.04
47:8:77:LYS:HB2	47:8:78:LEU:HA	1.37	1.04
1:f:243:TYR:OH	1:f:322:ASP:C	1.99	1.04
5:s:306:ILE:CG2	5:s:393:PRO:CB	2.35	1.04
37:V:52:ARG:NH2	46:C:39:THR:OG1	1.91	1.04
38:w:131:SER:HA	38:w:132:ASP:HB3	1.39	1.04
39:E:279:TYR:CE2	46:C:411:ARG:CD	2.41	1.04
46:C:51:LEU:HD13	46:C:56:LYS:HG2	1.07	1.04
51:A:302:ASN:HD22	51:A:306:ASP:HA	0.91	1.04
36:c:8:LEU:HD23	38:w:86:ARG:HE	1.23	1.03
1:f:1044:VAL:HG12	1:f:1220:LEU:HD12	1.06	1.03
5:s:166:TYR:HD1	5:s:167:THR:HG23	1.21	1.03
5:s:166:TYR:CD1	5:s:167:THR:HG23	1.92	1.03
51:A:151:LEU:O	51:A:338:VAL:HG22	1.58	1.03
51:A:152:VAL:HG11	51:A:293:THR:HG21	1.33	1.03
16:S:54:GLU:OE2	46:C:192:LYS:NZ	1.90	1.03
46:C:233:LEU:N	46:C:234:PRO:C	2.16	1.03
1:f:768:PHE:CB	1:f:773:THR:OG1	2.07	1.03
5:s:356:ARG:O	5:s:357:ALA:HB2	1.59	1.03
3:0:1361:C:OP1	46:C:53:ARG:HG3	1.57	1.03
39:E:279:TYR:CD2	46:C:411:ARG:CD	2.42	1.03
47:8:30:LEU:HD11	47:8:52:ALA:CB	1.84	1.03
1:f:240:PHE:O	1:f:240:PHE:HD1	1.40	1.02
5:s:306:ILE:HB	5:s:393:PRO:CB	1.85	1.02
39:E:279:TYR:CZ	46:C:411:ARG:CD	2.42	1.02
39:E:279:TYR:CD1	46:C:411:ARG:CD	2.42	1.02
46:C:51:LEU:CD1	46:C:56:LYS:HG2	1.87	1.02
51:A:12:ALA:HB1	51:A:13:PRO:HD3	1.40	1.02
16:S:54:GLU:OE2	46:C:192:LYS:CE	2.06	1.02
47:8:30:LEU:HD13	47:8:52:ALA:CB	1.86	1.02
7:n:282:LEU:HD23	7:n:286:VAL:CG2	1.88	1.02
46:C:329:GLN:HG3	46:C:330:GLN:H	1.25	1.02
1:f:807:MET:CE	1:f:855:ASP:OD1	2.07	1.02
51:A:302:ASN:ND2	51:A:306:ASP:HA	1.74	1.02
1:f:1259:CYS:HB3	1:f:1260:TYR:CA	1.89	1.02
47:8:78:LEU:HD21	51:A:106:THR:HA	1.40	1.02
5:s:315:PHE:O	5:s:316:GLN:HB2	1.59	1.01
47:8:8:ARG:NH2	48:W:75:LYS:HB3	1.74	1.01
1:f:261:LEU:CG	1:f:295:ASN:HD22	1.73	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:s:149:SER:CB	5:s:164:ILE:O	2.08	1.01
5:s:298:THR:CA	5:s:299:VAL:HG22	1.90	1.01
28:5:456:VAL:HG21	28:5:461:ARG:HG3	1.39	1.01
47:8:75:ARG:CA	47:8:76:ASN:HB3	1.89	1.01
3:0:228:G:H21	26:J:160:SER:CB	1.73	1.01
5:s:306:ILE:CB	5:s:393:PRO:HB3	1.89	1.01
16:S:66:ARG:HD2	46:C:194:LYS:NZ	1.75	1.01
39:E:279:TYR:CE1	46:C:411:ARG:CD	2.43	1.01
5:s:306:ILE:CB	5:s:393:PRO:HB2	1.89	1.01
47:8:62:ILE:HG21	47:8:64:VAL:CG2	1.91	1.01
28:5:79:LYS:HZ1	28:5:357:GLN:NE2	1.58	1.00
36:c:8:LEU:HD21	38:w:86:ARG:NE	1.74	1.00
1:f:243:TYR:OH	1:f:322:ASP:O	1.76	1.00
5:s:332:ARG:HA	5:s:334:LYS:H	1.11	1.00
1:f:5:TYR:OH	1:f:92:GLU:HB3	1.62	1.00
28:5:61:VAL:CB	55:5:502:GNP:O3G	2.09	1.00
39:E:279:TYR:CG	46:C:411:ARG:CD	2.44	1.00
51:A:377:TYR:CD2	51:A:435:LEU:CD1	2.44	1.00
2:1:75:A:H61	28:5:282:ARG:NH2	1.47	1.00
28:5:65:LYS:HB2	55:5:502:GNP:O2B	1.62	1.00
1:f:1032:LEU:HD13	1:f:1220:LEU:HD11	1.40	0.99
28:5:88:ILE:HD11	28:5:90:ILE:HD11	1.42	0.99
38:w:71:ARG:HA	38:w:74:TRP:CH2	1.96	0.99
1:f:1254:ALA:C	1:f:1255:GLN:CA	2.34	0.99
1:f:1595:ILE:HD11	1:f:1628:GLY:H	1.20	0.99
5:s:331:ARG:HG3	5:s:342:PRO:HG3	1.40	0.99
28:5:85:VAL:HG11	37:V:21:LEU:CD2	1.91	0.99
28:5:383:PHE:CE1	40:Y:240:LEU:CD2	2.46	0.99
3:0:1478:U:O4	46:C:232:ARG:CZ	2.11	0.99
28:5:390:GLY:HA3	28:5:461:ARG:HH11	1.26	0.99
47:8:8:ARG:HH12	48:W:76:THR:HB	1.25	0.99
48:W:75:LYS:CB	48:W:76:THR:HG22	1.91	0.99
1:f:832:TYR:CB	46:C:11:ASP:HB2	1.92	0.99
47:8:75:ARG:HA	47:8:76:ASN:HB3	1.04	0.99
5:s:306:ILE:HB	5:s:393:PRO:HB3	1.39	0.99
36:c:8:LEU:HD21	38:w:86:ARG:CD	1.92	0.99
37:V:58:PHE:O	37:V:62:TRP:NE1	1.95	0.98
40:Y:331:PHE:HE2	40:Y:337:LYS:HD3	1.26	0.98
28:5:88:ILE:HD12	28:5:90:ILE:HD11	1.30	0.98
28:5:400:LYS:HZ3	28:5:401:ARG:NH1	1.61	0.98
51:A:377:TYR:CD2	51:A:435:LEU:HD13	1.99	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:824:G:OP2	26:J:115:LYS:NZ	1.96	0.98
20:X:40:HIS:H	20:X:41:VAL:HG12	1.26	0.98
51:A:150:PRO:HG3	51:A:311:LEU:CD1	1.93	0.98
47:8:6:LYS:N	48:W:77:GLN:CD	2.20	0.98
1:f:234:GLY:C	1:f:235:LEU:O	1.96	0.98
1:f:1267:LEU:CD2	1:f:1719:MET:SD	2.51	0.98
28:5:281:LEU:H	28:5:281:LEU:HD22	1.26	0.98
46:C:51:LEU:HD13	46:C:56:LYS:CG	1.94	0.98
7:n:283:ASP:OD1	7:n:287:LYS:NZ	1.96	0.98
28:5:85:VAL:HG11	37:V:21:LEU:HD21	1.00	0.98
47:8:42:PRO:HB2	47:8:44:TYR:N	1.78	0.98
47:8:77:LYS:HD3	51:A:96:HIS:HD2	1.29	0.98
3:0:1478:U:O4	46:C:232:ARG:NH2	1.97	0.98
28:5:400:LYS:HD2	46:C:20:HIS:H	0.84	0.97
5:s:298:THR:HA	5:s:299:VAL:HG23	1.45	0.97
38:w:71:ARG:CA	38:w:74:TRP:CH2	2.47	0.97
1:f:1266:PRO:O	1:f:1401:GLU:CA	2.12	0.97
51:A:301:LYS:H	51:A:301:LYS:HZ3	1.08	0.97
1:f:902:ARG:HH21	1:f:956:HIS:CE1	1.82	0.97
47:8:62:ILE:HG23	47:8:64:VAL:N	1.77	0.97
1:f:259:PHE:C	1:f:259:PHE:CB	2.37	0.97
1:f:297:THR:HG22	1:f:298:ASP:C	1.89	0.97
28:5:383:PHE:CE1	40:Y:240:LEU:HD23	1.99	0.97
1:f:1032:LEU:HD13	1:f:1220:LEU:CD1	1.95	0.97
47:8:40:TRP:HH2	47:8:87:GLY:CA	1.76	0.97
1:f:3:SER:OG	27:h:70:ASP:OD1	1.83	0.97
28:5:201:LEU:HD12	55:5:502:GNP:N2	1.79	0.97
47:8:30:LEU:HA	47:8:33:LEU:HD23	1.47	0.97
3:0:1478:U:O4	46:C:232:ARG:NH1	1.98	0.96
11:m:51:VAL:O	11:m:52:LEU:HD12	1.63	0.96
37:V:66:GLY:O	37:V:67:THR:HG23	1.63	0.96
46:C:234:PRO:CG	51:A:44:TRP:HE1	1.74	0.96
1:f:785:LYS:CD	1:f:889:LEU:HD21	1.95	0.96
1:f:834:PHE:CD1	46:C:5:PHE:CZ	2.53	0.96
39:E:279:TYR:CE1	46:C:411:ARG:NE	2.33	0.96
1:f:261:LEU:CG	1:f:295:ASN:ND2	2.29	0.96
1:f:1068:ASN:CB	1:f:1122:GLN:NE2	2.27	0.96
46:C:329:GLN:HB2	46:C:331:ARG:CD	1.95	0.96
1:f:837:ILE:HD12	46:C:9:ASP:HB3	1.47	0.96
40:Y:337:LYS:O	40:Y:337:LYS:HD2	1.66	0.96
37:V:24:GLN:O	37:V:102:ASN:OD1	1.83	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:223:GLY:CA	40:Y:229:ARG:HH22	1.79	0.95
39:E:279:TYR:CD2	46:C:411:ARG:NE	2.34	0.95
8:p:279:GLN:NE2	51:A:410:ASN:C	2.25	0.95
36:c:8:LEU:HD11	38:w:88:PHE:CE2	2.00	0.95
48:W:75:LYS:HE2	48:W:75:LYS:HA	1.46	0.95
39:E:279:TYR:CG	46:C:411:ARG:NE	2.34	0.95
1:f:832:TYR:CB	46:C:11:ASP:CB	2.42	0.95
1:f:1071:VAL:O	1:f:1148:ASP:O	1.83	0.95
16:S:63:LYS:HE3	46:C:192:LYS:HD2	1.46	0.95
28:5:400:LYS:NZ	28:5:401:ARG:NH1	2.14	0.95
51:A:48:MET:HE3	51:A:48:MET:C	1.91	0.95
47:8:8:ARG:NH1	48:W:75:LYS:HD3	1.82	0.95
7:n:125:LYS:CD	40:Y:321:GLU:OE1	2.15	0.95
1:f:1044:VAL:HG12	1:f:1220:LEU:CD1	1.97	0.95
5:s:331:ARG:O	5:s:333:PHE:HB2	1.63	0.95
48:W:40:VAL:HG21	48:W:75:LYS:HE3	1.46	0.95
1:f:792:LEU:O	1:f:792:LEU:HD23	1.65	0.95
37:V:18:GLN:O	37:V:22:GLU:OE2	1.84	0.94
39:E:279:TYR:CD1	46:C:411:ARG:NE	2.34	0.94
5:s:305:THR:HB	5:s:358:LYS:HB2	1.50	0.94
28:5:178:LEU:HD12	28:5:396:ASP:CG	1.92	0.94
28:5:273:PRO:HB3	28:5:275:GLU:HG3	1.44	0.94
28:5:275:GLU:OE2	28:5:276:VAL:N	2.00	0.94
28:5:393:LYS:HZ3	46:C:21:ASP:HB3	0.79	0.94
39:E:279:TYR:CZ	46:C:411:ARG:NE	2.35	0.94
46:C:31:ILE:CG2	46:C:35:TRP:HB2	1.98	0.94
1:f:1203:LYS:HB2	1:f:1215:ASP:OD1	1.67	0.94
7:n:266:TYR:HE2	7:n:268:ILE:HD11	1.33	0.94
46:C:234:PRO:HG3	51:A:44:TRP:CD1	2.03	0.94
28:5:219:ASP:CB	28:5:225:ASN:HD21	1.75	0.94
39:E:279:TYR:CE2	46:C:411:ARG:NE	2.35	0.94
1:f:1071:VAL:CG1	1:f:1147:ILE:HG12	1.98	0.94
3:0:1476:U:C4	46:C:232:ARG:NH2	2.36	0.94
28:5:65:LYS:HE3	28:5:144:GLY:N	1.82	0.94
28:5:281:LEU:HD23	28:5:282:ARG:H	1.33	0.94
47:8:49:ASP:OD2	47:8:74:ASN:ND2	2.00	0.94
51:A:151:LEU:HD21	51:A:294:ARG:HE	1.32	0.94
1:f:769:ASP:HB3	1:f:770:PRO:CD	1.96	0.94
16:S:76:THR:HG21	51:A:41:PRO:HB3	1.49	0.94
37:V:53:ARG:NH2	46:C:37:GLU:CG	2.31	0.94
46:C:232:ARG:C	46:C:234:PRO:HA	1.92	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:151:LEU:CD2	51:A:294:ARG:NE	2.30	0.94
28:5:412:GLN:O	28:5:413:ILE:HG13	1.67	0.93
46:C:191:GLN:NE2	46:C:192:LYS:N	2.14	0.93
5:s:304:ALA:O	5:s:305:THR:HG22	1.68	0.93
28:5:61:VAL:HG23	55:5:502:GNP:PG	2.08	0.93
51:A:148:ASN:ND2	51:A:303:PRO:CD	2.31	0.93
1:f:240:PHE:HD1	1:f:240:PHE:C	1.75	0.93
1:f:243:TYR:HH	1:f:322:ASP:C	1.75	0.93
1:f:297:THR:HG23	1:f:298:ASP:HB3	1.48	0.93
3:0:230:G:H5'	26:J:157:PHE:CZ	2.03	0.93
40:Y:331:PHE:CE2	40:Y:337:LYS:HD3	2.04	0.93
5:s:306:ILE:HD11	5:s:369:MET:CE	1.99	0.93
5:s:356:ARG:CG	5:s:357:ALA:H	1.82	0.93
7:n:125:LYS:CE	40:Y:321:GLU:OE1	2.17	0.93
7:n:206:GLU:O	7:n:208:ASN:N	2.00	0.93
38:w:71:ARG:C	38:w:74:TRP:CZ3	2.47	0.93
46:C:233:LEU:N	46:C:234:PRO:CA	2.32	0.93
48:W:76:THR:CB	48:W:77:GLN:HB2	1.99	0.93
3:0:1701:G:H21	6:j:94:LYS:HE3	1.32	0.93
1:f:1630:GLY:O	1:f:1656:ILE:HG13	1.69	0.92
7:n:266:TYR:CE2	7:n:268:ILE:HD11	2.03	0.92
28:5:391:ARG:HH12	46:C:25:GLU:HG2	1.32	0.92
2:1:75:A:N6	28:5:282:ARG:HH22	1.67	0.92
20:X:38:LYS:CB	20:X:39:LYS:HA	1.93	0.92
1:f:768:PHE:HB3	1:f:773:THR:OG1	1.69	0.92
5:s:149:SER:CB	5:s:165:PRO:HA	1.98	0.92
1:f:834:PHE:CE1	46:C:5:PHE:CZ	2.58	0.92
1:f:1259:CYS:HB3	1:f:1260:TYR:HA	0.93	0.92
2:1:75:A:C2	28:5:285:VAL:CG1	2.53	0.92
5:s:305:THR:HB	5:s:358:LYS:HA	1.51	0.92
47:8:40:TRP:HE1	47:8:83:HIS:HB2	1.35	0.92
20:X:38:LYS:HB3	20:X:39:LYS:CA	1.98	0.92
2:1:75:A:C8	28:5:329:LYS:HD3	2.05	0.92
1:f:786:LEU:HD23	1:f:786:LEU:O	1.70	0.92
37:V:58:PHE:O	37:V:62:TRP:CD1	2.23	0.92
46:C:51:LEU:HD12	46:C:56:LYS:HD3	1.51	0.92
1:f:302:ALA:CA	1:f:303:ASN:OD1	2.18	0.91
5:s:149:SER:HB3	5:s:165:PRO:HA	1.51	0.91
18:U:51:LEU:HD21	18:U:98:MET:HE2	1.51	0.91
37:V:25:LYS:HA	37:V:102:ASN:HB3	1.50	0.91
51:A:219:ARG:NH2	51:A:437:ILE:HG23	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:c:8:LEU:HD23	38:w:86:ARG:NE	1.75	0.91
16:S:45:THR:HG21	16:S:58:ASN:N	1.85	0.91
28:5:219:ASP:HB2	28:5:225:ASN:HD22	1.29	0.91
5:s:306:ILE:CG1	5:s:369:MET:HE1	2.00	0.91
37:V:50:ASN:OD1	37:V:52:ARG:HG2	1.71	0.91
47:8:62:ILE:CG2	47:8:64:VAL:CG2	2.48	0.91
8:p:279:GLN:NE2	51:A:410:ASN:HA	1.86	0.91
39:E:198:THR:OG1	51:A:6:PRO:CG	2.19	0.91
7:n:326:TYR:CE2	37:V:77:VAL:HG22	2.06	0.90
37:V:50:ASN:HD21	37:V:52:ARG:CD	1.82	0.90
37:V:50:ASN:CG	37:V:52:ARG:HG2	1.95	0.90
5:s:306:ILE:CD1	5:s:369:MET:CE	2.49	0.90
28:5:413:ILE:HD11	28:5:436:LEU:HD13	1.52	0.90
18:U:71:ARG:HH11	18:U:71:ARG:HG3	1.36	0.90
28:5:79:LYS:NZ	28:5:357:GLN:NE2	2.18	0.90
47:8:6:LYS:N	48:W:77:GLN:HG2	1.84	0.90
1:f:235:LEU:O	1:f:236:SER:OG	1.89	0.90
5:s:306:ILE:HG22	5:s:394:TYR:HD1	1.30	0.90
7:n:209:ARG:HG3	7:n:209:ARG:HH11	1.36	0.90
1:f:909:ARG:NH1	1:f:991:LYS:HE3	1.86	0.90
5:s:331:ARG:HG2	5:s:342:PRO:CB	2.00	0.90
28:5:383:PHE:CZ	40:Y:240:LEU:HD21	2.05	0.90
28:5:65:LYS:HE3	28:5:144:GLY:CA	2.01	0.90
37:V:50:ASN:ND2	37:V:52:ARG:HD3	1.86	0.90
3:0:1440:U:N3	46:C:387:ILE:CG2	2.35	0.90
3:0:1861:G:O2'	51:A:296:GLN:O	1.90	0.90
5:s:331:ARG:NE	5:s:344:SER:OG	2.03	0.90
1:f:1195:LEU:HD23	1:f:1217:GLU:OE2	1.70	0.90
5:s:307:HIS:HB3	5:s:355:LEU:O	1.71	0.90
48:W:75:LYS:HD3	48:W:76:THR:HB	1.53	0.90
1:f:837:ILE:HD12	46:C:9:ASP:HB2	0.96	0.89
1:f:1109:LEU:CD2	1:f:1110:GLY:N	2.35	0.89
7:n:206:GLU:C	7:n:208:ASN:H	1.79	0.89
1:f:1624:ALA:O	1:f:1629:ILE:CG2	2.19	0.89
3:0:1478:U:C4	46:C:232:ARG:NH1	2.41	0.89
36:c:8:LEU:HD11	38:w:88:PHE:HE2	1.37	0.89
51:A:12:ALA:CB	51:A:13:PRO:CD	2.47	0.89
5:s:343:ILE:O	5:s:356:ARG:HB3	1.72	0.89
1:f:1108:ALA:HB1	1:f:1114:TYR:O	1.71	0.89
51:A:253:THR:HG23	51:A:381:ALA:HB2	1.51	0.89
1:f:240:PHE:C	1:f:240:PHE:CD1	2.47	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:1149:TYR:HD2	1:f:1177:PRO:HG2	1.37	0.89
5:s:306:ILE:CG1	5:s:393:PRO:HB3	2.03	0.89
18:U:98:MET:HE1	51:A:371:LYS:CB	2.01	0.89
28:5:197:ASN:O	55:5:502:GNP:O6	1.91	0.89
37:V:89:LYS:CD	37:V:103:LEU:HD21	2.03	0.89
46:C:232:ARG:C	46:C:234:PRO:C	2.40	0.89
7:n:125:LYS:HD2	40:Y:321:GLU:OE1	1.71	0.89
46:C:204:GLN:HA	46:C:207:LYS:CE	2.03	0.89
1:f:785:LYS:HD3	1:f:889:LEU:HD21	1.55	0.89
1:f:909:ARG:HH12	1:f:991:LYS:CE	1.86	0.89
5:s:297:HIS:O	5:s:299:VAL:HG22	1.72	0.89
5:s:331:ARG:CG	5:s:342:PRO:HB3	2.01	0.89
5:s:305:THR:HB	5:s:358:LYS:HB3	1.52	0.88
47:8:77:LYS:HD3	51:A:96:HIS:CD2	2.08	0.88
1:f:832:TYR:CZ	46:C:12:GLU:O	2.26	0.88
1:f:297:THR:CB	1:f:303:ASN:HB3	2.03	0.88
46:C:234:PRO:CB	51:A:44:TRP:CD1	2.56	0.88
48:W:188:THR:O	48:W:192:ARG:HG3	1.72	0.88
7:n:267:GLU:HG3	37:V:32:GLN:HE22	1.39	0.88
16:S:45:THR:CG2	16:S:58:ASN:HB2	1.90	0.88
1:f:1068:ASN:HA	1:f:1122:GLN:HE22	1.36	0.88
1:f:909:ARG:HH12	1:f:991:LYS:HE3	1.36	0.88
46:C:191:GLN:HE21	46:C:192:LYS:H	1.20	0.88
46:C:329:GLN:CB	46:C:331:ARG:HD3	2.02	0.88
51:A:148:ASN:ND2	51:A:303:PRO:HD2	1.86	0.88
5:s:306:ILE:HG21	5:s:393:PRO:HB2	0.88	0.88
5:s:331:ARG:CG	5:s:344:SER:OG	2.21	0.88
5:s:331:ARG:CG	5:s:342:PRO:CB	2.51	0.88
1:f:832:TYR:CD1	46:C:11:ASP:CB	2.55	0.88
1:f:1553:LEU:HD12	3:0:2176:C:N3	1.89	0.88
7:n:118:ASN:ND2	40:Y:265:ARG:HH12	1.49	0.88
16:S:54:GLU:OE2	46:C:192:LYS:HE3	1.71	0.87
51:A:253:THR:CG2	51:A:381:ALA:CA	2.52	0.87
37:V:95:GLU:O	37:V:97:MET:N	2.08	0.87
47:8:81:SER:HB2	47:8:83:HIS:CD2	2.09	0.87
5:s:318:ASP:HB3	5:s:383:ARG:O	1.73	0.87
37:V:99:THR:O	37:V:101:GLN:HG2	1.74	0.87
46:C:191:GLN:HE21	46:C:192:LYS:N	1.71	0.87
47:8:6:LYS:NZ	47:8:36:HIS:HB2	1.89	0.87
1:f:240:PHE:O	1:f:240:PHE:CD1	2.27	0.87
47:8:80:GLY:O	51:A:109:PRO:HA	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:1267:LEU:HD22	1:f:1719:MET:SD	2.14	0.87
1:f:261:LEU:CD1	1:f:295:ASN:ND2	2.37	0.87
2:1:75:A:H2	28:5:285:VAL:CG1	1.87	0.87
3:0:368:G:O3'	46:C:127:ARG:HD3	1.75	0.87
1:f:743:ARG:NE	1:f:743:ARG:HA	1.89	0.87
37:V:53:ARG:CZ	46:C:37:GLU:HG3	2.03	0.87
37:V:53:ARG:HH21	46:C:37:GLU:HG3	1.36	0.87
7:n:213:PRO:CD	38:w:135:PHE:CE1	2.57	0.87
51:A:258:ARG:O	51:A:271:ILE:HG23	1.74	0.87
5:s:305:THR:CB	5:s:358:LYS:CB	2.51	0.87
7:n:213:PRO:HD3	38:w:135:PHE:HE1	1.38	0.87
7:n:282:LEU:HD23	7:n:286:VAL:HG22	1.57	0.87
46:C:28:VAL:CG1	46:C:29:ALA:HA	2.04	0.86
3:0:1476:U:C5	46:C:232:ARG:CZ	2.58	0.86
11:m:73:GLN:HE21	11:m:80:LYS:HE2	1.39	0.86
48:W:69:ASN:OD1	48:W:82:ALA:O	1.94	0.86
1:f:292:ARG:NH1	1:f:308:ARG:NH2	2.23	0.86
5:s:356:ARG:HG2	5:s:357:ALA:N	1.89	0.86
18:U:51:LEU:HD23	18:U:98:MET:HG3	1.56	0.86
5:s:304:ALA:O	5:s:305:THR:CG2	2.23	0.86
28:5:458:LYS:HE3	28:5:458:LYS:HA	1.57	0.86
36:c:8:LEU:HD21	38:w:86:ARG:HD3	1.56	0.86
7:n:125:LYS:NZ	40:Y:364:GLN:NE2	1.94	0.86
28:5:457:GLU:HG2	46:C:25:GLU:OE1	1.76	0.86
5:s:305:THR:CA	5:s:358:LYS:HA	2.06	0.86
1:f:1595:ILE:CD1	1:f:1628:GLY:N	2.38	0.86
51:A:294:ARG:HH12	51:A:307:THR:HB	1.38	0.86
48:W:76:THR:OG1	48:W:77:GLN:HB2	1.75	0.86
3:0:368:G:O3'	46:C:127:ARG:CD	2.22	0.85
48:W:162:LEU:CD2	48:W:207:VAL:HG13	2.05	0.85
7:n:282:LEU:CD2	7:n:286:VAL:HG21	2.05	0.85
7:n:326:TYR:HE2	37:V:77:VAL:CG2	1.84	0.85
28:5:65:LYS:HE3	28:5:144:GLY:HA3	1.57	0.85
28:5:400:LYS:CD	46:C:20:HIS:H	1.80	0.85
16:S:56:GLN:NE2	46:C:191:GLN:OE1	2.09	0.85
5:s:306:ILE:HD11	5:s:369:MET:SD	2.15	0.85
5:s:332:ARG:HA	5:s:333:PHE:C	1.97	0.85
1:f:762:GLU:HG3	1:f:782:VAL:CG2	2.06	0.85
5:s:331:ARG:NH1	5:s:344:SER:HB3	1.91	0.85
47:8:42:PRO:HB2	47:8:43:MET:C	2.01	0.85
1:f:292:ARG:HD3	1:f:308:ARG:NH1	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:66:ARG:CD	46:C:194:LYS:HZ3	1.87	0.85
47:8:62:ILE:CG2	47:8:64:VAL:H	1.90	0.85
8:p:279:GLN:NE2	51:A:410:ASN:CA	2.39	0.84
1:f:837:ILE:HD11	46:C:10:SER:HB2	1.59	0.84
5:s:331:ARG:NH1	5:s:355:LEU:HD22	1.91	0.84
16:S:63:LYS:HD2	46:C:192:LYS:CG	2.06	0.84
28:5:271:ASN:HD22	28:5:274:GLY:H	1.25	0.84
48:W:74:ASN:OD1	48:W:75:LYS:N	2.11	0.84
5:s:306:ILE:CG2	5:s:394:TYR:CE1	2.60	0.84
1:f:297:THR:HG22	1:f:298:ASP:O	1.78	0.84
1:f:762:GLU:HG2	1:f:782:VAL:HG22	1.57	0.84
46:C:229:GLU:OE1	46:C:229:GLU:N	2.11	0.84
5:s:167:THR:HG21	13:o:120:VAL:O	1.77	0.84
7:n:282:LEU:CD2	7:n:286:VAL:CG2	2.56	0.84
28:5:223:GLY:HA2	40:Y:229:ARG:HH22	1.41	0.84
1:f:906:GLU:CD	28:5:204:GLU:HG3	2.02	0.84
1:f:1632:HIS:NE2	1:f:1641:ARG:NH2	2.24	0.84
7:n:282:LEU:HD23	7:n:286:VAL:HG21	1.59	0.84
28:5:220:SER:HA	40:Y:273:ARG:HH21	1.40	0.84
28:5:393:LYS:NZ	46:C:21:ASP:HB2	1.91	0.84
47:8:62:ILE:CG2	47:8:64:VAL:N	2.39	0.84
28:5:88:ILE:HD12	28:5:90:ILE:HG13	1.58	0.84
39:E:279:TYR:CE2	46:C:411:ARG:HD2	2.13	0.84
46:C:2:SER:HA	46:C:3:ASN:O	1.77	0.84
1:f:762:GLU:CG	1:f:782:VAL:CG2	2.54	0.83
1:f:1254:ALA:CA	1:f:1255:GLN:N	2.39	0.83
28:5:400:LYS:NZ	28:5:401:ARG:HH12	1.75	0.83
51:A:301:LYS:HZ3	51:A:301:LYS:N	1.75	0.83
5:s:148:THR:O	5:s:148:THR:HG23	1.78	0.83
5:s:331:ARG:O	5:s:333:PHE:HB3	1.75	0.83
5:s:347:ILE:HD12	28:5:271:ASN:HB2	1.60	0.83
5:s:343:ILE:O	5:s:356:ARG:NE	2.10	0.83
13:o:170:SER:O	13:o:176:ILE:CD1	2.25	0.83
28:5:351:ASP:OD2	28:5:352:PRO:CD	2.24	0.83
39:E:279:TYR:CG	46:C:411:ARG:HD3	2.13	0.83
48:W:43:PHE:CG	48:W:73:LEU:HD13	2.12	0.83
51:A:253:THR:HG21	51:A:381:ALA:CA	2.08	0.83
5:s:194:ILE:HG22	5:s:201:ILE:HG23	1.59	0.83
5:s:347:ILE:CD1	28:5:271:ASN:HB2	2.07	0.83
5:s:306:ILE:CG2	5:s:394:TYR:HD1	1.81	0.83
46:C:232:ARG:C	46:C:234:PRO:O	2.22	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:148:ASN:ND2	51:A:303:PRO:CG	2.41	0.83
5:s:305:THR:CB	5:s:358:LYS:HA	2.08	0.83
28:5:393:LYS:HZ2	46:C:21:ASP:CG	1.87	0.83
1:f:1068:ASN:CA	1:f:1122:GLN:NE2	2.42	0.83
2:1:25:G:H4'	7:n:255:ASN:HD21	1.42	0.83
2:1:71:U:H2'	2:1:72:A:H5''	1.61	0.83
2:1:75:A:H2	28:5:285:VAL:HG12	1.42	0.83
5:s:300:ARG:HH22	5:s:362:ARG:HH11	1.23	0.83
5:s:315:PHE:HE2	28:5:351:ASP:HB3	1.40	0.83
47:8:39:GLN:O	47:8:45:ILE:HD13	1.79	0.83
48:W:43:PHE:CD1	48:W:73:LEU:CD1	2.60	0.83
18:U:51:LEU:CD2	18:U:98:MET:HE2	2.07	0.83
47:8:62:ILE:CG2	47:8:64:VAL:HG23	2.07	0.83
1:f:138:ASP:OD2	1:f:139:MET:HG2	1.78	0.83
1:f:1549:ARG:HH11	1:f:1549:ARG:HG3	1.44	0.83
7:n:336:ALA:HA	7:n:339:GLN:HE21	1.41	0.83
28:5:455:LEU:CD2	28:5:459:ASN:H	1.92	0.83
7:n:213:PRO:HD2	38:w:135:PHE:CE1	2.14	0.82
16:S:76:THR:HG23	51:A:41:PRO:HB3	1.58	0.82
46:C:329:GLN:CB	46:C:331:ARG:CD	2.56	0.82
1:f:136:LEU:HG	1:f:136:LEU:O	1.77	0.82
1:f:1479:ILE:O	1:f:1483:LEU:HD13	1.79	0.82
5:s:315:PHE:HD2	28:5:351:ASP:OD1	1.62	0.82
1:f:304:PRO:HB2	1:f:305:TYR:CD2	2.13	0.82
13:o:170:SER:O	13:o:176:ILE:HD12	1.79	0.82
51:A:150:PRO:HD3	51:A:311:LEU:CD1	2.10	0.82
51:A:150:PRO:HD3	51:A:311:LEU:HD12	1.61	0.82
1:f:902:ARG:HH21	1:f:956:HIS:HE1	1.26	0.82
3:0:230:G:C5'	26:J:157:PHE:CZ	2.62	0.82
5:s:306:ILE:HG12	5:s:393:PRO:HB3	1.59	0.82
7:n:213:PRO:HD3	38:w:135:PHE:CE1	2.15	0.82
28:5:178:LEU:HD11	28:5:396:ASP:OD1	1.79	0.82
1:f:1535:ILE:HG23	1:f:1581:GLU:HG2	1.61	0.82
16:S:61:ALA:O	16:S:62:THR:HG23	1.79	0.82
47:8:42:PRO:N	47:8:43:MET:HA	1.93	0.82
5:s:305:THR:HA	5:s:358:LYS:HA	1.59	0.82
28:5:61:VAL:HB	55:5:502:GNP:O3G	1.77	0.82
37:V:52:ARG:HH22	37:V:53:ARG:HH11	1.24	0.82
1:f:1068:ASN:HA	1:f:1122:GLN:NE2	1.93	0.82
1:f:1496:VAL:HB	1:f:1657:PHE:CD1	2.15	0.82
1:f:1556:LYS:HG3	1:f:1557:ARG:HG3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Y:230:ARG:H	40:Y:230:ARG:HD3	1.45	0.81
1:f:766:LYS:HB3	1:f:778:THR:HG1	1.46	0.81
5:s:315:PHE:HE1	28:5:321:LEU:HD11	1.45	0.81
11:m:73:GLN:HE22	11:m:80:LYS:HE2	1.00	0.81
16:S:57:CYS:HB2	16:S:64:LEU:HD21	1.59	0.81
38:w:34:GLN:NE2	38:w:35:GLU:HB3	1.96	0.81
5:s:150:ALA:O	5:s:163:ILE:HG23	1.79	0.81
5:s:319:GLY:HA3	28:5:351:ASP:OD2	1.79	0.81
6:j:133:GLN:NE2	6:j:138:LYS:HG2	1.95	0.81
13:o:21:GLU:HA	51:A:434:GLN:HE22	1.46	0.81
28:5:172:PHE:HB3	28:5:173:PRO:HD3	1.60	0.81
1:f:755:ALA:HB1	1:f:789:TRP:CZ2	2.16	0.81
48:W:43:PHE:HB3	48:W:73:LEU:HD12	1.60	0.81
5:s:356:ARG:O	5:s:357:ALA:CB	2.25	0.81
1:f:303:ASN:CB	1:f:304:PRO:HD2	2.10	0.81
7:n:118:ASN:HD21	40:Y:265:ARG:HH11	1.23	0.81
28:5:454:ARG:O	28:5:460:PHE:HA	1.80	0.81
1:f:1483:LEU:HD21	1:f:1657:PHE:CZ	2.16	0.81
1:f:1541:ALA:HB1	1:f:1545:ARG:HH12	1.46	0.81
7:n:335:LYS:O	7:n:339:GLN:HG2	1.81	0.81
18:U:83:ARG:HH21	18:U:83:ARG:HG3	1.44	0.81
28:5:383:PHE:HE1	40:Y:240:LEU:HD23	1.46	0.81
1:f:307:LEU:HG	1:f:308:ARG:N	1.96	0.81
3:0:228:G:N2	26:J:160:SER:CB	2.43	0.81
47:8:30:LEU:CD1	47:8:52:ALA:HB1	2.11	0.81
51:A:150:PRO:CD	51:A:311:LEU:CD1	2.59	0.81
1:f:1237:TYR:CE1	1:f:1261:ILE:CG2	2.64	0.80
38:w:164:LEU:O	38:w:167:PHE:HB2	1.80	0.80
28:5:271:ASN:OD1	28:5:281:LEU:CA	2.29	0.80
3:0:228:G:N2	26:J:160:SER:OG	2.14	0.80
28:5:186:ILE:HD12	28:5:465:TRP:HB3	1.64	0.80
48:W:43:PHE:CB	48:W:73:LEU:HD12	2.10	0.80
1:f:1108:ALA:CB	1:f:1114:TYR:O	2.28	0.80
1:f:1263:ASP:N	1:f:1263:ASP:OD1	2.07	0.80
48:W:76:THR:H	48:W:77:GLN:C	1.88	0.80
5:s:331:ARG:CZ	5:s:344:SER:HB3	2.12	0.80
28:5:393:LYS:NZ	46:C:21:ASP:CG	2.40	0.80
38:w:75:ILE:HD13	38:w:96:VAL:HG11	1.61	0.80
27:h:72:GLU:O	27:h:73:TYR:C	2.25	0.80
28:5:455:LEU:HD21	28:5:458:LYS:N	1.97	0.80
46:C:31:ILE:HB	46:C:36:PHE:HE2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:294:ALA:O	1:f:295:ASN:HB2	1.79	0.80
7:n:206:GLU:HG3	38:w:133:TYR:CG	2.17	0.80
51:A:253:THR:CB	51:A:381:ALA:HB3	2.09	0.80
2:1:75:A:C2	28:5:285:VAL:HG11	2.16	0.80
3:0:230:G:H5'	26:J:157:PHE:CE1	2.17	0.80
28:5:455:LEU:HD21	28:5:459:ASN:H	1.47	0.80
40:Y:284:ASP:OD2	40:Y:288:ASP:OD1	2.00	0.80
1:f:150:PHE:CD1	1:f:196:VAL:HB	2.16	0.80
1:f:774:LEU:HD12	1:f:774:LEU:O	1.80	0.80
1:f:793:VAL:HG23	1:f:797:GLN:HE21	1.44	0.80
1:f:1237:TYR:HB2	1:f:1262:ARG:O	1.82	0.79
3:0:1701:G:N2	6:j:94:LYS:HE3	1.97	0.79
3:0:1861:G:H21	51:A:296:GLN:CD	1.90	0.79
5:s:331:ARG:CA	5:s:342:PRO:HG3	2.11	0.79
28:5:147:VAL:HG11	37:V:17:VAL:HG22	1.63	0.79
47:8:30:LEU:O	47:8:33:LEU:HG	1.81	0.79
1:f:1149:TYR:CD2	1:f:1177:PRO:HG2	2.18	0.79
1:f:1629:ILE:O	1:f:1629:ILE:CG2	2.30	0.79
2:1:75:A:H62	28:5:282:ARG:NH2	1.76	0.79
1:f:1032:LEU:CD1	1:f:1220:LEU:HD11	2.12	0.79
18:U:98:MET:CE	51:A:371:LYS:CA	2.30	0.79
46:C:51:LEU:CD1	46:C:56:LYS:CG	2.58	0.79
1:f:150:PHE:CD2	1:f:198:PHE:CZ	2.70	0.79
1:f:785:LYS:HD2	1:f:889:LEU:HD21	1.64	0.79
28:5:456:VAL:C	28:5:457:GLU:HG3	2.06	0.79
1:f:297:THR:HG21	1:f:303:ASN:HB3	0.81	0.79
5:s:356:ARG:CG	5:s:357:ALA:N	2.43	0.79
11:m:80:LYS:O	11:m:81:ILE:CG1	2.28	0.79
28:5:412:GLN:O	28:5:413:ILE:CG1	2.27	0.79
1:f:1535:ILE:HG23	1:f:1581:GLU:CG	2.12	0.79
5:s:331:ARG:CZ	5:s:344:SER:CB	2.60	0.79
28:5:390:GLY:HA3	28:5:461:ARG:NH1	1.97	0.79
7:n:266:TYR:HE2	7:n:268:ILE:CD1	1.95	0.79
47:8:78:LEU:CD2	51:A:106:THR:HA	2.11	0.79
48:W:76:THR:HG23	48:W:77:GLN:CB	2.13	0.79
36:c:8:LEU:CD2	38:w:86:ARG:CZ	2.61	0.79
46:C:329:GLN:HG3	46:C:330:GLN:N	1.97	0.79
5:s:169:ILE:O	5:s:170:THR:HG23	1.83	0.79
5:s:300:ARG:NH2	5:s:362:ARG:HH11	1.80	0.79
5:s:315:PHE:CE1	28:5:321:LEU:HD11	2.18	0.78
7:n:142:LEU:HD12	40:Y:332:ILE:O	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:33:SER:CB	20:X:34:HIS:HA	2.12	0.78
5:s:331:ARG:HH11	5:s:355:LEU:HD22	1.47	0.78
16:S:38:CYS:SG	16:S:64:LEU:CD2	2.71	0.78
46:C:53:ARG:C	46:C:54:ASN:CA	2.56	0.78
47:8:8:ARG:HH12	48:W:75:LYS:HD3	1.48	0.78
47:8:80:GLY:O	51:A:109:PRO:CA	2.31	0.78
5:s:306:ILE:HG23	5:s:394:TYR:CD1	2.17	0.78
28:5:223:GLY:CA	40:Y:229:ARG:NH2	2.46	0.78
51:A:257:LEU:HD12	51:A:257:LEU:H	1.49	0.78
46:C:2:SER:N	46:C:3:ASN:HB2	1.99	0.78
47:8:77:LYS:CB	47:8:78:LEU:HA	2.06	0.78
51:A:292:LYS:H	51:A:292:LYS:CD	1.96	0.78
1:f:739:ARG:HA	1:f:742:ASN:HD21	0.70	0.78
46:C:232:ARG:C	46:C:234:PRO:CA	2.55	0.78
1:f:902:ARG:HD3	28:5:205:VAL:HG13	1.64	0.78
7:n:326:TYR:HE2	37:V:77:VAL:HG22	1.46	0.78
51:A:28:MET:N	51:A:28:MET:SD	2.57	0.78
5:s:298:THR:CA	5:s:299:VAL:CG2	2.54	0.78
7:n:209:ARG:HB3	38:w:136:VAL:HG11	1.63	0.78
11:m:53:GLU:OE2	11:m:55:ILE:HD11	1.83	0.78
28:5:65:LYS:CE	28:5:144:GLY:HA3	2.14	0.78
7:n:212:GLU:HA	38:w:135:PHE:CD1	2.18	0.77
7:n:287:LYS:NZ	38:w:133:TYR:OH	2.17	0.77
51:A:377:TYR:CD2	51:A:435:LEU:HD12	2.18	0.77
16:S:78:CYS:O	51:A:39:ILE:HD11	1.84	0.77
1:f:187:MET:CB	1:f:193:ARG:NH2	2.47	0.77
1:f:1525:THR:O	1:f:1529:ALA:HB2	1.84	0.77
28:5:65:LYS:HD2	55:5:502:GNP:O2G	1.84	0.77
5:s:148:THR:O	5:s:149:SER:OG	2.00	0.77
28:5:271:ASN:OD1	28:5:281:LEU:HB2	1.83	0.77
1:f:1556:LYS:HA	1:f:1557:ARG:CG	2.13	0.77
3:0:282:C:H4'	26:J:183:ASN:ND2	2.00	0.77
46:C:2:SER:HA	46:C:3:ASN:C	2.09	0.77
46:C:431:HIS:C	46:C:435:LEU:HD23	2.09	0.77
5:s:306:ILE:O	5:s:357:ALA:HB3	1.83	0.77
7:n:326:TYR:CE2	37:V:77:VAL:CG1	2.67	0.77
13:o:177:LYS:HA	13:o:177:LYS:CE	2.14	0.77
47:8:40:TRP:HZ2	47:8:83:HIS:O	1.66	0.77
37:V:53:ARG:CZ	46:C:37:GLU:CG	2.63	0.77
48:W:75:LYS:HE2	48:W:75:LYS:CA	2.15	0.77
1:f:151:ILE:HD11	1:f:261:LEU:HD13	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:302:ALA:HA	1:f:303:ASN:OD1	1.84	0.77
46:C:34:LYS:H	46:C:34:LYS:HD2	1.49	0.77
47:8:39:GLN:O	47:8:45:ILE:CD1	2.33	0.77
1:f:243:TYR:HB2	1:f:244:TYR:O	1.85	0.77
1:f:307:LEU:CD1	1:f:308:ARG:HG2	2.14	0.77
1:f:1254:ALA:C	1:f:1255:GLN:HA	2.10	0.77
46:C:234:PRO:HB3	51:A:44:TRP:CD1	2.20	0.77
38:w:71:ARG:CA	38:w:74:TRP:HZ3	1.82	0.76
51:A:378:ARG:HD3	51:A:379:ARG:HG3	1.67	0.76
3:0:1476:U:O4	46:C:232:ARG:NH2	2.18	0.76
5:s:306:ILE:HG22	5:s:394:TYR:HA	1.65	0.76
48:W:71:ALA:CB	48:W:77:GLN:O	2.30	0.76
51:A:252:GLU:OE1	51:A:382:GLN:HB3	1.85	0.76
18:U:45:ASP:OD1	18:U:45:ASP:N	2.17	0.76
5:s:169:ILE:HG23	5:s:205:LYS:HE2	1.67	0.76
47:8:8:ARG:NH1	48:W:75:LYS:CD	2.49	0.76
47:8:62:ILE:CG2	47:8:64:VAL:HG22	2.12	0.76
48:W:78:GLY:O	48:W:81:ASP:HB2	1.85	0.76
51:A:7:GLU:OE2	51:A:7:GLU:HA	1.85	0.76
47:8:42:PRO:CD	47:8:43:MET:HA	2.15	0.76
48:W:43:PHE:CD2	48:W:73:LEU:HD13	2.21	0.76
1:f:1491:MET:SD	1:f:1671:ARG:NH1	2.59	0.76
7:n:125:LYS:HE2	40:Y:321:GLU:OE1	1.83	0.76
27:h:72:GLU:O	27:h:75:LYS:N	2.19	0.76
28:5:182:LYS:CE	28:5:389:VAL:HG11	2.16	0.76
47:8:42:PRO:CB	47:8:45:ILE:H	1.99	0.76
47:8:73:TRP:C	47:8:76:ASN:HB2	2.11	0.76
46:C:52:SER:O	46:C:56:LYS:HE2	1.86	0.76
28:5:88:ILE:HD13	28:5:90:ILE:HD11	1.66	0.75
1:f:129:TYR:O	1:f:132:ALA:CB	2.33	0.75
28:5:186:ILE:HD12	28:5:465:TRP:CB	2.15	0.75
51:A:146:LEU:HB2	51:A:300:GLU:HG3	1.68	0.75
46:C:28:VAL:HG13	46:C:29:ALA:HA	1.68	0.75
1:f:259:PHE:CD1	1:f:260:ILE:N	2.55	0.75
13:o:177:LYS:HA	13:o:177:LYS:HE3	1.66	0.75
1:f:1549:ARG:HG3	1:f:1549:ARG:NH1	2.00	0.75
7:n:131:GLU:OE2	7:n:135:ARG:CZ	2.35	0.75
1:f:1068:ASN:HB2	1:f:1122:GLN:NE2	2.02	0.75
28:5:273:PRO:CB	28:5:275:GLU:HG3	2.17	0.75
46:C:204:GLN:O	46:C:207:LYS:HG2	1.87	0.75
16:S:61:ALA:O	16:S:62:THR:CG2	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:186:ILE:CD1	28:5:465:TRP:HB3	2.17	0.75
51:A:150:PRO:HD3	51:A:311:LEU:CG	2.16	0.75
1:f:1630:GLY:C	1:f:1656:ILE:HG13	2.09	0.75
47:8:75:ARG:CA	47:8:76:ASN:HB2	2.07	0.75
1:f:137:CYS:O	1:f:302:ALA:CB	2.30	0.75
1:f:739:ARG:HD3	1:f:742:ASN:OD1	1.87	0.75
46:C:234:PRO:HG2	51:A:44:TRP:HE1	1.51	0.75
28:5:147:VAL:HG12	37:V:17:VAL:HG22	1.66	0.74
37:V:52:ARG:NH2	46:C:39:THR:HG1	1.82	0.74
51:A:151:LEU:HD22	51:A:294:ARG:HE	1.45	0.74
1:f:1266:PRO:C	1:f:1401:GLU:HA	2.09	0.74
11:m:96:GLU:C	11:m:97:ASN:HD22	1.94	0.74
51:A:371:LYS:NZ	51:A:371:LYS:HB3	2.03	0.74
27:h:69:GLU:HG2	27:h:70:ASP:N	2.03	0.74
38:w:131:SER:CA	38:w:132:ASP:HB3	2.15	0.74
46:C:9:ASP:HA	46:C:10:SER:CB	2.17	0.74
47:8:78:LEU:HD21	51:A:106:THR:CA	2.16	0.74
51:A:294:ARG:NH1	51:A:307:THR:CB	2.50	0.74
1:f:1267:LEU:HD23	1:f:1719:MET:SD	2.27	0.74
5:s:306:ILE:CD1	5:s:369:MET:HE1	2.18	0.74
7:n:255:ASN:O	7:n:262:LEU:HD12	1.88	0.74
51:A:375:ASP:OD1	51:A:378:ARG:NE	2.20	0.74
1:f:184:LEU:HD13	1:f:235:LEU:HG	1.68	0.74
1:f:1109:LEU:HD12	1:f:1130:THR:HG1	1.50	0.74
1:f:1629:ILE:O	1:f:1629:ILE:HG23	1.87	0.74
1:f:1397:LEU:CD1	1:f:1401:GLU:OE2	2.35	0.74
28:5:271:ASN:HD22	28:5:274:GLY:N	1.84	0.74
51:A:292:LYS:NZ	51:A:292:LYS:HB3	2.02	0.74
47:8:8:ARG:CZ	48:W:75:LYS:HD3	2.18	0.74
47:8:35:GLU:OE2	47:8:39:GLN:HA	1.87	0.74
1:f:768:PHE:HB2	1:f:773:THR:OG1	1.87	0.73
1:f:1195:LEU:HD23	1:f:1217:GLU:CD	2.11	0.73
1:f:1483:LEU:HD21	1:f:1657:PHE:HZ	1.50	0.73
5:s:347:ILE:O	28:5:272:LYS:HE3	1.86	0.73
37:V:49:LEU:CD2	46:C:31:ILE:HG21	2.18	0.73
47:8:77:LYS:HB2	47:8:78:LEU:CA	2.18	0.73
46:C:204:GLN:CA	46:C:207:LYS:HE2	2.16	0.73
51:A:12:ALA:CB	51:A:13:PRO:HD2	2.16	0.73
1:f:295:ASN:CG	1:f:303:ASN:HD22	1.97	0.73
11:m:40:PRO:HB3	11:m:81:ILE:CD1	2.18	0.73
1:f:187:MET:CB	1:f:193:ARG:HH21	1.91	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:s:306:ILE:HG12	5:s:393:PRO:CB	2.18	0.73
7:n:135:ARG:HH21	40:Y:332:ILE:HG12	1.51	0.73
1:f:1075:LEU:HD21	1:f:1128:PRO:HD3	1.71	0.73
51:A:292:LYS:HE2	51:A:292:LYS:N	2.02	0.73
1:f:1068:ASN:HB3	1:f:1122:GLN:HE22	1.52	0.73
5:s:300:ARG:HH22	5:s:362:ARG:NH1	1.86	0.73
40:Y:331:PHE:HE2	40:Y:337:LYS:CD	2.00	0.73
51:A:294:ARG:CZ	51:A:307:THR:HB	2.18	0.73
46:C:56:LYS:O	46:C:60:GLU:OE1	2.05	0.73
5:s:195:ASP:CG	13:o:184:ARG:HH12	1.97	0.73
46:C:234:PRO:CG	51:A:44:TRP:CD1	2.63	0.73
2:1:73:C:OP1	28:5:268:PHE:CE2	2.42	0.73
5:s:320:VAL:HG23	5:s:321:ASN:N	2.03	0.73
46:C:51:LEU:HD12	46:C:56:LYS:CD	2.19	0.73
51:A:427:ASP:OD1	51:A:428:PRO:CD	2.34	0.73
1:f:5:TYR:CE2	6:j:94:LYS:HG3	2.24	0.73
2:1:73:C:OP1	28:5:268:PHE:HE2	1.71	0.73
18:U:98:MET:CE	51:A:371:LYS:CB	2.65	0.73
40:Y:227:VAL:HG13	40:Y:229:ARG:HD3	1.69	0.73
47:8:8:ARG:HH21	47:8:8:ARG:HB3	1.54	0.73
47:8:33:LEU:HD12	47:8:33:LEU:C	2.14	0.73
5:s:331:ARG:NH2	28:5:279:GLU:OE2	2.22	0.72
28:5:182:LYS:HZ1	28:5:389:VAL:CG1	1.94	0.72
28:5:307:GLN:HE21	28:5:321:LEU:HD11	1.52	0.72
1:f:1108:ALA:HB2	1:f:1113:ASP:CG	2.12	0.72
1:f:1238:ILE:HD11	1:f:1264:LEU:HD12	1.69	0.72
11:m:40:PRO:HB3	11:m:81:ILE:HD11	1.70	0.72
13:o:51:ARG:NH2	51:A:367:SER:O	2.20	0.72
18:U:98:MET:HE1	51:A:371:LYS:HA	0.75	0.72
28:5:456:VAL:CG2	28:5:461:ARG:HG3	2.19	0.72
1:f:834:PHE:CD1	46:C:5:PHE:HZ	2.03	0.72
46:C:9:ASP:HA	46:C:10:SER:HB2	1.70	0.72
46:C:234:PRO:CB	51:A:44:TRP:NE1	2.51	0.72
48:W:162:LEU:HD13	48:W:207:VAL:CG1	2.18	0.72
46:C:490:LYS:HD2	51:A:29:LYS:NZ	2.03	0.72
1:f:1218:VAL:HG12	1:f:1219:HIS:H	1.53	0.72
1:f:297:THR:CG2	1:f:298:ASP:HB3	2.19	0.72
1:f:1174:LEU:O	1:f:1176:CYS:N	2.21	0.72
1:f:1267:LEU:O	1:f:1401:GLU:HB3	1.89	0.72
7:n:142:LEU:HD11	40:Y:332:ILE:C	2.14	0.72
28:5:223:GLY:HA2	40:Y:229:ARG:NH2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:223:GLY:C	40:Y:229:ARG:HH22	1.92	0.72
48:W:73:LEU:HD21	48:W:88:PHE:CE2	2.25	0.72
3:0:1478:U:C4	46:C:232:ARG:NH2	2.53	0.72
28:5:79:LYS:NZ	28:5:357:GLN:OE1	2.13	0.72
47:8:39:GLN:C	47:8:45:ILE:CD1	2.62	0.72
1:f:5:TYR:OH	6:j:94:LYS:HD3	1.90	0.72
1:f:1151:ILE:HG23	1:f:1179:VAL:O	1.90	0.72
5:s:304:ALA:C	5:s:305:THR:CG2	2.61	0.72
47:8:38:VAL:O	47:8:45:ILE:HD11	1.89	0.72
51:A:151:LEU:O	51:A:338:VAL:HG23	1.88	0.72
5:s:331:ARG:C	5:s:333:PHE:HB3	2.14	0.71
13:o:22:ILE:HG12	51:A:434:GLN:OE1	1.90	0.71
48:W:40:VAL:HG21	48:W:75:LYS:CE	2.20	0.71
1:f:259:PHE:C	1:f:259:PHE:CD1	2.67	0.71
37:V:94:ASP:OD1	37:V:95:GLU:HG2	1.90	0.71
47:8:24:LYS:HD2	47:8:24:LYS:N	2.05	0.71
47:8:81:SER:HB2	47:8:83:HIS:HD2	1.55	0.71
51:A:48:MET:HE3	51:A:48:MET:O	1.90	0.71
7:n:209:ARG:HG3	7:n:209:ARG:NH1	1.98	0.71
38:w:34:GLN:C	38:w:35:GLU:HG2	2.12	0.71
46:C:31:ILE:HG23	46:C:35:TRP:CD1	2.25	0.71
28:5:85:VAL:CG1	37:V:21:LEU:CD2	2.61	0.71
37:V:96:ASN:O	46:C:31:ILE:HD11	1.90	0.71
38:w:135:PHE:O	38:w:136:VAL:HG12	1.90	0.71
5:s:167:THR:CG2	13:o:120:VAL:O	2.39	0.71
46:C:31:ILE:HG23	46:C:35:TRP:HD1	1.55	0.71
1:f:1556:LYS:HA	1:f:1557:ARG:HG3	1.73	0.71
5:s:306:ILE:HG23	5:s:394:TYR:CE1	2.24	0.71
7:n:202:SER:O	7:n:207:ARG:HB2	1.91	0.71
7:n:268:ILE:HG22	7:n:269:GLN:O	1.88	0.71
47:8:6:LYS:N	48:W:77:GLN:HG3	2.01	0.71
28:5:244:GLU:O	28:5:248:HIS:CD2	2.44	0.71
1:f:149:PHE:HZ	1:f:261:LEU:HD13	1.55	0.71
3:0:1701:G:N2	6:j:94:LYS:CE	2.54	0.71
47:8:35:GLU:HG3	47:8:39:GLN:HB3	1.72	0.71
5:s:304:ALA:C	5:s:305:THR:HG23	2.15	0.70
11:m:80:LYS:C	11:m:81:ILE:HG13	2.16	0.70
47:8:39:GLN:O	47:8:76:ASN:ND2	2.22	0.70
51:A:253:THR:CG2	51:A:381:ALA:N	2.54	0.70
51:A:294:ARG:HH12	51:A:307:THR:CB	2.03	0.70
1:f:834:PHE:CD2	46:C:6:ASP:OD1	2.44	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:955:LYS:HE3	1:f:989:GLN:NE2	2.06	0.70
46:C:232:ARG:O	46:C:235:TYR:O	2.09	0.70
51:A:375:ASP:OD1	51:A:378:ARG:HD2	1.90	0.70
51:A:399:LYS:HG2	51:A:425:THR:HG22	1.72	0.70
1:f:755:ALA:CB	1:f:789:TRP:CH2	2.74	0.70
1:f:955:LYS:HE3	1:f:989:GLN:HG3	1.74	0.70
5:s:315:PHE:CE2	28:5:351:ASP:HB3	2.25	0.70
46:C:190:ILE:C	46:C:191:GLN:HG3	2.15	0.70
47:8:42:PRO:HD2	47:8:43:MET:HA	1.73	0.70
1:f:1624:ALA:C	1:f:1629:ILE:O	2.35	0.70
5:s:315:PHE:CZ	28:5:321:LEU:HD21	2.26	0.70
28:5:244:GLU:O	28:5:248:HIS:NE2	2.25	0.70
1:f:1237:TYR:CE1	1:f:1261:ILE:HG21	2.26	0.70
3:0:282:C:H5'	26:J:183:ASN:HB3	1.73	0.70
46:C:232:ARG:CA	46:C:234:PRO:HA	2.21	0.70
1:f:743:ARG:HA	1:f:743:ARG:HE	1.56	0.70
1:f:1542:GLN:HA	1:f:1542:GLN:NE2	2.05	0.70
3:0:816:C:H41	26:J:137:LYS:NZ	1.88	0.70
13:o:18:GLN:NE2	51:A:426:LYS:O	2.24	0.70
18:U:71:ARG:HG3	18:U:71:ARG:NH1	1.98	0.70
1:f:5:TYR:HH	1:f:92:GLU:HB3	1.56	0.70
1:f:1259:CYS:O	1:f:1485:GLU:HG3	1.92	0.70
39:E:240:GLN:O	39:E:244:GLU:HG3	1.92	0.70
47:8:27:VAL:HG21	47:8:62:ILE:HG13	1.74	0.69
8:p:279:GLN:HE22	51:A:410:ASN:C	1.95	0.69
40:Y:337:LYS:O	40:Y:337:LYS:CD	2.39	0.69
47:8:8:ARG:NH2	48:W:75:LYS:CB	2.51	0.69
47:8:36:HIS:HB2	47:8:37:GLY:HA2	1.72	0.69
1:f:257:PRO:C	1:f:258:GLU:HG3	2.17	0.69
13:o:177:LYS:HE3	13:o:177:LYS:CA	2.21	0.69
40:Y:230:ARG:HG3	40:Y:230:ARG:HH21	1.57	0.69
51:A:151:LEU:HA	51:A:293:THR:O	1.90	0.69
46:C:434:ILE:CD1	51:A:28:MET:HE3	2.22	0.69
47:8:8:ARG:HH12	48:W:76:THR:CB	2.01	0.69
51:A:257:LEU:HD12	51:A:257:LEU:N	2.04	0.69
1:f:1494:THR:O	1:f:1655:VAL:HA	1.93	0.69
38:w:131:SER:HA	38:w:132:ASP:CB	2.12	0.69
51:A:219:ARG:HH21	51:A:437:ILE:HG23	1.56	0.69
1:f:292:ARG:HD3	1:f:308:ARG:CZ	2.23	0.69
1:f:789:TRP:HA	1:f:789:TRP:HE3	1.58	0.69
1:f:792:LEU:O	1:f:792:LEU:CD2	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:369:C:OP2	46:C:127:ARG:HD2	1.92	0.69
5:s:331:ARG:HG3	5:s:342:PRO:CG	2.11	0.69
11:m:51:VAL:C	11:m:52:LEU:HD12	2.17	0.69
28:5:172:PHE:CB	28:5:173:PRO:HD3	2.22	0.69
28:5:393:LYS:HZ3	46:C:21:ASP:HB2	1.45	0.69
36:c:8:LEU:HD12	36:c:8:LEU:O	1.93	0.69
38:w:163:PRO:O	38:w:164:LEU:HB2	1.91	0.69
1:f:202:LEU:H	1:f:243:TYR:HD1	1.38	0.69
3:0:1440:U:C4	46:C:387:ILE:CG2	2.76	0.69
46:C:232:ARG:HG3	46:C:233:LEU:HD23	1.75	0.69
48:W:76:THR:HG23	48:W:77:GLN:HB3	1.74	0.69
48:W:84:ARG:HD2	48:W:105:MET:CE	2.23	0.69
1:f:758:ARG:HD3	1:f:789:TRP:CZ2	2.28	0.69
1:f:786:LEU:HD23	1:f:786:LEU:C	2.17	0.69
48:W:43:PHE:CB	48:W:73:LEU:CD1	2.67	0.69
48:W:162:LEU:HD13	48:W:207:VAL:HG11	1.75	0.69
51:A:149:ARG:HD3	51:A:295:TYR:HB3	1.73	0.69
7:n:267:GLU:CG	37:V:32:GLN:HE22	2.06	0.68
37:V:89:LYS:HG3	37:V:103:LEU:HD22	1.73	0.68
47:8:369:PHE:H	47:8:370:GLY:HA2	1.57	0.68
51:A:298:LYS:HD3	51:A:298:LYS:H	1.58	0.68
1:f:286:ASN:HD21	1:f:306:ARG:NH1	1.91	0.68
1:f:1109:LEU:HD23	1:f:1110:GLY:CA	2.22	0.68
7:n:287:LYS:HB3	7:n:287:LYS:HZ3	1.57	0.68
51:A:150:PRO:HD3	51:A:311:LEU:HG	1.75	0.68
5:s:347:ILE:O	28:5:272:LYS:HE2	1.92	0.68
20:X:38:LYS:HD2	20:X:41:VAL:HG11	1.75	0.68
46:C:28:VAL:HA	46:C:29:ALA:O	1.93	0.68
5:s:315:PHE:HZ	28:5:321:LEU:HD21	1.58	0.68
5:s:320:VAL:HG23	5:s:321:ASN:H	1.56	0.68
13:o:170:SER:O	13:o:176:ILE:HD13	1.94	0.68
1:f:1254:ALA:CB	1:f:1255:GLN:N	2.56	0.68
3:0:2303:G:N2	37:V:63:GLY:CA	2.57	0.68
7:n:212:GLU:HA	38:w:135:PHE:CE1	2.29	0.68
47:8:8:ARG:HH21	47:8:8:ARG:CB	2.06	0.68
48:W:75:LYS:HB3	48:W:76:THR:CG2	2.03	0.68
1:f:774:LEU:H	7:n:207:ARG:HH12	1.40	0.68
7:n:266:TYR:CE2	7:n:268:ILE:CD1	2.72	0.68
46:C:431:HIS:O	46:C:435:LEU:HD22	1.89	0.68
1:f:1553:LEU:HG	1:f:1553:LEU:O	1.93	0.68
5:s:297:HIS:O	5:s:299:VAL:CG2	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:142:LEU:CD1	40:Y:332:ILE:C	2.67	0.68
18:U:46:GLN:HG3	18:U:46:GLN:O	1.92	0.68
37:V:25:LYS:HA	37:V:102:ASN:CB	2.23	0.68
47:8:42:PRO:HB3	47:8:45:ILE:H	1.57	0.68
5:s:306:ILE:HG21	5:s:394:TYR:CD1	2.28	0.68
28:5:458:LYS:O	28:5:459:ASN:ND2	2.27	0.68
46:C:28:VAL:HG12	46:C:29:ALA:HA	1.74	0.68
1:f:221:LYS:HB3	1:f:237:ILE:HD11	1.75	0.68
1:f:739:ARG:CA	1:f:742:ASN:ND2	2.33	0.68
3:0:1476:U:C5	46:C:232:ARG:NH2	2.61	0.68
46:C:28:VAL:HA	46:C:29:ALA:C	2.18	0.68
3:0:1863:U:H5'	51:A:301:LYS:HD3	1.74	0.68
7:n:213:PRO:CD	38:w:135:PHE:HE1	1.99	0.68
47:8:8:ARG:CZ	48:W:75:LYS:CD	2.72	0.68
51:A:296:GLN:HA	51:A:296:GLN:OE1	1.93	0.68
5:s:305:THR:CB	5:s:358:LYS:HB2	2.21	0.67
51:A:12:ALA:HB1	51:A:13:PRO:HD2	1.70	0.67
8:p:279:GLN:NE2	51:A:410:ASN:O	2.24	0.67
16:S:45:THR:HG21	16:S:58:ASN:CB	2.20	0.67
46:C:9:ASP:CA	46:C:10:SER:HB2	2.23	0.67
2:1:25:G:H4'	7:n:255:ASN:ND2	2.09	0.67
5:s:332:ARG:H	5:s:342:PRO:HG2	1.58	0.67
28:5:270:ILE:O	28:5:281:LEU:HB2	1.93	0.67
1:f:243:TYR:HH	1:f:323:LYS:HA	1.42	0.67
1:f:793:VAL:HG21	1:f:882:GLU:HG3	1.76	0.67
1:f:1235:LYS:HB3	1:f:1704:HIS:HD2	1.60	0.67
3:0:825:C:C6	26:J:118:ILE:HD13	2.29	0.67
28:5:351:ASP:CG	28:5:352:PRO:CD	2.62	0.67
28:5:400:LYS:HG2	46:C:21:ASP:OD2	1.93	0.67
1:f:1549:ARG:NH2	1:f:1575:ASP:HB2	2.09	0.67
46:C:189:VAL:O	46:C:190:ILE:HD12	1.95	0.67
1:f:1546:ARG:HH12	1:f:1547:LYS:HB2	1.58	0.67
7:n:326:TYR:CE2	37:V:77:VAL:HG11	2.30	0.67
46:C:31:ILE:HB	46:C:36:PHE:CE2	2.29	0.67
46:C:233:LEU:N	46:C:234:PRO:HA	2.03	0.67
1:f:295:ASN:HB3	1:f:296:TYR:HA	1.76	0.67
11:m:97:ASN:HD22	11:m:97:ASN:N	1.93	0.67
18:U:73:MET:HE3	51:A:435:LEU:HD13	1.77	0.67
39:E:279:TYR:CD2	46:C:411:ARG:HD2	2.27	0.67
1:f:855:ASP:HB3	1:f:856:PRO:CD	2.25	0.67
48:W:76:THR:CG2	48:W:77:GLN:HB2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:282:C:H4'	26:J:183:ASN:CG	2.21	0.66
3:0:1440:U:C4	46:C:387:ILE:HG22	2.30	0.66
46:C:29:ALA:C	46:C:30:GLN:HG3	2.20	0.66
48:W:84:ARG:HD2	48:W:105:MET:HE2	1.77	0.66
3:0:1529:U:H5	48:W:165:TRP:HE1	1.42	0.66
5:s:315:PHE:CD2	28:5:351:ASP:OD1	2.47	0.66
7:n:266:TYR:HE2	7:n:268:ILE:CG1	2.08	0.66
20:X:33:SER:HB3	20:X:34:HIS:HA	1.77	0.66
28:5:412:GLN:HG3	28:5:413:ILE:H	1.60	0.66
40:Y:230:ARG:HD3	40:Y:230:ARG:N	2.09	0.66
46:C:191:GLN:NE2	46:C:192:LYS:H	1.84	0.66
51:A:147:HIS:HA	51:A:300:GLU:HB3	1.78	0.66
1:f:261:LEU:HD11	1:f:295:ASN:ND2	2.10	0.66
37:V:50:ASN:ND2	37:V:52:ARG:CG	2.59	0.66
37:V:98:ALA:O	37:V:100:GLU:N	2.28	0.66
47:8:39:GLN:H	47:8:39:GLN:CD	2.03	0.66
2:1:75:A:H61	28:5:282:ARG:HH21	1.42	0.66
28:5:281:LEU:CD2	28:5:282:ARG:H	2.07	0.66
28:5:383:PHE:CE1	40:Y:240:LEU:HD21	2.22	0.66
38:w:34:GLN:HE21	38:w:35:GLU:CG	2.08	0.66
46:C:234:PRO:HG3	51:A:44:TRP:CE2	2.31	0.66
1:f:768:PHE:HB3	1:f:773:THR:HG1	1.59	0.66
47:8:40:TRP:CZ2	47:8:83:HIS:O	2.49	0.66
1:f:1041:SER:HB3	1:f:1178:PHE:CZ	2.30	0.66
28:5:457:GLU:HG2	46:C:25:GLU:CD	2.20	0.66
40:Y:328:PHE:O	40:Y:332:ILE:HG13	1.96	0.66
1:f:832:TYR:CG	46:C:11:ASP:HB2	2.22	0.66
28:5:455:LEU:HD21	28:5:458:LYS:H	1.59	0.66
51:A:375:ASP:OD1	51:A:378:ARG:CD	2.43	0.66
1:f:792:LEU:HD23	1:f:795:ALA:HB3	1.78	0.66
1:f:832:TYR:OH	46:C:12:GLU:O	2.13	0.66
1:f:1188:THR:HG23	1:f:1219:HIS:NE2	2.11	0.66
1:f:1254:ALA:HB3	1:f:1255:GLN:N	2.11	0.66
39:E:245:THR:HG1	51:A:7:GLU:CD	1.98	0.66
39:E:279:TYR:CE1	46:C:411:ARG:CG	2.78	0.66
46:C:6:ASP:N	46:C:7:VAL:HA	2.11	0.66
47:8:8:ARG:NH1	48:W:76:THR:HB	2.03	0.66
3:0:1530:C:O2	3:0:1533:C:C4	2.49	0.66
28:5:172:PHE:HB3	28:5:173:PRO:CD	2.26	0.66
39:E:245:THR:CB	51:A:7:GLU:OE1	2.43	0.66
37:V:52:ARG:HH22	37:V:53:ARG:HD3	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:377:TYR:HD2	51:A:435:LEU:HD13	1.54	0.66
5:s:306:ILE:CG1	5:s:393:PRO:CB	2.67	0.65
5:s:332:ARG:CA	5:s:334:LYS:H	1.99	0.65
28:5:458:LYS:HA	28:5:458:LYS:CE	2.24	0.65
3:0:2303:G:N2	37:V:63:GLY:HA2	2.11	0.65
39:E:245:THR:CG2	51:A:13:PRO:HB3	2.27	0.65
39:E:279:TYR:CD2	39:E:279:TYR:CB	2.76	0.65
47:8:79:ARG:HG2	47:8:84:LEU:HD13	1.77	0.65
1:f:1496:VAL:HG11	1:f:1657:PHE:CE1	2.32	0.65
1:f:768:PHE:CB	1:f:773:THR:HG1	2.08	0.65
1:f:762:GLU:HG2	1:f:785:LYS:NZ	2.12	0.65
5:s:331:ARG:NE	5:s:344:SER:CB	2.60	0.65
5:s:356:ARG:HH21	5:s:356:ARG:HG3	1.60	0.65
1:f:133:ARG:HH11	1:f:309:ARG:NH2	1.95	0.65
1:f:1195:LEU:CG	1:f:1217:GLU:OE1	2.45	0.65
5:s:149:SER:HB2	5:s:165:PRO:HA	1.76	0.65
1:f:93:GLU:O	1:f:96:LEU:N	2.30	0.65
7:n:125:LYS:HD3	7:n:125:LYS:H	1.62	0.65
7:n:254:GLY:C	7:n:255:ASN:OD1	2.40	0.65
38:w:34:GLN:HE21	38:w:35:GLU:HG2	1.62	0.65
1:f:184:LEU:HD13	1:f:235:LEU:CG	2.25	0.65
1:f:1127:VAL:CG1	1:f:1128:PRO:HD2	2.27	0.65
28:5:226:ILE:HG23	28:5:227:PRO:HD2	1.79	0.65
37:V:49:LEU:HD21	46:C:31:ILE:HG21	1.79	0.65
51:A:377:TYR:CG	51:A:435:LEU:HD12	2.31	0.65
36:c:8:LEU:CD1	38:w:88:PHE:HE2	2.10	0.64
1:f:769:ASP:HB3	1:f:770:PRO:HD2	1.79	0.64
5:s:307:HIS:CB	5:s:355:LEU:O	2.43	0.64
51:A:371:LYS:HB3	51:A:371:LYS:HZ3	1.59	0.64
18:U:98:MET:HE2	51:A:371:LYS:HA	1.69	0.64
7:n:328:ALA:O	7:n:329:GLN:HG2	1.98	0.64
16:S:61:ALA:C	16:S:62:THR:HG23	2.22	0.64
1:f:292:ARG:CD	1:f:308:ARG:HH12	2.10	0.64
1:f:832:TYR:HB3	46:C:11:ASP:CG	2.22	0.64
27:h:71:GLU:OE1	27:h:74:LYS:NZ	2.23	0.64
46:C:234:PRO:HB3	51:A:44:TRP:HD1	1.60	0.64
51:A:302:ASN:HB2	51:A:305:PRO:O	1.98	0.64
5:s:165:PRO:O	5:s:168:GLU:HB2	1.98	0.64
5:s:195:ASP:CG	13:o:184:ARG:NH1	2.55	0.64
28:5:383:PHE:CZ	40:Y:240:LEU:CD2	2.75	0.64
46:C:130:ASP:CG	46:C:131:PHE:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:133:ARG:NH2	1:f:307:LEU:HD23	2.12	0.64
38:w:137:ALA:O	38:w:139:ASN:N	2.31	0.64
48:W:75:LYS:HA	48:W:75:LYS:CE	2.17	0.64
1:f:307:LEU:HD12	1:f:308:ARG:HG2	1.79	0.64
39:E:245:THR:OG1	51:A:7:GLU:CD	2.39	0.64
1:f:5:TYR:OH	1:f:92:GLU:CB	2.43	0.64
47:8:62:ILE:HG22	47:8:64:VAL:HG23	1.80	0.64
37:V:52:ARG:NH1	46:C:39:THR:OG1	2.30	0.64
37:V:54:ILE:HG22	37:V:58:PHE:CE2	2.33	0.64
38:w:75:ILE:CD1	38:w:96:VAL:HG11	2.26	0.64
1:f:1546:ARG:HG3	1:f:1546:ARG:HH11	1.62	0.63
46:C:435:LEU:HD22	46:C:435:LEU:N	2.13	0.63
46:C:490:LYS:HD2	51:A:29:LYS:HZ3	1.63	0.63
46:C:490:LYS:HE3	51:A:29:LYS:HZ1	1.62	0.63
47:8:83:HIS:ND1	51:A:113:LYS:HE2	2.13	0.63
1:f:755:ALA:CB	1:f:789:TRP:CZ2	2.80	0.63
5:s:195:ASP:OD1	13:o:184:ARG:NH1	2.32	0.63
51:A:450:ILE:HG23	51:A:451:MET:H	1.63	0.63
1:f:793:VAL:HG23	1:f:797:GLN:NE2	2.12	0.63
1:f:739:ARG:O	1:f:742:ASN:ND2	2.32	0.63
1:f:774:LEU:C	7:n:207:ARG:HH22	2.06	0.63
1:f:840:PHE:CE1	46:C:1:MET:SD	2.91	0.63
7:n:300:LYS:HA	7:n:300:LYS:CE	2.29	0.63
10:u:119:ARG:CZ	38:w:162:ASP:OD1	2.47	0.63
46:C:34:LYS:HD2	46:C:34:LYS:N	2.12	0.63
51:A:377:TYR:CG	51:A:435:LEU:CD1	2.81	0.63
1:f:792:LEU:C	1:f:795:ALA:H	2.06	0.63
28:5:281:LEU:HD23	28:5:282:ARG:N	2.09	0.63
28:5:326:LEU:HD11	28:5:349:THR:HG23	1.80	0.63
39:E:279:TYR:CD1	46:C:411:ARG:HD3	2.34	0.63
46:C:435:LEU:CD2	46:C:435:LEU:H	2.10	0.63
46:C:490:LYS:CD	51:A:29:LYS:HZ1	2.11	0.63
1:f:762:GLU:CD	1:f:782:VAL:HG22	2.22	0.63
1:f:789:TRP:HA	1:f:789:TRP:CE3	2.34	0.63
1:f:1267:LEU:H	1:f:1401:GLU:HB3	1.63	0.63
7:n:334:SER:O	7:n:337:ARG:HG3	1.98	0.63
28:5:63:HIS:CE1	28:5:170:GLU:HG3	2.33	0.63
1:f:1075:LEU:CD2	1:f:1128:PRO:HD3	2.28	0.63
1:f:1632:HIS:CE1	1:f:1641:ARG:CZ	2.82	0.63
5:s:310:ILE:HD11	5:s:376:MET:HE1	1.81	0.63
16:S:45:THR:CG2	16:S:58:ASN:H	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:275:GLU:OE2	28:5:276:VAL:HG22	1.98	0.63
1:f:792:LEU:O	1:f:795:ALA:HB3	1.99	0.63
3:0:369:C:P	46:C:127:ARG:HD2	2.39	0.63
28:5:194:ILE:HD12	28:5:226:ILE:HG21	1.81	0.63
40:Y:229:ARG:HG2	40:Y:229:ARG:HH21	1.62	0.63
1:f:297:THR:C	1:f:299:ALA:HB2	2.24	0.63
10:u:116:ARG:O	10:u:119:ARG:HD3	1.99	0.63
37:V:26:VAL:HB	37:V:102:ASN:O	1.98	0.63
1:f:902:ARG:NH2	1:f:956:HIS:CE1	2.62	0.62
1:f:1235:LYS:HB3	1:f:1704:HIS:CD2	2.34	0.62
1:f:1556:LYS:CG	1:f:1557:ARG:HG3	2.29	0.62
28:5:281:LEU:O	28:5:282:ARG:HB2	1.97	0.62
37:V:50:ASN:ND2	37:V:52:ARG:CD	2.54	0.62
46:C:231:THR:O	46:C:232:ARG:HB3	1.98	0.62
51:A:298:LYS:HD3	51:A:298:LYS:N	2.14	0.62
1:f:149:PHE:HE1	1:f:261:LEU:HB2	1.64	0.62
1:f:789:TRP:HZ3	1:f:792:LEU:HD12	1.64	0.62
2:l:75:A:H61	28:5:282:ARG:HH22	1.25	0.62
7:n:266:TYR:CE2	7:n:268:ILE:CG1	2.82	0.62
7:n:333:ARG:O	7:n:334:SER:C	2.41	0.62
16:S:78:CYS:O	51:A:39:ILE:CD1	2.46	0.62
28:5:400:LYS:HZ1	28:5:401:ARG:HH12	1.47	0.62
11:m:54:LYS:HD2	11:m:96:GLU:OE2	1.98	0.62
28:5:349:THR:O	28:5:350:LEU:HB2	1.99	0.62
46:C:435:LEU:HD22	46:C:435:LEU:H	1.63	0.62
51:A:294:ARG:HH21	51:A:294:ARG:CG	2.12	0.62
1:f:91:ASP:OD2	1:f:92:GLU:N	2.33	0.62
1:f:1195:LEU:HG	1:f:1217:GLU:OE1	1.98	0.62
5:s:318:ASP:O	5:s:384:GLY:HA2	1.98	0.62
16:S:37:LYS:HE2	51:A:36:THR:HG21	1.79	0.62
1:f:240:PHE:HA	1:f:241:SER:CB	2.29	0.62
1:f:774:LEU:H	7:n:207:ARG:NH1	1.97	0.62
1:f:1595:ILE:HD11	1:f:1628:GLY:CA	2.28	0.62
48:W:76:THR:CA	48:W:77:GLN:HB2	2.28	0.62
1:f:292:ARG:CZ	1:f:308:ARG:NH2	2.63	0.62
16:S:66:ARG:CD	46:C:194:LYS:NZ	2.56	0.62
20:X:33:SER:HB3	20:X:34:HIS:CA	2.27	0.62
37:V:48:ALA:CB	46:C:36:PHE:HE1	2.13	0.62
38:w:34:GLN:HE21	38:w:35:GLU:CB	2.12	0.62
47:8:39:GLN:OE1	47:8:39:GLN:N	2.17	0.62
48:W:76:THR:HG23	48:W:77:GLN:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:s:356:ARG:CD	5:s:357:ALA:H	2.13	0.62
28:5:147:VAL:HG13	37:V:17:VAL:HG22	1.72	0.62
28:5:412:GLN:OE1	37:V:12:GLN:OE1	2.17	0.62
1:f:243:TYR:OH	1:f:323:LYS:CB	2.30	0.62
1:f:769:ASP:HB3	1:f:770:PRO:HD3	1.82	0.62
1:f:1237:TYR:HE1	1:f:1261:ILE:CG2	2.12	0.62
5:s:166:TYR:O	5:s:167:THR:OG1	2.13	0.62
5:s:332:ARG:HG3	5:s:342:PRO:HG2	1.81	0.62
46:C:212:THR:OG1	46:C:254:LEU:HD22	1.99	0.62
47:8:35:GLU:HA	47:8:36:HIS:C	2.25	0.62
1:f:1268:SER:CB	1:f:1716:LYS:CD	2.78	0.62
3:0:825:C:H2'	26:J:118:ILE:HD11	1.81	0.61
18:U:98:MET:CE	51:A:371:LYS:HB2	2.30	0.61
28:5:197:ASN:HD21	55:5:502:GNP:C8	2.02	0.61
47:8:42:PRO:HB3	47:8:45:ILE:N	2.14	0.61
46:C:490:LYS:CE	51:A:29:LYS:NZ	2.63	0.61
1:f:197:VAL:HG13	1:f:237:ILE:HG13	1.82	0.61
1:f:1632:HIS:HE1	1:f:1641:ARG:NE	1.92	0.61
28:5:271:ASN:OD1	28:5:281:LEU:HA	1.99	0.61
46:C:31:ILE:HG21	46:C:35:TRP:HB2	1.78	0.61
1:f:840:PHE:CD1	46:C:1:MET:SD	2.93	0.61
1:f:1068:ASN:HB2	1:f:1122:GLN:HE22	1.49	0.61
1:f:1127:VAL:HG13	1:f:1128:PRO:HD2	1.82	0.61
47:8:41:GLY:N	47:8:42:PRO:HA	2.15	0.61
1:f:259:PHE:CA	1:f:259:PHE:O	2.45	0.61
1:f:909:ARG:O	1:f:912:GLN:N	2.33	0.61
7:n:209:ARG:HB3	38:w:136:VAL:CG1	2.30	0.61
28:5:461:ARG:O	28:5:462:LEU:C	2.43	0.61
2:1:75:A:N6	28:5:282:ARG:HH21	1.93	0.61
48:W:79:ASP:C	48:W:81:ASP:H	2.07	0.61
51:A:149:ARG:HD2	51:A:295:TYR:O	2.00	0.61
1:f:151:ILE:HD13	1:f:261:LEU:HD22	1.83	0.61
3:0:814:C:C5	26:J:105:ILE:HG21	2.35	0.61
6:j:99:LYS:HG3	6:j:99:LYS:O	2.00	0.61
40:Y:229:ARG:HH21	40:Y:229:ARG:CG	2.13	0.61
47:8:81:SER:CB	47:8:83:HIS:HD2	2.13	0.61
10:u:119:ARG:HH11	10:u:119:ARG:CG	2.14	0.61
16:S:57:CYS:CB	16:S:64:LEU:HD21	2.28	0.61
28:5:154:ASN:OD1	28:5:419:THR:HG23	2.01	0.61
28:5:455:LEU:HD21	28:5:459:ASN:N	2.15	0.61
1:f:5:TYR:CZ	6:j:94:LYS:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:837:ILE:CD1	46:C:10:SER:HB2	2.31	0.61
47:8:79:ARG:C	47:8:81:SER:H	2.09	0.61
48:W:73:LEU:CD2	48:W:88:PHE:HE2	2.13	0.61
1:f:1265:HIS:NE2	1:f:1289:GLU:OE2	2.34	0.60
20:X:41:VAL:HG21	20:X:45:GLY:O	2.01	0.60
28:5:197:ASN:ND2	55:5:502:GNP:C5	2.61	0.60
37:V:28:ILE:HD11	37:V:88:ILE:O	2.00	0.60
48:W:162:LEU:CD2	48:W:206:ILE:O	2.49	0.60
51:A:148:ASN:HD21	51:A:303:PRO:HD2	1.64	0.60
1:f:1521:ARG:CG	1:f:1521:ARG:HH11	2.14	0.60
28:5:198:LYS:HG2	55:5:502:GNP:C6	2.30	0.60
28:5:412:GLN:NE2	37:V:12:GLN:OE1	2.34	0.60
37:V:66:GLY:O	37:V:67:THR:CG2	2.43	0.60
37:V:98:ALA:C	37:V:100:GLU:H	2.07	0.60
46:C:490:LYS:CD	51:A:29:LYS:NZ	2.64	0.60
1:f:746:ASP:OD2	46:C:4:PHE:HD2	1.85	0.60
1:f:785:LYS:HD2	1:f:889:LEU:CD2	2.31	0.60
46:C:434:ILE:HD11	51:A:28:MET:HE3	1.83	0.60
46:C:490:LYS:HE3	51:A:29:LYS:NZ	2.16	0.60
51:A:292:LYS:HE2	51:A:292:LYS:CA	2.31	0.60
1:f:743:ARG:HG3	11:m:52:LEU:HG	1.84	0.60
28:5:390:GLY:CA	28:5:461:ARG:HH11	2.08	0.60
37:V:33:ARG:O	37:V:34:LYS:HB3	2.00	0.60
37:V:99:THR:C	37:V:100:GLU:HG2	2.26	0.60
38:w:34:GLN:NE2	38:w:35:GLU:CB	2.64	0.60
47:8:30:LEU:HD11	47:8:52:ALA:CA	2.31	0.60
1:f:1521:ARG:NH1	1:f:1521:ARG:HG2	2.15	0.60
1:f:1525:THR:O	1:f:1529:ALA:CB	2.50	0.60
1:f:1535:ILE:CG2	1:f:1581:GLU:HG2	2.32	0.60
1:f:1630:GLY:O	1:f:1656:ILE:CG1	2.47	0.60
7:n:287:LYS:HZ3	7:n:287:LYS:CB	2.14	0.60
40:Y:230:ARG:HH21	40:Y:230:ARG:CG	2.14	0.60
51:A:36:THR:O	51:A:36:THR:HG22	2.01	0.60
51:A:149:ARG:HH11	51:A:149:ARG:CG	2.13	0.60
1:f:1237:TYR:HE1	1:f:1261:ILE:HG21	1.63	0.60
5:s:149:SER:HB2	5:s:164:ILE:C	2.15	0.60
27:h:72:GLU:C	27:h:74:LYS:N	2.59	0.60
5:s:331:ARG:HG2	5:s:344:SER:OG	1.98	0.60
7:n:255:ASN:OD1	7:n:255:ASN:N	2.35	0.60
37:V:99:THR:C	37:V:101:GLN:H	2.10	0.60
1:f:1109:LEU:CD1	1:f:1130:THR:OG1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:s:331:ARG:HD2	5:s:344:SER:CB	2.31	0.60
46:C:231:THR:O	46:C:231:THR:HG22	2.01	0.60
51:A:293:THR:HG22	51:A:293:THR:O	2.01	0.60
51:A:301:LYS:H	51:A:301:LYS:NZ	1.93	0.60
2:1:75:A:C2	28:5:285:VAL:HG12	2.28	0.60
6:j:133:GLN:HE22	6:j:138:LYS:HG2	1.67	0.60
28:5:271:ASN:HD22	28:5:274:GLY:CA	2.13	0.60
46:C:295:ARG:HD3	51:A:44:TRP:HZ2	1.66	0.60
48:W:85:LYS:HE3	48:W:106:GLU:OE1	2.02	0.60
51:A:292:LYS:H	51:A:292:LYS:HD2	1.67	0.60
1:f:902:ARG:HH11	28:5:205:VAL:CG1	2.15	0.59
1:f:1268:SER:HB3	1:f:1716:LYS:HD2	1.83	0.59
5:s:194:ILE:CG2	5:s:201:ILE:HG23	2.31	0.59
51:A:149:ARG:HD3	51:A:295:TYR:O	1.99	0.59
20:X:42:ASN:OD1	20:X:42:ASN:O	2.21	0.59
47:8:41:GLY:H	47:8:42:PRO:HA	1.67	0.59
1:f:1075:LEU:HD21	1:f:1128:PRO:CD	2.32	0.59
3:0:825:C:C5	26:J:118:ILE:HD13	2.37	0.59
5:s:356:ARG:CD	5:s:357:ALA:N	2.66	0.59
46:C:234:PRO:CB	51:A:44:TRP:HE1	2.13	0.59
1:f:762:GLU:HG2	1:f:785:LYS:HZ3	1.65	0.59
1:f:1259:CYS:O	1:f:1485:GLU:CD	2.45	0.59
3:0:1863:U:H5	51:A:306:ASP:HB3	1.66	0.59
5:s:166:TYR:CE1	5:s:167:THR:HG23	2.36	0.59
1:f:5:TYR:CE1	1:f:93:GLU:OE1	2.55	0.59
1:f:1496:VAL:HG21	1:f:1657:PHE:CZ	2.36	0.59
1:f:1549:ARG:HH11	1:f:1549:ARG:CG	2.14	0.59
3:0:1341:A:OP2	7:n:333:ARG:HD3	2.02	0.59
28:5:61:VAL:HA	55:5:502:GNP:O3G	2.02	0.59
46:C:490:LYS:CE	51:A:29:LYS:HZ1	2.14	0.59
48:W:73:LEU:CD2	48:W:88:PHE:CE2	2.86	0.59
1:f:1565:ASP:OD2	7:n:335:LYS:HE3	2.03	0.59
5:s:356:ARG:HD2	5:s:357:ALA:N	2.18	0.59
11:m:73:GLN:HE22	11:m:80:LYS:NZ	2.00	0.59
16:S:62:THR:O	16:S:63:LYS:HB2	2.03	0.59
37:V:52:ARG:NH1	37:V:56:ARG:HH22	2.00	0.59
38:w:35:GLU:HG3	38:w:35:GLU:O	2.02	0.59
47:8:10:CYS:O	47:8:13:LYS:N	2.36	0.59
51:A:253:THR:CG2	51:A:381:ALA:H	2.13	0.59
1:f:855:ASP:HB3	1:f:856:PRO:HD3	1.83	0.59
5:s:315:PHE:CE2	28:5:351:ASP:CB	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:147:VAL:HA	28:5:459:ASN:OD1	2.03	0.59
37:V:52:ARG:HH11	37:V:56:ARG:HH22	1.51	0.59
1:f:2:SER:O	1:f:6:ARG:HD2	2.03	0.59
1:f:749:ILE:HG21	46:C:5:PHE:CE1	2.38	0.59
1:f:1068:ASN:HB3	1:f:1122:GLN:NE2	2.15	0.59
1:f:1218:VAL:HG12	1:f:1219:HIS:N	2.17	0.59
1:f:1221:LEU:O	1:f:1222:PRO:N	2.30	0.59
1:f:1265:HIS:CD2	1:f:1289:GLU:OE1	2.56	0.59
7:n:266:TYR:CE2	7:n:268:ILE:HG13	2.38	0.59
7:n:323:SER:O	7:n:324:ALA:HB2	2.02	0.59
1:f:297:THR:HG21	1:f:303:ASN:CA	2.33	0.58
7:n:206:GLU:C	7:n:208:ASN:N	2.48	0.58
7:n:210:LEU:O	38:w:135:PHE:O	2.21	0.58
37:V:52:ARG:HH21	37:V:53:ARG:HD3	1.64	0.58
51:A:292:LYS:HB3	51:A:292:LYS:HZ3	1.67	0.58
5:s:316:GLN:O	5:s:318:ASP:N	2.31	0.58
7:n:328:ALA:O	7:n:329:GLN:CG	2.51	0.58
28:5:273:PRO:HB3	28:5:275:GLU:CG	2.27	0.58
28:5:383:PHE:HE1	40:Y:240:LEU:CD2	2.03	0.58
46:C:232:ARG:O	46:C:234:PRO:C	2.45	0.58
1:f:6:ARG:HH22	27:h:72:GLU:HG3	1.66	0.58
1:f:1041:SER:OG	1:f:1178:PHE:CE2	2.49	0.58
7:n:118:ASN:OD1	7:n:118:ASN:O	2.21	0.58
28:5:61:VAL:CA	55:5:502:GNP:O3G	2.50	0.58
47:8:38:VAL:HG12	47:8:42:PRO:O	2.04	0.58
51:A:253:THR:HG23	51:A:253:THR:O	2.02	0.58
28:5:223:GLY:C	28:5:225:ASN:H	2.10	0.58
47:8:30:LEU:HD13	47:8:52:ALA:HB1	1.75	0.58
48:W:40:VAL:CG2	48:W:75:LYS:CE	2.69	0.58
1:f:834:PHE:CD2	46:C:10:SER:OG	2.56	0.58
3:0:368:G:O2'	46:C:127:ARG:HG2	2.03	0.58
1:f:1521:ARG:N	1:f:1521:ARG:HD3	2.18	0.58
7:n:338:LEU:O	7:n:341:MET:HG3	2.04	0.58
28:5:412:GLN:C	28:5:413:ILE:HG13	2.29	0.58
47:8:36:HIS:CB	47:8:37:GLY:HA2	2.31	0.58
51:A:302:ASN:CB	51:A:305:PRO:O	2.52	0.58
1:f:292:ARG:HD3	1:f:308:ARG:HH12	1.66	0.58
1:f:1195:LEU:HB3	1:f:1217:GLU:OE1	2.04	0.58
16:S:63:LYS:CE	46:C:192:LYS:HD2	2.28	0.58
46:C:431:HIS:O	46:C:435:LEU:HD21	1.90	0.58
1:f:151:ILE:HG12	1:f:261:LEU:CB	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:182:LYS:HE2	28:5:389:VAL:HG21	1.84	0.58
1:f:1632:HIS:HE2	1:f:1641:ARG:HH21	1.42	0.58
3:0:1440:U:C4	46:C:387:ILE:HG21	2.38	0.58
3:0:1861:G:H21	51:A:296:GLN:NE2	2.01	0.58
5:s:306:ILE:HG21	5:s:394:TYR:CE1	2.39	0.58
28:5:174:GLN:HB3	28:5:175:PRO:HD2	1.86	0.58
38:w:71:ARG:HB3	38:w:74:TRP:CH2	2.34	0.58
3:0:816:C:H5	26:J:137:LYS:CE	2.17	0.57
5:s:149:SER:O	5:s:150:ALA:HB2	2.03	0.57
1:f:150:PHE:CE2	1:f:198:PHE:CZ	2.92	0.57
1:f:779:ASN:OD1	1:f:896:LEU:HD12	2.03	0.57
3:0:1478:U:C5	46:C:232:ARG:NH1	2.56	0.57
5:s:331:ARG:HA	5:s:342:PRO:HG3	1.85	0.57
7:n:288:CYS:HB3	7:n:309:CYS:SG	2.44	0.57
1:f:197:VAL:CG1	1:f:237:ILE:HG13	2.35	0.57
28:5:67:THR:HG21	55:5:502:GNP:C8	2.34	0.57
28:5:219:ASP:OD2	28:5:225:ASN:CG	2.44	0.57
28:5:220:SER:CA	40:Y:273:ARG:HH21	2.14	0.57
1:f:941:ARG:HH11	40:Y:292:LYS:HB2	1.69	0.57
5:s:297:HIS:C	5:s:299:VAL:HG22	2.29	0.57
7:n:131:GLU:OE2	7:n:135:ARG:NH1	2.38	0.57
16:S:57:CYS:HB2	16:S:64:LEU:CD2	2.34	0.57
28:5:279:GLU:O	28:5:280:ASN:HB3	2.05	0.57
1:f:203:LEU:N	1:f:243:TYR:CD1	2.60	0.57
46:C:130:ASP:CG	46:C:131:PHE:N	2.63	0.57
1:f:193:ARG:HE	1:f:195:HIS:CD2	2.22	0.57
5:s:166:TYR:CD1	5:s:167:THR:N	2.73	0.57
11:m:96:GLU:O	11:m:97:ASN:HB2	2.03	0.57
28:5:400:LYS:CE	28:5:401:ARG:NH1	2.67	0.57
1:f:769:ASP:OD2	38:w:127:LYS:HE3	2.04	0.57
28:5:219:ASP:CB	28:5:225:ASN:HD22	1.94	0.57
46:C:38:VAL:O	46:C:38:VAL:HG22	2.05	0.57
48:W:76:THR:H	48:W:77:GLN:CA	2.17	0.57
1:f:807:MET:HE3	1:f:855:ASP:OD1	2.01	0.57
1:f:1539:ALA:O	1:f:1543:GLU:HG3	2.04	0.57
1:f:221:LYS:HB3	1:f:237:ILE:CD1	2.35	0.57
1:f:1268:SER:HB3	1:f:1716:LYS:CD	2.35	0.57
1:f:1534:ARG:O	1:f:1537:ARG:N	2.38	0.57
47:8:8:ARG:NH2	48:W:75:LYS:CG	2.68	0.57
1:f:746:ASP:OD2	46:C:4:PHE:CD2	2.57	0.57
1:f:755:ALA:HB2	1:f:789:TRP:CH2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:297:THR:CB	1:f:303:ASN:CB	2.81	0.56
1:f:1041:SER:O	1:f:1042:ALA:HB2	2.04	0.56
1:f:1068:ASN:HB2	1:f:1122:GLN:CD	2.29	0.56
16:S:76:THR:HG21	51:A:41:PRO:CB	2.31	0.56
37:V:18:GLN:O	37:V:18:GLN:HG2	2.05	0.56
51:A:146:LEU:CB	51:A:300:GLU:HG3	2.35	0.56
1:f:243:TYR:CZ	1:f:323:LYS:HA	2.33	0.56
1:f:792:LEU:HA	1:f:795:ALA:HB2	1.87	0.56
1:f:1632:HIS:CD2	1:f:1641:ARG:HH21	2.20	0.56
7:n:142:LEU:HD13	40:Y:332:ILE:HA	1.88	0.56
47:8:27:VAL:HG11	47:8:66:ARG:CZ	2.35	0.56
1:f:1259:CYS:O	1:f:1485:GLU:CG	2.53	0.56
1:f:1546:ARG:NH1	1:f:1547:LYS:HB2	2.20	0.56
7:n:326:TYR:HD2	37:V:77:VAL:HG21	0.79	0.56
16:S:60:CYS:O	16:S:61:ALA:HB3	2.06	0.56
20:X:38:LYS:HB2	20:X:38:LYS:HZ2	1.70	0.56
47:8:35:GLU:CG	47:8:39:GLN:HB3	2.35	0.56
1:f:770:PRO:HB3	28:5:170:GLU:C	2.31	0.56
48:W:73:LEU:HD21	48:W:88:PHE:CZ	2.40	0.56
1:f:792:LEU:HA	1:f:795:ALA:CB	2.34	0.56
3:0:230:G:C5'	26:J:157:PHE:HZ	2.18	0.56
5:s:148:THR:O	5:s:148:THR:CG2	2.50	0.56
20:X:33:SER:CB	20:X:34:HIS:CA	2.79	0.56
1:f:1546:ARG:NH1	1:f:1547:LYS:CA	2.69	0.56
3:0:825:C:C6	26:J:118:ILE:CD1	2.89	0.56
20:X:41:VAL:CG2	20:X:45:GLY:O	2.54	0.56
38:w:73:VAL:C	38:w:74:TRP:HE3	2.13	0.56
47:8:62:ILE:HG23	47:8:64:VAL:CA	2.35	0.56
1:f:1071:VAL:HA	1:f:1122:GLN:O	2.06	0.56
7:n:327:SER:O	7:n:328:ALA:HB3	2.05	0.56
7:n:328:ALA:C	7:n:329:GLN:CG	2.79	0.56
46:C:5:PHE:O	46:C:5:PHE:CD1	2.59	0.56
51:A:253:THR:HG22	51:A:381:ALA:N	2.19	0.56
1:f:1108:ALA:O	1:f:1109:LEU:HB2	2.06	0.56
1:f:1109:LEU:CD2	1:f:1110:GLY:O	2.54	0.56
5:s:316:GLN:C	5:s:318:ASP:H	2.11	0.56
26:J:238:ALA:HA	29:P:247:LYS:HE3	1.88	0.56
1:f:93:GLU:O	1:f:94:GLU:C	2.48	0.56
1:f:292:ARG:CD	1:f:308:ARG:NH1	2.63	0.56
1:f:309:ARG:CG	1:f:310:GLN:N	2.68	0.56
1:f:1242:PRO:CD	1:f:1260:TYR:CE1	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:1508:VAL:HG11	1:f:1631:MET:SD	2.45	0.56
38:w:34:GLN:HE22	38:w:35:GLU:HB3	1.71	0.56
46:C:329:GLN:CG	46:C:330:GLN:N	2.67	0.56
1:f:1075:LEU:HD21	1:f:1128:PRO:HG3	1.88	0.56
1:f:93:GLU:CD	1:f:93:GLU:H	2.13	0.55
1:f:1072:VAL:O	1:f:1123:VAL:HG13	2.05	0.55
10:u:119:ARG:HG3	10:u:119:ARG:NH1	2.21	0.55
16:S:79:GLY:HA2	51:A:38:ALA:HA	1.89	0.55
46:C:419:ARG:HG2	51:A:13:PRO:HA	1.88	0.55
28:5:390:GLY:CA	28:5:461:ARG:NH1	2.68	0.55
46:C:232:ARG:HA	46:C:234:PRO:HA	1.88	0.55
1:f:1632:HIS:CE1	1:f:1641:ARG:NH2	2.74	0.55
37:V:52:ARG:NH1	37:V:56:ARG:NH2	2.54	0.55
1:f:149:PHE:HZ	1:f:261:LEU:CD1	2.19	0.55
18:U:83:ARG:HH21	18:U:83:ARG:CG	2.14	0.55
51:A:103:ARG:HE	51:A:259:ARG:HE	1.53	0.55
1:f:202:LEU:N	1:f:243:TYR:HD1	2.03	0.55
1:f:303:ASN:HB2	1:f:304:PRO:HD2	1.89	0.55
1:f:762:GLU:CD	1:f:782:VAL:CG2	2.80	0.55
1:f:855:ASP:CB	1:f:856:PRO:CD	2.84	0.55
1:f:1109:LEU:HD13	1:f:1127:VAL:HB	1.88	0.55
37:V:52:ARG:CZ	46:C:39:THR:HG1	2.14	0.55
28:5:88:ILE:CD1	28:5:90:ILE:CG1	2.66	0.55
1:f:240:PHE:HA	1:f:241:SER:OG	2.06	0.55
1:f:834:PHE:CE2	46:C:6:ASP:OD1	2.59	0.55
1:f:955:LYS:CE	1:f:989:GLN:NE2	2.69	0.55
1:f:1556:LYS:HA	1:f:1557:ARG:HG2	1.89	0.55
28:5:281:LEU:HD22	28:5:281:LEU:N	2.02	0.55
46:C:431:HIS:C	46:C:435:LEU:CD2	2.73	0.55
51:A:7:GLU:HB2	51:A:13:PRO:HD3	1.89	0.55
51:A:294:ARG:HH21	51:A:294:ARG:HG3	1.72	0.55
1:f:137:CYS:C	1:f:302:ALA:HB1	2.27	0.55
1:f:906:GLU:OE2	28:5:204:GLU:HG3	2.06	0.55
51:A:149:ARG:HH11	51:A:149:ARG:CB	2.20	0.55
1:f:785:LYS:HG2	1:f:786:LEU:N	2.21	0.55
28:5:455:LEU:HD23	28:5:459:ASN:H	1.68	0.55
46:C:434:ILE:HD13	51:A:28:MET:HE3	1.89	0.55
46:C:490:LYS:HB3	51:A:29:LYS:HZ1	1.72	0.55
1:f:1235:LYS:HD3	1:f:1704:HIS:CD2	2.42	0.55
1:f:1268:SER:CB	1:f:1716:LYS:HD3	2.36	0.55
3:0:1478:U:C4	46:C:232:ARG:CZ	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:142:LEU:HD13	40:Y:332:ILE:O	1.95	0.55
7:n:212:GLU:O	7:n:214:LYS:HG3	2.07	0.55
7:n:328:ALA:C	7:n:329:GLN:HG3	2.32	0.55
37:V:50:ASN:CG	37:V:52:ARG:CG	2.75	0.55
39:E:245:THR:HG21	51:A:13:PRO:HB3	1.89	0.55
47:8:81:SER:CB	47:8:83:HIS:CD2	2.86	0.55
1:f:739:ARG:C	1:f:742:ASN:ND2	2.65	0.54
1:f:1254:ALA:HB3	1:f:1255:GLN:H	1.71	0.54
1:f:1553:LEU:HA	3:0:2176:C:H42	1.71	0.54
16:S:59:GLY:O	16:S:60:CYS:HB2	2.06	0.54
46:C:490:LYS:HB3	51:A:29:LYS:HE3	1.89	0.54
51:A:399:LYS:CG	51:A:425:THR:HG22	2.37	0.54
1:f:303:ASN:CB	1:f:304:PRO:CD	2.82	0.54
1:f:1494:THR:HG1	1:f:1672:SER:HB2	1.68	0.54
1:f:1517:GLU:HB3	1:f:1521:ARG:NH2	2.22	0.54
7:n:300:LYS:HE2	7:n:305:MET:O	2.06	0.54
27:h:71:GLU:OE1	27:h:71:GLU:HA	2.07	0.54
47:8:27:VAL:HG22	47:8:62:ILE:HD11	1.90	0.54
1:f:1496:VAL:HG21	1:f:1657:PHE:CE1	2.42	0.54
5:s:331:ARG:HG3	5:s:342:PRO:CB	2.36	0.54
13:o:166:ALA:HA	13:o:176:ILE:HD11	1.90	0.54
3:0:1408:U:OP1	46:C:271:LEU:HD11	2.07	0.54
46:C:295:ARG:CZ	51:A:44:TRP:CZ2	2.90	0.54
47:8:38:VAL:O	47:8:38:VAL:HG12	2.07	0.54
1:f:746:ASP:OD1	46:C:5:PHE:HD2	1.90	0.54
18:U:83:ARG:HG3	18:U:83:ARG:NH2	2.20	0.54
18:U:98:MET:HE1	51:A:371:LYS:HB2	1.87	0.54
37:V:53:ARG:NH2	46:C:37:GLU:CD	2.65	0.54
1:f:744:ASP:OD1	11:m:97:ASN:OD1	2.24	0.54
1:f:1546:ARG:HG3	1:f:1546:ARG:NH1	2.20	0.54
48:W:76:THR:CA	48:W:77:GLN:CB	2.85	0.54
1:f:902:ARG:HD3	28:5:205:VAL:CG1	2.36	0.54
1:f:1268:SER:HB2	1:f:1716:LYS:CD	2.37	0.54
3:0:1529:U:H5	48:W:165:TRP:NE1	2.04	0.54
28:5:281:LEU:H	28:5:281:LEU:CD2	2.10	0.54
46:C:51:LEU:CD1	46:C:56:LYS:CD	2.86	0.54
47:8:42:PRO:CB	47:8:45:ILE:N	2.68	0.54
51:A:148:ASN:HD22	51:A:303:PRO:CG	2.19	0.54
1:f:774:LEU:O	1:f:774:LEU:CD1	2.54	0.54
1:f:1549:ARG:HH21	1:f:1573:MET:HG3	1.73	0.54
3:0:282:C:H5'	26:J:183:ASN:CB	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:C:189:VAL:C	46:C:190:ILE:HG13	2.33	0.54
47:8:40:TRP:NE1	47:8:83:HIS:HB2	2.14	0.54
1:f:832:TYR:CB	46:C:11:ASP:CG	2.81	0.54
1:f:1070:LYS:HD3	1:f:1148:ASP:OD2	2.08	0.54
3:0:2303:G:H21	37:V:63:GLY:HA2	1.72	0.54
18:U:51:LEU:CD2	18:U:98:MET:CE	2.83	0.54
51:A:399:LYS:CD	51:A:425:THR:HG22	2.38	0.54
1:f:1242:PRO:HD2	1:f:1260:TYR:CE1	2.43	0.54
5:s:318:ASP:O	5:s:384:GLY:CA	2.56	0.54
5:s:331:ARG:HD2	5:s:344:SER:HG	1.69	0.54
7:n:249:GLU:HA	7:n:249:GLU:OE2	2.06	0.54
16:S:63:LYS:CE	46:C:192:LYS:HB2	2.38	0.54
37:V:50:ASN:ND2	37:V:52:ARG:HG2	2.22	0.54
1:f:832:TYR:CD1	46:C:11:ASP:CG	2.85	0.53
1:f:906:GLU:OE1	28:5:204:GLU:CG	2.41	0.53
1:f:1521:ARG:HH11	1:f:1521:ARG:HG2	1.71	0.53
5:s:317:CYS:O	5:s:318:ASP:HB2	2.08	0.53
47:8:10:CYS:O	47:8:11:LEU:C	2.50	0.53
5:s:320:VAL:CG2	5:s:321:ASN:H	2.21	0.53
38:w:130:HIS:C	38:w:130:HIS:CD2	2.86	0.53
1:f:5:TYR:OH	6:j:94:LYS:CD	2.56	0.53
7:n:326:TYR:HE2	37:V:77:VAL:CG1	2.20	0.53
16:S:63:LYS:HE2	46:C:192:LYS:HB2	1.90	0.53
28:5:61:VAL:HG23	55:5:502:GNP:N3B	2.24	0.53
28:5:431:PRO:HD2	40:Y:203:GLU:O	2.08	0.53
38:w:136:VAL:HG13	38:w:138:GLU:HB2	1.90	0.53
2:1:71:U:C2'	2:1:72:A:H5''	2.36	0.53
28:5:220:SER:HA	40:Y:273:ARG:NH2	2.17	0.53
46:C:203:ALA:O	46:C:206:SER:HB2	2.08	0.53
1:f:746:ASP:OD1	46:C:4:PHE:HB3	2.08	0.53
1:f:1068:ASN:HB2	1:f:1122:GLN:OE1	2.09	0.53
3:0:268:C:C5'	26:J:174:LYS:HE3	2.39	0.53
3:0:1974:G:H2'	3:0:1975:G:H5'	1.90	0.53
5:s:149:SER:H	5:s:166:TYR:HB2	1.72	0.53
7:n:288:CYS:CB	7:n:309:CYS:SG	2.97	0.53
38:w:130:HIS:HD2	38:w:131:SER:O	1.92	0.53
48:W:76:THR:OG1	48:W:77:GLN:OE1	2.27	0.53
3:0:816:C:H5	26:J:137:LYS:HZ2	1.57	0.53
5:s:320:VAL:CG2	5:s:321:ASN:N	2.71	0.53
5:s:332:ARG:CA	5:s:333:PHE:C	2.74	0.53
28:5:270:ILE:C	28:5:281:LEU:HB2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2068:A:H61	34:O:148:ALA:HB3	1.74	0.53
5:s:331:ARG:CD	5:s:344:SER:CB	2.84	0.53
7:n:118:ASN:CG	40:Y:265:ARG:NH1	2.30	0.53
16:S:57:CYS:HA	16:S:64:LEU:HD11	1.91	0.53
28:5:390:GLY:HA3	28:5:461:ARG:HD3	1.91	0.53
1:f:256:GLU:O	1:f:258:GLU:HG3	2.08	0.53
1:f:786:LEU:C	1:f:786:LEU:CD2	2.82	0.53
5:s:356:ARG:HG3	5:s:356:ARG:NH2	2.23	0.53
28:5:147:VAL:HG22	28:5:459:ASN:HD21	1.73	0.53
37:V:54:ILE:CG2	37:V:58:PHE:CE2	2.92	0.53
46:C:329:GLN:C	46:C:331:ARG:H	2.17	0.53
3:O:816:C:H41	26:J:137:LYS:HZ2	1.53	0.53
11:m:51:VAL:C	11:m:52:LEU:CD1	2.82	0.53
28:5:186:ILE:HD12	28:5:465:TRP:HB2	1.88	0.53
47:8:42:PRO:HB2	47:8:45:ILE:H	1.72	0.53
1:f:297:THR:HG22	1:f:298:ASP:CA	2.38	0.53
5:s:332:ARG:CA	5:s:334:LYS:N	2.52	0.53
1:f:789:TRP:CZ3	1:f:792:LEU:HD12	2.43	0.52
7:n:330:VAL:HG13	7:n:330:VAL:O	2.09	0.52
48:W:76:THR:N	48:W:77:GLN:CB	2.72	0.52
1:f:774:LEU:HD22	1:f:900:ASN:OD1	2.09	0.52
1:f:1546:ARG:HH12	1:f:1547:LYS:CB	2.22	0.52
5:s:307:HIS:CD2	5:s:356:ARG:HA	2.44	0.52
7:n:205:THR:OG1	7:n:207:ARG:NE	2.41	0.52
28:5:454:ARG:O	28:5:460:PHE:CA	2.55	0.52
37:V:52:ARG:HH22	37:V:53:ARG:NH1	2.02	0.52
46:C:241:TRP:CZ3	46:C:313:LEU:HD11	2.43	0.52
1:f:206:TRP:CG	1:f:207:GLU:HA	2.44	0.52
1:f:739:ARG:O	1:f:742:ASN:CG	2.51	0.52
1:f:955:LYS:HE3	1:f:989:GLN:HE21	1.72	0.52
3:O:228:G:N2	26:J:160:SER:HB3	2.21	0.52
5:s:169:ILE:O	5:s:170:THR:CG2	2.54	0.52
16:S:38:CYS:SG	16:S:64:LEU:HD23	2.47	0.52
39:E:279:TYR:CE2	46:C:411:ARG:CZ	2.92	0.52
46:C:34:LYS:O	46:C:37:GLU:N	2.43	0.52
51:A:258:ARG:O	51:A:271:ILE:CG2	2.54	0.52
1:f:309:ARG:HG2	1:f:310:GLN:N	2.24	0.52
20:X:38:LYS:CB	20:X:38:LYS:NZ	2.72	0.52
36:c:10:ARG:NH1	38:w:35:GLU:HB2	2.24	0.52
48:W:70:LEU:O	48:W:71:ALA:HB3	2.08	0.52
1:f:1494:THR:OG1	1:f:1672:SER:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:C:1:MET:C	46:C:3:ASN:HB2	2.35	0.52
46:C:685:VAL:HG21	50:H:282:HIS:CD2	2.45	0.52
51:A:152:VAL:HG22	51:A:293:THR:HB	1.92	0.52
51:A:292:LYS:NZ	51:A:292:LYS:CB	2.73	0.52
1:f:955:LYS:HE3	1:f:989:GLN:CG	2.39	0.52
3:0:368:G:O3'	46:C:127:ARG:HD2	2.05	0.52
5:s:315:PHE:HE2	28:5:351:ASP:CB	2.15	0.52
48:W:40:VAL:HG22	48:W:75:LYS:HE3	1.82	0.52
5:s:342:PRO:C	5:s:356:ARG:HE	2.18	0.52
28:5:412:GLN:CD	37:V:12:GLN:OE1	2.52	0.52
46:C:31:ILE:N	46:C:31:ILE:CD1	2.73	0.52
51:A:375:ASP:O	51:A:378:ARG:HD2	2.10	0.52
13:o:26:ASP:OD2	51:A:368:GLN:HG3	2.10	0.52
16:S:45:THR:CG2	16:S:58:ASN:CA	2.87	0.52
20:X:40:HIS:O	20:X:40:HIS:ND1	2.43	0.52
46:C:34:LYS:H	46:C:34:LYS:CD	2.13	0.52
51:A:148:ASN:HD21	51:A:303:PRO:CD	2.21	0.52
1:f:193:ARG:HB2	1:f:195:HIS:HB2	1.91	0.52
1:f:302:ALA:C	1:f:303:ASN:CG	2.67	0.52
3:0:1531:A:H4'	3:0:1532:G:OP2	2.10	0.52
37:V:24:GLN:O	37:V:102:ASN:CG	2.49	0.52
38:w:34:GLN:C	38:w:34:GLN:HE21	2.18	0.52
47:8:8:ARG:NH2	47:8:8:ARG:CB	2.73	0.52
51:A:292:LYS:H	51:A:292:LYS:CE	2.23	0.52
1:f:1496:VAL:HG11	1:f:1657:PHE:HE1	1.74	0.52
2:1:71:U:H2'	2:1:72:A:C5'	2.37	0.52
3:0:2303:G:N2	37:V:63:GLY:HA3	2.23	0.52
3:0:2303:G:H21	37:V:63:GLY:CA	2.23	0.52
7:n:206:GLU:HG3	38:w:133:TYR:CD2	2.45	0.52
46:C:6:ASP:H	46:C:7:VAL:HA	1.74	0.52
1:f:264:ASP:OD1	1:f:265:GLY:N	2.43	0.51
1:f:1108:ALA:O	1:f:1126:THR:HG22	2.10	0.51
45:T:137:ARG:NH1	45:T:137:ARG:HG2	2.25	0.51
46:C:435:LEU:CD2	46:C:435:LEU:N	2.73	0.51
47:8:24:LYS:N	47:8:24:LYS:CD	2.73	0.51
1:f:297:THR:HG21	1:f:303:ASN:HA	1.93	0.51
1:f:1042:ALA:CB	1:f:1218:VAL:O	2.57	0.51
7:n:336:ALA:O	7:n:339:GLN:HG3	2.09	0.51
13:o:177:LYS:NZ	13:o:180:ASP:HB3	2.25	0.51
46:C:230:ASP:OD1	46:C:231:THR:N	2.43	0.51
51:A:12:ALA:HB3	51:A:13:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:242:SER:O	1:f:323:LYS:HE2	2.10	0.51
1:f:1043:VAL:HG23	1:f:1180:ALA:C	2.35	0.51
7:n:287:LYS:NZ	7:n:287:LYS:CB	2.73	0.51
13:o:177:LYS:HE3	13:o:177:LYS:C	2.36	0.51
28:5:391:ARG:HH12	46:C:25:GLU:CG	2.13	0.51
1:f:909:ARG:O	1:f:910:LEU:C	2.53	0.51
1:f:941:ARG:NH1	40:Y:288:ASP:O	2.41	0.51
1:f:1549:ARG:HH21	1:f:1573:MET:CG	2.24	0.51
26:J:190:LEU:HB2	26:J:194:ALA:HB2	1.92	0.51
37:V:52:ARG:HH12	37:V:56:ARG:HH12	1.56	0.51
37:V:94:ASP:OD1	37:V:95:GLU:N	2.43	0.51
39:E:279:TYR:CZ	46:C:411:ARG:CZ	2.92	0.51
40:Y:230:ARG:N	40:Y:230:ARG:CD	2.73	0.51
51:A:301:LYS:HZ3	51:A:301:LYS:CA	2.22	0.51
1:f:1397:LEU:HD12	1:f:1401:GLU:OE2	2.10	0.51
5:s:300:ARG:NH2	5:s:362:ARG:NH1	2.52	0.51
28:5:220:SER:CA	40:Y:273:ARG:NH2	2.73	0.51
37:V:48:ALA:HB1	46:C:36:PHE:HE1	1.75	0.51
1:f:307:LEU:HG	1:f:308:ARG:HG2	1.93	0.51
1:f:309:ARG:CG	1:f:310:GLN:H	2.24	0.51
1:f:1144:VAL:HG11	1:f:1174:LEU:HD13	1.91	0.51
1:f:1546:ARG:NH1	1:f:1547:LYS:HA	2.26	0.51
2:1:75:A:N3	28:5:285:VAL:HG11	2.26	0.51
5:s:310:ILE:HD11	5:s:376:MET:CE	2.40	0.51
7:n:125:LYS:CD	7:n:125:LYS:H	2.23	0.51
46:C:274:LYS:H	46:C:275:ARG:CA	2.23	0.51
47:8:6:LYS:C	47:8:7:THR:CG2	2.83	0.51
51:A:151:LEU:HD22	51:A:294:ARG:NE	2.14	0.51
3:0:1467:U:H2'	3:0:1468:U:H5''	1.92	0.51
28:5:172:PHE:CB	28:5:173:PRO:CD	2.85	0.51
51:A:148:ASN:CG	51:A:303:PRO:HD2	2.35	0.51
38:w:160:LEU:O	38:w:161:ASP:HB2	2.10	0.51
51:A:42:SER:O	51:A:46:GLU:HG3	2.11	0.51
1:f:133:ARG:HH21	1:f:307:LEU:CD2	2.23	0.51
1:f:138:ASP:CG	1:f:139:MET:HG2	2.35	0.51
1:f:771:GLY:CA	1:f:772:TYR:HB3	2.41	0.51
1:f:1195:LEU:CB	1:f:1217:GLU:OE1	2.58	0.51
1:f:1235:LYS:HD3	1:f:1704:HIS:HD2	1.76	0.51
1:f:1702:LEU:HD13	1:f:1704:HIS:NE2	2.25	0.51
3:0:816:C:H41	26:J:137:LYS:HZ1	1.59	0.51
3:0:1866:A:H2	51:A:294:ARG:HH22	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:151:LEU:HD21	51:A:294:ARG:NE	2.14	0.51
1:f:150:PHE:CE2	1:f:258:GLU:OE1	2.64	0.51
1:f:262:MET:HG2	1:f:293:LYS:HE2	1.92	0.51
51:A:149:ARG:CG	51:A:149:ARG:NH1	2.73	0.51
51:A:149:ARG:NH1	51:A:149:ARG:HG3	2.26	0.51
1:f:6:ARG:HH22	27:h:72:GLU:CG	2.24	0.50
7:n:341:MET:C	7:n:341:MET:SD	2.94	0.50
1:f:5:TYR:OH	6:j:94:LYS:HG3	2.11	0.50
1:f:1149:TYR:HE2	1:f:1177:PRO:HB2	1.76	0.50
1:f:1259:CYS:O	1:f:1485:GLU:OE1	2.29	0.50
37:V:17:VAL:O	37:V:19:ASP:N	2.44	0.50
47:8:41:GLY:N	47:8:42:PRO:CA	2.73	0.50
51:A:258:ARG:HD2	51:A:274:LEU:HG	1.94	0.50
1:f:150:PHE:CD2	1:f:198:PHE:CE2	3.00	0.50
1:f:755:ALA:HB1	1:f:789:TRP:CH2	2.44	0.50
1:f:1043:VAL:HG23	1:f:1180:ALA:O	2.12	0.50
10:u:119:ARG:CG	10:u:119:ARG:NH1	2.73	0.50
28:5:455:LEU:CD2	28:5:458:LYS:H	2.23	0.50
38:w:32:ASP:OD2	38:w:35:GLU:CD	2.54	0.50
40:Y:229:ARG:CB	40:Y:229:ARG:CZ	2.89	0.50
46:C:228:GLU:HB3	46:C:229:GLU:OE1	2.10	0.50
1:f:753:MET:HA	1:f:756:ILE:HD12	1.93	0.50
18:U:71:ARG:HH11	18:U:71:ARG:CG	2.13	0.50
28:5:226:ILE:CG2	28:5:227:PRO:HD2	2.42	0.50
37:V:61:ARG:NH1	37:V:91:PHE:CE1	2.79	0.50
39:E:279:TYR:CZ	46:C:411:ARG:CG	2.94	0.50
1:f:742:ASN:HA	1:f:745:ARG:HE	1.77	0.50
1:f:834:PHE:CE1	46:C:5:PHE:CE2	3.00	0.50
1:f:1397:LEU:HG	1:f:1401:GLU:OE2	2.12	0.50
1:f:1491:MET:SD	1:f:1671:ARG:CZ	3.00	0.50
37:V:34:LYS:O	37:V:36:LYS:N	2.44	0.50
51:A:25:MET:HB3	51:A:26:ASP:HA	1.94	0.50
1:f:150:PHE:HE1	1:f:196:VAL:HG21	1.77	0.50
1:f:739:ARG:O	1:f:740:THR:C	2.55	0.50
1:f:1521:ARG:CG	1:f:1521:ARG:NH1	2.73	0.50
1:f:1549:ARG:HH21	1:f:1575:ASP:HB2	1.77	0.50
3:0:816:C:H5	26:J:137:LYS:NZ	2.10	0.50
18:U:96:GLY:HA3	51:A:371:LYS:HE3	1.93	0.50
27:h:71:GLU:O	27:h:72:GLU:HB2	2.12	0.50
28:5:65:LYS:NZ	28:5:144:GLY:HA3	2.27	0.50
40:Y:230:ARG:CG	40:Y:230:ARG:NH2	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:8:16:THR:HG21	48:W:194:ILE:CD1	2.41	0.50
1:f:1546:ARG:HH11	1:f:1547:LYS:N	2.09	0.50
28:5:456:VAL:O	28:5:457:GLU:HG3	2.11	0.50
47:8:8:ARG:NH1	48:W:76:THR:CB	2.68	0.50
51:A:294:ARG:CG	51:A:294:ARG:NH2	2.73	0.50
1:f:133:ARG:NH2	1:f:307:LEU:CD2	2.75	0.50
1:f:1397:LEU:O	1:f:1401:GLU:OE1	2.28	0.50
23:d:146:ILE:HD12	23:d:225:LEU:HB3	1.94	0.50
38:w:136:VAL:C	38:w:138:GLU:H	2.19	0.50
47:8:8:ARG:NH2	48:W:75:LYS:HD3	2.26	0.50
48:W:162:LEU:HD22	48:W:207:VAL:CG1	2.22	0.50
1:f:797:GLN:HG3	1:f:798:LEU:H	1.77	0.49
2:l:25:G:O2'	7:n:255:ASN:ND2	2.39	0.49
7:n:125:LYS:CD	7:n:125:LYS:N	2.74	0.49
20:X:38:LYS:HB2	20:X:38:LYS:NZ	2.25	0.49
28:5:430:ASN:ND2	40:Y:205:THR:HG21	2.27	0.49
47:8:42:PRO:N	47:8:43:MET:CA	2.73	0.49
1:f:746:ASP:OD1	46:C:5:PHE:CD2	2.66	0.49
1:f:773:THR:O	1:f:774:LEU:HG	2.12	0.49
1:f:1534:ARG:O	1:f:1535:ILE:C	2.54	0.49
5:s:305:THR:CG2	5:s:358:LYS:HB2	2.41	0.49
28:5:85:VAL:HB	28:5:88:ILE:HG12	1.93	0.49
37:V:34:LYS:NZ	37:V:35:GLY:N	2.60	0.49
1:f:2:SER:HA	1:f:5:TYR:HD2	1.77	0.49
16:S:38:CYS:SG	16:S:64:LEU:HD21	2.51	0.49
46:C:53:ARG:O	46:C:54:ASN:HA	2.11	0.49
47:8:40:TRP:CH2	47:8:87:GLY:CA	2.68	0.49
47:8:41:GLY:CA	47:8:42:PRO:C	2.85	0.49
48:W:141:VAL:HG12	48:W:142:ILE:H	1.77	0.49
51:A:151:LEU:HD23	51:A:294:ARG:HD3	1.94	0.49
51:A:152:VAL:CG2	51:A:293:THR:HG21	2.42	0.49
1:f:3:SER:N	27:h:70:ASP:OD1	2.43	0.49
1:f:739:ARG:O	1:f:741:THR:N	2.45	0.49
1:f:1632:HIS:HE2	1:f:1641:ARG:NH2	2.03	0.49
10:u:68:ILE:HD12	10:u:68:ILE:H	1.77	0.49
28:5:413:ILE:HG22	28:5:415:VAL:HG23	1.94	0.49
37:V:59:GLN:O	37:V:62:TRP:O	2.31	0.49
46:C:4:PHE:O	46:C:5:PHE:HB3	2.12	0.49
46:C:229:GLU:O	46:C:230:ASP:HB3	2.11	0.49
47:8:6:LYS:O	47:8:7:THR:HG22	2.13	0.49
47:8:42:PRO:O	47:8:45:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:1221:LEU:C	1:f:1222:PRO:CD	2.78	0.49
47:8:73:TRP:O	47:8:76:ASN:CG	2.54	0.49
48:W:70:LEU:HD13	48:W:86:VAL:HG21	1.93	0.49
6:j:133:GLN:HE21	6:j:138:LYS:HG2	1.76	0.49
37:V:99:THR:C	37:V:100:GLU:CG	2.85	0.49
1:f:1632:HIS:ND1	1:f:1641:ARG:HB2	2.28	0.49
28:5:79:LYS:CE	28:5:357:GLN:OE1	2.61	0.49
48:W:69:ASN:ND2	48:W:70:LEU:O	2.46	0.49
1:f:902:ARG:HE	1:f:956:HIS:CE1	2.31	0.49
1:f:1238:ILE:CD1	1:f:1264:LEU:HD12	2.40	0.49
7:n:125:LYS:HZ2	40:Y:364:GLN:NE2	2.04	0.49
10:u:14:VAL:HG22	10:u:15:ARG:H	1.78	0.49
28:5:219:ASP:OD1	40:Y:229:ARG:HG2	2.13	0.49
46:C:192:LYS:HG2	46:C:193:GLY:N	2.28	0.49
46:C:295:ARG:NH1	51:A:44:TRP:CZ2	2.81	0.49
1:f:306:ARG:N	1:f:306:ARG:C	2.61	0.49
1:f:1068:ASN:CB	1:f:1122:GLN:CD	2.86	0.49
40:Y:331:PHE:HZ	40:Y:337:LYS:HZ3	1.60	0.49
46:C:233:LEU:CD1	46:C:235:TYR:OH	2.61	0.49
46:C:329:GLN:CB	46:C:331:ARG:HD2	2.43	0.49
47:8:17:LEU:CD2	47:8:25:GLU:OE1	2.60	0.49
1:f:758:ARG:HD3	1:f:789:TRP:CH2	2.46	0.48
1:f:837:ILE:CD1	46:C:9:ASP:HB3	2.21	0.48
1:f:1632:HIS:CE1	1:f:1641:ARG:HH21	2.21	0.48
5:s:306:ILE:CD1	5:s:306:ILE:C	2.86	0.48
36:c:8:LEU:C	36:c:10:ARG:H	2.20	0.48
38:w:34:GLN:NE2	38:w:35:GLU:CG	2.75	0.48
39:E:132:TYR:H	39:E:135:ALA:H	1.61	0.48
48:W:75:LYS:HD3	48:W:76:THR:CB	2.33	0.48
1:f:136:LEU:O	1:f:136:LEU:CG	2.43	0.48
1:f:295:ASN:CB	1:f:296:TYR:HA	2.42	0.48
5:s:343:ILE:N	5:s:356:ARG:HE	2.10	0.48
28:5:65:LYS:CD	55:5:502:GNP:O2G	2.59	0.48
38:w:166:THR:O	38:w:168:ASP:N	2.46	0.48
46:C:189:VAL:C	46:C:190:ILE:CG1	2.86	0.48
47:8:75:ARG:CB	47:8:76:ASN:HB3	2.42	0.48
51:A:148:ASN:HD22	51:A:303:PRO:HG3	1.76	0.48
51:A:253:THR:HG23	51:A:381:ALA:H	1.78	0.48
1:f:1071:VAL:HG11	1:f:1147:ILE:CG1	2.20	0.48
3:0:1992:A:H3'	3:0:1993:U:H5'	1.94	0.48
7:n:206:GLU:O	38:w:133:TYR:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:206:GLU:OE2	7:n:208:ASN:HB2	2.14	0.48
28:5:455:LEU:CD2	28:5:458:LYS:N	2.73	0.48
37:V:89:LYS:CG	37:V:103:LEU:CD2	2.57	0.48
39:E:241:SER:HA	39:E:244:GLU:OE1	2.13	0.48
46:C:331:ARG:HA	46:C:332:LYS:HB3	1.95	0.48
1:f:902:ARG:HH11	28:5:205:VAL:HG12	1.78	0.48
1:f:1397:LEU:HD11	1:f:1401:GLU:OE2	2.13	0.48
3:0:230:G:H5''	26:J:157:PHE:CZ	2.48	0.48
10:u:119:ARG:HE	38:w:164:LEU:HD23	1.78	0.48
43:G:121:MET:HE1	43:G:141:THR:HB	1.96	0.48
47:8:44:TYR:O	47:8:48:LEU:HD13	2.12	0.48
51:A:152:VAL:HG11	51:A:293:THR:CG2	2.11	0.48
1:f:834:PHE:HD2	46:C:10:SER:OG	1.94	0.48
1:f:955:LYS:HE3	1:f:989:GLN:CD	2.38	0.48
1:f:1039:ARG:HD3	1:f:1177:PRO:HG2	1.95	0.48
7:n:206:GLU:OE1	7:n:294:ILE:HG13	2.13	0.48
27:h:123:VAL:HG12	27:h:125:ASP:H	1.78	0.48
28:5:219:ASP:OD1	28:5:219:ASP:O	2.31	0.48
28:5:252:PRO:HG2	28:5:254:ARG:NH1	2.28	0.48
36:c:8:LEU:HD22	38:w:86:ARG:CZ	2.42	0.48
47:8:24:LYS:HD2	47:8:24:LYS:H	1.74	0.48
7:n:326:TYR:HD1	7:n:327:SER:N	2.12	0.48
18:U:78:SER:CB	51:A:126:GLN:HG2	2.44	0.48
47:8:62:ILE:HG22	47:8:64:VAL:N	2.26	0.48
1:f:5:TYR:OH	6:j:94:LYS:CG	2.61	0.48
1:f:1268:SER:HB2	1:f:1716:LYS:CG	2.44	0.48
3:0:47:A:H4'	3:0:48:G:H5''	1.96	0.48
28:5:307:GLN:NE2	28:5:321:LEU:HD11	2.26	0.48
40:Y:229:ARG:NH2	40:Y:229:ARG:CB	2.77	0.48
47:8:53:GLU:HG3	47:8:98:HIS:CG	2.49	0.48
1:f:240:PHE:HB2	1:f:241:SER:HB2	1.95	0.48
1:f:292:ARG:HD2	1:f:308:ARG:HH12	1.79	0.48
1:f:307:LEU:CG	1:f:308:ARG:HG2	2.44	0.48
1:f:772:TYR:O	7:n:204:MET:HE2	2.14	0.48
5:s:306:ILE:HD11	5:s:369:MET:HE2	1.90	0.48
10:u:119:ARG:NH1	38:w:162:ASP:OD1	2.46	0.48
37:V:102:ASN:N	37:V:102:ASN:ND2	2.60	0.48
47:8:6:LYS:C	47:8:7:THR:HG23	2.38	0.48
1:f:762:GLU:OE2	1:f:782:VAL:HG23	2.14	0.48
3:0:1438:G:OP1	46:C:330:GLN:HA	2.14	0.48
7:n:314:ALA:HB1	55:5:502:GNP:O2'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:154:ASN:O	28:5:417:THR:HG23	2.14	0.48
28:5:456:VAL:HG22	28:5:459:ASN:O	2.14	0.48
46:C:95:LYS:HB3	46:C:96:GLU:HB2	1.95	0.48
46:C:232:ARG:O	46:C:234:PRO:O	2.32	0.48
47:8:78:LEU:HD12	47:8:79:ARG:H	1.79	0.48
3:0:814:C:H5	26:J:105:ILE:HG21	1.75	0.47
28:5:201:LEU:HD12	55:5:502:GNP:HN21	1.76	0.47
46:C:2:SER:CA	46:C:3:ASN:HB2	2.44	0.47
1:f:150:PHE:CD2	1:f:198:PHE:HZ	2.29	0.47
1:f:1039:ARG:HG2	1:f:1177:PRO:HB2	1.96	0.47
3:0:268:C:H5''	26:J:174:LYS:HE3	1.94	0.47
13:o:177:LYS:HE3	13:o:177:LYS:O	2.14	0.47
39:E:279:TYR:CE1	46:C:411:ARG:HG2	2.49	0.47
1:f:902:ARG:CD	28:5:205:VAL:HG13	2.39	0.47
1:f:1075:LEU:HD21	1:f:1128:PRO:CG	2.44	0.47
7:n:326:TYR:CE2	37:V:77:VAL:CB	2.95	0.47
11:m:81:ILE:HG22	11:m:82:ILE:O	2.14	0.47
11:m:96:GLU:C	11:m:97:ASN:ND2	2.69	0.47
28:5:172:PHE:CD1	28:5:213:LYS:HE2	2.50	0.47
39:E:145:VAL:H	39:E:146:VAL:HA	1.79	0.47
1:f:1629:ILE:O	1:f:1629:ILE:HG22	2.14	0.47
7:n:206:GLU:OE2	7:n:206:GLU:HA	2.13	0.47
51:A:371:LYS:CB	51:A:371:LYS:NZ	2.77	0.47
5:s:306:ILE:O	5:s:306:ILE:HD12	2.14	0.47
10:u:117:LYS:O	10:u:119:ARG:HD3	2.15	0.47
37:V:52:ARG:HH11	37:V:56:ARG:NH2	2.11	0.47
37:V:99:THR:C	37:V:101:GLN:N	2.73	0.47
45:T:137:ARG:HH11	45:T:137:ARG:CG	2.26	0.47
1:f:150:PHE:HD1	1:f:196:VAL:HB	1.75	0.47
1:f:771:GLY:HA3	1:f:772:TYR:CB	2.44	0.47
1:f:902:ARG:NH2	1:f:956:HIS:HE1	2.03	0.47
1:f:1491:MET:CE	1:f:1671:ARG:NH1	2.77	0.47
5:s:304:ALA:O	5:s:305:THR:HG23	2.10	0.47
28:5:281:LEU:HD23	28:5:283:GLY:N	2.29	0.47
1:f:243:TYR:CZ	1:f:322:ASP:O	2.65	0.47
1:f:785:LYS:CD	1:f:889:LEU:CD2	2.80	0.47
1:f:989:GLN:OE1	28:5:212:HIS:NE2	2.47	0.47
1:f:1496:VAL:CB	1:f:1657:PHE:CD1	2.94	0.47
7:n:326:TYR:HD1	7:n:327:SER:H	1.62	0.47
11:m:97:ASN:N	11:m:97:ASN:ND2	2.61	0.47
18:U:83:ARG:CG	18:U:83:ARG:NH2	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:V:17:VAL:C	37:V:19:ASP:N	2.73	0.47
37:V:96:ASN:OD1	37:V:96:ASN:N	2.41	0.47
46:C:3:ASN:O	46:C:4:PHE:HB2	2.15	0.47
46:C:190:ILE:O	46:C:191:GLN:HG3	2.13	0.47
46:C:330:GLN:O	46:C:331:ARG:C	2.54	0.47
49:I:303:TRP:CG	49:I:304:LEU:H	2.33	0.47
5:s:316:GLN:C	5:s:318:ASP:N	2.73	0.47
20:X:91:HIS:CE1	20:X:102:ARG:HH21	2.33	0.47
20:X:124:VAL:HG22	20:X:125:HIS:H	1.80	0.47
28:5:170:GLU:HB3	28:5:171:PRO:HD3	1.97	0.47
1:f:1077:PRO:HG3	1:f:1153:ASP:O	2.15	0.47
3:0:2008:G:H1	3:0:2131:A:H1'	1.80	0.47
5:s:324:ARG:HH22	28:5:278:ILE:CG2	2.28	0.47
10:u:117:LYS:O	10:u:119:ARG:HG2	2.14	0.47
1:f:909:ARG:NH1	1:f:991:LYS:CE	2.57	0.47
5:s:320:VAL:HG13	28:5:351:ASP:N	2.30	0.47
5:s:331:ARG:CG	5:s:344:SER:HG	2.27	0.47
7:n:203:ALA:O	7:n:293:LYS:HD2	2.15	0.47
37:V:49:LEU:HD21	46:C:31:ILE:HG12	1.96	0.47
38:w:133:TYR:CD2	38:w:133:TYR:N	2.83	0.47
47:8:73:TRP:O	47:8:76:ASN:CA	2.61	0.47
51:A:292:LYS:H	51:A:292:LYS:HE2	1.78	0.47
1:f:909:ARG:HH12	1:f:991:LYS:HE2	1.74	0.46
1:f:1595:ILE:CD1	1:f:1628:GLY:CA	2.92	0.46
31:L:51:VAL:HG13	31:L:52:ARG:H	1.81	0.46
46:C:230:ASP:CG	46:C:231:THR:N	2.73	0.46
48:W:76:THR:H	48:W:77:GLN:CB	2.28	0.46
1:f:297:THR:CG2	1:f:298:ASP:O	2.56	0.46
1:f:1041:SER:CB	1:f:1178:PHE:CZ	2.97	0.46
3:0:1361:C:OP1	46:C:53:ARG:CG	2.45	0.46
5:s:307:HIS:HB3	5:s:356:ARG:HA	1.98	0.46
10:u:119:ARG:NE	38:w:164:LEU:HD23	2.30	0.46
1:f:133:ARG:HH21	1:f:307:LEU:HD23	1.81	0.46
1:f:149:PHE:CE1	1:f:261:LEU:HB2	2.45	0.46
1:f:1546:ARG:HG3	1:f:1547:LYS:N	2.30	0.46
5:s:332:ARG:HG2	5:s:334:LYS:O	2.16	0.46
46:C:437:ASN:HD21	51:A:26:ASP:N	2.13	0.46
5:s:148:THR:OG1	13:o:122:ARG:NH1	2.46	0.46
5:s:307:HIS:HD2	5:s:356:ARG:HA	1.81	0.46
16:S:56:GLN:HB3	16:S:61:ALA:HA	1.97	0.46
25:a:84:LYS:H	25:a:84:LYS:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:8:83:HIS:CE1	51:A:113:LYS:HE2	2.51	0.46
1:f:1556:LYS:CA	1:f:1557:ARG:HG3	2.44	0.46
28:5:223:GLY:C	28:5:225:ASN:N	2.73	0.46
28:5:413:ILE:HD12	28:5:422:ALA:HB2	1.97	0.46
1:f:150:PHE:CE2	1:f:198:PHE:HZ	2.33	0.46
1:f:738:GLY:O	1:f:742:ASN:ND2	2.48	0.46
1:f:1039:ARG:CD	1:f:1177:PRO:HG3	2.45	0.46
3:0:230:G:H5''	26:J:157:PHE:HZ	1.81	0.46
5:s:315:PHE:O	5:s:316:GLN:CB	2.42	0.46
11:m:96:GLU:O	11:m:97:ASN:CB	2.64	0.46
27:h:69:GLU:O	27:h:71:GLU:N	2.49	0.46
47:8:42:PRO:HB3	47:8:45:ILE:HB	1.97	0.46
47:8:79:ARG:CG	47:8:84:LEU:HD13	2.44	0.46
48:W:79:ASP:C	48:W:81:ASP:N	2.73	0.46
1:f:1496:VAL:CB	1:f:1657:PHE:CE1	2.99	0.46
5:s:148:THR:O	5:s:149:SER:CB	2.63	0.46
28:5:65:LYS:HE2	55:5:502:GNP:O3G	2.15	0.46
46:C:490:LYS:CB	51:A:29:LYS:HZ1	2.28	0.46
47:8:77:LYS:CD	51:A:96:HIS:HD2	2.15	0.46
5:s:327:LEU:HD13	28:5:280:ASN:OD1	2.15	0.46
51:A:148:ASN:HA	51:A:301:LYS:O	2.16	0.46
51:A:302:ASN:N	51:A:302:ASN:OD1	2.48	0.46
1:f:151:ILE:CD1	1:f:261:LEU:HD13	2.43	0.46
1:f:1032:LEU:HD13	1:f:1220:LEU:HD12	1.92	0.46
5:s:149:SER:OG	5:s:150:ALA:N	2.48	0.46
7:n:249:GLU:CD	7:n:280:LYS:NZ	2.67	0.46
7:n:282:LEU:HD22	7:n:294:ILE:CD1	2.46	0.46
7:n:333:ARG:HB3	7:n:334:SER:H	1.58	0.46
28:5:281:LEU:CD2	28:5:282:ARG:N	2.73	0.46
37:V:12:GLN:HB3	37:V:13:GLN:H	1.63	0.46
1:f:743:ARG:NH2	1:f:746:ASP:OD2	2.49	0.46
1:f:768:PHE:CA	1:f:773:THR:OG1	2.64	0.46
7:n:205:THR:O	7:n:206:GLU:HB3	2.16	0.46
28:5:455:LEU:HD21	28:5:458:LYS:CA	2.45	0.46
46:C:418:LEU:O	51:A:15:THR:O	2.33	0.46
51:A:257:LEU:N	51:A:257:LEU:CD1	2.73	0.46
1:f:261:LEU:CD1	1:f:295:ASN:HD21	2.23	0.45
3:0:1207:G:H1	3:0:1300:U:H3	1.65	0.45
3:0:2032:C:H5	3:0:2045:G:H1	1.64	0.45
5:s:319:GLY:CA	28:5:351:ASP:OD2	2.58	0.45
28:5:182:LYS:CE	28:5:389:VAL:CG1	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:458:LYS:HG2	46:C:26:ARG:HG2	1.97	0.45
37:V:97:MET:HE2	37:V:97:MET:HB2	1.67	0.45
47:8:39:GLN:C	47:8:45:ILE:HD13	2.33	0.45
1:f:257:PRO:C	1:f:258:GLU:CG	2.85	0.45
7:n:135:ARG:NH2	40:Y:332:ILE:HG12	2.25	0.45
11:m:73:GLN:HE21	11:m:73:GLN:HB2	1.59	0.45
40:Y:229:ARG:NH2	40:Y:229:ARG:HB3	2.31	0.45
46:C:34:LYS:HA	46:C:34:LYS:HE3	1.98	0.45
47:8:41:GLY:HA3	47:8:42:PRO:C	2.41	0.45
1:f:769:ASP:C	1:f:771:GLY:N	2.73	0.45
21:B:103:ILE:H	21:B:103:ILE:HD12	1.80	0.45
37:V:54:ILE:HG22	37:V:58:PHE:HE2	1.78	0.45
46:C:181:ILE:HD12	46:C:208:LYS:HG2	1.97	0.45
50:H:297:LEU:HG	50:H:298:GLY:H	1.82	0.45
51:A:148:ASN:HD21	51:A:303:PRO:CG	2.23	0.45
51:A:297:MET:HB3	51:A:298:LYS:H	1.49	0.45
1:f:1149:TYR:C	1:f:1150:VAL:CA	2.79	0.45
5:s:305:THR:CB	5:s:358:LYS:HB3	2.34	0.45
1:f:294:ALA:CB	1:f:295:ASN:ND2	2.80	0.45
1:f:1214:ARG:O	1:f:1215:ASP:C	2.50	0.45
7:n:206:GLU:CG	38:w:133:TYR:CD2	2.99	0.45
28:5:421:GLY:HA2	37:V:12:GLN:HE22	1.81	0.45
45:T:51:HIS:CE1	45:T:55:HIS:CE1	3.04	0.45
1:f:93:GLU:CD	1:f:93:GLU:N	2.73	0.45
1:f:1494:THR:HG21	1:f:1674:VAL:HG23	1.98	0.45
20:X:34:HIS:CG	20:X:35:ASN:N	2.82	0.45
36:c:50:LYS:HB2	36:c:51:PRO:HD2	1.98	0.45
46:C:34:LYS:N	46:C:34:LYS:CD	2.73	0.45
51:A:151:LEU:HD23	51:A:294:ARG:CD	2.46	0.45
1:f:1483:LEU:HD21	1:f:1657:PHE:CE2	2.51	0.45
3:0:816:C:C5	26:J:137:LYS:NZ	2.85	0.45
6:j:133:GLN:HE22	6:j:138:LYS:CG	2.28	0.45
20:X:33:SER:HB2	20:X:34:HIS:HA	1.95	0.45
28:5:154:ASN:OD1	28:5:419:THR:CG2	2.62	0.45
36:c:9:ALA:O	36:c:10:ARG:NE	2.44	0.45
46:C:53:ARG:O	46:C:54:ASN:CA	2.65	0.45
46:C:274:LYS:H	46:C:275:ARG:HA	1.82	0.45
47:8:30:LEU:HD23	47:8:33:LEU:HD23	1.99	0.45
51:A:151:LEU:HD12	51:A:290:CYS:HB3	1.99	0.45
1:f:1237:TYR:HB3	1:f:1263:ASP:HA	1.99	0.45
5:s:305:THR:CB	5:s:358:LYS:CA	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:73:MET:HE1	51:A:435:LEU:HD22	1.98	0.45
18:U:98:MET:HE1	51:A:371:LYS:N	2.18	0.45
27:h:72:GLU:C	27:h:74:LYS:H	2.24	0.45
46:C:191:GLN:HE21	46:C:191:GLN:N	2.15	0.45
1:f:1109:LEU:HD23	1:f:1110:GLY:O	2.17	0.45
27:h:69:GLU:HG2	27:h:70:ASP:H	1.78	0.45
37:V:99:THR:O	37:V:99:THR:OG1	2.30	0.45
37:V:99:THR:O	37:V:101:GLN:N	2.50	0.45
48:W:75:LYS:CA	48:W:76:THR:HG22	2.46	0.45
46:C:234:PRO:O	46:C:235:TYR:CG	2.70	0.45
1:f:955:LYS:NZ	1:f:989:GLN:NE2	2.65	0.44
46:C:329:GLN:HA	46:C:331:ARG:HD2	1.99	0.44
1:f:834:PHE:CD1	46:C:5:PHE:CE1	3.03	0.44
1:f:902:ARG:CD	28:5:205:VAL:CG1	2.94	0.44
1:f:1041:SER:HB3	1:f:1178:PHE:CE1	2.52	0.44
28:5:412:GLN:HG3	28:5:413:ILE:N	2.29	0.44
46:C:28:VAL:CG1	46:C:29:ALA:CA	2.88	0.44
46:C:31:ILE:HG23	46:C:35:TRP:HB2	1.94	0.44
46:C:384:LEU:HD23	51:A:11:ASN:ND2	2.32	0.44
50:H:96:THR:HB	50:H:97:PRO:HD3	1.99	0.44
51:A:150:PRO:CG	51:A:311:LEU:CD1	2.59	0.44
51:A:292:LYS:N	51:A:292:LYS:CE	2.73	0.44
1:f:90:ALA:H	1:f:93:GLU:CG	2.30	0.44
1:f:309:ARG:HG3	1:f:310:GLN:H	1.82	0.44
38:w:130:HIS:CD2	38:w:131:SER:O	2.71	0.44
38:w:166:THR:C	38:w:168:ASP:N	2.73	0.44
46:C:6:ASP:CB	46:C:7:VAL:HA	2.46	0.44
46:C:331:ARG:CA	46:C:332:LYS:CB	2.95	0.44
51:A:302:ASN:ND2	51:A:306:ASP:OD1	2.50	0.44
1:f:1039:ARG:CD	1:f:1177:PRO:CG	2.96	0.44
7:n:205:THR:OG1	7:n:207:ARG:HG3	2.17	0.44
7:n:266:TYR:CD2	7:n:268:ILE:HG13	2.53	0.44
16:S:63:LYS:CD	46:C:192:LYS:CG	2.88	0.44
28:5:413:ILE:CD1	28:5:436:LEU:HD13	2.36	0.44
28:5:430:ASN:ND2	40:Y:205:THR:CG2	2.80	0.44
46:C:37:GLU:OE1	46:C:39:THR:N	2.24	0.44
1:f:1039:ARG:HD3	1:f:1177:PRO:CG	2.47	0.44
26:J:222:LEU:HB2	26:J:223:ALA:HA	1.99	0.44
50:H:51:LEU:HD22	50:H:51:LEU:H	1.82	0.44
1:f:793:VAL:HA	1:f:797:GLN:HG2	1.98	0.44
16:S:55:VAL:O	16:S:63:LYS:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:51:LEU:HD23	18:U:98:MET:CG	2.37	0.44
1:f:203:LEU:H	1:f:243:TYR:HB3	1.82	0.44
3:0:1212:U:O4	48:W:161:ARG:NH1	2.51	0.44
5:s:145:VAL:HG12	5:s:147:ASP:H	1.82	0.44
28:5:67:THR:HG22	28:5:68:VAL:N	2.31	0.44
28:5:244:GLU:HG2	28:5:248:HIS:NE2	2.32	0.44
28:5:271:ASN:ND2	28:5:274:GLY:H	2.05	0.44
46:C:6:ASP:CB	46:C:7:VAL:CA	2.96	0.44
1:f:132:ALA:HB1	1:f:306:ARG:HE	1.83	0.44
1:f:150:PHE:CE1	1:f:196:VAL:HG21	2.53	0.44
1:f:241:SER:HA	1:f:242:SER:HA	1.57	0.44
1:f:1126:THR:HG21	1:f:1130:THR:HG21	1.99	0.44
3:0:282:C:O4'	26:J:183:ASN:HB2	2.17	0.44
3:0:1212:U:O4	3:0:1531:A:N3	2.51	0.44
38:w:136:VAL:HG13	38:w:136:VAL:O	2.17	0.44
40:Y:232:ILE:HD13	40:Y:273:ARG:NH2	2.33	0.44
47:8:24:LYS:CD	47:8:24:LYS:H	2.28	0.44
5:s:331:ARG:HD3	5:s:331:ARG:N	2.33	0.44
45:T:137:ARG:HG2	45:T:137:ARG:HH11	1.83	0.44
46:C:28:VAL:HG12	46:C:29:ALA:CA	2.46	0.44
47:8:27:VAL:CG1	47:8:66:ARG:CZ	2.96	0.44
3:0:1652:G:H21	3:0:1982:G:H22	1.66	0.43
5:s:306:ILE:HD12	5:s:306:ILE:N	2.33	0.43
7:n:333:ARG:O	7:n:336:ALA:N	2.48	0.43
47:8:8:ARG:C	47:8:10:CYS:N	2.75	0.43
51:A:146:LEU:C	51:A:300:GLU:HG3	2.43	0.43
51:A:152:VAL:CB	51:A:293:THR:HG21	2.38	0.43
1:f:286:ASN:HD21	1:f:306:ARG:HH11	1.65	0.43
1:f:286:ASN:HD21	1:f:306:ARG:HH12	1.66	0.43
1:f:1258:ASN:O	1:f:1259:CYS:HB2	2.17	0.43
28:5:176:GLN:HG3	28:5:180:HIS:CE1	2.53	0.43
46:C:559:GLN:HE22	46:C:583:GLY:HA3	1.83	0.43
51:A:151:LEU:CA	51:A:293:THR:O	2.63	0.43
1:f:1214:ARG:C	1:f:1215:ASP:O	2.55	0.43
3:0:724:A:C2	3:0:734:G:N1	2.86	0.43
11:m:40:PRO:CB	11:m:81:ILE:CD1	2.93	0.43
31:L:65:THR:HG22	31:L:67:CYS:H	1.83	0.43
46:C:233:LEU:HD11	46:C:235:TYR:OH	2.18	0.43
47:8:194:ILE:H	47:8:194:ILE:HD12	1.83	0.43
51:A:151:LEU:HD23	51:A:294:ARG:NE	2.25	0.43
1:f:870:ARG:HH12	46:C:1:MET:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:1042:ALA:HA	1:f:1218:VAL:O	2.19	0.43
1:f:1526:ASN:O	1:f:1529:ALA:HB3	2.19	0.43
3:0:1478:U:H5	46:C:232:ARG:HH12	1.52	0.43
3:0:2303:G:C2	37:V:63:GLY:HA2	2.53	0.43
5:s:318:ASP:O	5:s:383:ARG:C	2.54	0.43
28:5:118:GLN:HB3	28:5:119:PRO:HD2	2.01	0.43
40:Y:284:ASP:CG	40:Y:288:ASP:OD1	2.61	0.43
47:8:80:GLY:O	51:A:109:PRO:N	2.51	0.43
51:A:48:MET:HE1	51:A:52:ALA:HB2	1.99	0.43
3:0:814:C:C6	26:J:105:ILE:HG21	2.53	0.43
5:s:149:SER:HA	5:s:166:TYR:N	2.34	0.43
5:s:166:TYR:C	5:s:167:THR:HG1	2.19	0.43
31:L:86:VAL:HG22	31:L:87:GLU:H	1.83	0.43
47:8:16:THR:HG21	48:W:194:ILE:HD11	2.00	0.43
48:W:84:ARG:NH1	48:W:105:MET:HE1	2.32	0.43
51:A:8:ILE:H	51:A:8:ILE:HG12	1.51	0.43
1:f:262:MET:HG3	1:f:263:SER:H	1.84	0.43
1:f:1060:MET:HE2	1:f:1123:VAL:HG11	2.01	0.43
3:0:1701:G:N2	6:j:94:LYS:NZ	2.66	0.43
28:5:208:GLN:O	28:5:209:ASP:C	2.59	0.43
32:M:113:GLN:HG3	32:M:114:VAL:H	1.83	0.43
46:C:24:VAL:HG13	46:C:27:LYS:HB2	1.99	0.43
46:C:331:ARG:HA	46:C:332:LYS:CB	2.49	0.43
46:C:433:ALA:O	46:C:436:TYR:HB3	2.19	0.43
1:f:285:ASN:OD1	1:f:291:ARG:NH2	2.51	0.43
1:f:1149:TYR:OH	1:f:1179:VAL:HG23	2.18	0.43
28:5:270:ILE:O	28:5:271:ASN:CG	2.62	0.43
37:V:53:ARG:CZ	46:C:37:GLU:CD	2.92	0.43
47:8:33:LEU:C	47:8:33:LEU:CD1	2.85	0.43
1:f:1203:LYS:CB	1:f:1215:ASP:OD1	2.54	0.43
1:f:1644:VAL:CG1	1:f:1656:ILE:HD12	2.49	0.43
3:0:1881:G:H22	9:r:32:GLN:HE21	1.66	0.43
5:s:193:ARG:O	5:s:194:ILE:HG23	2.18	0.43
20:X:124:VAL:HG23	20:X:152:TYR:HB2	2.01	0.43
37:V:48:ALA:HB1	46:C:36:PHE:CE1	2.54	0.43
37:V:93:LEU:HD12	37:V:93:LEU:HA	1.86	0.43
47:8:8:ARG:C	47:8:10:CYS:H	2.26	0.43
51:A:67:LEU:H	51:A:67:LEU:HD12	1.84	0.43
1:f:785:LYS:NZ	1:f:785:LYS:CB	2.82	0.43
3:0:821:C:C2	26:J:152:PHE:HZ	2.37	0.43
32:M:198:GLU:CD	32:M:198:GLU:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:O:63:ALA:HB3	34:O:64:PRO:HD3	2.01	0.43
51:A:149:ARG:CD	51:A:295:TYR:HB3	2.45	0.43
1:f:1546:ARG:HH11	1:f:1547:LYS:CA	2.32	0.43
23:d:159:HIS:H	23:d:159:HIS:CD2	2.35	0.43
38:w:73:VAL:C	38:w:74:TRP:CE3	2.95	0.43
46:C:432:LEU:CA	46:C:435:LEU:HD23	2.49	0.43
47:8:35:GLU:CD	47:8:35:GLU:H	2.27	0.43
1:f:92:GLU:HB2	6:j:94:LYS:HD3	2.00	0.42
7:n:326:TYR:CE2	37:V:77:VAL:HG13	2.52	0.42
37:V:17:VAL:C	37:V:19:ASP:H	2.26	0.42
46:C:26:ARG:O	46:C:27:LYS:C	2.62	0.42
1:f:52:ILE:HD12	1:f:52:ILE:H	1.83	0.42
1:f:1071:VAL:HB	1:f:1147:ILE:HA	2.01	0.42
1:f:1644:VAL:HG11	1:f:1656:ILE:CD1	2.49	0.42
1:f:1735:ILE:H	1:f:1735:ILE:HD12	1.84	0.42
3:0:1360:A:O3'	46:C:52:SER:OG	2.36	0.42
46:C:384:LEU:HD23	51:A:11:ASN:CG	2.44	0.42
47:8:40:TRP:CD1	47:8:40:TRP:O	2.70	0.42
47:8:40:TRP:HA	47:8:45:ILE:HD12	2.00	0.42
1:f:1237:TYR:CD1	1:f:1261:ILE:CG2	3.02	0.42
3:0:1913:U:H3'	3:0:1914:U:H5'	2.01	0.42
5:s:350:PRO:HB3	28:5:268:PHE:HE1	1.84	0.42
16:S:45:THR:CG2	16:S:58:ASN:N	2.65	0.42
18:U:96:GLY:CA	51:A:371:LYS:HE3	2.50	0.42
28:5:79:LYS:HZ2	28:5:357:GLN:NE2	2.15	0.42
37:V:61:ARG:C	37:V:62:TRP:CG	2.96	0.42
45:T:137:ARG:NH1	45:T:137:ARG:CG	2.82	0.42
47:8:13:LYS:O	47:8:17:LEU:HD13	2.18	0.42
47:8:33:LEU:O	47:8:34:SER:C	2.62	0.42
47:8:36:HIS:HB2	47:8:37:GLY:CA	2.39	0.42
47:8:79:ARG:C	47:8:81:SER:N	2.73	0.42
47:8:369:PHE:H	47:8:370:GLY:CA	2.30	0.42
1:f:93:GLU:O	1:f:95:ARG:N	2.52	0.42
1:f:1064:LEU:HD23	1:f:1122:GLN:CD	2.44	0.42
1:f:1546:ARG:NH1	1:f:1547:LYS:CB	2.82	0.42
1:f:1549:ARG:NH2	1:f:1573:MET:CG	2.83	0.42
28:5:194:ILE:HD12	28:5:226:ILE:CG2	2.49	0.42
30:i:120:VAL:HA	30:i:121:ALA:HB2	2.01	0.42
36:c:10:ARG:HD3	36:c:10:ARG:HA	1.76	0.42
37:V:105:ILE:HG22	37:V:107:SER:H	1.84	0.42
46:C:232:ARG:HA	51:A:47:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:1644:VAL:HG11	1:f:1656:ILE:HD11	2.00	0.42
7:n:323:SER:O	7:n:324:ALA:CB	2.66	0.42
45:T:136:GLY:O	45:T:137:ARG:HB2	2.19	0.42
46:C:34:LYS:C	46:C:36:PHE:N	2.77	0.42
47:8:42:PRO:HD2	47:8:43:MET:CA	2.45	0.42
47:8:79:ARG:O	47:8:81:SER:N	2.53	0.42
1:f:92:GLU:CB	6:j:94:LYS:HD3	2.50	0.42
1:f:139:MET:CE	1:f:142:HIS:NE2	2.83	0.42
1:f:1304:VAL:HB	1:f:1306:TRP:HB3	2.02	0.42
1:f:1541:ALA:HB1	1:f:1545:ARG:NH1	2.25	0.42
10:u:116:ARG:O	10:u:119:ARG:CD	2.66	0.42
10:u:119:ARG:HD2	38:w:164:LEU:HD23	2.02	0.42
48:W:75:LYS:HA	48:W:76:THR:HA	1.73	0.42
48:W:76:THR:CG2	48:W:77:GLN:CB	2.85	0.42
1:f:762:GLU:CG	1:f:785:LYS:NZ	2.81	0.42
7:n:212:GLU:HA	38:w:135:PHE:HD1	1.80	0.42
13:o:165:ASN:O	13:o:176:ILE:CD1	2.67	0.42
16:S:45:THR:HG21	16:S:58:ASN:CA	2.45	0.42
46:C:191:GLN:NE2	46:C:191:GLN:C	2.73	0.42
47:8:6:LYS:O	47:8:7:THR:CG2	2.68	0.42
47:8:30:LEU:HA	47:8:33:LEU:CD2	2.34	0.42
48:W:162:LEU:HD21	48:W:206:ILE:O	2.18	0.42
1:f:149:PHE:HD1	1:f:259:PHE:O	2.02	0.42
1:f:1265:HIS:CE1	1:f:1289:GLU:OE2	2.73	0.42
1:f:1511:VAL:HG11	1:f:1629:ILE:HD11	2.02	0.42
1:f:1627:ARG:HB2	1:f:1629:ILE:HG22	2.02	0.42
3:0:196:U:C2	3:0:197:C:C5	3.07	0.42
3:0:943:G:H21	20:X:44:SER:HB3	1.85	0.42
3:0:1530:C:O2	3:0:1533:C:C5	2.73	0.42
5:s:146:ASN:O	5:s:147:ASP:HB2	2.19	0.42
40:Y:229:ARG:NH2	40:Y:229:ARG:CG	2.73	0.42
48:W:162:LEU:HD22	48:W:206:ILE:O	2.19	0.42
51:A:258:ARG:CD	51:A:274:LEU:HG	2.50	0.42
1:f:90:ALA:H	1:f:93:GLU:HG2	1.84	0.42
1:f:292:ARG:CZ	1:f:308:ARG:HH22	2.33	0.42
1:f:294:ALA:HB3	1:f:295:ASN:ND2	2.35	0.42
1:f:1126:THR:HB	1:f:1127:VAL:H	1.52	0.42
1:f:1218:VAL:CG1	1:f:1219:HIS:N	2.83	0.42
5:s:147:ASP:O	5:s:166:TYR:HD2	2.03	0.42
28:5:79:LYS:NZ	28:5:357:GLN:HE22	2.12	0.42
1:f:1109:LEU:HB3	1:f:1110:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:1437:C:OP1	46:C:268:SER:CB	2.68	0.42
3:0:1437:C:OP1	46:C:268:SER:HB2	2.20	0.42
5:s:300:ARG:O	5:s:301:ASN:HB2	2.19	0.42
28:5:171:PRO:HD2	28:5:174:GLN:HE21	1.84	0.42
28:5:172:PHE:CD1	28:5:213:LYS:CE	3.03	0.42
1:f:832:TYR:CD2	46:C:11:ASP:HB3	2.40	0.41
1:f:1496:VAL:CG1	1:f:1657:PHE:CE1	3.01	0.41
1:f:1624:ALA:C	1:f:1629:ILE:HG22	2.31	0.41
3:0:1969:U:H2'	3:0:1970:U:H5'	2.02	0.41
37:V:98:ALA:C	37:V:100:GLU:N	2.73	0.41
46:C:432:LEU:HA	46:C:435:LEU:HD23	2.02	0.41
47:8:17:LEU:HD21	47:8:25:GLU:OE1	2.19	0.41
1:f:240:PHE:CA	1:f:241:SER:CB	2.98	0.41
1:f:789:TRP:CE3	1:f:789:TRP:CA	3.02	0.41
13:o:18:GLN:NE2	51:A:426:LYS:C	2.78	0.41
13:o:18:GLN:HE21	51:A:426:LYS:HA	1.85	0.41
13:o:26:ASP:OD2	51:A:368:GLN:CG	2.68	0.41
18:U:68:VAL:HG22	18:U:69:ARG:H	1.85	0.41
18:U:76:GLU:HG2	51:A:219:ARG:NH1	2.35	0.41
28:5:182:LYS:HE3	28:5:389:VAL:CG1	2.50	0.41
28:5:400:LYS:CE	28:5:401:ARG:HH11	2.33	0.41
28:5:400:LYS:HD3	28:5:400:LYS:HA	1.67	0.41
28:5:400:LYS:HE3	46:C:20:HIS:O	2.19	0.41
28:5:413:ILE:HD11	28:5:436:LEU:CD1	2.35	0.41
38:w:166:THR:C	38:w:168:ASP:H	2.28	0.41
43:G:136:TRP:CD2	50:H:237:LEU:HD22	2.54	0.41
47:8:331:ALA:O	47:8:334:ALA:HB3	2.20	0.41
1:f:138:ASP:N	1:f:302:ALA:HB1	2.35	0.41
18:U:98:MET:HE3	51:A:371:LYS:HB2	2.00	0.41
37:V:29:ARG:HE	37:V:29:ARG:HB2	1.66	0.41
40:Y:227:VAL:CG1	40:Y:229:ARG:HD3	2.44	0.41
48:W:73:LEU:HD22	48:W:88:PHE:HE2	1.85	0.41
1:f:133:ARG:HH11	1:f:309:ARG:CZ	2.34	0.41
1:f:1039:ARG:HD2	1:f:1177:PRO:HG3	2.02	0.41
1:f:1311:SER:HB3	1:f:1312:LEU:HA	2.02	0.41
18:U:71:ARG:HE	51:A:378:ARG:HG3	1.85	0.41
28:5:79:LYS:HE2	28:5:357:GLN:OE1	2.21	0.41
28:5:182:LYS:HE3	28:5:389:VAL:HG11	2.00	0.41
28:5:209:ASP:O	28:5:210:GLN:C	2.64	0.41
37:V:34:LYS:HZ3	37:V:35:GLY:N	2.19	0.41
37:V:52:ARG:HG3	37:V:53:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:C:31:ILE:HG22	46:C:35:TRP:HB2	1.95	0.41
47:8:8:ARG:NH1	48:W:75:LYS:HD2	2.35	0.41
47:8:38:VAL:CG1	47:8:42:PRO:O	2.68	0.41
1:f:138:ASP:HA	1:f:139:MET:HA	0.67	0.41
37:V:53:ARG:NE	46:C:37:GLU:CB	2.83	0.41
37:V:89:LYS:CD	37:V:103:LEU:CD2	2.86	0.41
39:E:313:LEU:CB	39:E:314:GLY:HA2	2.50	0.41
46:C:204:GLN:O	46:C:207:LYS:CG	2.62	0.41
47:8:30:LEU:HD11	47:8:52:ALA:HA	2.00	0.41
51:A:294:ARG:HD3	51:A:294:ARG:HA	1.57	0.41
2:1:71:U:O2'	5:s:348:VAL:HG13	2.20	0.41
28:5:457:GLU:O	28:5:458:LYS:HB2	2.21	0.41
37:V:28:ILE:CD1	37:V:88:ILE:O	2.67	0.41
46:C:475:GLN:H	46:C:476:ARG:HB2	1.85	0.41
47:8:42:PRO:HB3	47:8:45:ILE:CB	2.50	0.41
47:8:42:PRO:C	47:8:45:ILE:HG13	2.46	0.41
1:f:1397:LEU:CG	1:f:1401:GLU:OE2	2.68	0.41
3:0:1977:G:H3'	3:0:1978:A:H5''	2.01	0.41
5:s:341:ILE:H	5:s:342:PRO:CD	2.32	0.41
28:5:280:ASN:HA	28:5:281:LEU:HA	1.56	0.41
46:C:346:LEU:H	46:C:347:GLY:C	2.29	0.41
47:8:38:VAL:O	47:8:45:ILE:CD1	2.63	0.41
47:8:531:LEU:O	47:8:535:PRO:HD2	2.20	0.41
51:A:8:ILE:HB	51:A:9:PHE:H	1.73	0.41
1:f:989:GLN:HE22	28:5:212:HIS:CD2	2.39	0.41
3:0:816:C:H5	26:J:137:LYS:HE3	1.85	0.41
5:s:169:ILE:HG23	5:s:205:LYS:CE	2.43	0.41
18:U:76:GLU:HG2	51:A:219:ARG:HH11	1.86	0.41
47:8:17:LEU:HG	47:8:25:GLU:HG3	1.52	0.41
48:W:79:ASP:O	48:W:81:ASP:N	2.54	0.41
51:A:148:ASN:ND2	51:A:303:PRO:HG2	2.33	0.41
1:f:298:ASP:O	1:f:302:ALA:O	2.39	0.41
1:f:739:ARG:O	1:f:742:ASN:N	2.54	0.41
1:f:1108:ALA:HB3	1:f:1114:TYR:O	2.13	0.41
1:f:1109:LEU:HD22	1:f:1110:GLY:O	2.21	0.41
1:f:1238:ILE:HD11	1:f:1264:LEU:CD1	2.45	0.41
3:0:772:U:C2	3:0:774:C:C5	3.09	0.41
28:5:280:ASN:HD22	28:5:281:LEU:HD13	1.85	0.41
46:C:31:ILE:N	46:C:31:ILE:HD12	2.36	0.41
46:C:34:LYS:HE3	46:C:34:LYS:CA	2.50	0.41
46:C:230:ASP:OD1	46:C:232:ARG:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:8:39:GLN:C	47:8:45:ILE:HD11	2.41	0.41
47:8:53:GLU:OE1	47:8:53:GLU:HA	2.20	0.41
48:W:40:VAL:HG23	48:W:75:LYS:HE3	1.87	0.41
48:W:84:ARG:HA	48:W:107:MET:HA	2.02	0.41
51:A:220:GLY:CA	51:A:253:THR:HB	2.51	0.41
1:f:5:TYR:HH	6:j:94:LYS:HD3	1.84	0.41
1:f:303:ASN:OD1	1:f:303:ASN:N	2.45	0.41
1:f:1108:ALA:HB1	1:f:1114:TYR:H	1.86	0.41
1:f:1265:HIS:NE2	1:f:1289:GLU:CD	2.78	0.41
36:c:10:ARG:HH12	38:w:35:GLU:HB2	1.84	0.41
47:8:39:GLN:CD	47:8:39:GLN:N	2.73	0.41
1:f:706:ILE:HG21	11:m:136:GLN:HB3	2.03	0.40
5:s:149:SER:O	5:s:150:ALA:CB	2.68	0.40
5:s:332:ARG:H	5:s:332:ARG:HG3	1.51	0.40
46:C:29:ALA:C	46:C:30:GLN:CG	2.93	0.40
1:f:292:ARG:HD3	1:f:308:ARG:NH2	2.35	0.40
1:f:758:ARG:HD3	1:f:789:TRP:HZ2	1.84	0.40
3:0:1476:U:H5	46:C:232:ARG:CZ	2.25	0.40
3:0:1866:A:H2	51:A:294:ARG:NH2	2.19	0.40
28:5:88:ILE:O	28:5:88:ILE:HG13	2.22	0.40
28:5:178:LEU:CD1	28:5:396:ASP:CG	2.69	0.40
28:5:282:ARG:O	28:5:283:GLY:O	2.29	0.40
40:Y:331:PHE:CE2	40:Y:337:LYS:NZ	2.89	0.40
47:8:261:SER:H	47:8:263:HIS:HB2	1.86	0.40
1:f:133:ARG:HH11	1:f:309:ARG:HH21	1.69	0.40
1:f:1072:VAL:H	1:f:1123:VAL:HG22	1.86	0.40
5:s:347:ILE:HD12	28:5:271:ASN:CB	2.40	0.40
10:u:119:ARG:HH11	10:u:119:ARG:HG3	1.79	0.40
39:E:244:GLU:HA	39:E:245:THR:HA	1.92	0.40
46:C:329:GLN:CA	46:C:331:ARG:H	2.34	0.40
46:C:494:LEU:HD12	51:A:29:LYS:HE3	2.02	0.40
47:8:42:PRO:CB	47:8:43:MET:C	2.85	0.40
48:W:162:LEU:CD1	48:W:207:VAL:CG1	2.94	0.40
1:f:1553:LEU:CD1	3:0:2176:C:N3	2.74	0.40
5:s:315:PHE:HA	28:5:351:ASP:OD1	2.22	0.40
5:s:319:GLY:HA3	28:5:351:ASP:HA	2.04	0.40
7:n:212:GLU:HA	7:n:213:PRO:HD2	1.87	0.40
14:q:21:ASP:HB3	14:q:52:ARG:HH21	1.87	0.40
26:J:157:PHE:HB3	26:J:159:ALA:H	1.87	0.40
48:W:76:THR:N	48:W:77:GLN:HB3	2.36	0.40
51:A:149:ARG:HH11	51:A:149:ARG:HB2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:256:GLU:O	1:f:257:PRO:C	2.64	0.40
1:f:296:TYR:CD1	1:f:296:TYR:N	2.88	0.40
1:f:1494:THR:CG2	1:f:1674:VAL:HG23	2.51	0.40
3:0:1322:G:H4'	46:C:47:ARG:HE	1.86	0.40
7:n:283:ASP:HA	7:n:287:LYS:HZ3	1.86	0.40
37:V:64:CYS:HB3	37:V:65:ASN:H	1.74	0.40
47:8:7:THR:HA	47:8:10:CYS:SG	2.62	0.40
47:8:305:SER:HB3	47:8:306:HIS:HA	2.03	0.40
51:A:294:ARG:NH2	51:A:307:THR:HB	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	f	1519/2174 (70%)	1094 (72%)	295 (19%)	130 (9%)	0	4
4	y	121/137 (88%)	109 (90%)	10 (8%)	2 (2%)	7	30
5	s	293/418 (70%)	207 (71%)	51 (17%)	35 (12%)	0	2
6	j	77/150 (51%)	68 (88%)	6 (8%)	3 (4%)	2	16
7	n	223/343 (65%)	179 (80%)	33 (15%)	11 (5%)	1	12
8	p	308/318 (97%)	268 (87%)	31 (10%)	9 (3%)	3	21
9	r	138/149 (93%)	101 (73%)	29 (21%)	8 (6%)	1	9
10	u	134/153 (88%)	87 (65%)	33 (25%)	14 (10%)	0	2
11	m	140/143 (98%)	120 (86%)	18 (13%)	2 (1%)	9	34
12	Z	171/221 (77%)	145 (85%)	20 (12%)	6 (4%)	3	18
13	o	188/190 (99%)	147 (78%)	33 (18%)	8 (4%)	2	14
14	q	198/211 (94%)	168 (85%)	28 (14%)	2 (1%)	12	41
15	R	139/151 (92%)	121 (87%)	15 (11%)	3 (2%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	S	80/86 (93%)	69 (86%)	9 (11%)	2 (2%)	4	24
17	t	102/112 (91%)	82 (80%)	19 (19%)	1 (1%)	12	41
18	U	66/91 (72%)	54 (82%)	10 (15%)	2 (3%)	3	21
19	v	133/144 (92%)	121 (91%)	10 (8%)	2 (2%)	8	33
20	X	146/173 (84%)	121 (83%)	20 (14%)	5 (3%)	3	19
21	B	177/190 (93%)	149 (84%)	23 (13%)	5 (3%)	4	22
22	F	205/245 (84%)	180 (88%)	23 (11%)	2 (1%)	12	41
23	d	221/263 (84%)	191 (86%)	28 (13%)	2 (1%)	14	43
24	g	81/247 (33%)	68 (84%)	12 (15%)	1 (1%)	10	37
25	a	68/110 (62%)	56 (82%)	12 (18%)	0	100	100
26	J	171/257 (66%)	132 (77%)	24 (14%)	15 (9%)	0	4
27	h	119/141 (84%)	96 (81%)	19 (16%)	4 (3%)	3	19
28	5	417/477 (87%)	325 (78%)	62 (15%)	30 (7%)	1	6
29	P	247/250 (99%)	219 (89%)	25 (10%)	3 (1%)	10	37
30	i	119/141 (84%)	91 (76%)	16 (13%)	12 (10%)	0	3
31	L	97/117 (83%)	75 (77%)	20 (21%)	2 (2%)	5	27
32	M	198/214 (92%)	160 (81%)	31 (16%)	7 (4%)	3	18
33	N	91/161 (56%)	78 (86%)	10 (11%)	3 (3%)	3	19
34	O	138/167 (83%)	103 (75%)	27 (20%)	8 (6%)	1	9
35	b	127/145 (88%)	108 (85%)	18 (14%)	1 (1%)	16	46
36	c	58/66 (88%)	47 (81%)	10 (17%)	1 (2%)	7	30
37	V	95/109 (87%)	70 (74%)	15 (16%)	10 (10%)	0	2
38	w	145/166 (87%)	105 (72%)	30 (21%)	10 (7%)	1	7
39	E	389/407 (96%)	288 (74%)	46 (12%)	55 (14%)	0	1
40	Y	172/379 (45%)	139 (81%)	27 (16%)	6 (4%)	3	18
41	Q	55/57 (96%)	40 (73%)	8 (14%)	7 (13%)	0	1
42	D	31/34 (91%)	25 (81%)	5 (16%)	1 (3%)	3	19
43	G	306/345 (89%)	254 (83%)	33 (11%)	19 (6%)	1	8
44	K	199/203 (98%)	185 (93%)	10 (5%)	4 (2%)	6	28
45	T	130/152 (86%)	100 (77%)	21 (16%)	9 (7%)	1	7
46	C	694/716 (97%)	490 (71%)	82 (12%)	122 (18%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	8	574/762 (75%)	462 (80%)	57 (10%)	55 (10%)	0	3
48	W	215/254 (85%)	181 (84%)	27 (13%)	7 (3%)	3	19
49	I	342/489 (70%)	302 (88%)	21 (6%)	19 (6%)	1	10
50	H	295/334 (88%)	231 (78%)	41 (14%)	23 (8%)	1	5
51	A	481/502 (96%)	341 (71%)	89 (18%)	51 (11%)	0	2
52	l	256/273 (94%)	216 (84%)	30 (12%)	10 (4%)	2	16
All	All	11089/13737 (81%)	8768 (79%)	1572 (14%)	749 (7%)	2	7

All (749) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	f	56	THR
1	f	91	ASP
1	f	190	ARG
1	f	203	LEU
1	f	235	LEU
1	f	241	SER
1	f	245	SER
1	f	247	ALA
1	f	295	ASN
1	f	297	THR
1	f	302	ALA
1	f	305	TYR
1	f	306	ARG
1	f	307	LEU
1	f	680	LYS
1	f	706	ILE
1	f	713	ILE
1	f	721	GLU
1	f	732	ALA
1	f	772	TYR
1	f	803	PHE
1	f	834	PHE
1	f	861	LYS
1	f	982	LEU
1	f	1022	ALA
1	f	1039	ARG
1	f	1108	ALA
1	f	1109	LEU
1	f	1114	TYR

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Mol	Chain	Res	Type
1	f	1117	PHE
1	f	1122	GLN
1	f	1149	TYR
1	f	1161	ASN
1	f	1221	LEU
1	f	1252	ILE
1	f	1259	CYS
1	f	1265	HIS
1	f	1267	LEU
1	f	1285	LEU
1	f	1305	VAL
1	f	1313	GLN
1	f	1333	ALA
1	f	1340	GLU
1	f	1403	LEU
1	f	1440	GLU
1	f	1468	PHE
1	f	1474	PHE
1	f	1559	THR
1	f	1587	ASP
1	f	1694	ALA
1	f	1723	MET
1	f	1816	LEU
1	f	1837	PHE
5	s	301	ASN
5	s	316	GLN
5	s	318	ASP
5	s	357	ALA
5	s	363	GLU
7	n	207	ARG
7	n	323	SER
7	n	324	ALA
7	n	334	SER
8	p	66	HIS
8	p	176	ASN
10	u	57	ALA
10	u	103	MET
10	u	117	LYS
18	U	78	SER
26	J	94	VAL
26	J	155	PRO
26	J	160	SER

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Mol	Chain	Res	Type
26	J	184	ASN
27	h	73	TYR
28	5	90	ILE
28	5	172	PHE
28	5	351	ASP
28	5	399	ALA
28	5	413	ILE
30	i	83	ASP
31	L	51	VAL
33	N	19	THR
33	N	93	ALA
36	c	53	GLU
37	V	96	ASN
37	V	99	THR
38	w	71	ARG
38	w	125	ASP
38	w	138	GLU
38	w	161	ASP
39	E	22	TYR
39	E	39	GLN
39	E	62	ALA
39	E	63	GLN
39	E	65	ALA
39	E	93	ASP
39	E	116	MET
39	E	126	TYR
39	E	150	ILE
39	E	214	PRO
39	E	231	PHE
39	E	246	VAL
39	E	281	TYR
39	E	284	PRO
39	E	320	LEU
39	E	341	HIS
39	E	346	ILE
40	Y	288	ASP
40	Y	366	ALA
41	Q	10	ARG
41	Q	41	ARG
43	G	221	GLU
43	G	275	LYS
43	G	279	SER

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Mol	Chain	Res	Type
44	K	183	ALA
46	C	4	PHE
46	C	5	PHE
46	C	10	SER
46	C	11	ASP
46	C	15	ASP
46	C	20	HIS
46	C	51	LEU
46	C	74	HIS
46	C	103	TRP
46	C	128	PRO
46	C	147	ILE
46	C	167	GLU
46	C	169	GLN
46	C	173	GLU
46	C	191	GLN
46	C	192	LYS
46	C	196	ALA
46	C	197	ALA
46	C	258	ASN
46	C	282	LEU
46	C	283	CYS
46	C	284	GLY
46	C	305	ASP
46	C	319	ASP
46	C	324	VAL
46	C	332	LYS
46	C	346	LEU
46	C	353	ALA
46	C	358	TYR
46	C	369	VAL
46	C	375	GLU
46	C	394	CYS
46	C	396	ALA
46	C	454	ILE
46	C	469	HIS
46	C	476	ARG
46	C	489	LEU
46	C	501	TYR
46	C	504	HIS
46	C	505	ALA
46	C	526	LYS

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Mol	Chain	Res	Type
46	C	529	GLU
46	C	542	ASN
46	C	546	TYR
46	C	556	PHE
46	C	572	TYR
46	C	581	ASN
46	C	582	MET
46	C	585	TRP
46	C	592	ASP
46	C	612	TYR
46	C	613	ASN
46	C	623	VAL
47	8	22	ASN
47	8	62	ILE
47	8	68	PHE
47	8	76	ASN
47	8	112	ALA
47	8	117	PRO
47	8	127	LEU
47	8	130	VAL
47	8	160	ALA
47	8	202	PHE
47	8	206	LEU
47	8	208	SER
47	8	279	ILE
47	8	283	PRO
47	8	306	HIS
47	8	334	ALA
47	8	346	LYS
47	8	352	GLU
47	8	468	GLU
47	8	546	SER
49	I	175	SER
49	I	216	SER
49	I	219	LYS
49	I	303	TRP
49	I	351	LYS
49	I	430	VAL
50	H	46	SER
50	H	96	THR
50	H	171	PRO
50	H	182	LEU

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Mol	Chain	Res	Type
50	H	199	THR
50	H	203	ASN
50	H	204	ILE
50	H	245	ALA
50	H	300	ARG
51	A	4	GLU
51	A	12	ALA
51	A	271	ILE
51	A	304	PHE
51	A	305	PRO
51	A	321	ALA
51	A	355	ASP
51	A	404	SER
51	A	451	MET
51	A	455	LYS
52	l	146	TYR
1	f	144	SER
1	f	165	SER
1	f	194	PHE
1	f	228	GLU
1	f	257	PRO
1	f	271	LEU
1	f	317	ASP
1	f	724	LYS
1	f	740	THR
1	f	802	GLU
1	f	977	MET
1	f	1042	ALA
1	f	1071	VAL
1	f	1078	ALA
1	f	1101	PRO
1	f	1121	CYS
1	f	1175	PRO
1	f	1215	ASP
1	f	1284	SER
1	f	1368	GLU
1	f	1402	ALA
1	f	1439	GLN
1	f	1465	SER
1	f	1475	ILE
1	f	1628	GLY
5	s	124	VAL

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Mol	Chain	Res	Type
5	s	239	ILE
5	s	305	THR
5	s	313	THR
5	s	317	CYS
5	s	335	ALA
5	s	362	ARG
6	j	76	LYS
7	n	165	SER
8	p	131	ASN
8	p	277	GLU
9	r	130	CYS
9	r	141	ARG
13	o	39	ALA
16	S	60	CYS
16	S	62	THR
19	v	40	MET
19	v	57	ALA
20	X	41	VAL
20	X	43	MET
21	B	131	ARG
26	J	75	TRP
26	J	110	ASN
26	J	164	LYS
26	J	183	ASN
26	J	204	ASN
27	h	70	ASP
28	5	223	GLY
28	5	269	ASP
28	5	277	ASP
28	5	279	GLU
28	5	358	ASP
28	5	429	LYS
28	5	457	GLU
28	5	462	LEU
30	i	69	ILE
30	i	96	GLN
30	i	121	ALA
32	M	141	ILE
33	N	45	PRO
34	O	104	SER
35	b	79	PHE
37	V	18	GLN

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Mol	Chain	Res	Type
37	V	35	GLY
38	w	167	PHE
39	E	13	ASP
39	E	46	ALA
39	E	47	GLU
39	E	92	ILE
39	E	107	GLU
39	E	132	TYR
39	E	211	VAL
39	E	216	PHE
39	E	233	ILE
39	E	279	TYR
39	E	319	ILE
39	E	389	GLN
39	E	393	VAL
41	Q	33	ARG
41	Q	40	CYS
43	G	75	CYS
43	G	93	PRO
43	G	149	SER
43	G	213	LYS
43	G	245	ALA
43	G	252	LYS
45	T	133	VAL
46	C	8	SER
46	C	12	GLU
46	C	27	LYS
46	C	38	VAL
46	C	44	ALA
46	C	47	ARG
46	C	114	ASP
46	C	157	ASP
46	C	160	SER
46	C	174	LYS
46	C	230	ASP
46	C	234	PRO
46	C	243	ARG
46	C	259	PRO
46	C	261	ILE
46	C	280	ASP
46	C	298	GLN
46	C	318	VAL

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Mol	Chain	Res	Type
46	C	334	GLY
46	C	351	GLN
46	C	373	VAL
46	C	389	ASN
46	C	410	TYR
46	C	429	SER
46	C	466	ASN
46	C	468	ASN
46	C	549	LEU
46	C	620	THR
47	8	21	GLY
47	8	60	GLN
47	8	67	PHE
47	8	115	GLU
47	8	188	LYS
47	8	191	ILE
47	8	213	ILE
47	8	322	GLY
47	8	369	PHE
47	8	476	HIS
47	8	486	SER
47	8	551	LEU
48	W	80	ASP
49	I	274	LYS
49	I	350	TYR
49	I	437	THR
50	H	130	TYR
50	H	243	ASN
51	A	3	PHE
51	A	25	MET
51	A	39	ILE
51	A	63	ASP
51	A	73	LEU
51	A	117	ASP
51	A	170	GLU
51	A	200	THR
51	A	292	LYS
51	A	390	LEU
52	l	21	THR
52	l	38	CYS
1	f	94	GLU
1	f	177	ILE

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Mol	Chain	Res	Type
1	f	697	LYS
1	f	722	TRP
1	f	774	LEU
1	f	918	ALA
1	f	981	THR
1	f	984	PRO
1	f	995	GLU
1	f	997	PRO
1	f	1049	SER
1	f	1128	PRO
1	f	1245	ALA
1	f	1250	LYS
1	f	1258	ASN
1	f	1467	SER
1	f	1535	ILE
1	f	1751	HIS
1	f	1851	ALA
5	s	149	SER
5	s	263	ASP
5	s	284	PRO
5	s	314	CYS
5	s	343	ILE
5	s	356	ARG
5	s	393	PRO
6	j	78	LYS
7	n	328	ALA
8	p	94	TRP
8	p	253	CYS
8	p	306	ASP
10	u	11	GLN
10	u	35	LYS
10	u	75	PRO
10	u	79	LYS
12	Z	69	THR
12	Z	193	PRO
13	o	3	ALA
13	o	36	PRO
14	q	134	LEU
20	X	34	HIS
22	F	7	GLY
23	d	238	ALA
26	J	140	PRO

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Mol	Chain	Res	Type
28	5	66	SER
28	5	120	ASP
28	5	173	PRO
28	5	268	PHE
28	5	270	ILE
28	5	314	GLY
28	5	350	LEU
30	i	18	GLU
30	i	80	ARG
30	i	87	GLU
32	M	147	LYS
32	M	187	ILE
32	M	196	GLU
37	V	22	GLU
37	V	24	GLN
37	V	62	TRP
37	V	74	ALA
38	w	136	VAL
39	E	15	HIS
39	E	94	ALA
39	E	110	GLY
39	E	148	TYR
39	E	217	LYS
39	E	232	ASP
39	E	265	ARG
39	E	266	SER
39	E	277	ASN
39	E	296	GLN
39	E	391	ARG
40	Y	231	CYS
43	G	89	ALA
43	G	91	PRO
44	K	177	ALA
44	K	187	ASP
45	T	56	ALA
45	T	134	ILE
46	C	25	GLU
46	C	37	GLU
46	C	100	VAL
46	C	194	LYS
46	C	264	LYS
46	C	265	GLU

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Mol	Chain	Res	Type
46	C	266	VAL
46	C	273	SER
46	C	274	LYS
46	C	303	ALA
46	C	331	ARG
46	C	465	SER
46	C	481	VAL
46	C	485	ASP
47	8	57	SER
47	8	77	LYS
47	8	132	PRO
47	8	214	VAL
47	8	216	THR
47	8	217	ASP
47	8	220	HIS
47	8	280	THR
47	8	409	SER
47	8	454	THR
48	W	77	GLN
48	W	159	LYS
49	I	298	PRO
49	I	301	LEU
49	I	337	PRO
50	H	58	ALA
50	H	59	THR
50	H	175	SER
50	H	206	ARG
50	H	296	PRO
51	A	17	GLY
51	A	40	ALA
51	A	52	ALA
51	A	81	GLY
51	A	82	PRO
51	A	130	ALA
51	A	159	LYS
51	A	185	GLU
51	A	188	THR
51	A	262	GLU
51	A	337	ALA
51	A	339	GLN
51	A	363	LYS
51	A	379	ARG

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Mol	Chain	Res	Type
52	l	150	ARG
52	l	168	ASP
52	l	169	LEU
1	f	230	ASP
1	f	232	LYS
1	f	769	ASP
1	f	800	GLU
1	f	860	ALA
1	f	1226	LYS
1	f	1233	ASP
1	f	1264	LEU
1	f	1525	THR
5	s	300	ARG
5	s	338	GLU
5	s	341	ILE
5	s	395	ALA
6	j	121	PRO
7	n	293	LYS
7	n	333	ARG
8	p	78	ASN
8	p	278	ALA
9	r	122	LEU
9	r	126	ASP
9	r	139	SER
10	u	43	TYR
10	u	84	PHE
10	u	91	PRO
12	Z	59	ARG
12	Z	106	ALA
13	o	48	ARG
18	U	83	ARG
20	X	33	SER
24	g	47	ASN
26	J	161	THR
26	J	163	LYS
26	J	180	THR
27	h	71	GLU
28	5	310	ALA
28	5	352	PRO
28	5	353	THR
29	P	242	ALA
30	i	89	SER

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Mol	Chain	Res	Type
30	i	92	ASP
31	L	85	LEU
32	M	113	GLN
34	O	77	ILE
34	O	81	VAL
34	O	99	LYS
37	V	63	GLY
37	V	100	GLU
38	w	147	ASP
38	w	156	ASN
39	E	14	LYS
39	E	97	SER
39	E	127	TYR
39	E	149	GLU
39	E	151	ASP
39	E	152	GLN
39	E	213	PHE
39	E	239	TYR
39	E	261	ASN
39	E	262	LYS
40	Y	339	ALA
40	Y	356	PRO
41	Q	31	VAL
43	G	76	TYR
43	G	247	LEU
43	G	254	LYS
45	T	22	PHE
45	T	137	ARG
46	C	30	GLN
46	C	34	LYS
46	C	94	HIS
46	C	180	ASP
46	C	209	ARG
46	C	322	ASP
46	C	323	SER
46	C	329	GLN
46	C	330	GLN
46	C	364	LEU
46	C	383	GLU
46	C	568	LYS
46	C	665	VAL
47	8	58	GLN

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Mol	Chain	Res	Type
47	8	187	LEU
47	8	210	ILE
47	8	257	THR
47	8	304	CYS
47	8	366	ALA
47	8	472	GLU
48	W	131	THR
49	I	423	LEU
50	H	84	PRO
50	H	95	GLU
51	A	58	PHE
51	A	79	ARG
51	A	138	ALA
51	A	426	LYS
51	A	472	SER
52	l	79	TYR
1	f	166	VAL
1	f	173	PRO
1	f	209	ALA
1	f	315	VAL
1	f	707	ARG
1	f	795	ALA
1	f	1079	ARG
1	f	1099	LYS
1	f	1103	ARG
1	f	1361	HIS
1	f	1750	ARG
1	f	1772	ASN
1	f	1855	PRO
5	s	150	ALA
5	s	166	TYR
5	s	306	ILE
5	s	330	GLY
5	s	332	ARG
5	s	381	ALA
7	n	164	SER
10	u	17	LEU
10	u	53	VAL
11	m	97	ASN
12	Z	23	LYS
13	o	11	LYS
13	o	67	ARG

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Mol	Chain	Res	Type
13	o	152	LEU
21	B	90	ASP
26	J	147	ASN
26	J	175	VAL
28	5	161	ALA
28	5	233	ALA
28	5	280	ASN
34	O	13	ARG
34	O	15	ILE
34	O	33	LYS
39	E	78	THR
39	E	87	LEU
39	E	131	ARG
41	Q	30	ALA
43	G	12	PRO
43	G	60	ARG
43	G	163	GLU
44	K	132	LYS
45	T	28	GLU
45	T	45	HIS
45	T	107	ARG
46	C	208	LYS
46	C	232	ARG
46	C	386	VAL
46	C	498	PRO
46	C	500	ALA
47	8	114	GLY
47	8	347	GLU
48	W	56	ILE
48	W	119	TRP
49	I	215	LEU
49	I	275	PHE
49	I	325	GLU
49	I	343	PRO
49	I	346	THR
50	H	40	ARG
50	H	301	ILE
51	A	64	GLU
51	A	84	ARG
51	A	98	ALA
51	A	261	VAL
52	l	144	ILE

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Mol	Chain	Res	Type
1	f	205	ILE
1	f	303	ASN
1	f	805	PHE
1	f	806	ALA
1	f	1046	ALA
1	f	1534	ARG
4	y	64	VAL
5	s	299	VAL
5	s	331	ARG
11	m	14	VAL
15	R	134	GLN
20	X	14	ASP
21	B	171	VAL
27	h	140	LEU
28	5	175	PRO
28	5	272	LYS
30	i	67	ARG
30	i	93	GLN
32	M	199	ILE
38	w	113	VAL
41	Q	21	HIS
42	D	3	THR
43	G	130	ALA
46	C	52	SER
46	C	96	GLU
46	C	165	GLY
46	C	548	PRO
46	C	630	TYR
46	C	647	GLU
49	I	428	TYR
50	H	177	MET
50	H	191	TYR
50	H	205	LEU
51	A	174	SER
51	A	357	VAL
51	A	403	LEU
4	y	94	PRO
7	n	331	GLY
15	R	37	VAL
17	t	43	VAL
28	5	174	GLN
38	w	163	PRO

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Mol	Chain	Res	Type
40	Y	358	VAL
43	G	177	ILE
46	C	113	PRO
46	C	547	GLN
47	8	80	GLY
47	8	284	ASP
48	W	142	ILE
51	A	8	ILE
51	A	30	VAL
52	l	44	ILE
52	l	45	ILE
1	f	1819	ILE
5	s	233	VAL
9	r	96	VAL
10	u	80	ILE
10	u	134	GLY
29	P	70	ALA
30	i	86	PRO
39	E	105	VAL
1	f	23	VAL
1	f	1782	VAL
9	r	61	VAL
12	Z	91	VAL
13	o	156	PRO
15	R	116	ILE
21	B	16	ARG
21	B	126	VAL
28	5	125	PRO
32	M	92	VAL
51	A	308	GLN
51	A	329	ILE
1	f	1601	VAL
1	f	1605	VAL
5	s	229	ILE
5	s	348	VAL
7	n	330	VAL
9	r	106	VAL
14	q	51	VAL
23	d	203	VAL
46	C	477	MET
47	8	424	ILE
51	A	20	PRO

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Mol	Chain	Res	Type
5	s	339	PRO
22	F	155	ALA
29	P	111	VAL
34	O	32	VAL
45	T	136	GLY
47	8	42	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	
1	f	1318/1862 (71%)	1272 (96%)	46 (4%)	32	58
4	y	104/116 (90%)	104 (100%)	0	100	100
5	s	252/362 (70%)	240 (95%)	12 (5%)	23	52
6	j	69/123 (56%)	65 (94%)	4 (6%)	18	47
7	n	196/289 (68%)	182 (93%)	14 (7%)	13	41
8	p	262/268 (98%)	259 (99%)	3 (1%)	65	75
9	r	113/121 (93%)	113 (100%)	0	100	100
10	u	117/132 (89%)	108 (92%)	9 (8%)	12	38
11	m	116/117 (99%)	112 (97%)	4 (3%)	32	59
12	Z	143/184 (78%)	143 (100%)	0	100	100
13	o	160/160 (100%)	157 (98%)	3 (2%)	50	68
14	q	188/195 (96%)	186 (99%)	2 (1%)	65	75
15	R	125/132 (95%)	125 (100%)	0	100	100
16	S	70/73 (96%)	69 (99%)	1 (1%)	59	72
17	t	87/93 (94%)	86 (99%)	1 (1%)	65	75
18	U	57/74 (77%)	50 (88%)	7 (12%)	4	20
19	v	103/112 (92%)	102 (99%)	1 (1%)	68	75
20	X	137/157 (87%)	134 (98%)	3 (2%)	45	65
21	B	159/165 (96%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	F	182/212 (86%)	181 (100%)	1 (0%)	81	82
23	d	187/208 (90%)	187 (100%)	0	100	100
24	g	68/197 (34%)	65 (96%)	3 (4%)	25	53
25	a	64/96 (67%)	63 (98%)	1 (2%)	55	71
26	J	138/191 (72%)	127 (92%)	11 (8%)	11	37
27	h	103/120 (86%)	101 (98%)	2 (2%)	50	68
28	5	358/408 (88%)	338 (94%)	20 (6%)	19	47
29	P	204/205 (100%)	201 (98%)	3 (2%)	57	71
30	i	110/124 (89%)	104 (94%)	6 (6%)	19	48
31	L	89/104 (86%)	88 (99%)	1 (1%)	65	75
32	M	167/179 (93%)	164 (98%)	3 (2%)	51	69
33	N	84/125 (67%)	82 (98%)	2 (2%)	43	65
34	O	118/139 (85%)	117 (99%)	1 (1%)	73	78
35	b	110/123 (89%)	109 (99%)	1 (1%)	70	77
36	c	49/53 (92%)	47 (96%)	2 (4%)	27	55
37	V	86/97 (89%)	68 (79%)	18 (21%)	1	5
38	w	125/137 (91%)	117 (94%)	8 (6%)	16	44
39	E	334/350 (95%)	327 (98%)	7 (2%)	47	66
40	Y	152/327 (46%)	146 (96%)	6 (4%)	28	56
41	Q	49/49 (100%)	46 (94%)	3 (6%)	17	46
42	D	30/31 (97%)	29 (97%)	1 (3%)	33	59
43	G	260/289 (90%)	257 (99%)	3 (1%)	63	74
44	K	176/178 (99%)	174 (99%)	2 (1%)	65	75
45	T	111/131 (85%)	109 (98%)	2 (2%)	51	69
46	C	616/628 (98%)	585 (95%)	31 (5%)	22	50
47	8	485/648 (75%)	467 (96%)	18 (4%)	30	57
48	W	194/217 (89%)	186 (96%)	8 (4%)	27	55
49	I	300/430 (70%)	295 (98%)	5 (2%)	53	70
50	H	266/299 (89%)	263 (99%)	3 (1%)	65	75
51	A	425/441 (96%)	384 (90%)	41 (10%)	8	30
52	l	217/230 (94%)	215 (99%)	2 (1%)	70	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9633/11701 (82%)	9308 (97%)	325 (3%)	33 59

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	3	SER
1	f	25	ILE
1	f	88	ILE
1	f	89	VAL
1	f	93	GLU
1	f	137	CYS
1	f	138	ASP
1	f	240	PHE
1	f	303	ASN
1	f	305	TYR
1	f	722	TRP
1	f	743	ARG
1	f	772	TYR
1	f	785	LYS
1	f	789	TRP
1	f	831	LEU
1	f	855	ASP
1	f	906	GLU
1	f	909	ARG
1	f	941	ARG
1	f	1068	ASN
1	f	1101	PRO
1	f	1115	HIS
1	f	1122	GLN
1	f	1217	GLU
1	f	1251	LYS
1	f	1263	ASP
1	f	1264	LEU
1	f	1285	LEU
1	f	1306	TRP
1	f	1327	PRO
1	f	1521	ARG
1	f	1525	THR
1	f	1530	LEU
1	f	1532	LYS
1	f	1545	ARG
1	f	1546	ARG

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Mol	Chain	Res	Type
1	f	1549	ARG
1	f	1551	SER
1	f	1552	THR
1	f	1588	VAL
1	f	1598	LYS
1	f	1631	MET
1	f	1705	LEU
1	f	1820	LEU
1	f	1852	HIS
5	s	168	GLU
5	s	194	ILE
5	s	195	ASP
5	s	267	GLU
5	s	283	LEU
5	s	302	ASP
5	s	306	ILE
5	s	315	PHE
5	s	316	GLN
5	s	318	ASP
5	s	324	ARG
5	s	332	ARG
6	j	73	LYS
6	j	74	LYS
6	j	94	LYS
6	j	99	LYS
7	n	125	LYS
7	n	209	ARG
7	n	210	LEU
7	n	255	ASN
7	n	267	GLU
7	n	287	LYS
7	n	291	CYS
7	n	293	LYS
7	n	300	LYS
7	n	309	CYS
7	n	332	LYS
7	n	333	ARG
7	n	335	LYS
7	n	341	MET
8	p	32	VAL
8	p	279	GLN
8	p	311	VAL

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Mol	Chain	Res	Type
10	u	16	LEU
10	u	26	LYS
10	u	37	VAL
10	u	39	ILE
10	u	84	PHE
10	u	97	GLU
10	u	119	ARG
10	u	131	ARG
10	u	137	THR
11	m	73	GLN
11	m	80	LYS
11	m	82	ILE
11	m	97	ASN
13	o	51	ARG
13	o	154	THR
13	o	177	LYS
14	q	122	THR
14	q	154	VAL
16	S	64	LEU
17	t	104	VAL
18	U	45	ASP
18	U	46	GLN
18	U	48	GLN
18	U	71	ARG
18	U	83	ARG
18	U	94	LYS
18	U	98	MET
19	v	131	ASP
20	X	33	SER
20	X	35	ASN
20	X	38	LYS
22	F	79	VAL
24	g	49	VAL
24	g	85	ILE
24	g	86	LYS
25	a	79	VAL
26	J	94	VAL
26	J	102	ARG
26	J	103	TYR
26	J	105	ILE
26	J	107	PHE
26	J	150	VAL

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Mol	Chain	Res	Type
26	J	152	PHE
26	J	162	THR
26	J	183	ASN
26	J	222	LEU
26	J	233	ARG
27	h	68	CYS
27	h	71	GLU
28	5	65	LYS
28	5	67	THR
28	5	88	ILE
28	5	146	ASP
28	5	170	GLU
28	5	209	ASP
28	5	234	GLN
28	5	275	GLU
28	5	281	LEU
28	5	321	LEU
28	5	349	THR
28	5	350	LEU
28	5	400	LYS
28	5	401	ARG
28	5	414	ASN
28	5	455	LEU
28	5	456	VAL
28	5	457	GLU
28	5	459	ASN
28	5	461	ARG
29	P	46	PHE
29	P	100	LEU
29	P	109	ILE
30	i	69	ILE
30	i	71	LEU
30	i	76	GLU
30	i	91	VAL
30	i	116	VAL
30	i	120	VAL
31	L	79	LEU
32	M	141	ILE
32	M	147	LYS
32	M	149	MET
33	N	8	ARG
33	N	18	PHE

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Mol	Chain	Res	Type
34	O	85	PRO
35	b	25	VAL
36	c	8	LEU
36	c	10	ARG
37	V	12	GLN
37	V	13	GLN
37	V	14	LYS
37	V	21	LEU
37	V	22	GLU
37	V	31	GLN
37	V	34	LYS
37	V	36	LYS
37	V	43	GLN
37	V	62	TRP
37	V	64	CYS
37	V	65	ASN
37	V	93	LEU
37	V	96	ASN
37	V	97	MET
37	V	100	GLU
37	V	101	GLN
37	V	102	ASN
38	w	34	GLN
38	w	86	ARG
38	w	125	ASP
38	w	133	TYR
38	w	135	PHE
38	w	140	ASP
38	w	164	LEU
38	w	166	THR
39	E	22	TYR
39	E	36	ARG
39	E	54	GLN
39	E	71	GLU
39	E	244	GLU
39	E	279	TYR
39	E	320	LEU
40	Y	229	ARG
40	Y	230	ARG
40	Y	242	GLU
40	Y	337	LYS
40	Y	354	VAL

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Mol	Chain	Res	Type
40	Y	364	GLN
41	Q	15	MET
41	Q	42	GLN
41	Q	55	LYS
42	D	3	THR
43	G	136	TRP
43	G	160	VAL
43	G	193	ILE
44	K	31	VAL
44	K	194	ARG
45	T	91	VAL
45	T	137	ARG
46	C	1	MET
46	C	2	SER
46	C	6	ASP
46	C	27	LYS
46	C	30	GLN
46	C	31	ILE
46	C	34	LYS
46	C	37	GLU
46	C	52	SER
46	C	60	GLU
46	C	149	LYS
46	C	189	VAL
46	C	190	ILE
46	C	191	GLN
46	C	207	LYS
46	C	209	ARG
46	C	211	LEU
46	C	229	GLU
46	C	232	ARG
46	C	233	LEU
46	C	243	ARG
46	C	274	LYS
46	C	287	GLN
46	C	296	ILE
46	C	307	TYR
46	C	331	ARG
46	C	434	ILE
46	C	435	LEU
46	C	464	TRP
46	C	481	VAL

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Mol	Chain	Res	Type
46	C	538	PHE
47	8	8	ARG
47	8	10	CYS
47	8	18	ARG
47	8	33	LEU
47	8	35	GLU
47	8	43	MET
47	8	75	ARG
47	8	77	LYS
47	8	79	ARG
47	8	82	GLN
47	8	163	HIS
47	8	172	LEU
47	8	263	HIS
47	8	419	LYS
47	8	452	VAL
47	8	495	LYS
47	8	564	GLN
47	8	569	ARG
48	W	39	GLU
48	W	76	THR
48	W	77	GLN
48	W	121	THR
48	W	161	ARG
48	W	165	TRP
48	W	192	ARG
48	W	207	VAL
49	I	144	ARG
49	I	337	PRO
49	I	338	LYS
49	I	412	ARG
49	I	434	ILE
50	H	51	LEU
50	H	259	MET
50	H	304	LEU
51	A	7	GLU
51	A	8	ILE
51	A	10	VAL
51	A	15	THR
51	A	28	MET
51	A	29	LYS
51	A	30	VAL

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Mol	Chain	Res	Type
51	A	32	LEU
51	A	35	LYS
51	A	44	TRP
51	A	48	MET
51	A	50	ASP
51	A	73	LEU
51	A	100	LYS
51	A	102	LYS
51	A	114	VAL
51	A	149	ARG
51	A	151	LEU
51	A	207	THR
51	A	226	LEU
51	A	252	GLU
51	A	257	LEU
51	A	292	LYS
51	A	293	THR
51	A	294	ARG
51	A	296	GLN
51	A	297	MET
51	A	301	LYS
51	A	302	ASN
51	A	307	THR
51	A	352	GLN
51	A	368	GLN
51	A	371	LYS
51	A	378	ARG
51	A	383	LYS
51	A	403	LEU
51	A	425	THR
51	A	435	LEU
51	A	437	ILE
51	A	473	ILE
51	A	479	MET
52	l	139	HIS
52	l	148	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (283) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	109	ASN
1	f	128	HIS

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Mol	Chain	Res	Type
1	f	172	GLN
1	f	175	HIS
1	f	179	ASN
1	f	195	HIS
1	f	254	GLN
1	f	286	ASN
1	f	288	HIS
1	f	691	HIS
1	f	723	HIS
1	f	742	ASN
1	f	797	GLN
1	f	839	GLN
1	f	850	HIS
1	f	884	HIS
1	f	928	HIS
1	f	956	HIS
1	f	965	ASN
1	f	976	ASN
1	f	989	GLN
1	f	1007	HIS
1	f	1068	ASN
1	f	1083	ASN
1	f	1122	GLN
1	f	1156	HIS
1	f	1190	GLN
1	f	1205	GLN
1	f	1229	GLN
1	f	1257	ASN
1	f	1351	ASN
1	f	1361	HIS
1	f	1542	GLN
1	f	1652	HIS
1	f	1679	HIS
1	f	1686	GLN
1	f	1704	HIS
1	f	1731	GLN
1	f	1747	ASN
1	f	1786	ASN
1	f	1808	HIS
1	f	1812	HIS
1	f	1821	GLN
1	f	1852	HIS

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Mol	Chain	Res	Type
5	s	160	HIS
5	s	186	ASN
5	s	266	HIS
5	s	282	HIS
5	s	307	HIS
6	j	90	HIS
6	j	133	GLN
7	n	139	HIS
7	n	208	ASN
7	n	276	ASN
7	n	339	GLN
8	p	12	HIS
8	p	144	HIS
8	p	242	GLN
8	p	279	GLN
8	p	307	ASN
9	r	32	GLN
9	r	34	ASN
9	r	44	GLN
9	r	65	HIS
9	r	83	GLN
9	r	100	GLN
9	r	138	HIS
10	u	11	GLN
10	u	98	HIS
10	u	118	ASN
10	u	121	HIS
11	m	8	HIS
11	m	36	GLN
11	m	61	GLN
11	m	73	GLN
11	m	97	ASN
11	m	110	HIS
12	Z	21	HIS
12	Z	116	HIS
12	Z	170	HIS
12	Z	179	GLN
13	o	10	ASN
13	o	18	GLN
13	o	27	HIS
13	o	60	ASN
13	o	81	HIS

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Mol	Chain	Res	Type
13	o	93	ASN
14	q	80	GLN
14	q	101	GLN
14	q	193	ASN
15	R	53	GLN
15	R	77	HIS
15	R	105	ASN
16	S	56	GLN
17	t	24	HIS
18	U	88	ASN
19	v	36	HIS
20	X	19	HIS
20	X	34	HIS
20	X	91	HIS
20	X	142	GLN
21	B	6	ASN
21	B	8	ASN
21	B	45	ASN
21	B	65	HIS
21	B	115	HIS
21	B	132	HIS
21	B	165	ASN
22	F	25	HIS
22	F	50	ASN
22	F	95	GLN
22	F	113	ASN
22	F	114	GLN
22	F	116	GLN
22	F	168	ASN
23	d	153	ASN
23	d	210	ASN
24	g	38	GLN
25	a	92	GLN
26	J	68	ASN
26	J	129	ASN
26	J	184	ASN
27	h	60	HIS
27	h	90	ASN
27	h	99	GLN
28	5	91	HIS
28	5	96	ASN
28	5	169	ASN

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Mol	Chain	Res	Type
28	5	180	HIS
28	5	208	GLN
28	5	307	GLN
28	5	403	GLN
28	5	430	ASN
28	5	449	HIS
29	P	15	GLN
29	P	122	GLN
30	i	25	ASN
30	i	48	ASN
30	i	56	HIS
30	i	74	GLN
30	i	90	HIS
30	i	93	GLN
31	L	69	ASN
32	M	38	HIS
32	M	73	GLN
32	M	84	GLN
32	M	124	HIS
32	M	195	ASN
33	N	51	GLN
33	N	65	GLN
33	N	70	HIS
33	N	76	ASN
33	N	98	HIS
34	O	38	HIS
35	b	113	HIS
36	c	16	ASN
36	c	42	GLN
37	V	13	GLN
37	V	18	GLN
37	V	31	GLN
37	V	32	GLN
37	V	43	GLN
37	V	50	ASN
37	V	101	GLN
38	w	34	GLN
38	w	54	GLN
38	w	98	HIS
38	w	130	HIS
39	E	182	GLN
39	E	197	ASN

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Mol	Chain	Res	Type
39	E	209	HIS
39	E	220	ASN
39	E	228	ASN
39	E	236	ASN
39	E	263	GLN
39	E	290	ASN
39	E	296	GLN
39	E	328	ASN
39	E	366	ASN
39	E	373	GLN
40	Y	267	HIS
40	Y	303	GLN
40	Y	364	GLN
41	Q	47	ASN
42	D	15	HIS
43	G	21	HIS
43	G	51	HIS
43	G	145	ASN
43	G	191	ASN
43	G	215	ASN
43	G	218	ASN
43	G	231	ASN
43	G	238	GLN
43	G	258	GLN
44	K	87	ASN
44	K	117	GLN
44	K	189	ASN
45	T	45	HIS
45	T	51	HIS
45	T	55	HIS
45	T	86	HIS
45	T	110	ASN
46	C	89	GLN
46	C	156	HIS
46	C	191	GLN
46	C	200	GLN
46	C	292	HIS
46	C	315	ASN
46	C	352	GLN
46	C	354	HIS
46	C	359	HIS
46	C	431	HIS

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Mol	Chain	Res	Type
46	C	437	ASN
46	C	475	GLN
46	C	503	GLN
46	C	504	HIS
46	C	506	GLN
46	C	533	HIS
46	C	559	GLN
46	C	614	ASN
46	C	633	ASN
46	C	669	ASN
46	C	674	GLN
47	8	83	HIS
47	8	98	HIS
47	8	107	HIS
47	8	109	ASN
47	8	149	GLN
47	8	218	ASN
47	8	220	HIS
47	8	251	HIS
47	8	270	GLN
47	8	310	HIS
47	8	350	ASN
47	8	426	GLN
47	8	444	GLN
47	8	494	HIS
47	8	523	HIS
47	8	542	HIS
47	8	576	ASN
48	W	49	ASN
48	W	52	GLN
48	W	69	ASN
48	W	101	GLN
48	W	168	HIS
48	W	172	ASN
48	W	204	ASN
48	W	234	HIS
49	I	188	HIS
49	I	280	GLN
49	I	287	HIS
49	I	369	GLN
49	I	370	GLN
49	I	401	HIS

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Mol	Chain	Res	Type
49	I	463	ASN
49	I	464	ASN
50	H	56	GLN
50	H	99	GLN
50	H	113	GLN
50	H	255	HIS
50	H	282	HIS
50	H	316	HIS
51	A	65	ASN
51	A	74	HIS
51	A	89	HIS
51	A	96	HIS
51	A	136	GLN
51	A	148	ASN
51	A	263	ASN
51	A	273	ASN
51	A	283	ASN
51	A	302	ASN
51	A	320	HIS
51	A	368	GLN
51	A	382	GLN
51	A	456	GLN
51	A	471	GLN
52	l	47	ASN
52	l	125	ASN
52	l	160	ASN
52	l	185	ASN
52	l	239	GLN
52	l	240	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	74/75 (98%)	11 (14%)	1 (1%)
3	0	2144/2319 (92%)	394 (18%)	28 (1%)
All	All	2218/2394 (92%)	405 (18%)	29 (1%)

All (405) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	16	U

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Mol	Chain	Res	Type
2	1	17	G
2	1	20	A
2	1	25	G
2	1	32	U
2	1	45	G
2	1	47	C
2	1	55	C
2	1	72	A
2	1	73	C
2	1	74	C
3	0	2	A
3	0	3	U
3	0	4	C
3	0	25	C
3	0	26	A
3	0	34	G
3	0	42	G
3	0	45	U
3	0	63	G
3	0	65	A
3	0	68	A
3	0	69	C
3	0	75	U
3	0	82	A
3	0	83	U
3	0	90	A
3	0	99	U
3	0	101	C
3	0	113	U
3	0	123	A
3	0	127	C
3	0	136	U
3	0	155	U
3	0	157	G
3	0	170	C
3	0	189	G
3	0	194	U
3	0	196	U
3	0	197	C
3	0	200	U
3	0	201	U
3	0	202	C

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Mol	Chain	Res	Type
3	0	204	G
3	0	207	G
3	0	214	C
3	0	215	A
3	0	217	C
3	0	218	C
3	0	227	U
3	0	228	G
3	0	230	G
3	0	249	A
3	0	252	G
3	0	253	U
3	0	254	A
3	0	255	A
3	0	256	A
3	0	257	A
3	0	258	C
3	0	270	C
3	0	271	C
3	0	272	G
3	0	273	G
3	0	274	C
3	0	278	A
3	0	281	A
3	0	288	A
3	0	306	U
3	0	308	C
3	0	309	G
3	0	316	A
3	0	320	G
3	0	325	U
3	0	326	U
3	0	328	U
3	0	329	U
3	0	330	A
3	0	331	U
3	0	344	G
3	0	345	A
3	0	346	C
3	0	357	C
3	0	362	C
3	0	364	G

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Mol	Chain	Res	Type
3	0	385	G
3	0	386	A
3	0	400	G
3	0	408	C
3	0	425	A
3	0	447	A
3	0	448	A
3	0	451	G
3	0	464	C
3	0	471	C
3	0	473	G
3	0	486	U
3	0	488	G
3	0	491	C
3	0	492	A
3	0	501	A
3	0	505	A
3	0	506	A
3	0	507	A
3	0	511	G
3	0	512	A
3	0	520	A
3	0	527	A
3	0	528	U
3	0	545	U
3	0	546	U
3	0	547	G
3	0	555	G
3	0	556	U
3	0	557	U
3	0	558	U
3	0	571	A
3	0	585	A
3	0	586	A
3	0	592	A
3	0	596	A
3	0	599	A
3	0	600	U
3	0	605	G
3	0	611	G
3	0	648	A
3	0	665	U

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Mol	Chain	Res	Type
3	0	673	A
3	0	674	A
3	0	676	G
3	0	694	A
3	0	695	G
3	0	696	G
3	0	704	A
3	0	707	C
3	0	709	C
3	0	714	G
3	0	715	U
3	0	717	U
3	0	718	A
3	0	723	C
3	0	729	C
3	0	734	G
3	0	737	U
3	0	738	G
3	0	739	G
3	0	740	U
3	0	741	G
3	0	743	C
3	0	745	C
3	0	747	U
3	0	762	U
3	0	763	G
3	0	770	C
3	0	772	U
3	0	773	U
3	0	774	C
3	0	775	A
3	0	776	G
3	0	785	A
3	0	786	A
3	0	791	G
3	0	793	A
3	0	796	G
3	0	797	G
3	0	810	U
3	0	811	U
3	0	812	A
3	0	813	U

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Mol	Chain	Res	Type
3	0	814	C
3	0	820	U
3	0	825	C
3	0	826	A
3	0	830	C
3	0	834	G
3	0	846	U
3	0	847	U
3	0	848	U
3	0	849	U
3	0	861	A
3	0	871	G
3	0	872	A
3	0	874	C
3	0	881	G
3	0	885	U
3	0	887	C
3	0	888	G
3	0	889	A
3	0	891	U
3	0	892	U
3	0	895	A
3	0	919	G
3	0	923	A
3	0	924	G
3	0	925	C
3	0	935	A
3	0	938	G
3	0	940	U
3	0	941	U
3	0	942	C
3	0	945	C
3	0	946	U
3	0	976	U
3	0	977	A
3	0	984	A
3	0	985	G
3	0	987	G
3	0	991	C
3	0	999	U
3	0	1071	G
3	0	1077	U

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Mol	Chain	Res	Type
3	0	1078	U
3	0	1183	U
3	0	1184	C
3	0	1190	A
3	0	1191	U
3	0	1195	G
3	0	1196	G
3	0	1197	A
3	0	1199	U
3	0	1202	A
3	0	1212	U
3	0	1216	G
3	0	1226	U
3	0	1273	A
3	0	1275	A
3	0	1291	A
3	0	1300	U
3	0	1304	U
3	0	1306	A
3	0	1328	A
3	0	1344	G
3	0	1345	A
3	0	1361	C
3	0	1364	C
3	0	1365	A
3	0	1366	A
3	0	1367	A
3	0	1368	C
3	0	1393	U
3	0	1394	U
3	0	1396	U
3	0	1397	G
3	0	1399	U
3	0	1400	C
3	0	1402	U
3	0	1411	U
3	0	1417	U
3	0	1418	U
3	0	1420	A
3	0	1423	A
3	0	1426	A
3	0	1427	U

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Mol	Chain	Res	Type
3	0	1429	U
3	0	1430	U
3	0	1432	C
3	0	1433	A
3	0	1438	G
3	0	1439	U
3	0	1440	U
3	0	1441	C
3	0	1451	C
3	0	1454	A
3	0	1456	G
3	0	1457	A
3	0	1459	U
3	0	1460	A
3	0	1461	U
3	0	1467	U
3	0	1468	U
3	0	1471	G
3	0	1477	A
3	0	1478	U
3	0	1481	U
3	0	1483	U
3	0	1485	U
3	0	1487	G
3	0	1491	U
3	0	1500	U
3	0	1502	C
3	0	1503	G
3	0	1512	C
3	0	1513	U
3	0	1514	U
3	0	1516	A
3	0	1521	G
3	0	1523	A
3	0	1525	A
3	0	1527	C
3	0	1528	C
3	0	1529	U
3	0	1530	C
3	0	1531	A
3	0	1532	G
3	0	1549	U

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Mol	Chain	Res	Type
3	0	1550	U
3	0	1563	U
3	0	1564	U
3	0	1565	G
3	0	1570	U
3	0	1580	G
3	0	1611	A
3	0	1623	G
3	0	1631	C
3	0	1633	A
3	0	1637	G
3	0	1658	U
3	0	1666	A
3	0	1669	A
3	0	1673	G
3	0	1674	G
3	0	1675	A
3	0	1676	A
3	0	1690	G
3	0	1691	G
3	0	1694	A
3	0	1695	G
3	0	1700	A
3	0	1702	G
3	0	1716	G
3	0	1718	G
3	0	1719	U
3	0	1728	G
3	0	1729	A
3	0	1731	C
3	0	1732	C
3	0	1773	A
3	0	1787	U
3	0	1788	U
3	0	1794	A
3	0	1819	U
3	0	1820	A
3	0	1833	G
3	0	1834	C
3	0	1835	C
3	0	1862	U
3	0	1863	U

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Mol	Chain	Res	Type
3	0	1879	C
3	0	1880	G
3	0	1881	G
3	0	1882	U
3	0	1883	A
3	0	1884	U
3	0	1888	C
3	0	1889	U
3	0	1890	U
3	0	1891	G
3	0	1908	A
3	0	1909	U
3	0	1914	U
3	0	1915	G
3	0	1935	U
3	0	1952	U
3	0	1955	G
3	0	1967	U
3	0	1971	C
3	0	1972	U
3	0	1975	G
3	0	1977	G
3	0	1978	A
3	0	1979	C
3	0	1980	A
3	0	1981	C
3	0	1982	G
3	0	1995	U
3	0	1996	C
3	0	1997	A
3	0	1998	G
3	0	1999	U
3	0	2013	A
3	0	2015	G
3	0	2016	A
3	0	2019	C
3	0	2021	U
3	0	2022	G
3	0	2028	C
3	0	2059	G
3	0	2075	C
3	0	2080	G

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Mol	Chain	Res	Type
3	0	2095	U
3	0	2097	A
3	0	2099	U
3	0	2100	G
3	0	2103	C
3	0	2107	C
3	0	2108	A
3	0	2112	A
3	0	2140	A
3	0	2158	C
3	0	2221	A
3	0	2232	U
3	0	2233	C
3	0	2279	A
3	0	2280	G
3	0	2283	G
3	0	2285	A
3	0	2288	A
3	0	2289	A
3	0	2292	U
3	0	2293	A
3	0	2315	G
3	0	2316	G
3	0	2317	A
3	0	2319	C
3	0	2322	U

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	73	C
3	0	68	A
3	0	122	A
3	0	200	U
3	0	217	C
3	0	251	A
3	0	325	U
3	0	693	G
3	0	785	A
3	0	812	A
3	0	923	A
3	0	945	C

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Mol	Chain	Res	Type
3	0	975	U
3	0	1070	C
3	0	1196	G
3	0	1299	C
3	0	1393	U
3	0	1450	G
3	0	1477	A
3	0	1528	C
3	0	1531	A
3	0	1579	A
3	0	1694	A
3	0	1977	G
3	0	1979	C
3	0	1980	A
3	0	1982	G
3	0	2073	C
3	0	2157	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	GNP	5	502	54	34,34,34	2.21	7 (20%)	47,54,54	1.07	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	GNP	5	502	54	-	6/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	5	502	GNP	PA-O3A	-7.78	1.51	1.59
55	5	502	GNP	PB-O3A	-7.57	1.49	1.59
55	5	502	GNP	PB-O2B	-3.67	1.47	1.56
55	5	502	GNP	PG-O3G	-2.48	1.50	1.56
55	5	502	GNP	PG-N3B	-2.26	1.57	1.63
55	5	502	GNP	PG-O2G	-2.21	1.50	1.56
55	5	502	GNP	PB-N3B	-2.15	1.57	1.63

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	5	502	GNP	O3G-PG-O1G	-3.59	104.44	113.45
55	5	502	GNP	O2B-PB-O1B	2.75	115.76	109.87
55	5	502	GNP	C3'-C2'-C1'	2.44	106.07	101.46
55	5	502	GNP	O2G-PG-O3G	2.12	113.29	107.59

There are no chirality outliers.

All (6) torsion outliers are listed below:

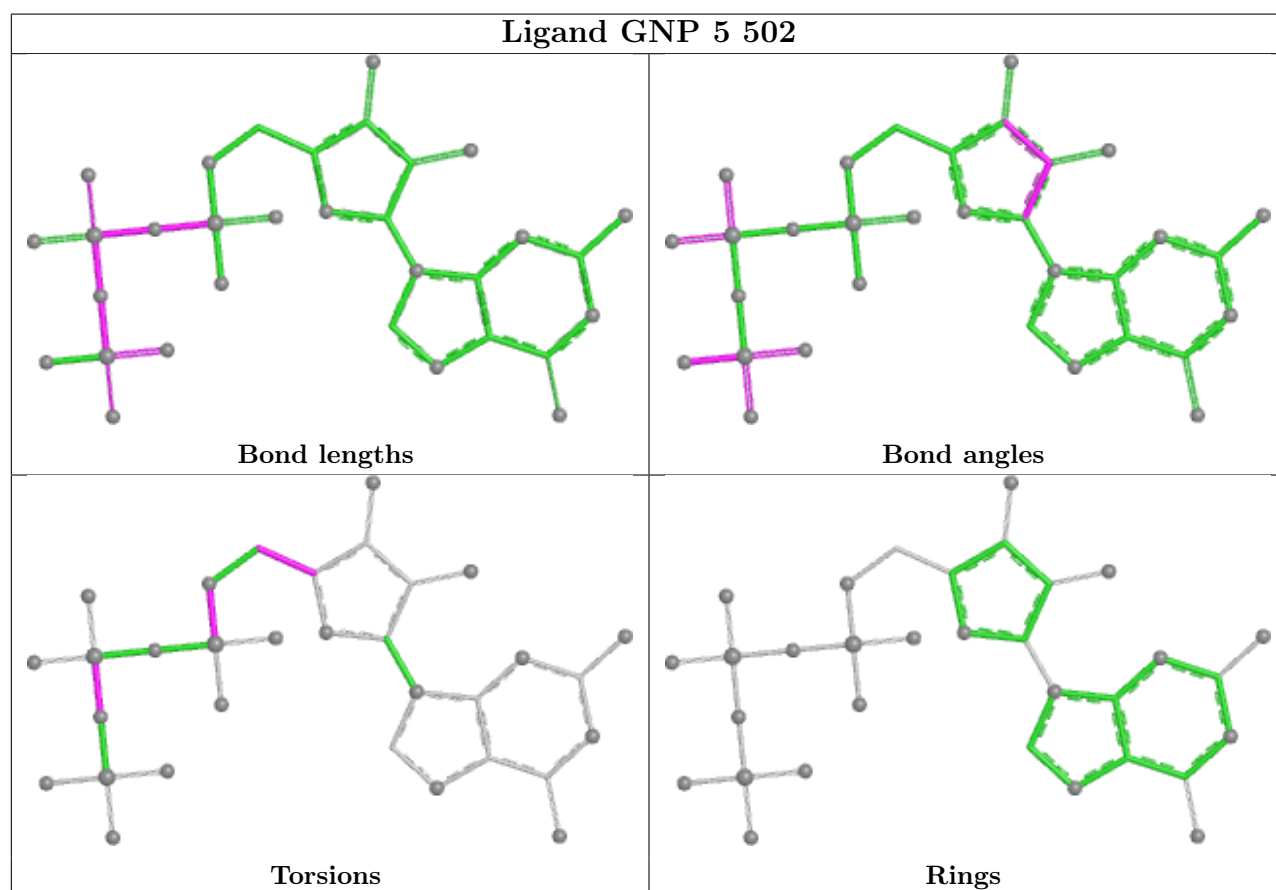
Mol	Chain	Res	Type	Atoms
55	5	502	GNP	PG-N3B-PB-O1B
55	5	502	GNP	PG-N3B-PB-O3A
55	5	502	GNP	C5'-O5'-PA-O3A
55	5	502	GNP	O4'-C4'-C5'-O5'
55	5	502	GNP	C3'-C4'-C5'-O5'
55	5	502	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	5	502	GNP	21	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	f	20
28	5	2
46	C	1
48	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	282:ARG	C	283:GLY	N	2.09
1	f	1149:TYR	C	1150:VAL	N	1.72
1	f	1221:LEU	C	1222:PRO	N	1.71
1	f	1254:ALA	C	1255:GLN	N	1.68
1	C	53:ARG	C	54:ASN	N	1.67
1	f	774:LEU	C	775:GLY	N	1.66
1	f	1127:VAL	C	1128:PRO	N	1.66
1	f	307:LEU	C	308:ARG	N	1.65
1	f	301:GLU	C	302:ALA	N	1.62
1	f	1492:GLY	C	1493:PRO	N	1.61
1	f	132:ALA	C	133:ARG	N	1.19
1	f	296:TYR	C	297:THR	N	1.19
1	5	253:THR	C	254:ARG	N	1.19
1	f	263:SER	C	264:ASP	N	1.18
1	f	304:PRO	C	305:TYR	N	1.15
1	W	165:TRP	C	166:VAL	N	1.15
1	f	198:PHE	C	199:PHE	N	1.14
1	f	199:PHE	C	200:ASP	N	1.14
1	f	131:THR	C	132:ALA	N	1.13
1	f	1214:ARG	C	1215:ASP	N	1.13
1	f	195:HIS	C	196:VAL	N	1.12
1	f	139:MET	C	140:PHE	N	1.11
1	f	194:PHE	C	195:HIS	N	1.08
1	f	234:GLY	C	235:LEU	N	1.06

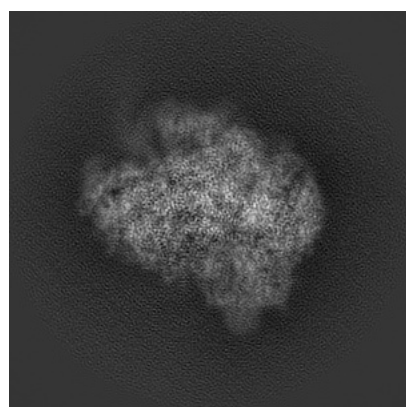
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11893. These allow visual inspection of the internal detail of the map and identification of artifacts.

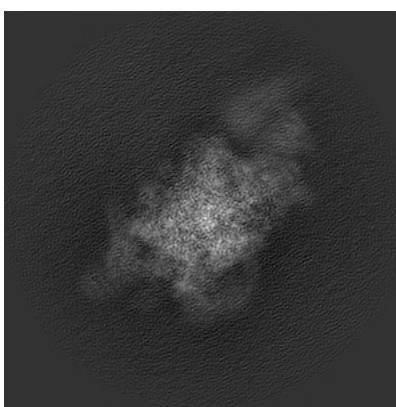
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

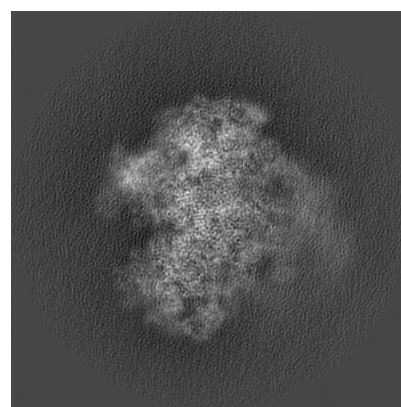
6.1.1 Primary map



X



Y

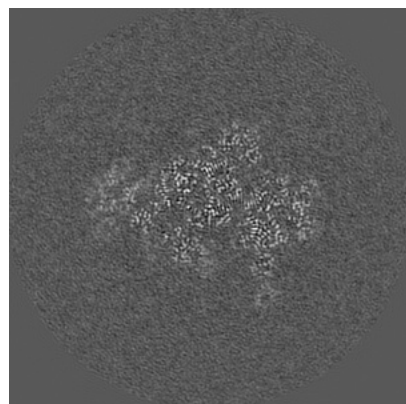


Z

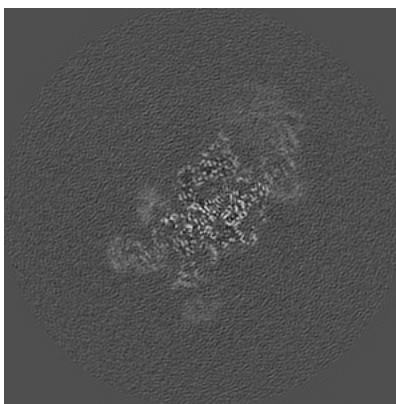
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

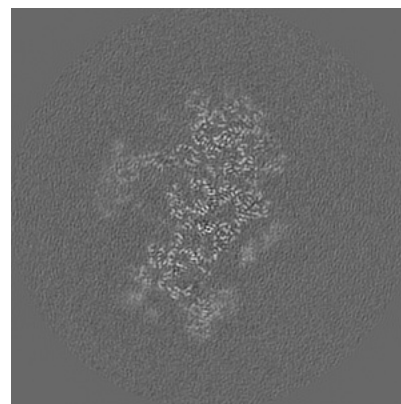
6.2.1 Primary map



X Index: 200



Y Index: 200

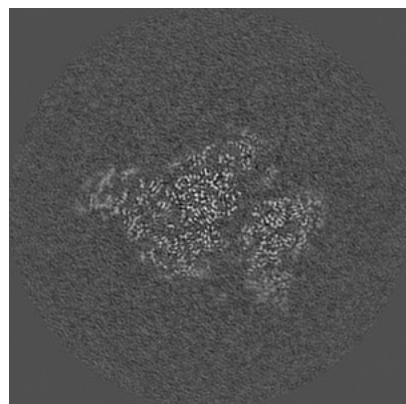


Z Index: 200

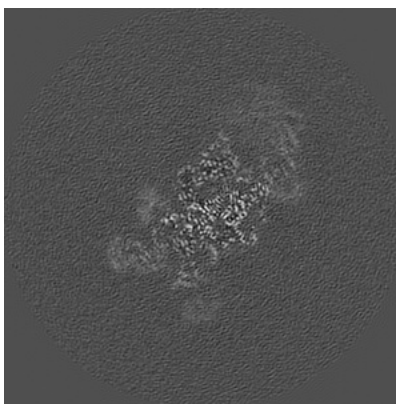
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

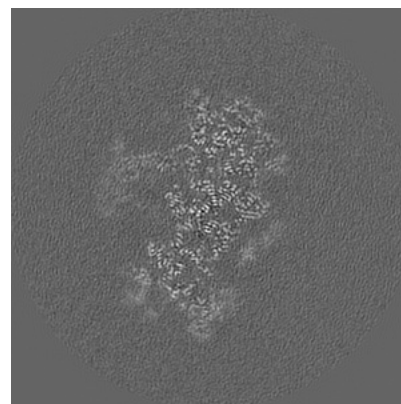
6.3.1 Primary map



X Index: 188



Y Index: 200

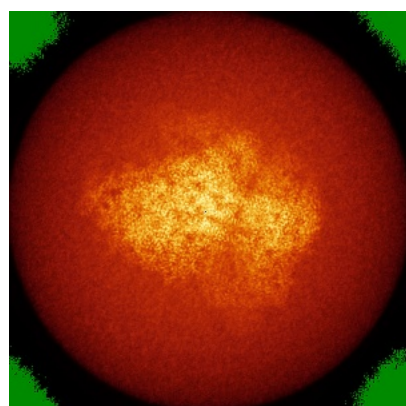


Z Index: 199

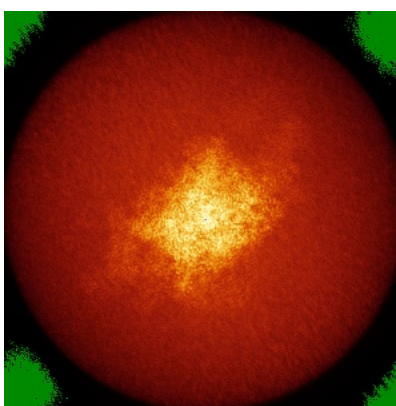
The images above show the largest variance slices of the map in three orthogonal directions.

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

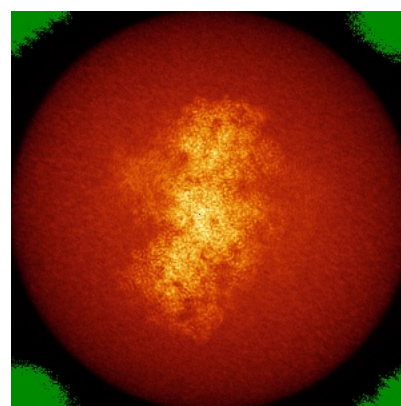
6.4.1 Primary map



X



Y

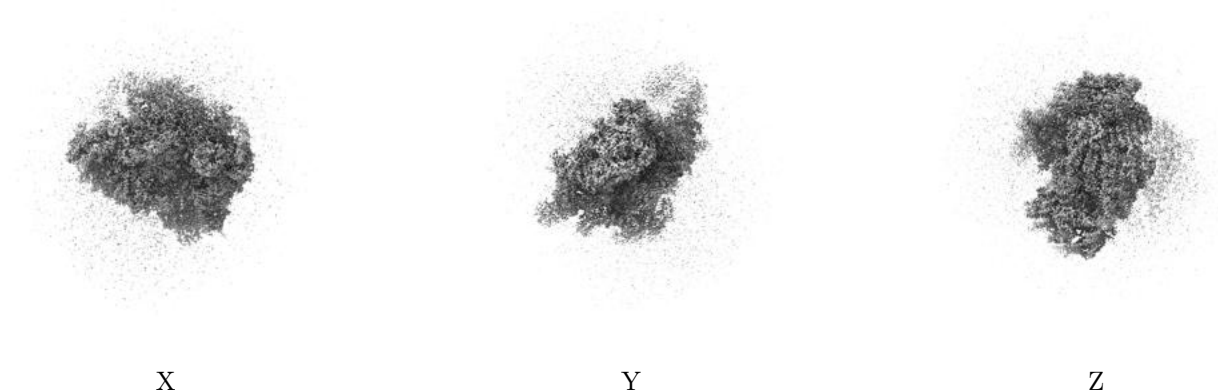


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0193. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

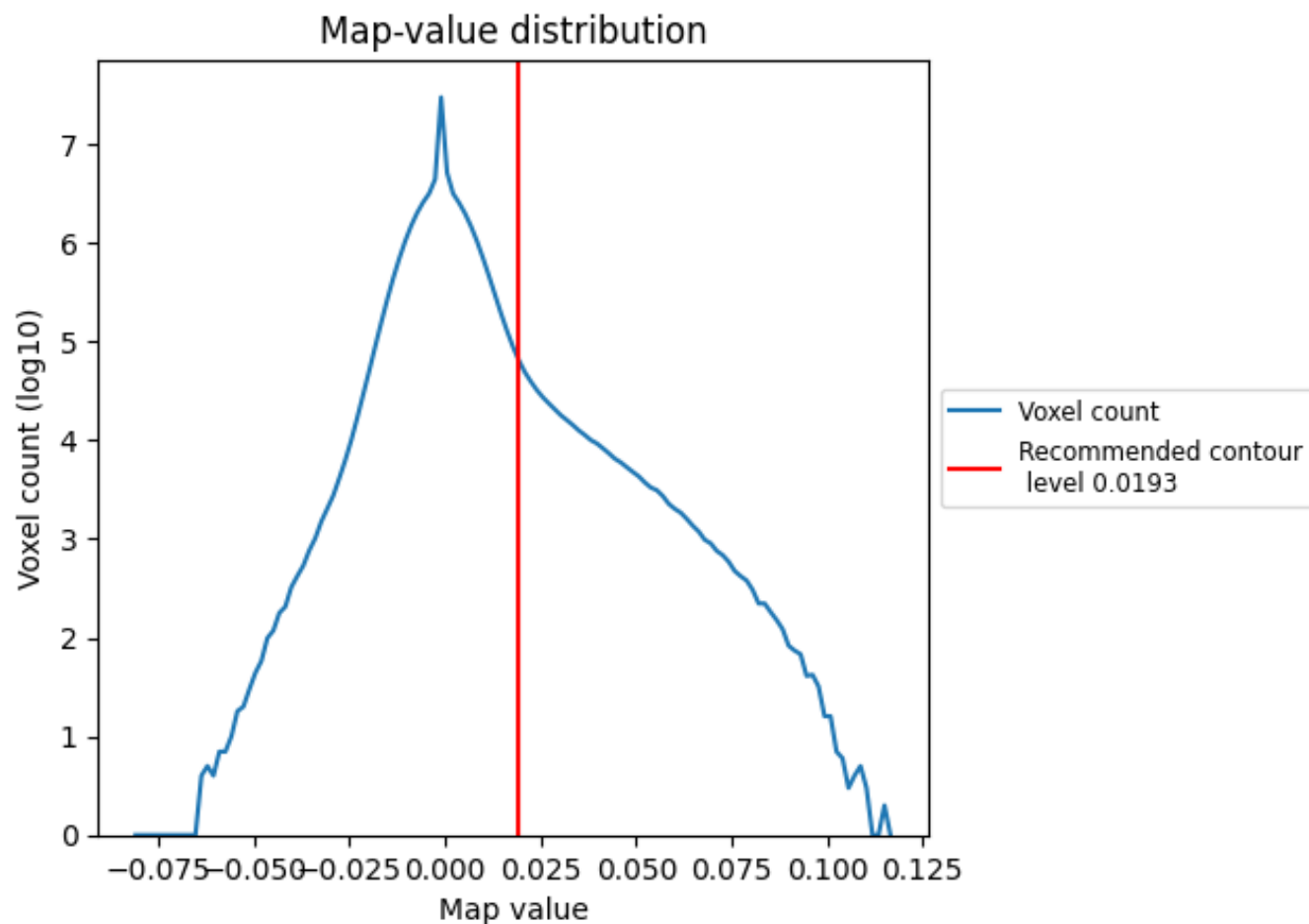
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

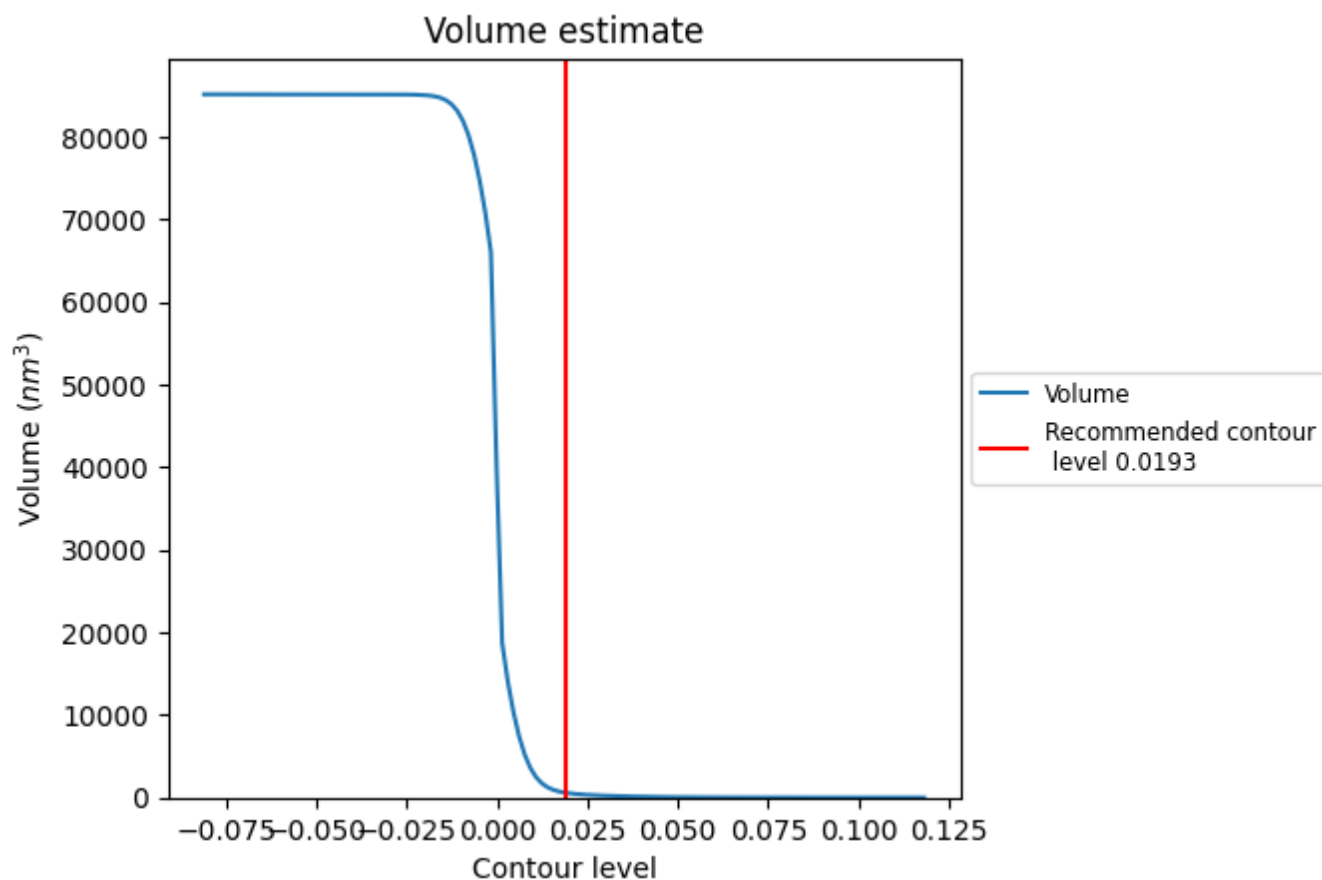
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

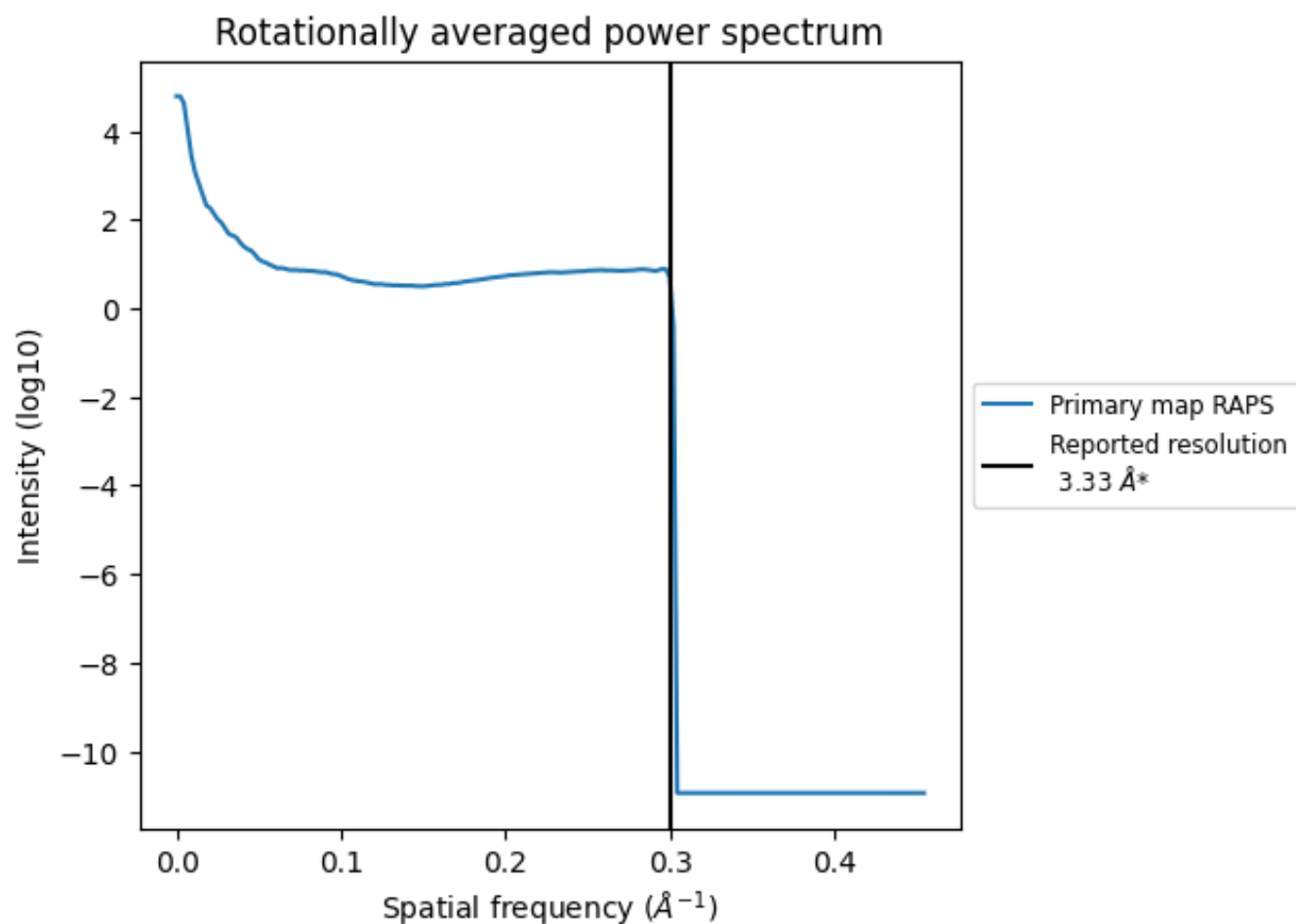
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 566 nm³; this corresponds to an approximate mass of 511 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.300 $\text{\AA}^{-1}$

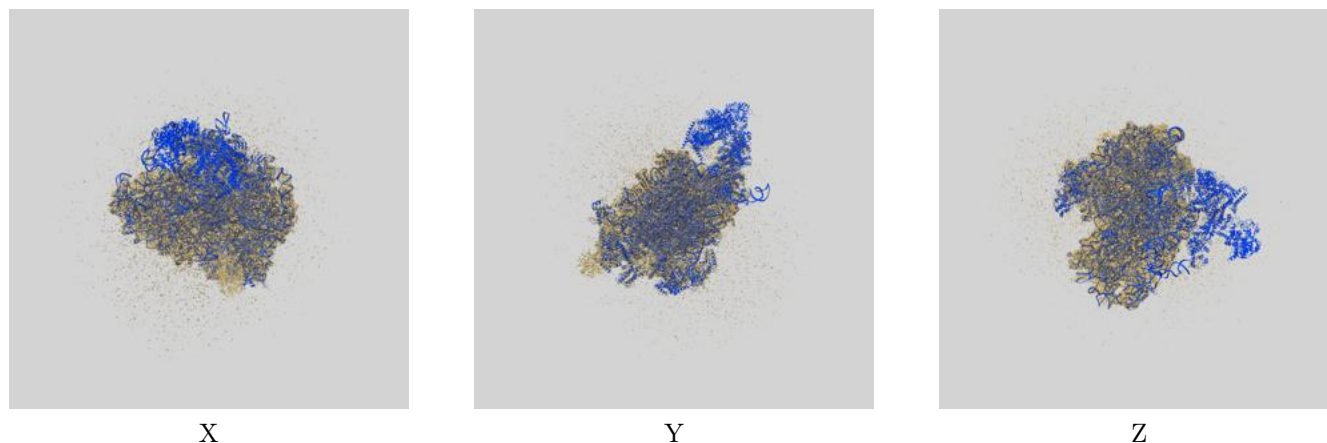
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

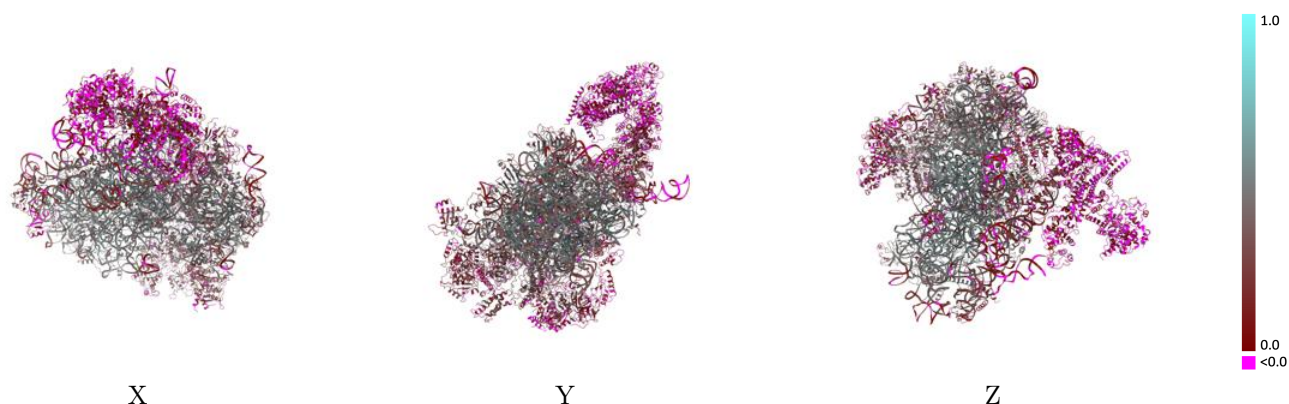
This section contains information regarding the fit between EMDB map EMD-11893 and PDB model 7ASE. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



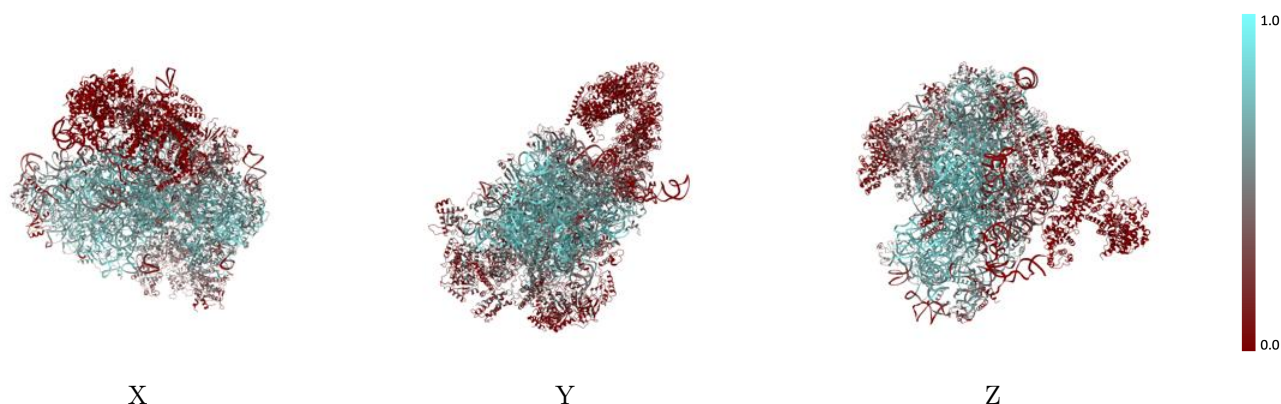
The images above show the 3D surface view of the map at the recommended contour level 0.0193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



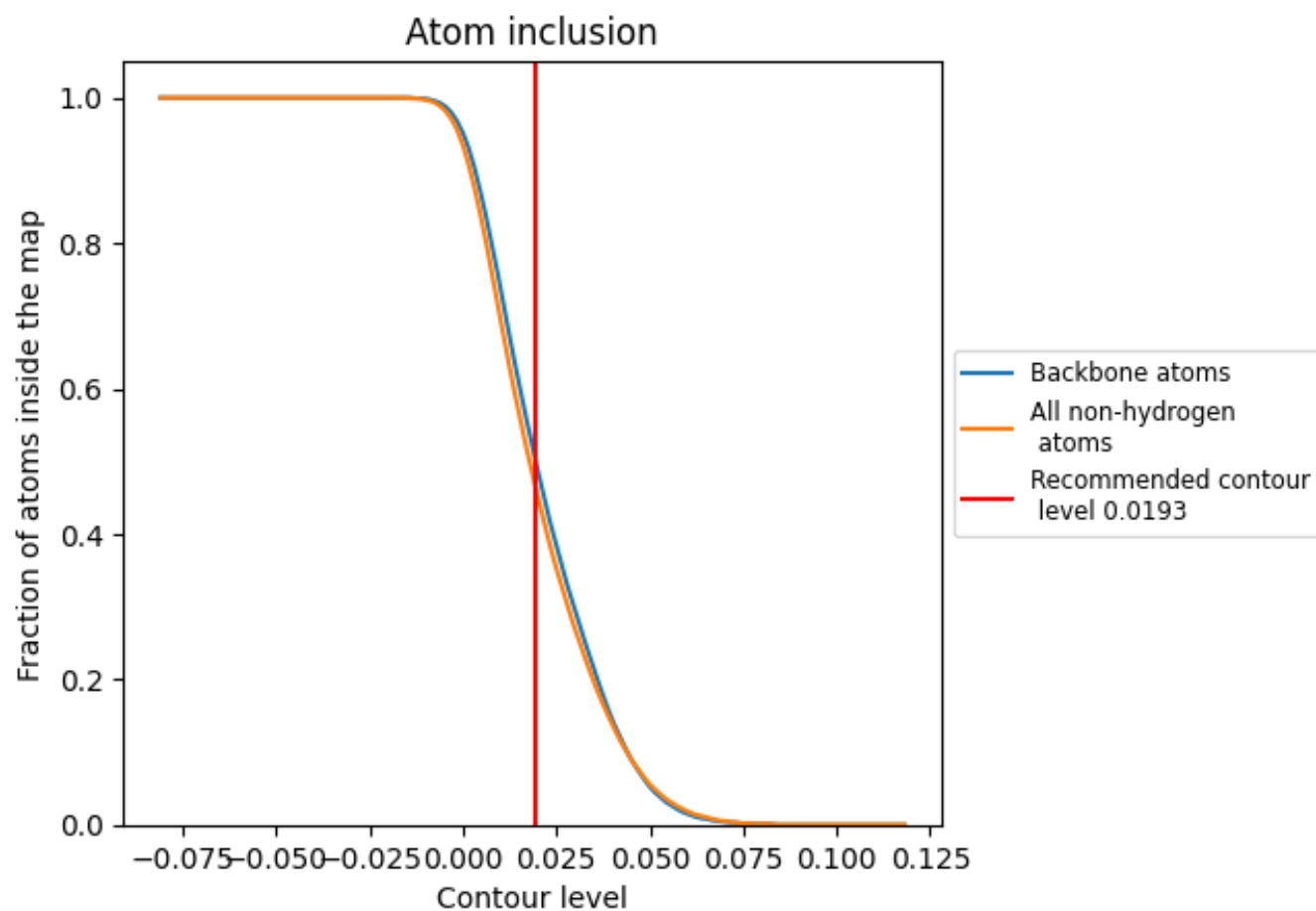
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0193).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4650	 0.3140
0	 0.6860	 0.4100
1	 0.6240	 0.3900
5	 0.1770	 0.1970
8	 0.1050	 0.1110
A	 0.1800	 0.2290
B	 0.6630	 0.4450
C	 0.1370	 0.1530
D	 0.6490	 0.4030
E	 0.0180	 0.0580
F	 0.6590	 0.4440
G	 0.0090	 0.0310
H	 0.0060	 0.0140
I	 0.0000	 0.0270
J	 0.2140	 0.1620
K	 0.0000	 0.0090
L	 0.5220	 0.3740
M	 0.5820	 0.4010
N	 0.5150	 0.3200
O	 0.5160	 0.2710
P	 0.5250	 0.3680
Q	 0.6170	 0.3660
R	 0.6710	 0.4560
S	 0.6560	 0.4530
T	 0.5680	 0.3920
U	 0.4510	 0.3740
V	 0.5590	 0.4390
W	 0.6410	 0.4440
X	 0.7030	 0.4570
Y	 0.0510	 0.1140
Z	 0.6630	 0.4390
a	 0.4440	 0.3150
b	 0.7230	 0.4770
c	 0.5110	 0.3610
d	 0.6770	 0.4640



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Chain	Atom inclusion	Q-score
f	 0.2540	 0.2210
g	 0.6680	 0.4600
h	 0.2370	 0.1980
i	 0.5450	 0.3570
j	 0.3190	 0.2750
l	 0.6780	 0.4450
m	 0.7000	 0.4630
n	 0.2780	 0.2490
o	 0.5770	 0.3930
p	 0.4880	 0.3530
q	 0.6080	 0.4110
r	 0.6470	 0.4160
s	 0.2070	 0.1950
t	 0.6920	 0.4720
u	 0.5260	 0.3220
v	 0.6550	 0.4420
w	 0.3930	 0.3050
y	 0.6420	 0.4190